



wwPDB X-ray Structure Validation Summary Report ⓘ

May 23, 2020 – 01:07 am BST

PDB ID : 4V5J
Title : Structure of the 70S ribosome bound to Release factor 2 and a substrate analog provides insights into catalysis of peptide release
Authors : Jin, H.; Kelley, A.C.; Loakes, D.; Ramakrishnan, V.
Deposited on : 2010-03-24
Resolution : 3.10 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

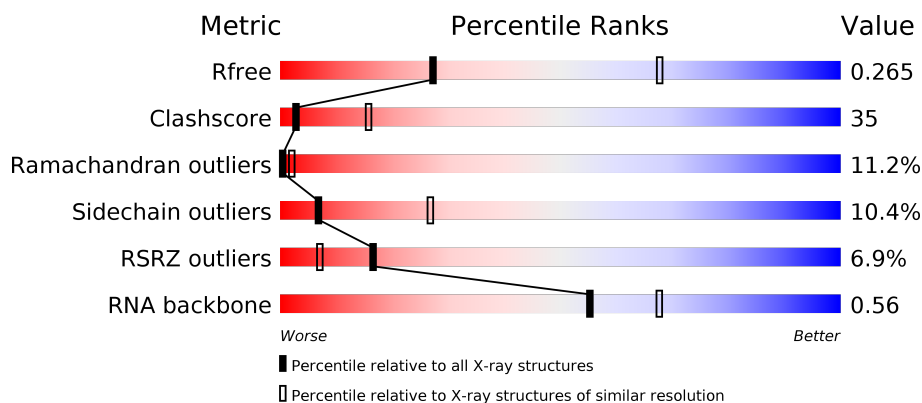
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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.



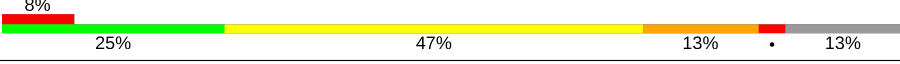
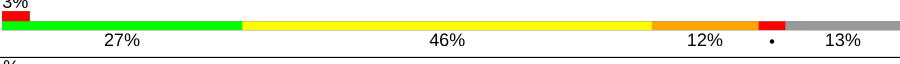
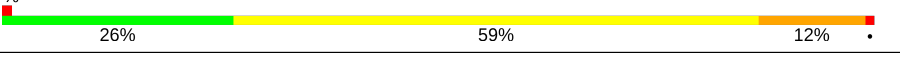
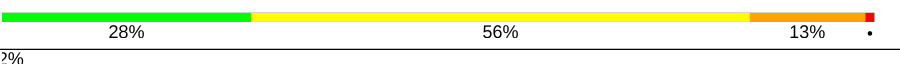
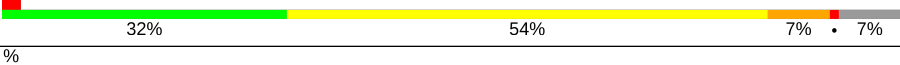
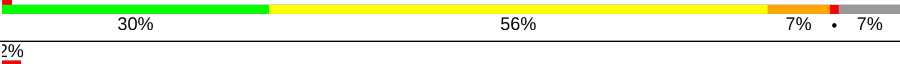
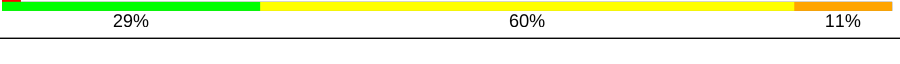


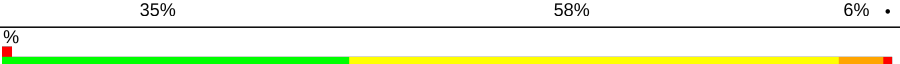
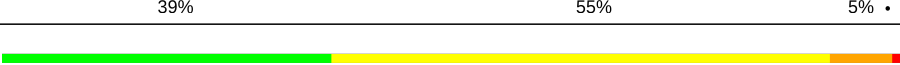
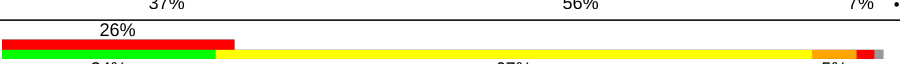
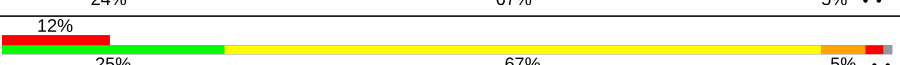
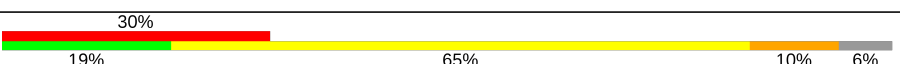
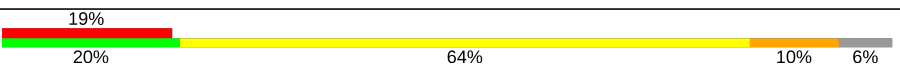
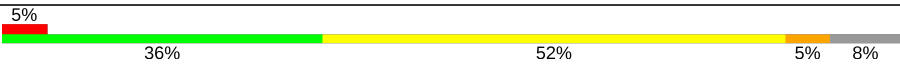

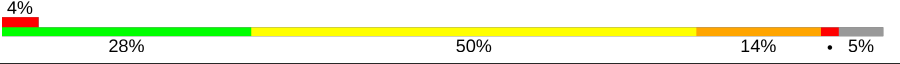
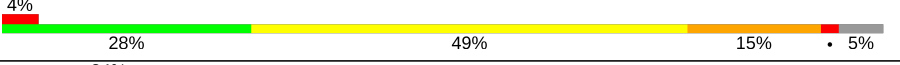
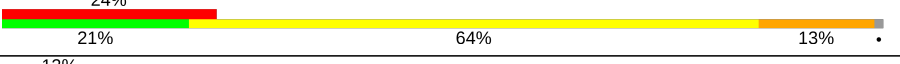
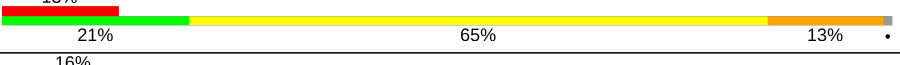
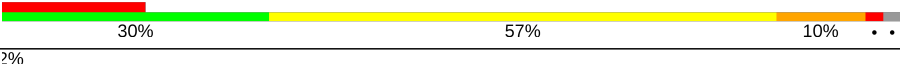



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)
RNA backbone	3102	1116 (3.40-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on 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	<div> <div>3%</div> <div>29%</div> <div>59%</div> <div>10%</div> </div>
1	CA	1522	<div> <div>2%</div> <div>29%</div> <div>59%</div> <div>10%</div> </div>
2	AB	256	<div> <div>9%</div> <div>19%</div> <div>57%</div> <div>14%</div> <div>8%</div> </div>
2	CB	256	<div> <div>7%</div> <div>19%</div> <div>57%</div> <div>14%</div> <div>8%</div> </div>

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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	

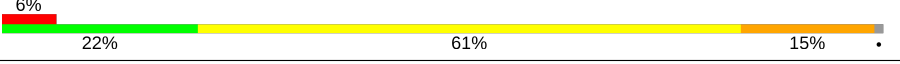
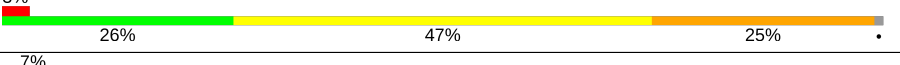

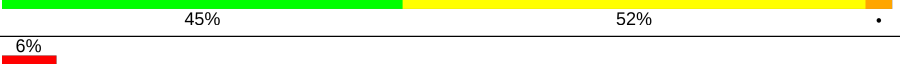

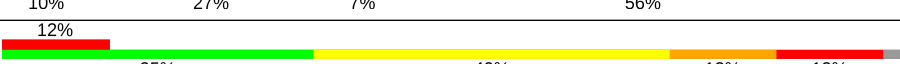
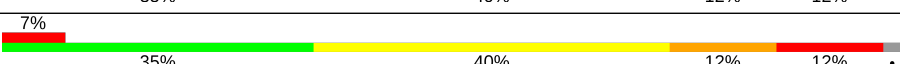
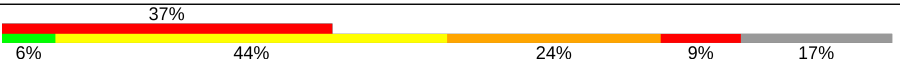



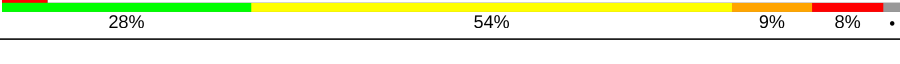


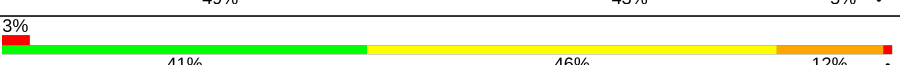
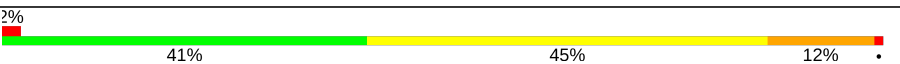


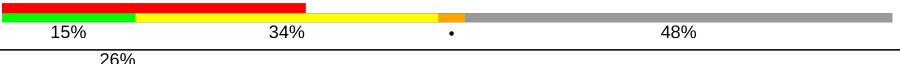
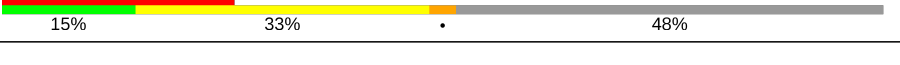

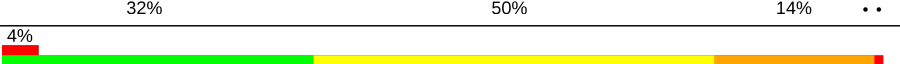



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Mol	Chain	Length	Quality of chain
15	CO	89	
16	AP	88	
16	CP	88	
17	AQ	105	
17	CQ	105	
18	AR	88	
18	CR	88	
19	AS	93	
19	CS	93	
20	AT	106	
20	CT	106	
21	AU	27	
21	CU	27	
22	AV	77	
22	AW	77	
22	CV	77	
22	CW	77	
23	AX	8	
23	CX	8	
24	AY	351	
24	CY	351	
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	2915	
35	DA	2915	
36	BB	122	
36	DB	122	
37	BC	229	
37	DC	229	
38	BD	276	
38	DD	276	
39	BE	206	

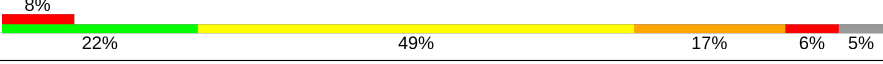
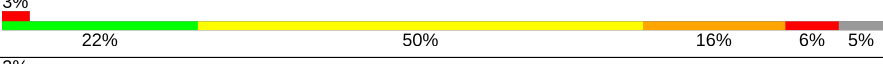
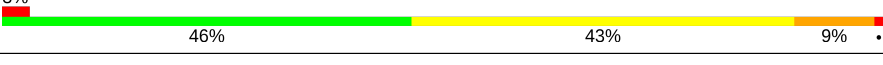
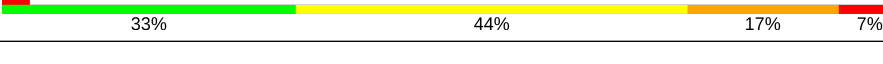


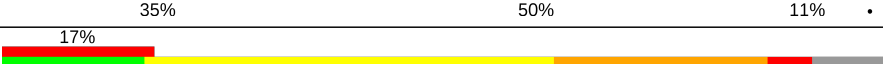
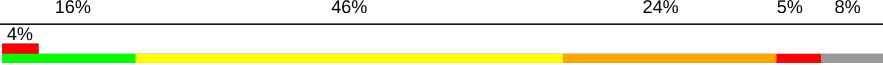
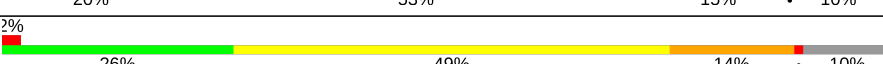
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Mol	Chain	Length	Quality of chain
39	DE	206	
40	BF	210	
40	DF	210	
41	BG	182	
41	DG	182	
42	BH	180	
42	DH	180	
43	BI	148	
43	DI	148	
44	BJ	130	
44	DJ	130	
45	BK	147	
45	DK	147	
46	BN	140	
46	DN	140	
47	BO	122	
47	DO	122	
48	BP	150	
48	DP	150	
49	BQ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

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Mol	Chain	Length	Quality of chain
52	BT	146	
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	

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
22	8AN	AV	76	-	-	X	-
22	PHA	AW	77	-	-	X	X
22	PHA	CW	77	-	-	X	-
59	MG	AA	1611	-	-	-	X
59	MG	AA	1630	-	-	-	X
59	MG	AA	1721	-	-	-	X
59	MG	AA	1727	-	-	-	X
59	MG	AA	1732	-	-	-	X
59	MG	AA	1748	-	-	-	X
59	MG	AA	1752	-	-	-	X
59	MG	AV	105	-	-	-	X
59	MG	AX	101	-	-	-	X
59	MG	B5	102	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
59	MG	BA	3010	-	-	-	X
59	MG	BA	3029	-	-	-	X
59	MG	BA	3039	-	-	-	X
59	MG	BA	3111	-	-	-	X
59	MG	BA	3127	-	-	-	X
59	MG	BA	3131	-	-	-	X
59	MG	BA	3149	-	-	-	X
59	MG	BA	3208	-	-	-	X
59	MG	BA	3209	-	-	-	X
59	MG	BA	3212	-	-	-	X
59	MG	BA	3217	-	-	-	X
59	MG	BA	3218	-	-	-	X
59	MG	BA	3273	-	-	-	X
59	MG	BA	3276	-	-	-	X
59	MG	BA	3277	-	-	-	X
59	MG	BA	3290	-	-	-	X
59	MG	BA	3313	-	-	-	X
59	MG	BA	3319	-	-	-	X
59	MG	BA	3344	-	-	-	X
59	MG	BA	3354	-	-	-	X
59	MG	BA	3357	-	-	-	X
59	MG	BG	201	-	-	-	X
59	MG	CA	1603	-	-	-	X
59	MG	CA	1632	-	-	-	X
59	MG	CA	1637	-	-	-	X
59	MG	CA	1638	-	-	-	X
59	MG	CA	1648	-	-	-	X
59	MG	CA	1675	-	-	-	X
59	MG	CA	1680	-	-	-	X
59	MG	CA	1699	-	-	-	X
59	MG	CA	1712	-	-	-	X
59	MG	CA	1714	-	-	-	X
59	MG	CA	1715	-	-	-	X
59	MG	CA	1748	-	-	-	X
59	MG	CL	202	-	-	-	X
59	MG	DA	3044	-	-	-	X
59	MG	DA	3095	-	-	-	X
59	MG	DA	3153	-	-	-	X
59	MG	DA	3197	-	-	-	X
59	MG	DA	3210	-	-	-	X
59	MG	DA	3215	-	-	-	X
59	MG	DA	3226	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
59	MG	DA	3244	-	-	-	X
59	MG	DA	3253	-	-	-	X
59	MG	DA	3258	-	-	-	X
59	MG	DA	3339	-	-	-	X
59	MG	DA	3356	-	-	-	X
59	MG	DB	201	-	-	-	X
59	MG	DP	201	-	-	-	X

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 305067 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	125	Total	C	N	O	S	0	0	1
			971	611	196	163	1			
12	CL	125	Total	C	N	O	S	0	0	1
			971	611	196	163	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AM	125	Total	C	N	O	S	0	0	1
			988	611	206	169	2			
13	CM	125	Total	C	N	O	S	0	0	1
			988	611	206	169	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	77	Total	C	N	O	P	0	0	0
			1630	732	292	531	75			
22	AW	77	Total	C	N	O	P	0	0	0
			1630	732	292	531	75			
22	CV	77	Total	C	N	O	P	0	0	0
			1630	732	292	531	75			
22	CW	77	Total	C	N	O	P	0	0	0
			1630	732	292	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
			165	76	29	53	7			
23	CX	8	Total	C	N	O	P	0	0	0
			165	76	29	53	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
			2801	1752	506	535	8			
24	CY	351	Total	C	N	O	S	0	0	0
			2801	1752	506	535	8			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	B0	83	Total	C	N	O	S	0	0	0
			657	407	139	110	1			
25	D0	83	Total	C	N	O	S	0	0	0
			657	407	139	110	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			
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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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	2901	Total	C	N	O	P	0	0	0
			62474	27806	11681	20087	2900			
35	DA	2901	Total	C	N	O	P	0	0	0
			62474	27806	11681	20087	2900			

- 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	120	Total	C	N	O	S	0	0	0
			937	590	174	172	1			
37	DC	120	Total	C	N	O	S	0	0	0
			937	590	174	172	1			

- 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			
43	DI	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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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			
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	185	Total 1468	C 936	N 262	O 268	S 2	0	0	1
58	DZ	185	Total 1468	C 936	N 262	O 268	S 2	0	0	1

- Molecule 59 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	BA	357	Total 357	Mg 357	0	0
59	CA	155	Total 155	Mg 155	0	0
59	DF	1	Total 1	Mg 1	0	0
59	CV	7	Total 7	Mg 7	0	0
59	AW	4	Total 4	Mg 4	0	0
59	B1	1	Total 1	Mg 1	0	0
59	CD	1	Total 1	Mg 1	0	0
59	AX	1	Total 1	Mg 1	0	0
59	AS	1	Total 1	Mg 1	0	0
59	B5	2	Total 2	Mg 2	0	0
59	BB	4	Total 4	Mg 4	0	0
59	BT	1	Total 1	Mg 1	0	0
59	DG	1	Total 1	Mg 1	0	0
59	BF	2	Total 2	Mg 2	0	0
59	AV	7	Total 7	Mg 7	0	0
59	BX	1	Total 1	Mg 1	0	0
59	AA	161	Total 161	Mg 161	0	0
59	CX	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	CN	1	Total 1	Mg 1	0	0
59	DD	1	Total 1	Mg 1	0	0
59	DH	1	Total 1	Mg 1	0	0
59	DS	1	Total 1	Mg 1	0	0
59	BG	1	Total 1	Mg 1	0	0
59	BY	1	Total 1	Mg 1	0	0
59	DX	1	Total 1	Mg 1	0	0
59	DA	359	Total 359	Mg 359	0	0
59	AL	1	Total 1	Mg 1	0	0
59	DE	1	Total 1	Mg 1	0	0
59	AY	1	Total 1	Mg 1	0	0
59	D1	1	Total 1	Mg 1	0	0
59	DP	1	Total 1	Mg 1	0	0
59	CW	4	Total 4	Mg 4	0	0
59	D5	2	Total 2	Mg 2	0	0
59	BD	2	Total 2	Mg 2	0	0
59	CS	1	Total 1	Mg 1	0	0
59	CL	2	Total 2	Mg 2	0	0
59	DB	4	Total 4	Mg 4	0	0

- Molecule 60 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	CN	1	Total 1	Zn 1	0	0
60	AN	1	Total 1	Zn 1	0	0
60	B9	1	Total 1	Zn 1	0	0
60	D9	1	Total 1	Zn 1	0	0
60	CD	1	Total 1	Zn 1	0	0
60	AD	1	Total 1	Zn 1	0	0

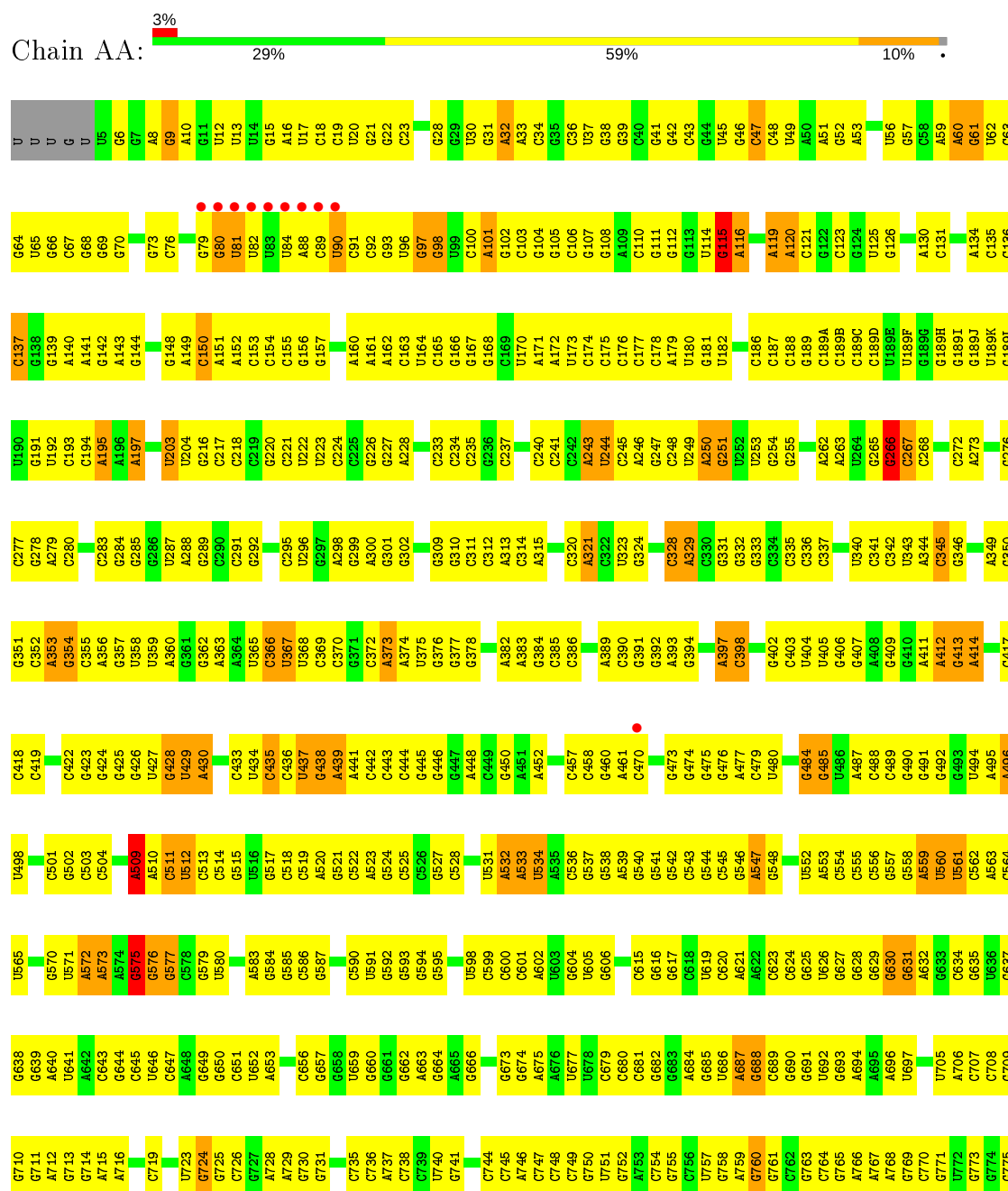
- Molecule 61 is water.

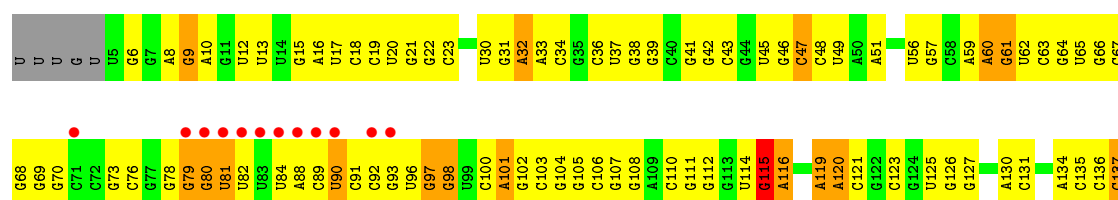
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	AV	1	Total 1	O 1	0	0
61	AY	1	Total 1	O 1	0	0
61	BA	1	Total 1	O 1	0	0

3 Residue-property plots

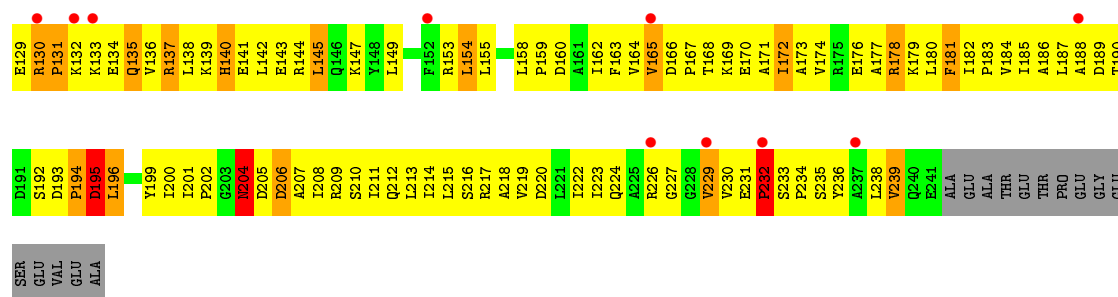
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

• Molecule 1: 16S Ribosomal RNA

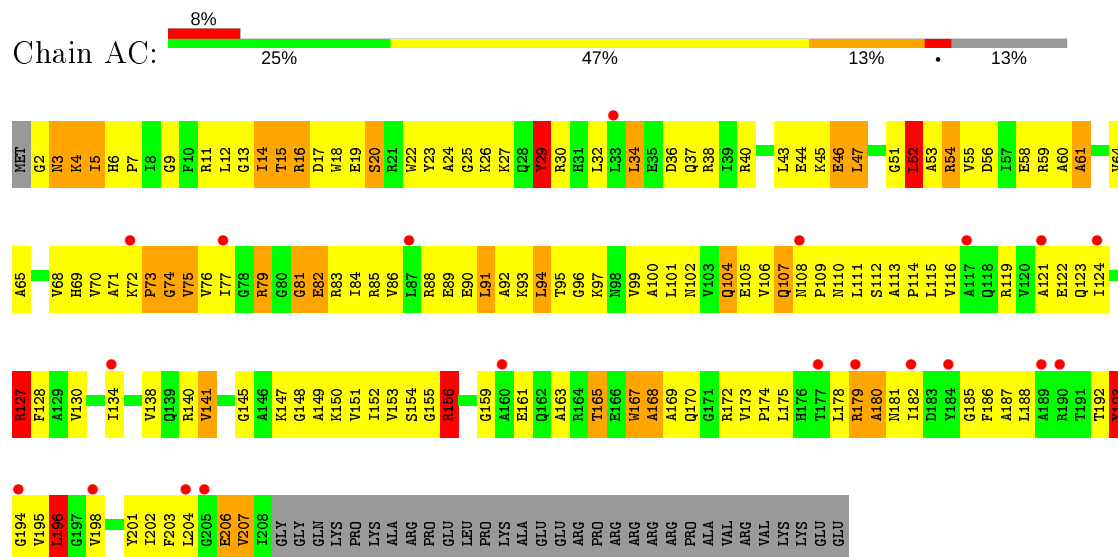




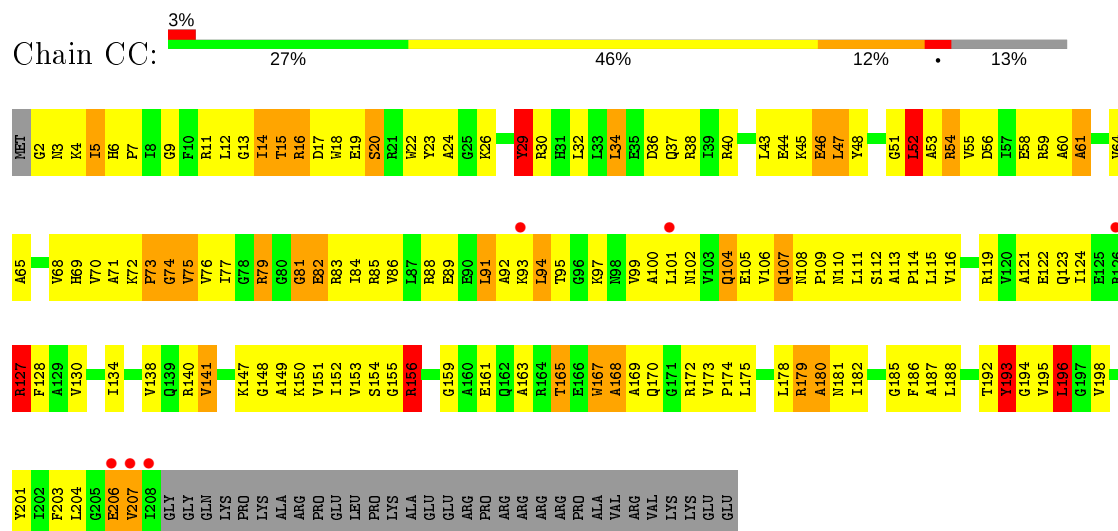
G1143	G1076	A1015	U952	G869	G785	A715	C643	G570	C501	G354	C277	G191	G138
G1144	G1077	A1016	G953	U870	A790	A716	G644	U571	C502	C355	G278	U192	G139
C1145	G1078	C1017	G954	G878	G793	G719	G645	A572	G502	A356	G279	C193	A140
A1146	G1079	C1018	U955	G879	U793	C719	U646	A573	C503	G357	C280	C194	A141
C1147	A1080	C1019	U956	C880	A794	U723	C647	A574	C504	U358	U359	A195	G142
U1148	G1081	U1020	U957	C881	C795	G724	A643	G575	A509	G360	C283	A196	A143
U1149	G1082	A958	A958	G881	C796	G725	G649	U576	C509	A361	G284	A197	G144
C1150	A959	U959	A959	C882	C797	G726	G650	U577	A510	G362	G285		
G1084	A1151	G1084	U960	C883	C797	C726	C651	C578	C511	G361			
A1152	U1085	G1024	U961	U884	G798	G727	U652	C578	C512	U429			
C1153	U1086	G1026	C962	G885	A802	A728	A653	A583	C513	A363	G289	U203	G148
	G1087	C1027	G963		G803	A729		G584	C514	U365	C290	U204	A149
A1157	G1088	U964	A964	G888	U804	A730	C856	G585	G515	G366	C291	U204	C150
C1158	G1089	C1029	U965		C805	G731	G657	C586	G516	U367	G292	G216	A151
U1159	G966	C1030	G966	C897	C806		G658	G587	C517	U368		C218	A152
G1160	G1094	C1030A	C967	G898		C735	U659		C518	C436	C295	C219	C154
C1161	U1095	C1030B	A968		A814	C736	G660	C590	C519	U437	U296	G220	C155
C1162	C1096	C1030C	A969	G902	A815	A737	G661	U591	A520	G371	A298	U222	G157
C1163	C1097	A1030D	C970		A816	C738	G662	G592	C521	C372	A299	U223	
G1164	C1098	G1031	G971	A908	C739	C739	A663	G593	C522	A373	A300	C224	
C1165	C1165	G1032	C972	A909	C817	U740	A675	G594	A523	A374	A300	C225	
G1166	A1101	G1033	C973	C910	G818	G741	A676	G595		U375	G302	G226	A161
A1168	A1102	A1034	A974	U911	C819	U742	U677	G604		G376	G302	G227	A162
G1169	C1103	A1035	A975	C912	U820	U743	U678	G605		G377			C163
A1169	G1104	G1036	G976	A913	C821	C744	G673	U598		G378	G309		C164
A1170	A1105	C1037	A977	A914	C826	C745	G674	C599		G378	G310		C165
C1172	G1106		A978		A746	C745	A675	C600		A382	C311		G166
G1173	C1107	U1040	C979	G917	U827	C747	A676	A602		A383	C312		G167
	A1108	A1041	C980	A918	U828	C747	U677	U603		G384	C313		G168
A1176	C1109	G1042	U981	A919	A829	C748	U677	U604		C385	C314		C169
G1177	A1110	C1043		U920	G829	C749	U678	G604		C386	A315		U170
G1178	A1111		C984	U921	U831	U751	C680	U605		U387			A171
A1179	C985	G1047	C985	G922	C832	G752	C681	G537		A321	C240		A172
A1180	A986	U1048	A986	A923	U833	A753	G682	C538		C322	C242		U173
G1181	C987	U1049	G987	C924	C834	C754	G683	G540		U323	C243		C174
G1182	G1117	G1050		G925	U835	G755	A684	G541		C390	U244		G175
	C1118	C1051	C990	G926	G836	G756	A685	G542		G391	C245		C176
A1188	U1121	U1052	U991	G927	U836	C757	G686	G542		C328	A246		C177
C1189	U1122	G1053	U992	G928	U839	C758	A687	C543		A329	G247		C178
G1190	A1123	C1054	G993	G929	C840	A759	G688	C544		C330	C248		A179
	C1124	A1055	A994	C930	U841	G760	C689	C545		G331	U249		U180
G1193	U1125	U1056		C931	C848	G761	G690	G546		A397	G181		G181
U1194	C1126	G1057	U997	C932			G691	C624		C398	G251		U182
C1195	G1127	U1058	U998	G933	G851	C764	U692	G625					
U1196	C1128	C1059	U999	C934	G852	G765	G693	U626		G402	G254		C186
G1197	U1129	G1061	A1001	C936	G853	A766	A694	G627		C403	G255		C187
C1198	A1130	U1062	G1001A	A937	G854	A767	A695	C628		U404			C188
U1199	C1131	C1063	G1001A	A938		A768	A696	G629		U405	A262		G189
C1200	A1132	G1064	G1002	G939	C857	G769	U697	G630		G406	A263		C189A
G1202	G1133	U1065	A1004	C940	G858	C770	U705	A632		G407	U264		C189B
C1203	C1134	C1066	G941	C937	G859	G771	A706	U633		A408	G265		C189C
A1204	A1067	C1006	G942	C942	A860	C634	C707	U634		G409	C266		C189D
U1205	U1136	G1068		A946	G861	G775	A706	C635		A411	C267		U189E
G1206	C1137			G947	C862	G776	C708	U636		A412	C268		U189F
C1207	G1138	C1071		G947	U863	A777	G709	G637		G413	A270		G189G
C1208	G1139	U1072		C948	G864		G710	U638		A414			G189H
	C1140	G1073		U949	A865	A781	G711	U639		A349	C271		G189I
U1211	C1141	U1074	U1012	A949	C866	A782	A712	A640		G351	C272		U189J
C1142	C1142	G1074	G1013	U950	G867	C783	G713	U641		C417	A273		G189L
		G1075	A1014	C954	C868	C784	G714	A642		C418			U190
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• Molecule 3: 30S RIBOSOMAL PROTEIN S3

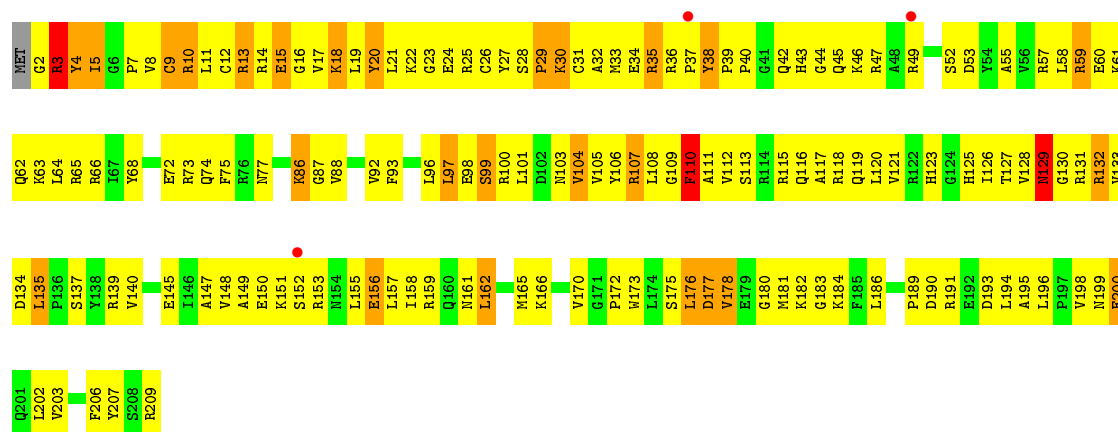


• Molecule 3: 30S RIBOSOMAL PROTEIN S3

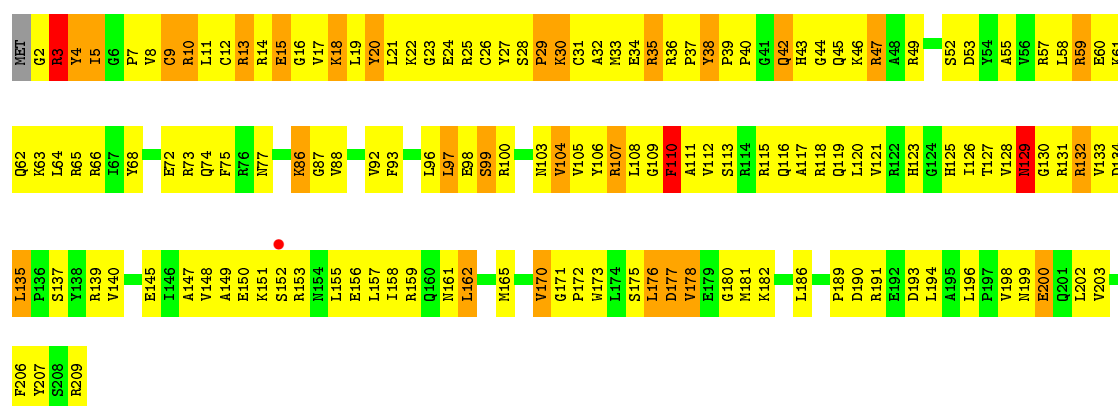
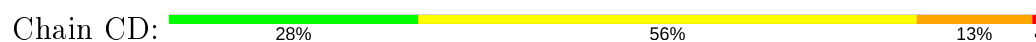


• Molecule 4: 30S RIBOSOMAL PROTEIN S4

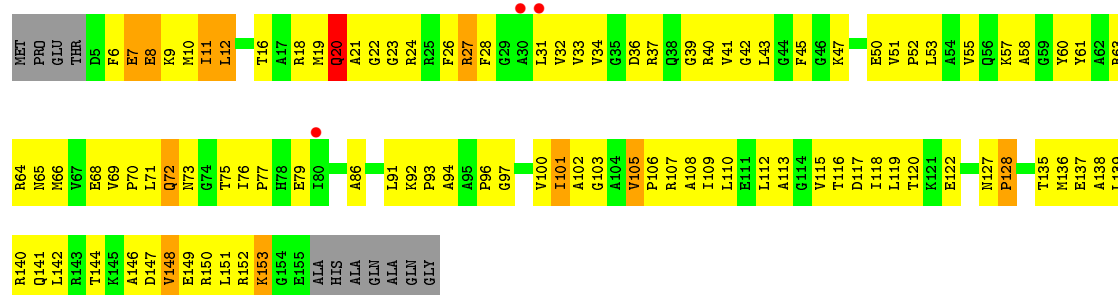




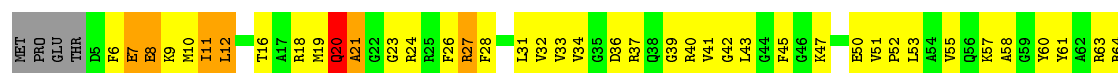
• Molecule 4: 30S RIBOSOMAL PROTEIN S4

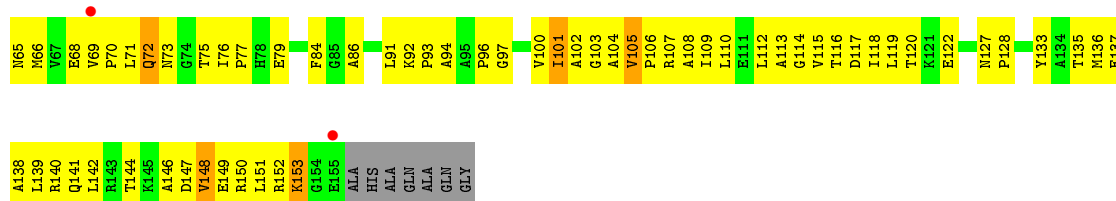


• Molecule 5: 30S RIBOSOMAL PROTEIN S5

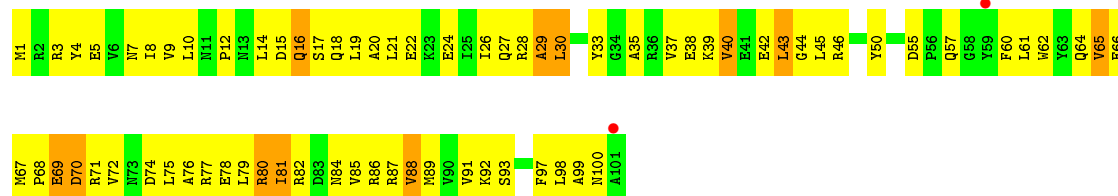


• Molecule 5: 30S RIBOSOMAL PROTEIN S5

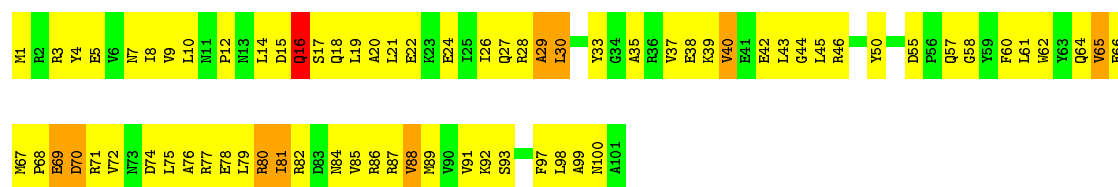




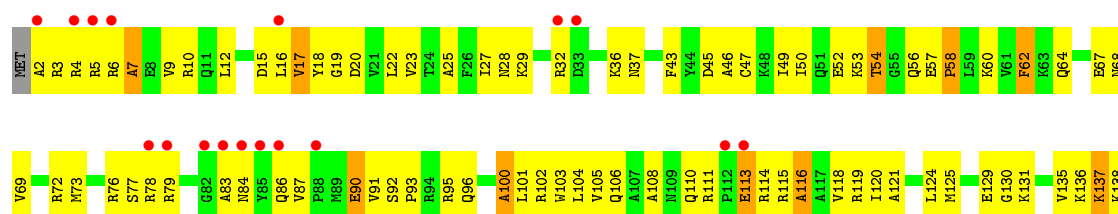
• Molecule 6: 30S RIBOSOMAL PROTEIN S6



• Molecule 6: 30S RIBOSOMAL PROTEIN S6

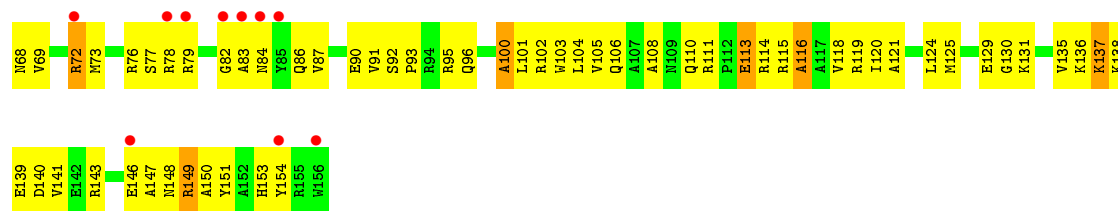


• Molecule 7: 30S RIBOSOMAL PROTEIN S7

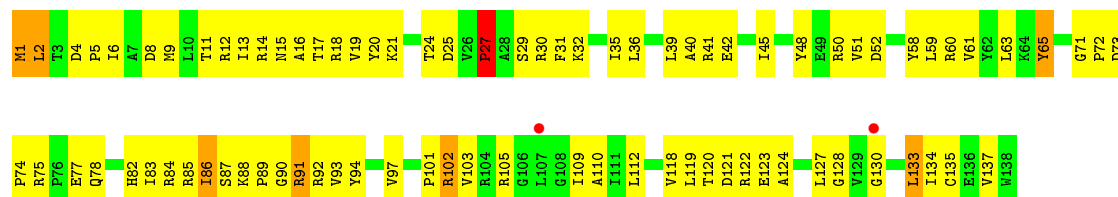


• Molecule 7: 30S RIBOSOMAL PROTEIN S7

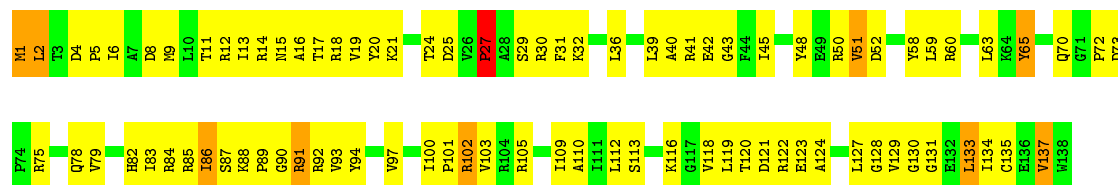




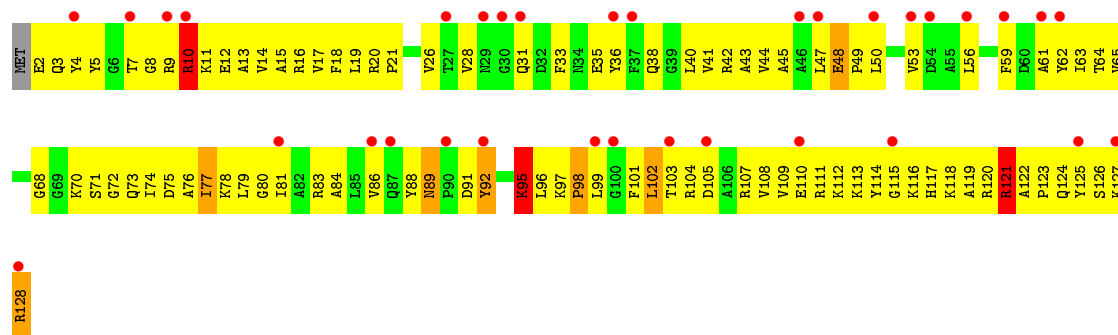
• Molecule 8: 30S RIBOSOMAL PROTEIN S8



• Molecule 8: 30S RIBOSOMAL PROTEIN S8

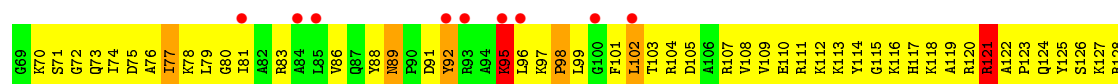


• Molecule 9: 30S RIBOSOMAL PROTEIN S9

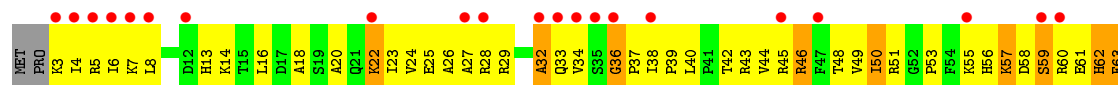


• Molecule 9: 30S RIBOSOMAL PROTEIN S9

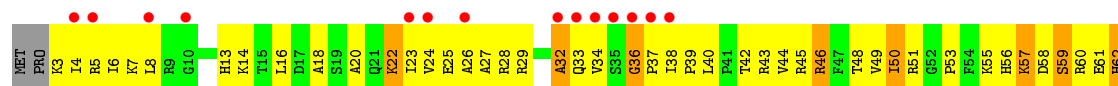




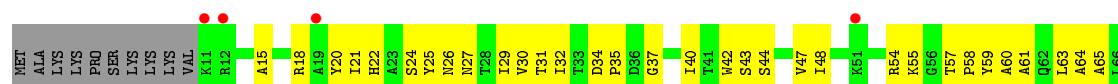
• Molecule 10: 30S RIBOSOMAL PROTEIN S10



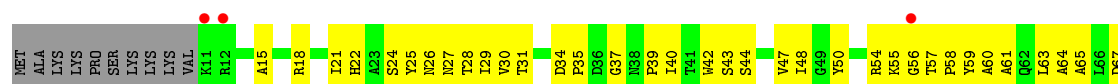
• Molecule 10: 30S RIBOSOMAL PROTEIN S10



• Molecule 11: 30S RIBOSOMAL PROTEIN S11

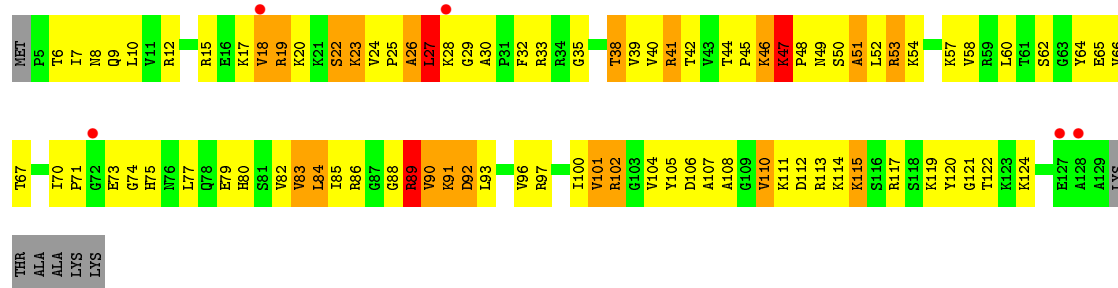


• Molecule 11: 30S RIBOSOMAL PROTEIN S11

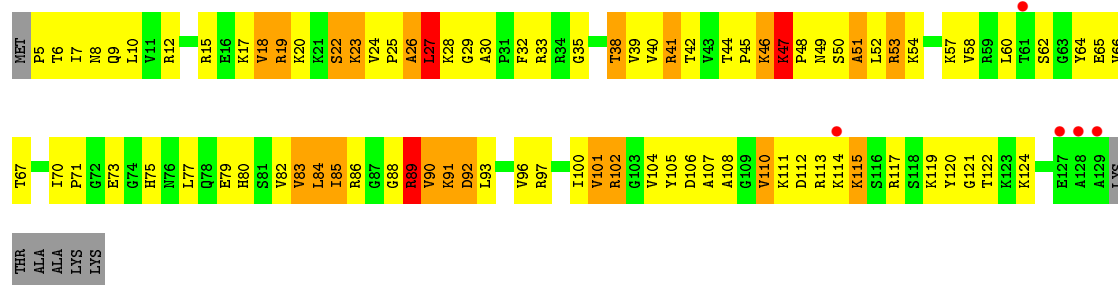


• Molecule 12: 30S RIBOSOMAL PROTEIN S12

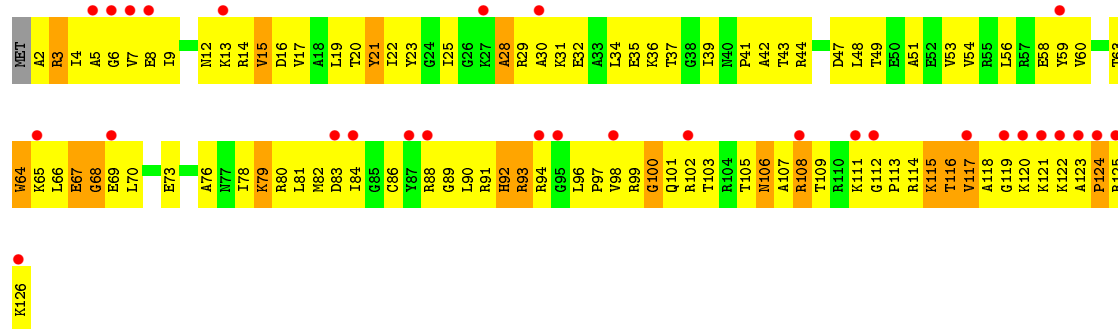




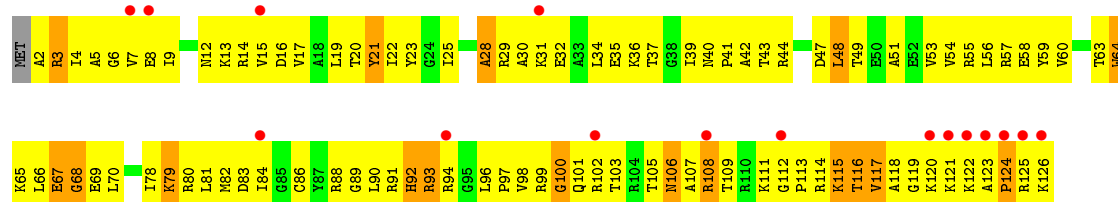
• Molecule 12: 30S RIBOSOMAL PROTEIN S12



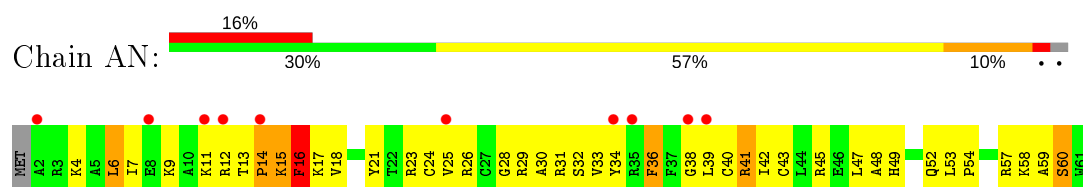
• Molecule 13: 30S RIBOSOMAL PROTEIN S13



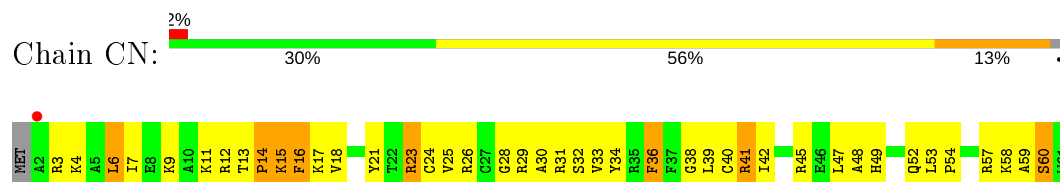
• Molecule 13: 30S RIBOSOMAL PROTEIN S13



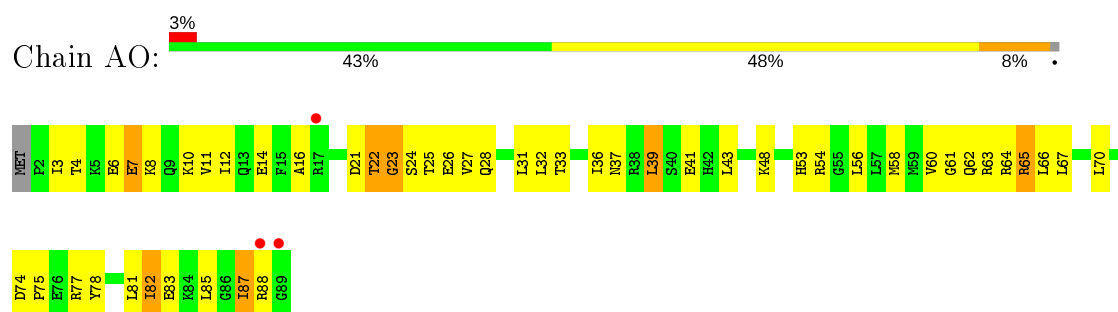
• Molecule 14: 30S RIBOSOMAL PROTEIN S14 TYPE Z



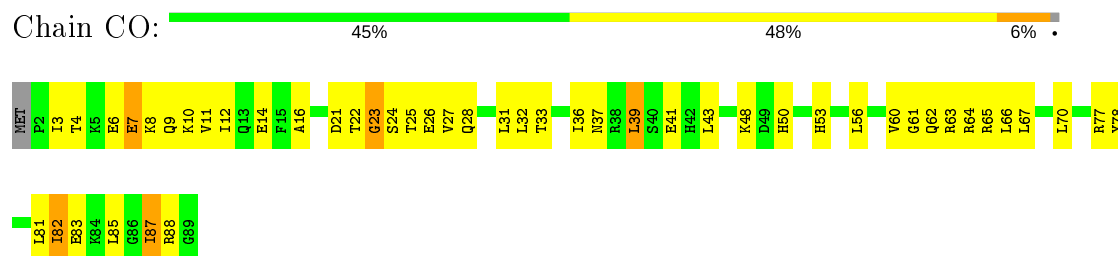
• Molecule 14: 30S RIBOSOMAL PROTEIN S14 TYPE Z



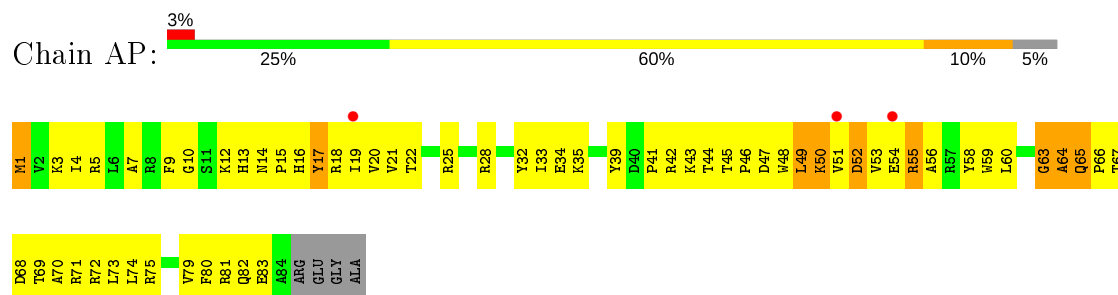
• Molecule 15: 30S RIBOSOMAL PROTEIN S15



• Molecule 15: 30S RIBOSOMAL PROTEIN S15

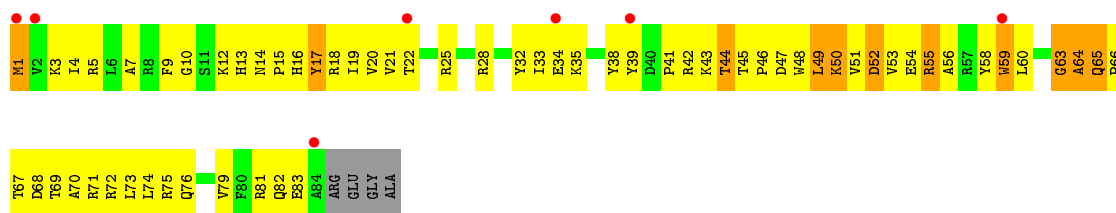


• Molecule 16: 30S RIBOSOMAL PROTEIN S16

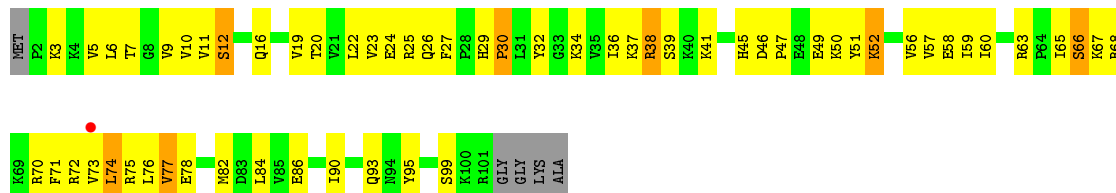


• Molecule 16: 30S RIBOSOMAL PROTEIN S16

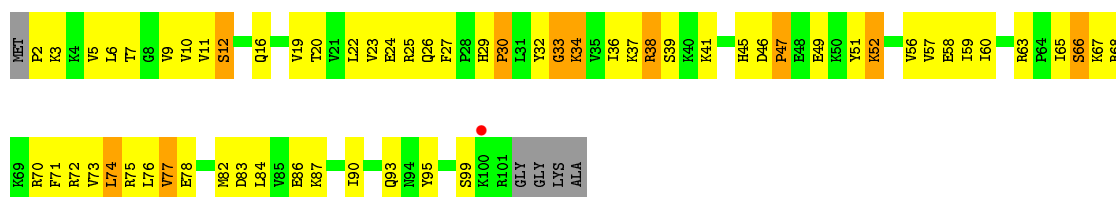




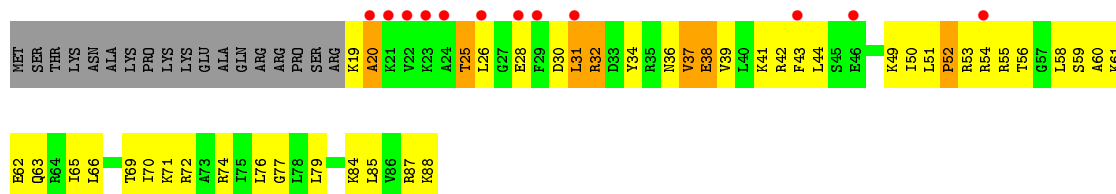
• Molecule 17: 30S RIBOSOMAL PROTEIN S17



• Molecule 17: 30S RIBOSOMAL PROTEIN S17



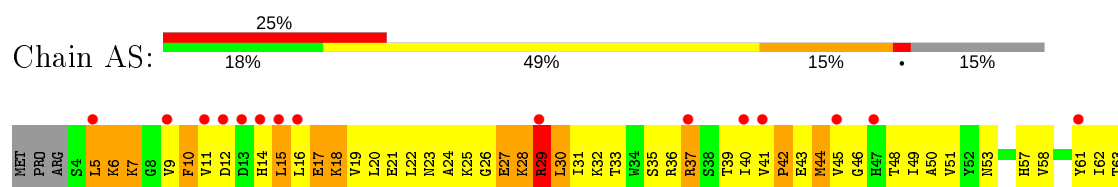
• Molecule 18: 30S RIBOSOMAL PROTEIN S18



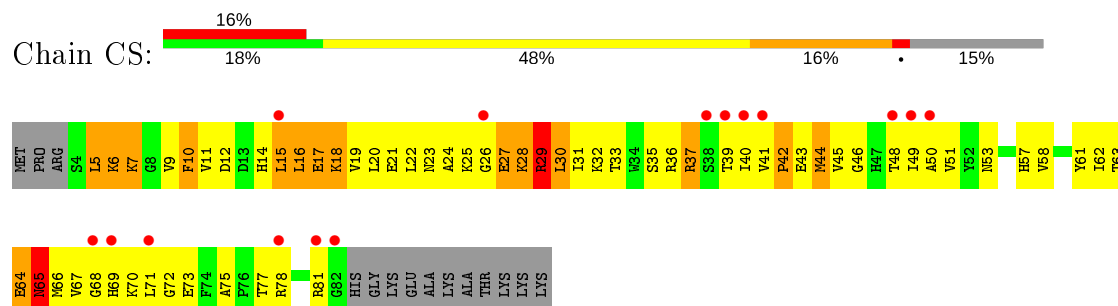
• Molecule 18: 30S RIBOSOMAL PROTEIN S18



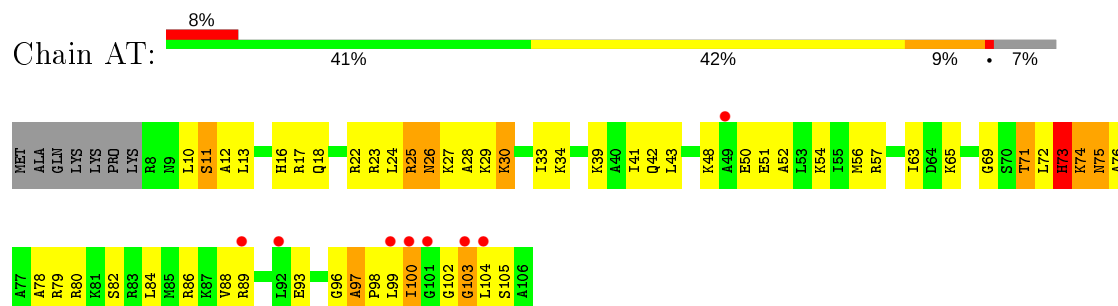
• Molecule 19: 30S RIBOSOMAL PROTEIN S19



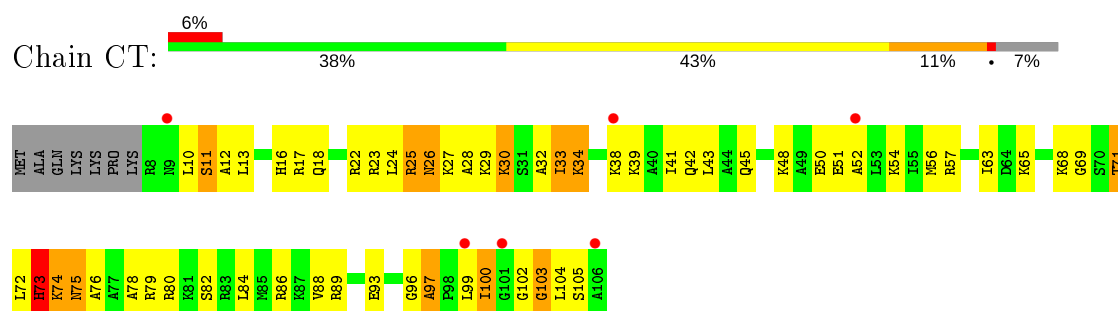
- Molecule 19: 30S RIBOSOMAL PROTEIN S19



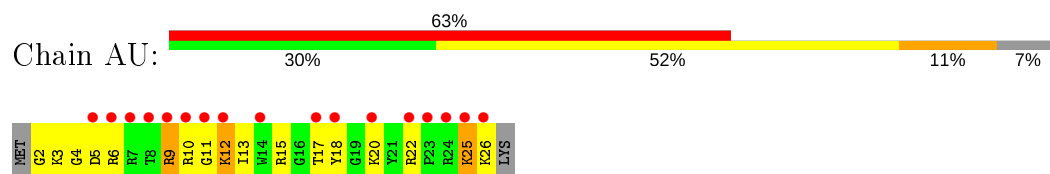
- Molecule 20: 30S RIBOSOMAL PROTEIN S20



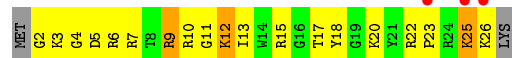
- Molecule 20: 30S RIBOSOMAL PROTEIN S20



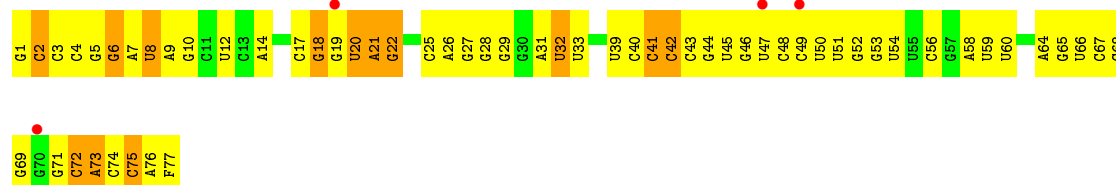
- Molecule 21: 30S RIBOSOMAL PROTEIN THX



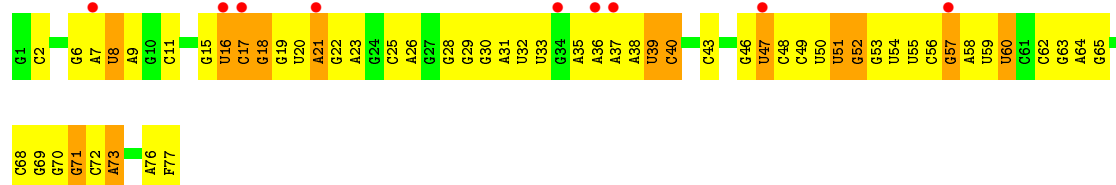
- Molecule 21: 30S RIBOSOMAL PROTEIN THX



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



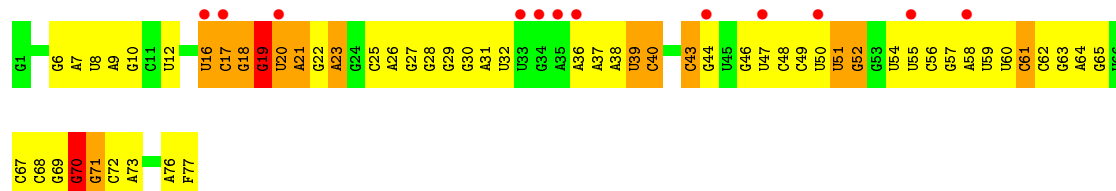
- Molecule 22: E-SITE TRNA PHE OR P-SITE TRNA PHE (UNMODIFIED BASES)



- 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

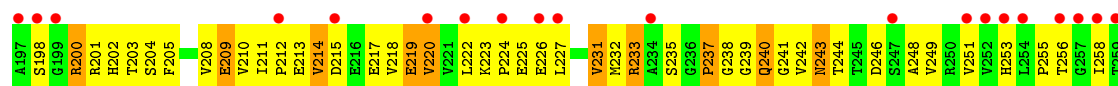
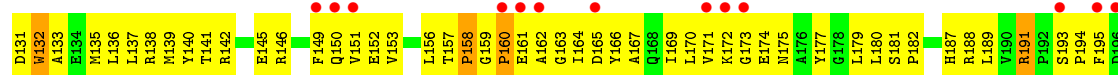
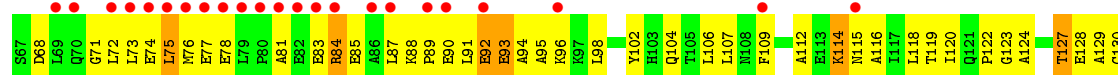
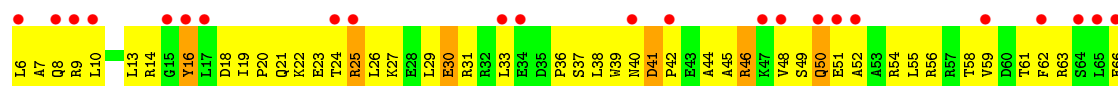




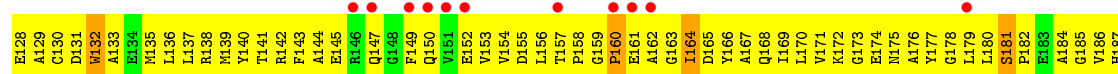
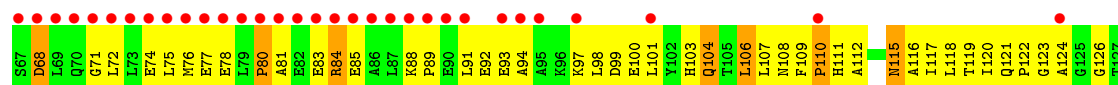
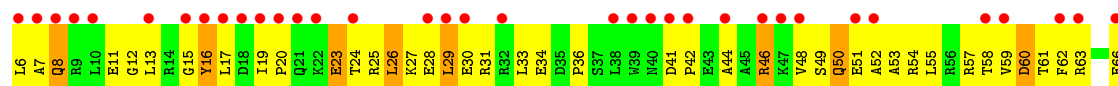
• Molecule 23: MRNA

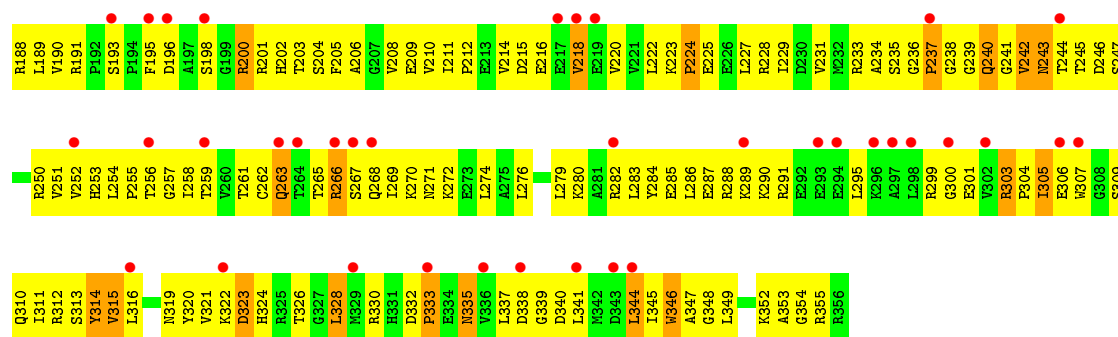


• Molecule 24: PEPTIDE CHAIN RELEASE FACTOR 2



• Molecule 24: PEPTIDE CHAIN RELEASE FACTOR 2

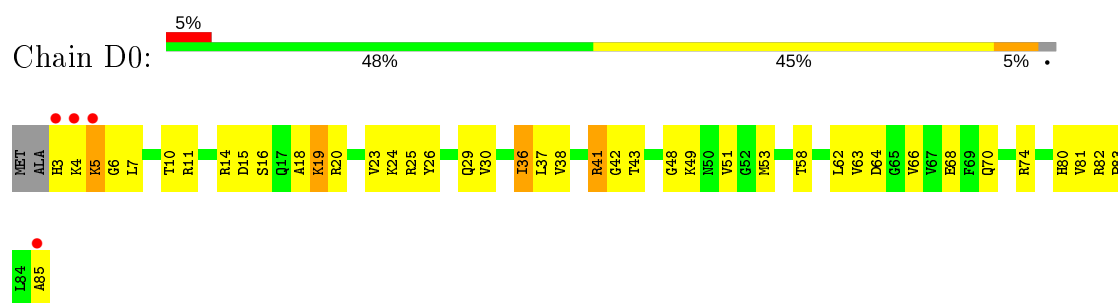




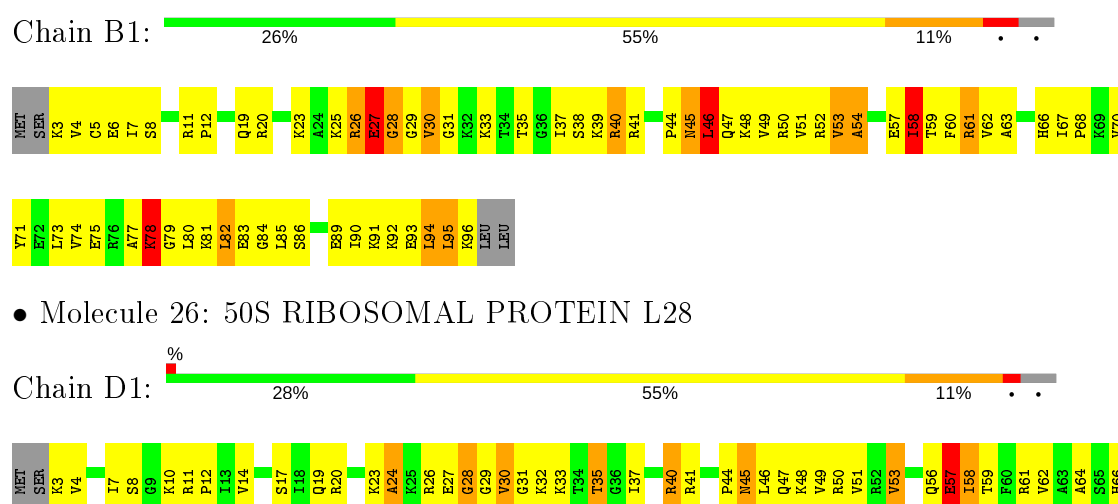
• Molecule 25: 50S RIBOSOMAL PROTEIN L27



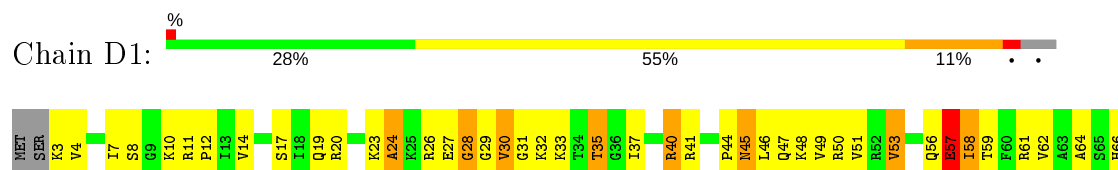
• Molecule 25: 50S RIBOSOMAL PROTEIN L27

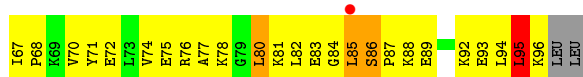


• Molecule 26: 50S RIBOSOMAL PROTEIN L28

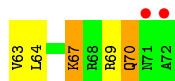
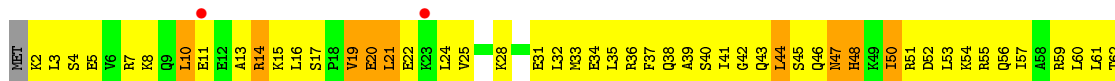


• Molecule 26: 50S RIBOSOMAL PROTEIN L28

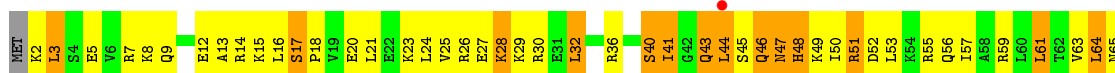




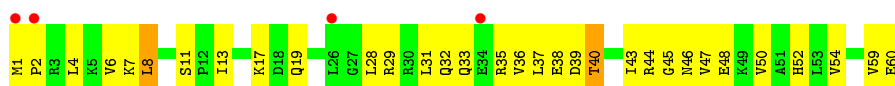
• Molecule 27: 50S RIBOSOMAL PROTEIN L29



• Molecule 27: 50S RIBOSOMAL PROTEIN L29



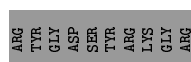
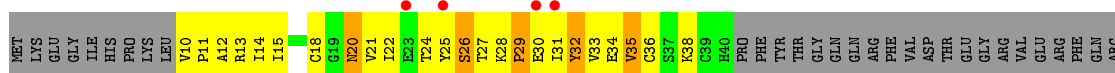
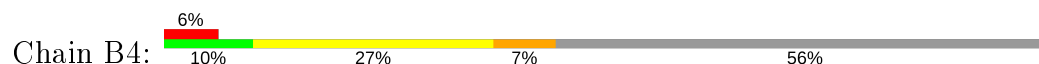
• Molecule 28: 50S RIBOSOMAL PROTEIN L30



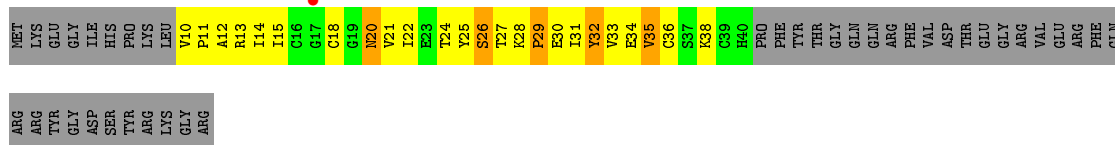
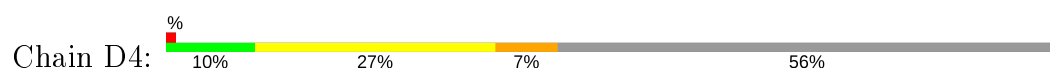
• Molecule 28: 50S RIBOSOMAL PROTEIN L30



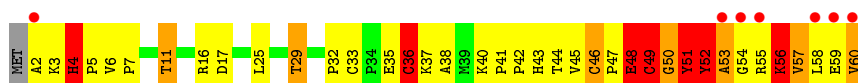
• Molecule 29: 50S RIBOSOMAL PROTEIN L31



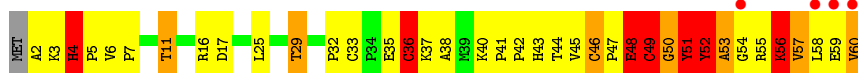
• Molecule 29: 50S RIBOSOMAL PROTEIN L31



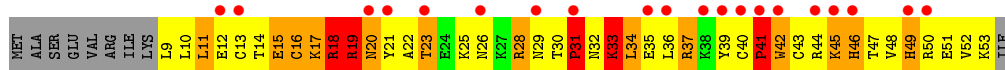
• Molecule 30: 50S RIBOSOMAL PROTEIN L32



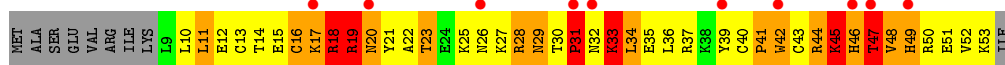
• Molecule 30: 50S RIBOSOMAL PROTEIN L32



• Molecule 31: 50S RIBOSOMAL PROTEIN L33



• Molecule 31: 50S RIBOSOMAL PROTEIN L33



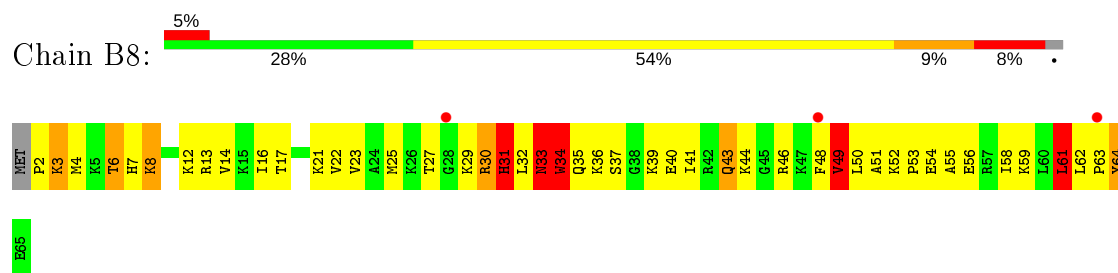
• Molecule 32: 50S RIBOSOMAL PROTEIN L34



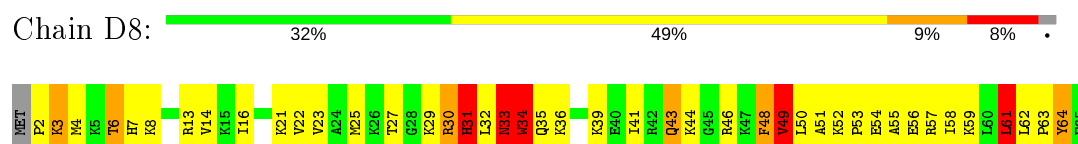
• Molecule 32: 50S RIBOSOMAL PROTEIN L34



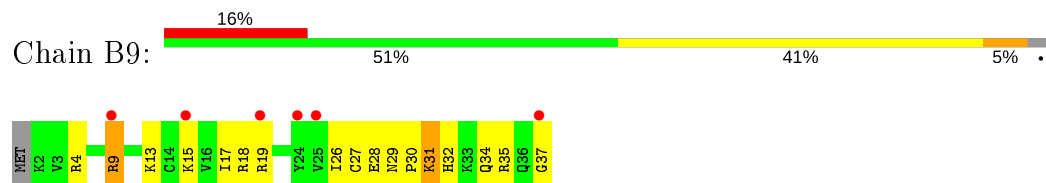
- Molecule 33: 50S RIBOSOMAL PROTEIN L35



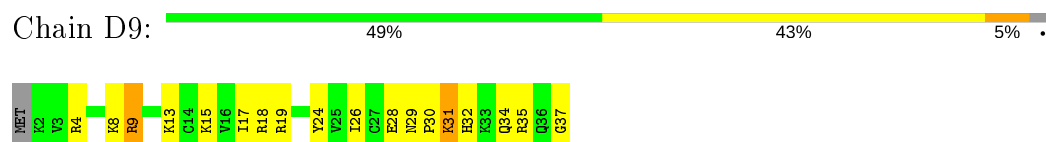
- Molecule 33: 50S RIBOSOMAL PROTEIN L35



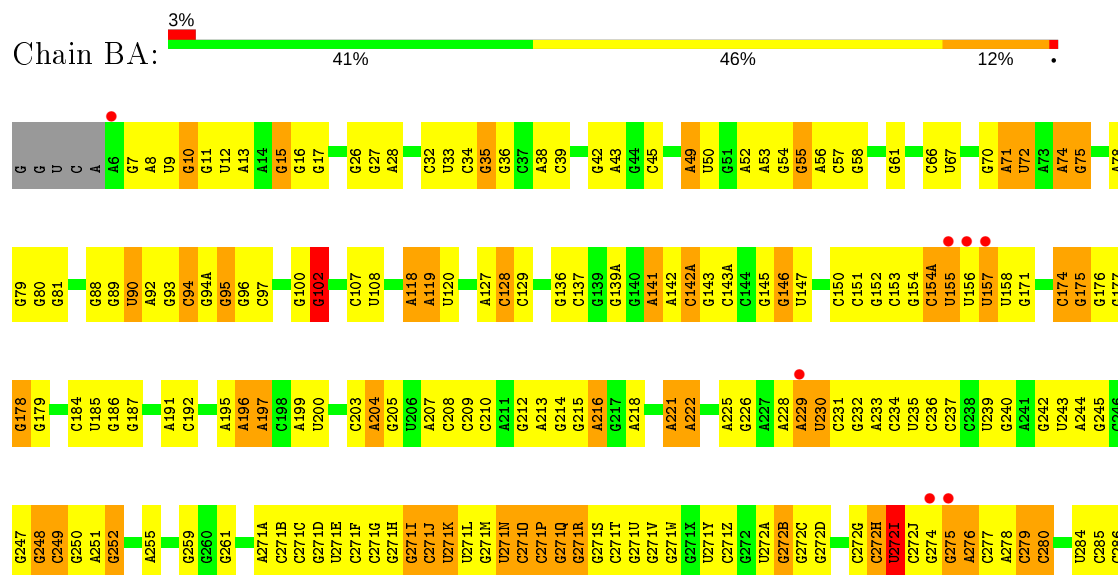
- Molecule 34: 50S RIBOSOMAL PROTEIN L36



- Molecule 34: 50S RIBOSOMAL PROTEIN L36

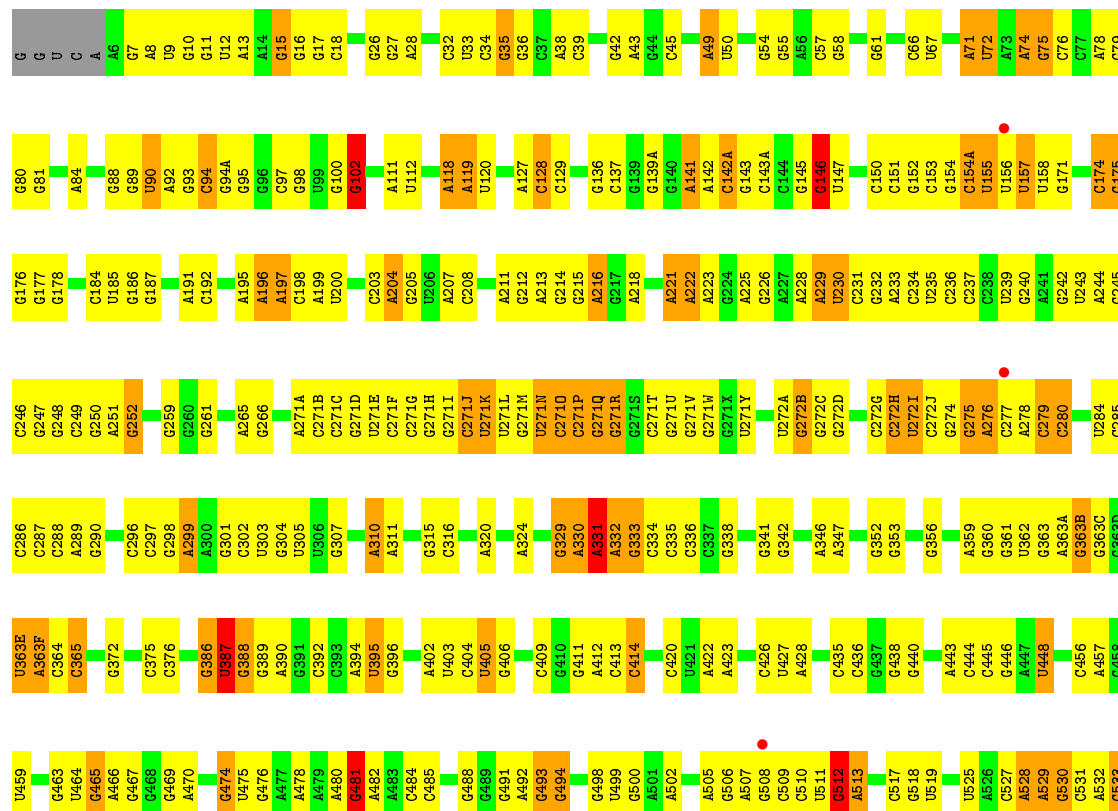


- Molecule 35: 23S RIBOSOMAL RNA



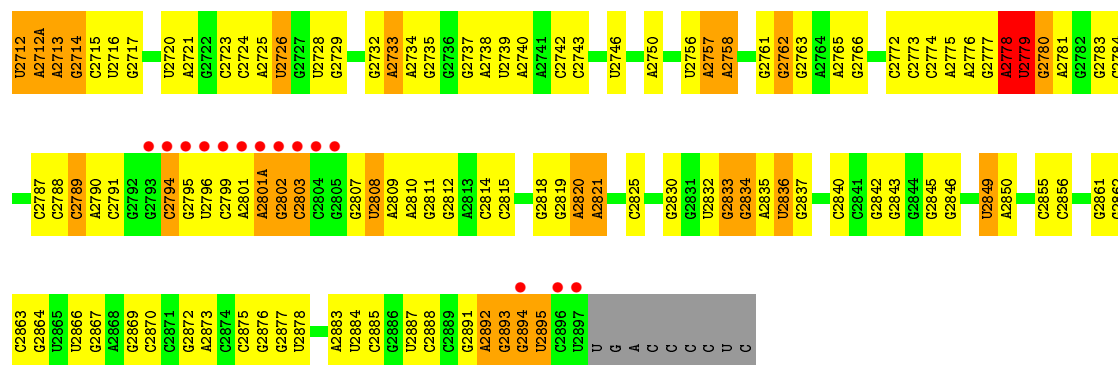
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A1272	C1181	C1109	C970	A896	C817	G660	G621	G553	U475	U387	A289
A1273	A1182	G1110	C970	C897	C818	C661	G622	G554	G476	G388	G290
A1274	A1111	G1111	A1050	C898	A819	G662	G623	U594	A477	G389	
G1275	G1186	G1112	G974	C899	U827	G663	G624	G558	A478	C392	C296
A1276	G1187	U1113	C975	U902	U828	C664	G625	G559	A479	C393	C297
G1277	A1188	G1114	G979	C903	A829	C665	U626	G599	A480	C394	G298
A1278	U1189	G1115	A980	G830	A829	A670	G627	U562	A481	A394	A299
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A1282	A1194	G1119	U907	U833	U833	G674	A631	U566	C485	G398	U303
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A1284	G1125	G1125	C909	U839	U839	A675	A633	G570	G488	A402	U305
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C1201	G1062	G1062	A910	C840	C840	A676	A633	A571	G490	U404	G307
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G1209	U1066	U1066	C915	G847	G847	A685	G638	U576	G494		
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G1218	G1075	G1075	G927	C856	C856	G695	G649	C584	A506	A423	G329
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G1222	G1079	G1079	G932	U860	U860	C698	A653	U588	C509	U428	G333
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G1226	G1083	G1083	G938	A866	A866	G708	C654B	C592	A513	G437	A346
G1227	A1084	A1084	A941	U869	U869	G709	G654C	G593	C517	G438	A347
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G1230	G1087	G1087	U943	C792	C792	G712	G654F	U597	U519	G442	G353
G1231	G1088	G1088	G944	G793	G793	G713	C654G	U598	U525	A443	
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G1237	A1094	A1094	G953	A878	A878	C719	C654M	C605	G530	U448	U362
G1238	U1094	U1094	A954	G879	G879	C720	C654N	U606	C531	G449	G363
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G1241	G1097	G1097	G957	G882	G882	G723	C654Q	A609	C534	G458	G366
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G1243	G1099	G1099	U959	G884	G884	A725	C654S	G611	A536	G463	G368
G1244	U1100	U1100	U960	A887	A887	G726	C654T	G612	C537	U464	U369
G1245	C1101	C1101	A961	C888	C888	G727	A654U	G613	G539	G465	A370
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G1247	C1043	C1043	G962	A890	A890	C730	A655	U614A	C541	G467	G372
G1248	G1044	G1044	U963	G892	G892	C731	G656	G614B	C542		
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WORLDWIDE
PDB
PROTEIN DATA BANK



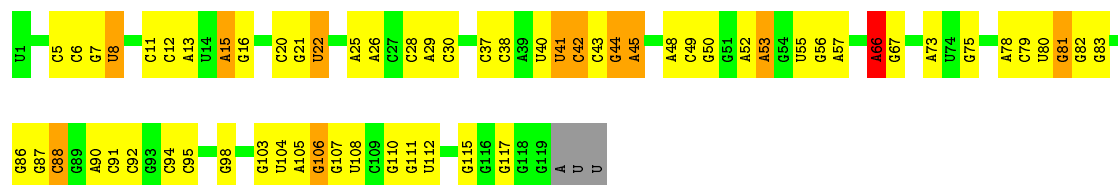


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G2648	G2481	G2565	G2482	U2406	G2252	A2169	C2105	U2028	G1936	G1846	C1766	U1679	C1574
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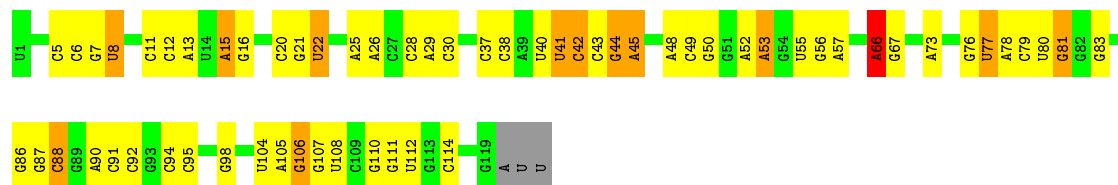
• Molecule 36: 5S RIBOSOMAL RNA

Chain BB: 46% 42% 9% ..



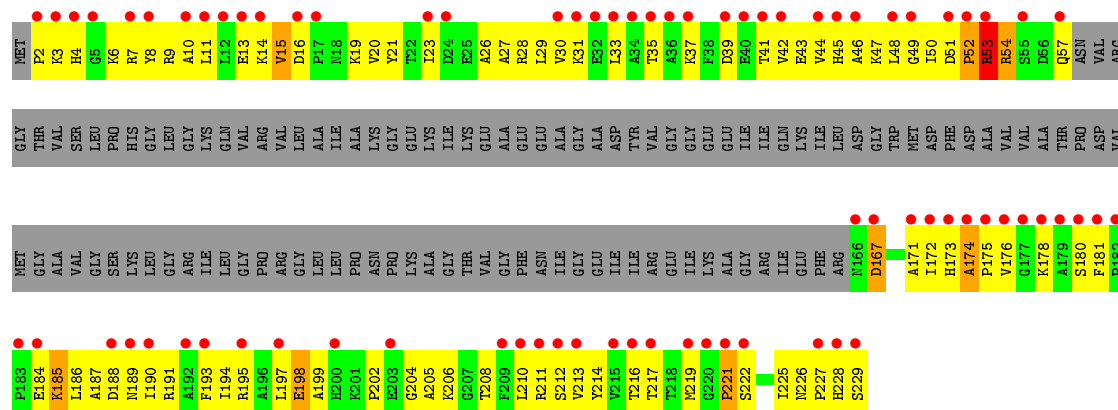
• Molecule 36: 5S RIBOSOMAL RNA

Chain DB: 48% 39% 10% ..

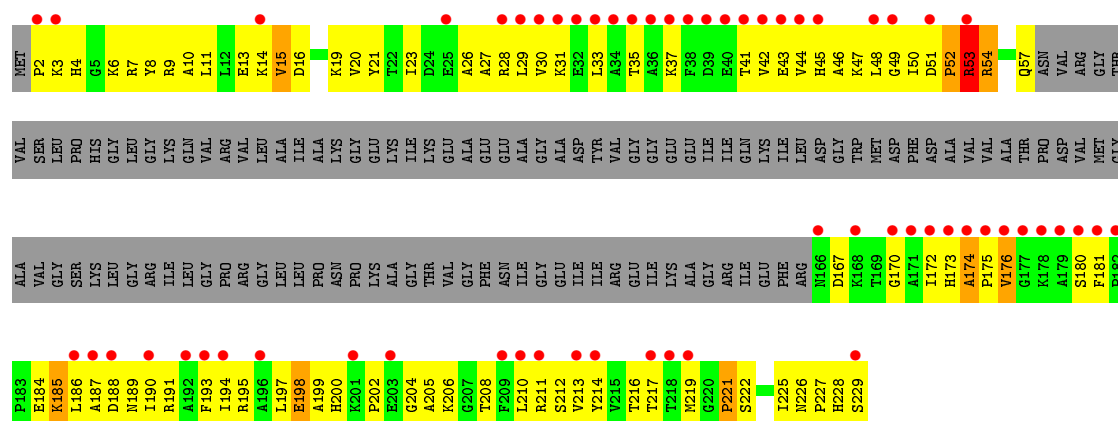


• Molecule 37: 50S RIBOSOMAL PROTEIN L1

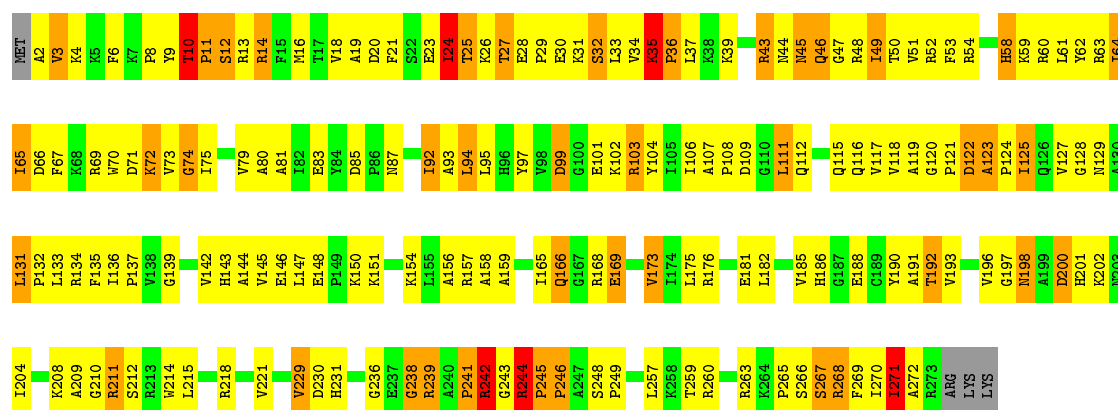
Chain BC: 15% 34% 48%



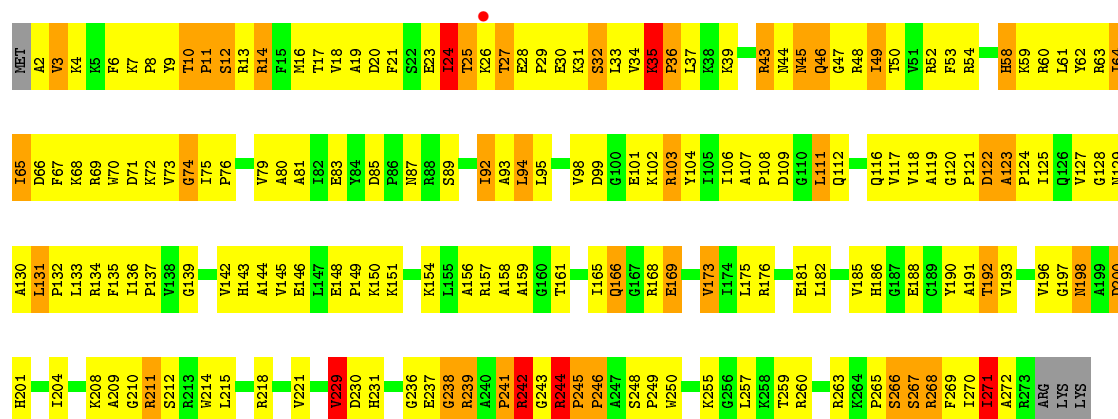
• Molecule 37: 50S RIBOSOMAL PROTEIN L1



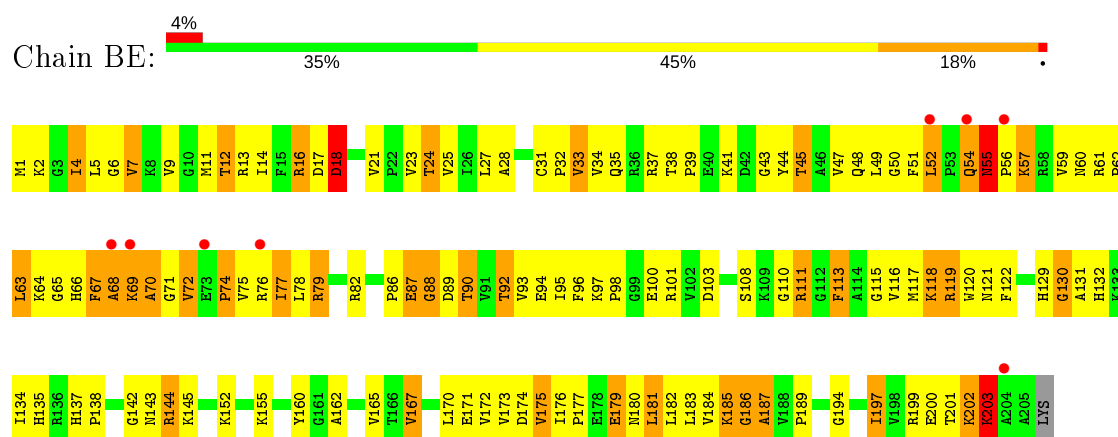
• Molecule 38: 50S RIBOSOMAL PROTEIN L2



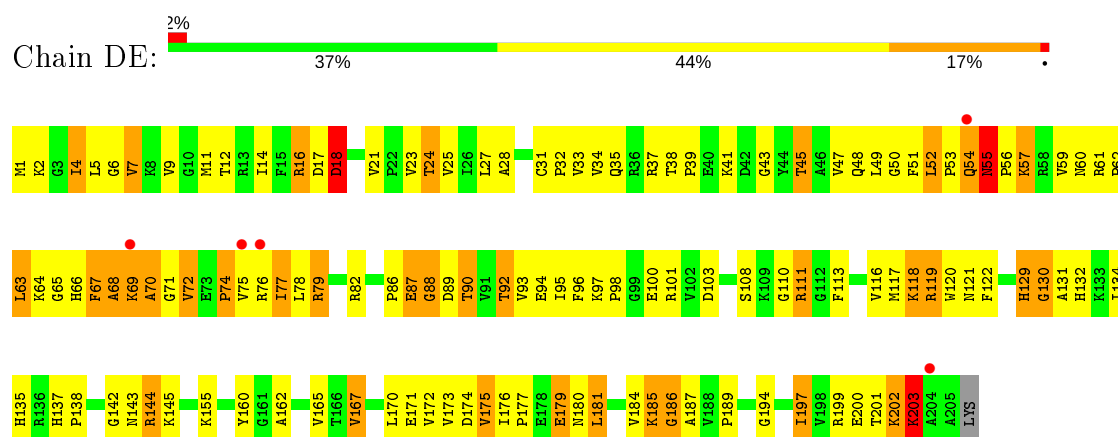
• Molecule 38: 50S RIBOSOMAL PROTEIN L2



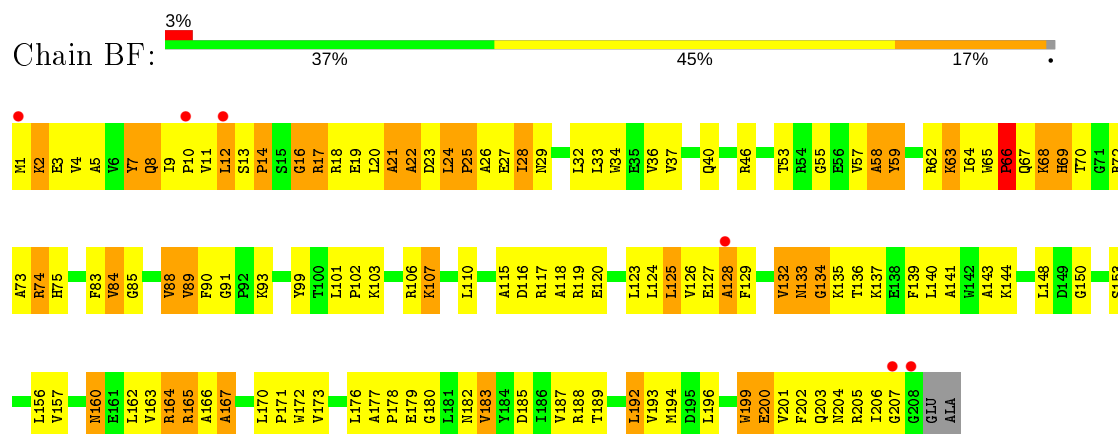
• Molecule 39: 50S RIBOSOMAL PROTEIN L3



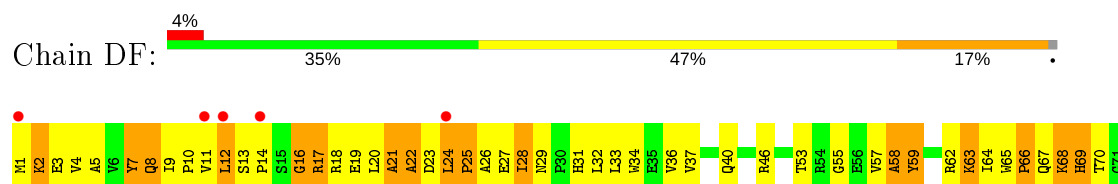
• Molecule 39: 50S RIBOSOMAL PROTEIN L3

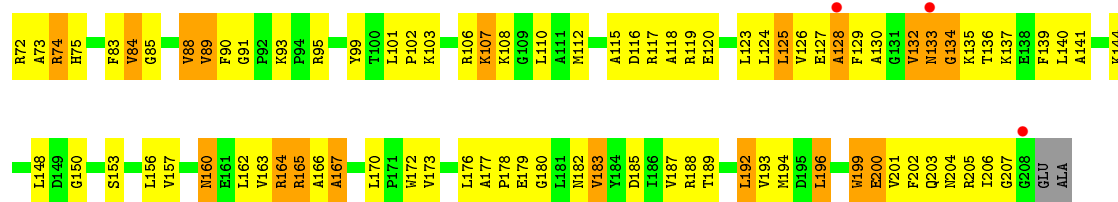


• Molecule 40: 50S RIBOSOMAL PROTEIN L4

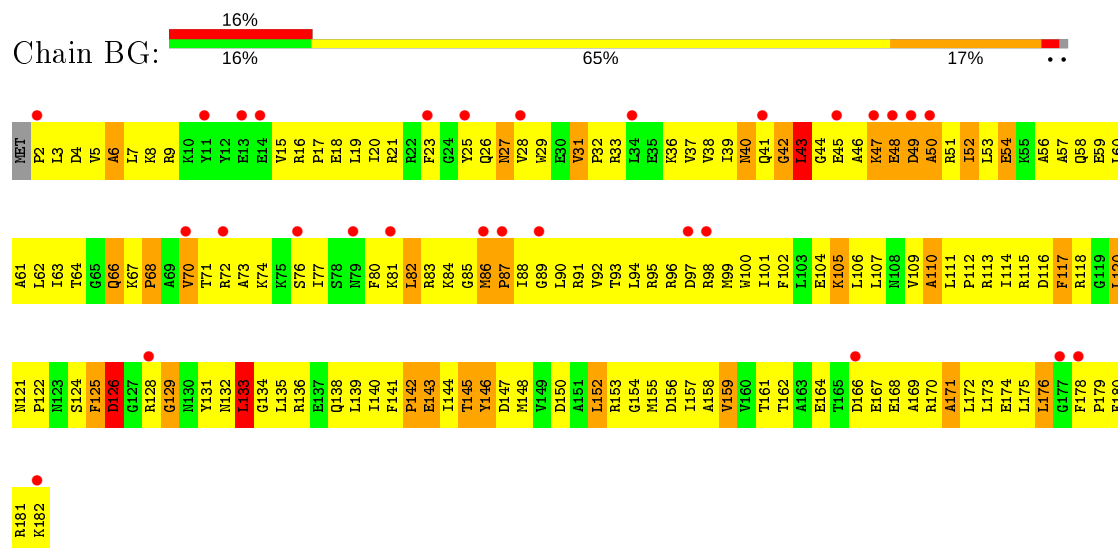


• Molecule 40: 50S RIBOSOMAL PROTEIN L4

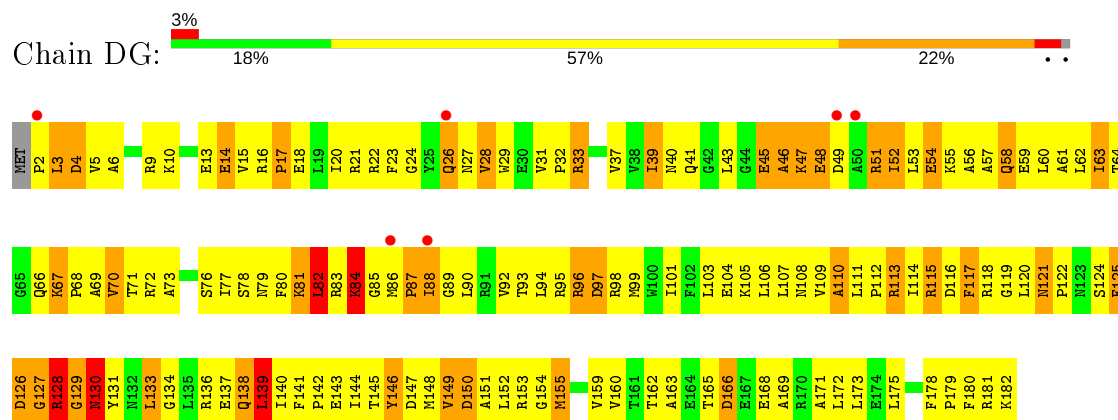




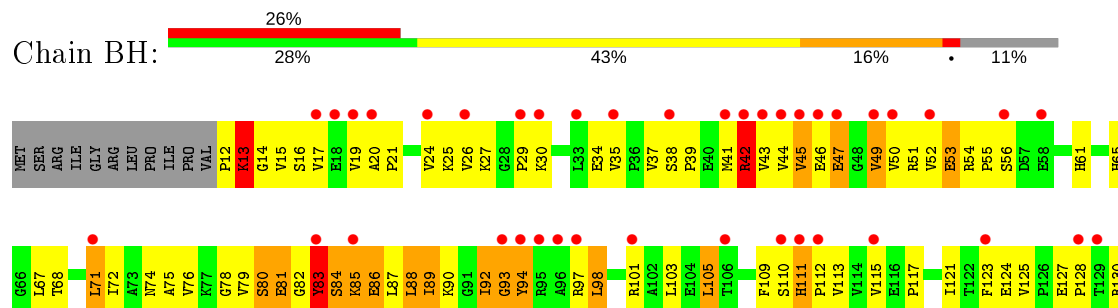
• Molecule 41: 50S RIBOSOMAL PROTEIN L5

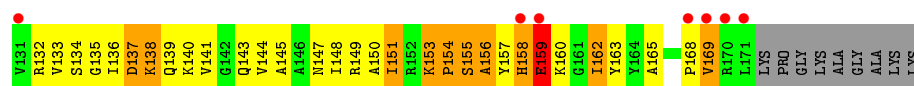


• Molecule 41: 50S RIBOSOMAL PROTEIN L5

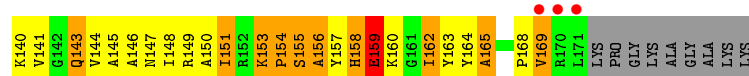
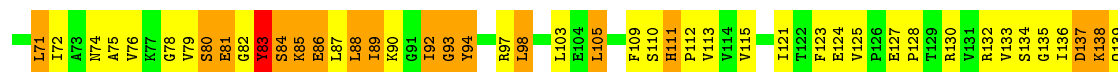
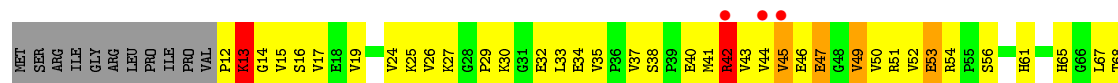


• Molecule 42: 50S RIBOSOMAL PROTEIN L6

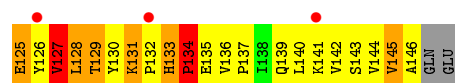
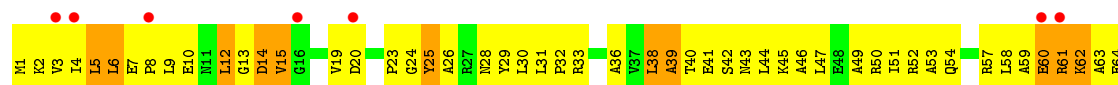




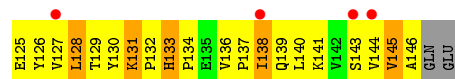
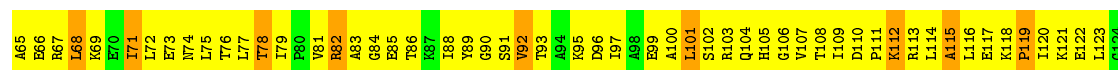
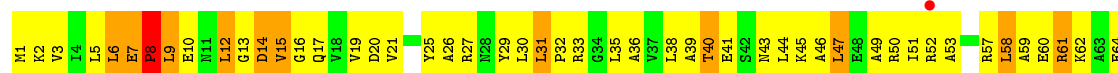
• Molecule 42: 50S RIBOSOMAL PROTEIN L6



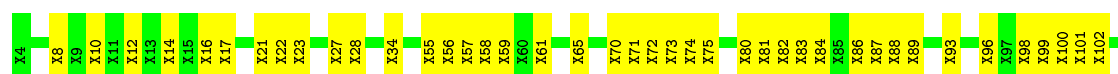
• Molecule 43: 50S RIBOSOMAL PROTEIN L9



• Molecule 43: 50S RIBOSOMAL PROTEIN L9



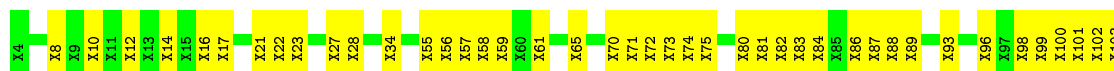
• Molecule 44: 50S RIBOSOMAL PROTEIN L10





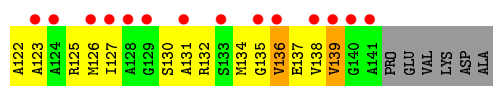
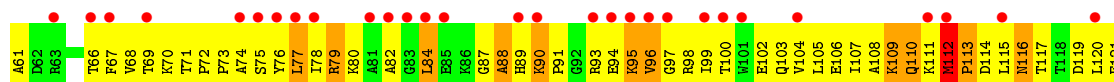
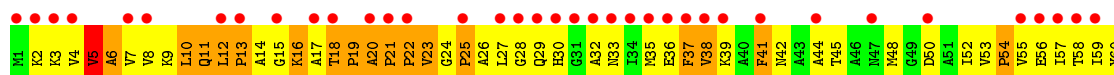
• Molecule 44: 50S RIBOSOMAL PROTEIN L10

Chain DJ: 62% 38%



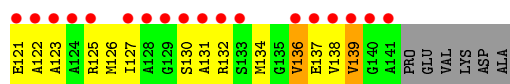
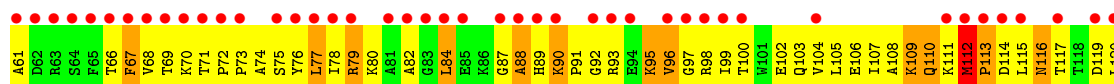
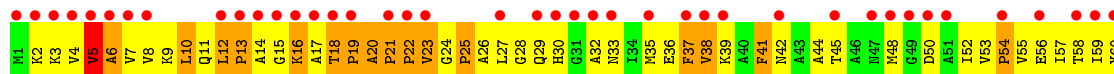
• Molecule 45: 50S RIBOSOMAL PROTEIN L11

Chain BK: 18% 54% 56% 20%



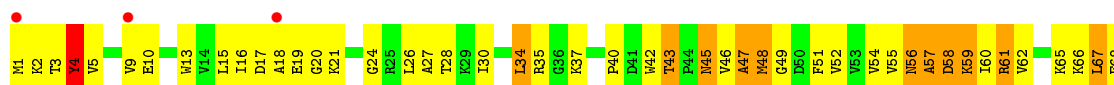
• Molecule 45: 50S RIBOSOMAL PROTEIN L11

Chain DK: 18% 70% 56% 20%



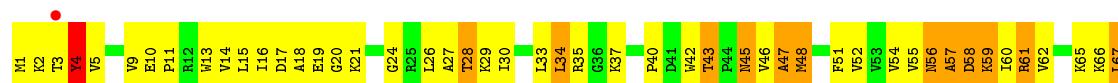
• Molecule 46: 50S RIBOSOMAL PROTEIN L13

Chain BN: 2% 40% 48% 11%





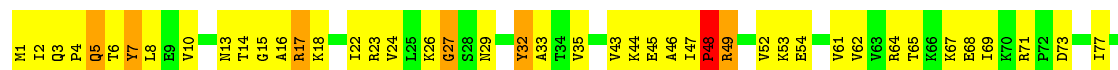
• Molecule 46: 50S RIBOSOMAL PROTEIN L13



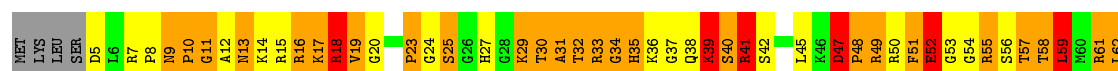
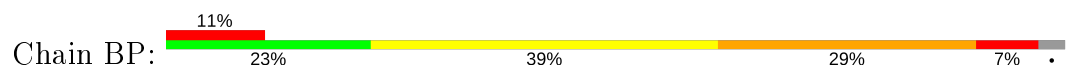
• Molecule 47: 50S RIBOSOMAL PROTEIN L14



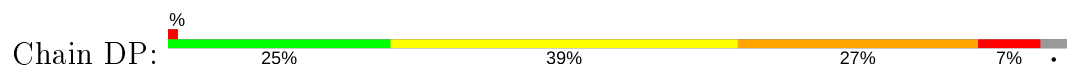
• Molecule 48: 50S RIBOSOMAL PROTEIN L15

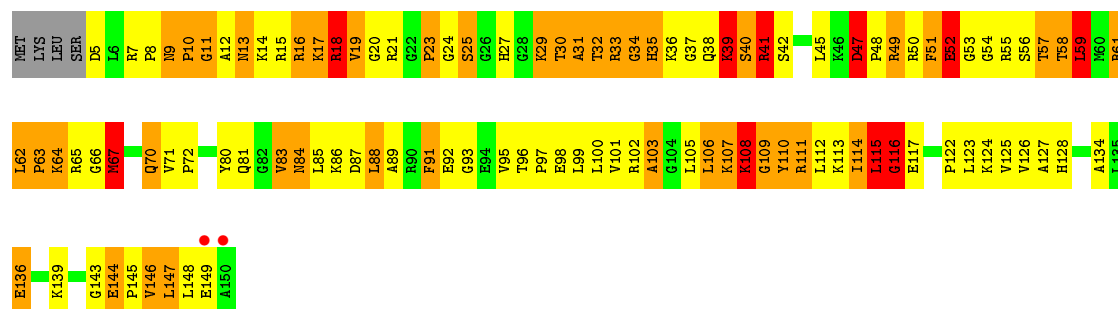


• Molecule 49: 50S RIBOSOMAL PROTEIN L16

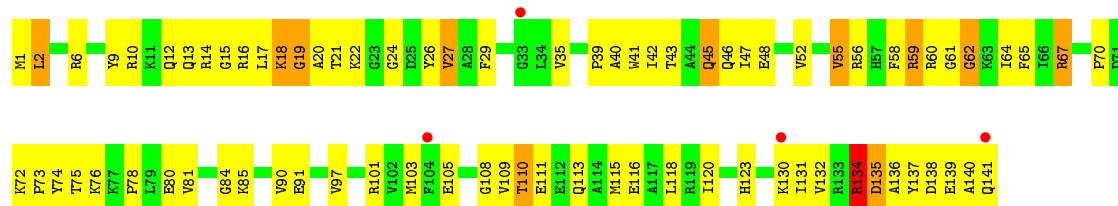


• Molecule 50: 50S RIBOSOMAL PROTEIN L17

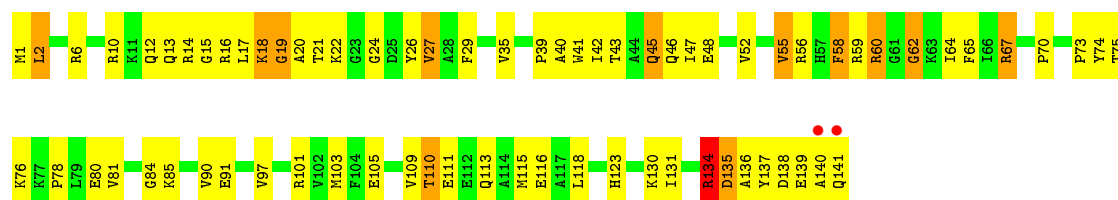




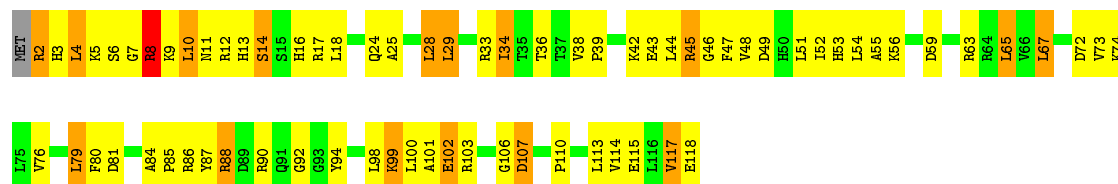
• Molecule 49: 50S RIBOSOMAL PROTEIN L16



• Molecule 49: 50S RIBOSOMAL PROTEIN L16

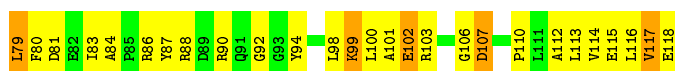


• Molecule 50: 50S RIBOSOMAL PROTEIN L17



• Molecule 50: 50S RIBOSOMAL PROTEIN L17

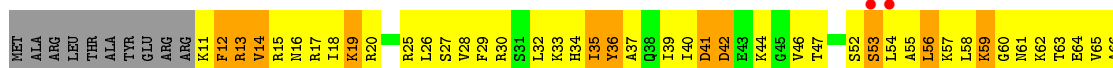




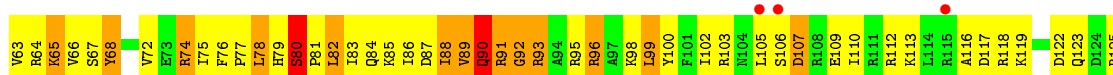
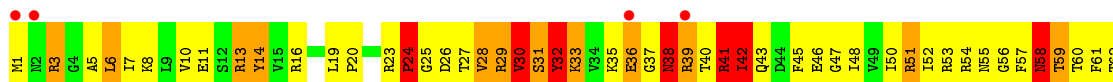
• Molecule 51: 50S RIBOSOMAL PROTEIN L18



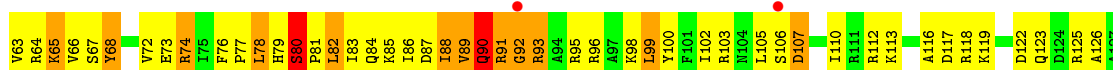
• Molecule 51: 50S RIBOSOMAL PROTEIN L18

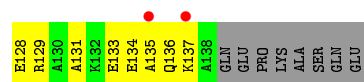


• Molecule 52: 50S RIBOSOMAL PROTEIN L19

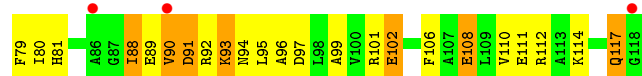


• Molecule 52: 50S RIBOSOMAL PROTEIN L19

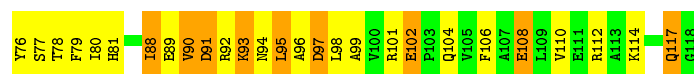
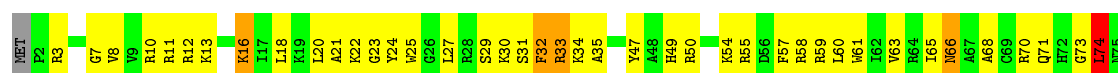




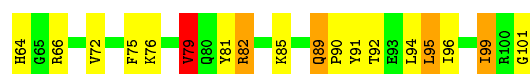
• Molecule 53: 50S RIBOSOMAL PROTEIN L20



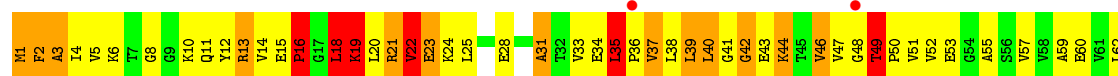
• Molecule 53: 50S RIBOSOMAL PROTEIN L20



• Molecule 54: 50S RIBOSOMAL PROTEIN L21

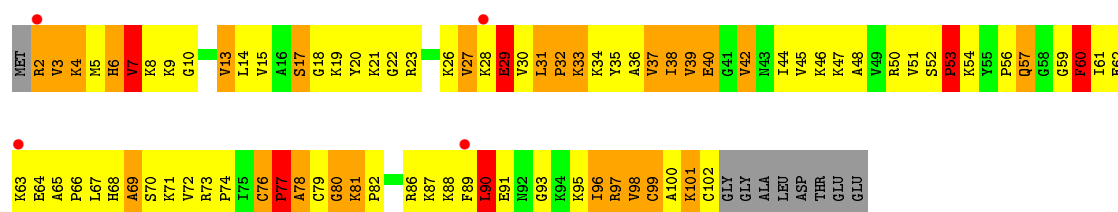
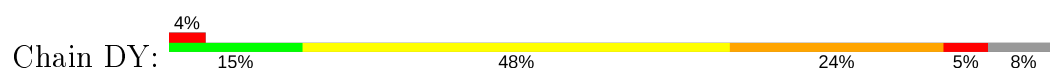


• Molecule 54: 50S RIBOSOMAL PROTEIN L21

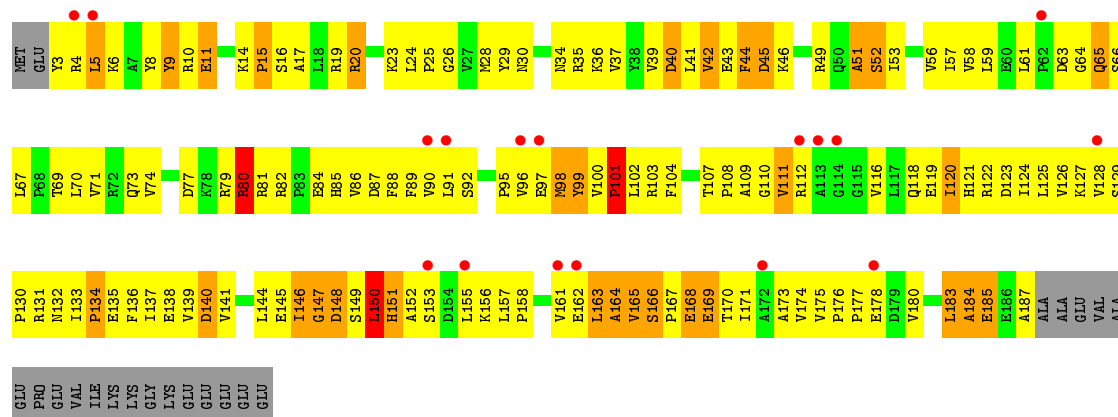


• Molecule 55: 50S RIBOSOMAL PROTEIN L22

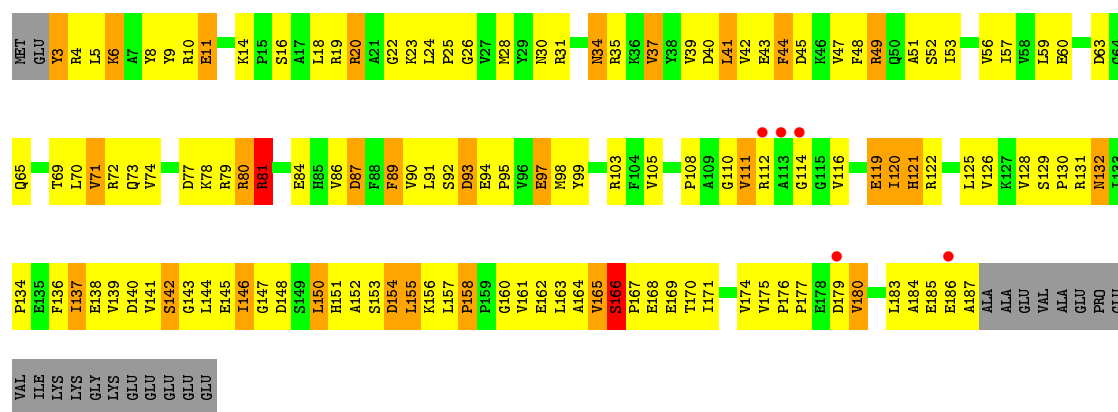




• Molecule 58: 50S RIBOSOMAL PROTEIN L25



• Molecule 58: 50S RIBOSOMAL PROTEIN L25



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	211.42Å 452.50Å 625.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.86 – 3.10 49.71 – 3.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.86-3.10) 99.6 (49.71-3.00)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 3.01Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.223 , 0.264 0.223 , 0.265	Depositor DCC
R_{free} test set	52374 reflections (4.44%)	wwPDB-VP
Wilson B-factor (Å ²)	55.0	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 79.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	305067	wwPDB-VP
Average B, all atoms (Å ²)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.49% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ZN, 8AN, PHA

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	0.37	0/36190	0.69	14/56486 (0.0%)
1	CA	0.39	0/36190	0.69	11/56486 (0.0%)
2	AB	0.31	0/1936	0.58	0/2611
2	CB	0.33	0/1936	0.58	0/2611
3	AC	0.32	0/1637	0.54	0/2207
3	CC	0.32	0/1637	0.54	0/2207
4	AD	0.33	0/1733	0.63	0/2318
4	CD	0.33	0/1733	0.62	0/2318
5	AE	0.34	0/1163	0.61	0/1566
5	CE	0.35	0/1163	0.62	0/1566
6	AF	0.32	0/856	0.63	0/1154
6	CF	0.34	0/856	0.64	0/1154
7	AG	0.30	0/1276	0.56	0/1709
7	CG	0.31	0/1276	0.56	0/1709
8	AH	0.32	0/1136	0.61	0/1527
8	CH	0.32	0/1136	0.62	0/1527
9	AI	0.31	0/1027	0.58	0/1372
9	CI	0.32	0/1027	0.58	0/1372
10	AJ	0.32	0/808	0.56	0/1087
10	CJ	0.33	0/808	0.56	0/1087
11	AK	0.32	0/900	0.58	0/1213
11	CK	0.36	0/900	0.59	0/1213
12	AL	0.36	0/987	0.67	0/1322
12	CL	0.36	0/987	0.67	0/1322
13	AM	0.30	0/994	0.56	0/1322
13	CM	0.32	0/994	0.56	0/1322
14	AN	0.31	0/501	0.53	0/664
14	CN	0.33	0/501	0.55	0/664
15	AO	0.32	0/745	0.57	0/992
15	CO	0.33	0/745	0.58	0/992
16	AP	0.36	0/717	0.58	0/965
16	CP	0.34	0/717	0.58	0/965

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AQ	0.33	0/837	0.61	0/1119
17	CQ	0.35	0/837	0.61	0/1119
18	AR	0.33	0/579	0.60	0/768
18	CR	0.34	0/579	0.60	0/768
19	AS	0.34	0/643	0.56	0/867
19	CS	0.34	0/643	0.57	0/867
20	AT	0.29	0/765	0.58	0/1007
20	CT	0.29	0/765	0.58	0/1007
21	AU	0.41	0/213	0.49	0/279
21	CU	0.42	0/213	0.50	0/279
22	AV	0.38	0/1784	0.70	0/2780
22	AW	0.35	0/1784	0.71	0/2780
22	CV	0.44	0/1784	0.69	0/2780
22	CW	0.36	0/1784	0.70	0/2780
23	AX	0.39	0/184	0.74	0/284
23	CX	0.45	0/184	0.76	0/284
24	AY	0.31	0/2849	0.60	0/3848
24	CY	0.33	0/2849	0.66	0/3848
25	B0	0.36	0/666	0.63	0/885
25	D0	0.42	0/666	0.67	0/885
26	B1	0.41	0/739	0.73	1/983 (0.1%)
26	D1	0.50	0/739	0.79	0/983
27	B2	0.36	0/600	0.60	0/793
27	D2	0.46	0/600	0.79	0/793
28	B3	0.34	0/473	0.61	0/636
28	D3	0.43	0/473	0.65	0/636
29	B4	0.38	0/229	0.61	0/311
29	D4	0.40	0/229	0.62	0/311
30	B5	0.49	0/473	0.94	2/639 (0.3%)
30	D5	0.71	2/473 (0.4%)	1.01	2/639 (0.3%)
31	B6	0.48	0/387	0.79	0/517
31	D6	0.54	0/388	0.77	0/520
32	B7	0.46	0/427	0.67	0/563
32	D7	0.53	0/427	0.70	0/563
33	B8	0.50	0/516	0.78	0/681
33	D8	0.59	0/516	0.81	0/681
34	B9	0.33	0/302	0.63	0/397
34	D9	0.44	0/302	0.68	0/397
35	BA	0.46	1/69972 (0.0%)	0.74	51/109237 (0.0%)
35	DA	0.60	1/69972 (0.0%)	0.76	63/109237 (0.1%)
36	BB	0.37	0/2853	0.73	0/4451
36	DB	0.50	0/2853	0.74	0/4451
37	BC	0.27	0/956	0.51	0/1288

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
37	DC	0.27	0/956	0.51	0/1288
38	BD	0.42	0/2155	0.77	1/2907 (0.0%)
38	DD	0.49	0/2155	0.80	2/2907 (0.1%)
39	BE	0.42	0/1597	0.77	0/2155
39	DE	0.52	0/1597	0.80	0/2155
40	BF	0.41	0/1659	0.72	1/2246 (0.0%)
40	DF	0.49	0/1659	0.76	1/2246 (0.0%)
41	BG	0.32	0/1498	0.62	0/2013
41	DG	0.39	0/1499	0.75	2/2016 (0.1%)
42	BH	0.35	0/1246	0.70	0/1684
42	DH	0.43	0/1246	0.73	0/1684
43	BI	0.36	0/1147	0.68	0/1553
43	DI	0.35	0/1147	0.74	0/1553
45	BK	0.33	0/1057	0.58	0/1432
45	DK	0.34	0/1057	0.58	0/1432
46	BN	0.37	0/1132	0.76	1/1527 (0.1%)
46	DN	0.47	0/1132	0.80	1/1527 (0.1%)
47	BO	0.42	0/943	0.69	0/1269
47	DO	0.47	0/943	0.71	0/1269
48	BP	0.44	0/1131	0.99	7/1504 (0.5%)
48	DP	0.55	0/1131	1.04	7/1504 (0.5%)
49	BQ	0.37	0/1143	0.66	0/1527
49	DQ	0.46	0/1143	0.69	0/1527
50	BR	0.39	0/974	0.73	2/1302 (0.2%)
50	DR	0.48	0/974	0.77	2/1302 (0.2%)
51	BS	0.39	0/779	0.70	0/1038
51	DS	0.48	0/779	0.73	0/1038
52	BT	0.43	0/1156	0.81	3/1544 (0.2%)
52	DT	0.48	0/1156	0.83	3/1544 (0.2%)
53	BU	0.41	0/975	0.68	1/1297 (0.1%)
53	DU	0.54	0/975	0.75	2/1297 (0.2%)
54	BV	0.38	0/790	0.73	0/1057
54	DV	0.48	0/790	0.79	0/1057
55	BW	0.39	0/907	0.70	0/1216
55	DW	0.48	0/907	0.74	0/1216
56	BX	0.41	0/740	0.70	0/995
56	DX	0.49	0/740	0.73	0/995
57	BY	0.44	0/789	0.75	0/1053
57	DY	0.52	0/789	0.77	1/1053 (0.1%)
58	BZ	0.36	0/1500	0.65	0/2037
58	DZ	0.42	0/1500	0.71	0/2037
All	All	0.46	4/328312 (0.0%)	0.72	181/489974 (0.0%)

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	1	15
1	CA	1	17
22	AW	0	1
22	CV	0	1
22	CW	0	3
30	B5	0	2
30	D5	0	2
35	BA	5	59
35	DA	6	77
36	BB	0	2
36	DB	0	3
All	All	13	182

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	D5	49	CYS	CB-SG	5.59	1.91	1.82
35	DA	2685	G	C6-O6	5.54	1.29	1.24
35	BA	1899	G	C2-N2	-5.53	1.29	1.34
30	D5	51	TYR	CD1-CE1	5.27	1.47	1.39

The worst 5 of 181 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	BA	1992	G	C2'-C3'-O3'	10.98	133.66	109.50
35	DA	1992	G	C2'-C3'-O3'	10.73	133.11	109.50
35	DA	331	A	C2'-C3'-O3'	9.84	131.14	109.50
35	BA	331	A	C2'-C3'-O3'	9.40	130.19	109.50
35	DA	1653	G	C2'-C3'-O3'	9.16	129.65	109.50

5 of 13 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	AA	1504	G	C3'
35	BA	587	C	C3'
35	BA	1300	U	C3'
35	BA	1799	G	C3'
35	BA	1819	A	C3'

5 of 182 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	21	G	Sidechain
1	AA	575	G	Sidechain
1	AA	587	G	Sidechain
1	AA	760	G	Sidechain
1	AA	832	C	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	16314	1204	0
1	CA	32329	0	16316	1222	0
2	AB	1901	0	1951	258	0
2	CB	1901	0	1951	259	0
3	AC	1613	0	1677	199	0
3	CC	1613	0	1677	196	0
4	AD	1703	0	1763	219	0
4	CD	1703	0	1763	207	0
5	AE	1147	0	1207	125	0
5	CE	1147	0	1207	125	0
6	AF	843	0	857	88	0
6	CF	843	0	857	95	0
7	AG	1257	0	1296	113	0
7	CG	1257	0	1296	121	0
8	AH	1116	0	1177	118	0
8	CH	1116	0	1177	113	0
9	AI	1011	0	1041	126	0
9	CI	1011	0	1041	129	0
10	AJ	795	0	840	146	0
10	CJ	795	0	840	144	0
11	AK	885	0	904	74	0
11	CK	885	0	904	77	0
12	AL	971	0	1057	122	0
12	CL	971	0	1057	124	0
13	AM	988	0	1055	161	0
13	CM	988	0	1055	153	0
14	AN	492	0	530	66	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	CN	492	0	529	65	0
15	AO	734	0	771	55	0
15	CO	734	0	771	52	0
16	AP	701	0	720	81	0
16	CP	701	0	720	87	0
17	AQ	824	0	891	62	0
17	CQ	824	0	891	63	0
18	AR	574	0	644	59	0
18	CR	574	0	644	59	0
19	AS	630	0	651	98	0
19	CS	630	0	651	100	0
20	AT	763	0	861	73	0
20	CT	763	0	861	78	0
21	AU	209	0	221	24	0
21	CU	209	0	221	26	0
22	AV	1630	0	831	76	0
22	AW	1630	0	831	101	0
22	CV	1630	0	831	65	0
22	CW	1630	0	832	110	0
23	AX	165	0	87	11	0
23	CX	165	0	87	17	0
24	AY	2801	0	2816	377	0
24	CY	2801	0	2816	430	0
25	B0	657	0	683	58	0
25	D0	657	0	683	55	0
26	B1	732	0	808	88	0
26	D1	732	0	808	80	0
27	B2	598	0	653	81	0
27	D2	598	0	653	77	0
28	B3	468	0	523	40	0
28	D3	468	0	523	42	0
29	B4	226	0	229	46	0
29	D4	226	0	229	45	0
30	B5	459	0	480	74	0
30	D5	459	0	480	74	0
31	B6	381	0	390	73	0
31	D6	381	0	389	149	0
32	B7	419	0	467	19	0
32	D7	419	0	467	22	0
33	B8	508	0	576	103	0
33	D8	508	0	576	103	0
34	B9	299	0	323	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	D9	299	0	323	24	0
35	BA	62474	0	31492	1876	0
35	DA	62474	0	31493	1854	0
36	BB	2551	0	1295	80	0
36	DB	2551	0	1295	70	0
37	BC	937	0	957	106	0
37	DC	937	0	957	108	0
38	BD	2105	0	2182	248	0
38	DD	2105	0	2182	254	0
39	BE	1564	0	1629	191	0
39	DE	1564	0	1629	192	0
40	BF	1624	0	1677	189	0
40	DF	1624	0	1677	188	0
41	BG	1474	0	1534	286	0
41	DG	1474	0	1535	240	0
42	BH	1223	0	1282	139	0
42	DH	1223	0	1282	145	0
43	BI	1132	0	1218	179	0
43	DI	1132	0	1218	181	0
44	BJ	651	0	151	34	0
44	DJ	651	0	151	34	0
45	BK	1038	0	1089	196	0
45	DK	1038	0	1089	192	0
46	BN	1105	0	1180	127	0
46	DN	1105	0	1180	134	0
47	BO	933	0	996	84	0
47	DO	933	0	996	93	0
48	BP	1114	0	1187	268	0
48	DP	1114	0	1187	263	0
49	BQ	1122	0	1179	127	0
49	DQ	1122	0	1179	110	0
50	BR	960	0	1021	93	0
50	DR	960	0	1021	94	0
51	BS	771	0	832	126	0
51	DS	771	0	832	121	0
52	BT	1142	0	1202	223	0
52	DT	1142	0	1202	228	0
53	BU	958	0	1015	103	0
53	DU	958	0	1015	109	0
54	BV	779	0	852	132	0
54	DV	779	0	852	133	0
55	BW	896	0	953	50	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	DW	896	0	953	50	0
56	BX	726	0	778	73	0
56	DX	726	0	778	70	0
57	BY	776	0	870	178	0
57	DY	776	0	870	190	0
58	BZ	1468	0	1492	228	0
58	DZ	1468	0	1492	188	0
59	AA	161	0	0	0	0
59	AL	1	0	0	0	0
59	AS	1	0	0	0	0
59	AV	7	0	0	0	0
59	AW	4	0	0	0	0
59	AX	1	0	0	0	0
59	AY	1	0	0	0	0
59	B1	1	0	0	0	0
59	B5	2	0	0	0	0
59	BA	357	0	0	0	0
59	BB	4	0	0	0	0
59	BD	2	0	0	0	0
59	BF	2	0	0	0	0
59	BG	1	0	0	0	0
59	BT	1	0	0	0	0
59	BX	1	0	0	0	0
59	BY	1	0	0	0	0
59	CA	155	0	0	0	0
59	CD	1	0	0	0	0
59	CL	2	0	0	0	0
59	CN	1	0	0	0	0
59	CS	1	0	0	0	0
59	CV	7	0	0	0	0
59	CW	4	0	0	0	0
59	CX	1	0	0	0	0
59	D1	1	0	0	0	0
59	D5	2	0	0	0	0
59	DA	359	0	0	0	0
59	DB	4	0	0	0	0
59	DD	1	0	0	0	0
59	DE	1	0	0	0	0
59	DF	1	0	0	0	0
59	DG	1	0	0	0	0
59	DH	1	0	0	0	0
59	DP	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	DS	1	0	0	0	0
59	DX	1	0	0	0	0
60	AD	1	0	0	0	0
60	AN	1	0	0	0	0
60	B9	1	0	0	0	0
60	CD	1	0	0	0	0
60	CN	1	0	0	0	0
60	D9	1	0	0	0	0
61	AV	1	0	0	0	0
61	AY	1	0	0	0	0
61	BA	1	0	0	1	0
All	All	305067	0	208379	18089	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 35.

The worst 5 of 18089 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)
24:CY:303:ARG:HH22	35:DA:1914:C:C1'	1.34	1.39
24:CY:303:ARG:NH2	35:DA:1914:C:H1'	1.33	1.39
31:D6:41:PRO:HD3	31:D6:46:HIS:CB	1.55	1.36
31:D6:46:HIS:CA	31:D6:47:THR:HG23	1.58	1.33
35:DA:1899:G:N2	35:DA:1902:C:H41	1.26	1.32

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	AB	233/256 (91%)	127 (54%)	71 (30%)	35 (15%)	0 0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	CB	233/256 (91%)	128 (55%)	70 (30%)	35 (15%)	0	0
3	AC	205/239 (86%)	129 (63%)	40 (20%)	36 (18%)	0	0
3	CC	205/239 (86%)	129 (63%)	42 (20%)	34 (17%)	0	0
4	AD	206/209 (99%)	139 (68%)	45 (22%)	22 (11%)	0	2
4	CD	206/209 (99%)	139 (68%)	44 (21%)	23 (11%)	0	2
5	AE	149/162 (92%)	115 (77%)	23 (15%)	11 (7%)	1	6
5	CE	149/162 (92%)	114 (76%)	24 (16%)	11 (7%)	1	6
6	AF	99/101 (98%)	70 (71%)	21 (21%)	8 (8%)	1	5
6	CF	99/101 (98%)	73 (74%)	18 (18%)	8 (8%)	1	5
7	AG	153/156 (98%)	117 (76%)	26 (17%)	10 (6%)	1	8
7	CG	153/156 (98%)	117 (76%)	27 (18%)	9 (6%)	1	10
8	AH	136/138 (99%)	106 (78%)	23 (17%)	7 (5%)	2	13
8	CH	136/138 (99%)	104 (76%)	24 (18%)	8 (6%)	1	10
9	AI	121/128 (94%)	86 (71%)	24 (20%)	11 (9%)	1	4
9	CI	121/128 (94%)	86 (71%)	24 (20%)	11 (9%)	1	4
10	AJ	97/105 (92%)	70 (72%)	22 (23%)	5 (5%)	2	12
10	CJ	97/105 (92%)	71 (73%)	21 (22%)	5 (5%)	2	12
11	AK	117/129 (91%)	86 (74%)	27 (23%)	4 (3%)	3	21
11	CK	117/129 (91%)	87 (74%)	26 (22%)	4 (3%)	3	21
12	AL	123/132 (93%)	84 (68%)	21 (17%)	18 (15%)	0	1
12	CL	123/132 (93%)	84 (68%)	21 (17%)	18 (15%)	0	1
13	AM	113/126 (90%)	71 (63%)	25 (22%)	17 (15%)	0	0
13	CM	113/126 (90%)	70 (62%)	26 (23%)	17 (15%)	0	0
14	AN	58/61 (95%)	40 (69%)	13 (22%)	5 (9%)	1	4
14	CN	58/61 (95%)	40 (69%)	12 (21%)	6 (10%)	0	3
15	AO	86/89 (97%)	66 (77%)	18 (21%)	2 (2%)	6	28
15	CO	86/89 (97%)	66 (77%)	18 (21%)	2 (2%)	6	28
16	AP	82/88 (93%)	58 (71%)	17 (21%)	7 (8%)	1	5
16	CP	82/88 (93%)	58 (71%)	16 (20%)	8 (10%)	0	3
17	AQ	98/105 (93%)	76 (78%)	13 (13%)	9 (9%)	1	4
17	CQ	98/105 (93%)	76 (78%)	12 (12%)	10 (10%)	0	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	AR	68/88 (77%)	45 (66%)	16 (24%)	7 (10%)	0	3
18	CR	68/88 (77%)	45 (66%)	15 (22%)	8 (12%)	0	1
19	AS	77/93 (83%)	44 (57%)	22 (29%)	11 (14%)	0	1
19	CS	77/93 (83%)	44 (57%)	22 (29%)	11 (14%)	0	1
20	AT	97/106 (92%)	63 (65%)	26 (27%)	8 (8%)	1	5
20	CT	97/106 (92%)	63 (65%)	24 (25%)	10 (10%)	0	3
21	AU	23/27 (85%)	16 (70%)	5 (22%)	2 (9%)	1	4
21	CU	23/27 (85%)	16 (70%)	5 (22%)	2 (9%)	1	4
24	AY	349/351 (99%)	263 (75%)	65 (19%)	21 (6%)	1	9
24	CY	349/351 (99%)	272 (78%)	55 (16%)	22 (6%)	1	8
25	B0	81/85 (95%)	69 (85%)	11 (14%)	1 (1%)	13	44
25	D0	81/85 (95%)	69 (85%)	11 (14%)	1 (1%)	13	44
26	B1	92/98 (94%)	64 (70%)	16 (17%)	12 (13%)	0	1
26	D1	92/98 (94%)	72 (78%)	12 (13%)	8 (9%)	1	4
27	B2	69/72 (96%)	46 (67%)	12 (17%)	11 (16%)	0	0
27	D2	69/72 (96%)	42 (61%)	16 (23%)	11 (16%)	0	0
28	B3	58/60 (97%)	52 (90%)	6 (10%)	0	100	100
28	D3	58/60 (97%)	52 (90%)	6 (10%)	0	100	100
29	B4	29/71 (41%)	16 (55%)	10 (34%)	3 (10%)	0	3
29	D4	29/71 (41%)	16 (55%)	10 (34%)	3 (10%)	0	3
30	B5	57/60 (95%)	41 (72%)	5 (9%)	11 (19%)	0	0
30	D5	57/60 (95%)	41 (72%)	5 (9%)	11 (19%)	0	0
31	B6	41/54 (76%)	18 (44%)	7 (17%)	16 (39%)	0	0
31	D6	43/54 (80%)	17 (40%)	9 (21%)	17 (40%)	0	0
32	B7	47/49 (96%)	47 (100%)	0	0	100	100
32	D7	47/49 (96%)	46 (98%)	1 (2%)	0	100	100
33	B8	62/65 (95%)	43 (69%)	11 (18%)	8 (13%)	0	1
33	D8	62/65 (95%)	44 (71%)	9 (14%)	9 (14%)	0	1
34	B9	34/37 (92%)	31 (91%)	2 (6%)	1 (3%)	4	24
34	D9	34/37 (92%)	31 (91%)	2 (6%)	1 (3%)	4	24
37	BC	116/229 (51%)	88 (76%)	19 (16%)	9 (8%)	1	5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	DC	116/229 (51%)	88 (76%)	19 (16%)	9 (8%)	1	5
38	BD	270/276 (98%)	203 (75%)	37 (14%)	30 (11%)	0	2
38	DD	270/276 (98%)	205 (76%)	37 (14%)	28 (10%)	0	3
39	BE	203/206 (98%)	146 (72%)	34 (17%)	23 (11%)	0	2
39	DE	203/206 (98%)	149 (73%)	32 (16%)	22 (11%)	0	2
40	BF	206/210 (98%)	149 (72%)	33 (16%)	24 (12%)	0	1
40	DF	206/210 (98%)	149 (72%)	34 (16%)	23 (11%)	0	2
41	BG	177/182 (97%)	98 (55%)	50 (28%)	29 (16%)	0	0
41	DG	179/182 (98%)	123 (69%)	26 (14%)	30 (17%)	0	0
42	BH	158/180 (88%)	105 (66%)	27 (17%)	26 (16%)	0	0
42	DH	158/180 (88%)	105 (66%)	28 (18%)	25 (16%)	0	0
43	BI	144/148 (97%)	86 (60%)	34 (24%)	24 (17%)	0	0
43	DI	144/148 (97%)	90 (62%)	40 (28%)	14 (10%)	0	3
45	BK	139/147 (95%)	78 (56%)	37 (27%)	24 (17%)	0	0
45	DK	139/147 (95%)	78 (56%)	37 (27%)	24 (17%)	0	0
46	BN	137/140 (98%)	105 (77%)	24 (18%)	8 (6%)	1	10
46	DN	137/140 (98%)	103 (75%)	26 (19%)	8 (6%)	1	10
47	BO	120/122 (98%)	101 (84%)	14 (12%)	5 (4%)	3	16
47	DO	120/122 (98%)	102 (85%)	12 (10%)	6 (5%)	2	13
48	BP	144/150 (96%)	71 (49%)	32 (22%)	41 (28%)	0	0
48	DP	144/150 (96%)	71 (49%)	33 (23%)	40 (28%)	0	0
49	BQ	139/141 (99%)	108 (78%)	25 (18%)	6 (4%)	2	16
49	DQ	139/141 (99%)	109 (78%)	23 (16%)	7 (5%)	2	13
50	BR	115/118 (98%)	92 (80%)	15 (13%)	8 (7%)	1	7
50	DR	115/118 (98%)	93 (81%)	14 (12%)	8 (7%)	1	7
51	BS	97/112 (87%)	51 (53%)	29 (30%)	17 (18%)	0	0
51	DS	97/112 (87%)	51 (53%)	28 (29%)	18 (19%)	0	0
52	BT	136/146 (93%)	84 (62%)	33 (24%)	19 (14%)	0	1
52	DT	136/146 (93%)	85 (62%)	32 (24%)	19 (14%)	0	1
53	BU	115/118 (98%)	97 (84%)	11 (10%)	7 (6%)	1	9
53	DU	115/118 (98%)	98 (85%)	9 (8%)	8 (7%)	1	7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
54	BV	99/101 (98%)	72 (73%)	12 (12%)	15 (15%)	0	0
54	DV	99/101 (98%)	72 (73%)	11 (11%)	16 (16%)	0	0
55	BW	111/113 (98%)	93 (84%)	10 (9%)	8 (7%)	1	6
55	DW	111/113 (98%)	93 (84%)	10 (9%)	8 (7%)	1	6
56	BX	91/96 (95%)	73 (80%)	10 (11%)	8 (9%)	1	4
56	DX	91/96 (95%)	73 (80%)	10 (11%)	8 (9%)	1	4
57	BY	99/110 (90%)	55 (56%)	17 (17%)	27 (27%)	0	0
57	DY	99/110 (90%)	54 (54%)	18 (18%)	27 (27%)	0	0
58	BZ	183/206 (89%)	107 (58%)	45 (25%)	31 (17%)	0	0
58	DZ	183/206 (89%)	127 (69%)	38 (21%)	18 (10%)	0	3
All	All	12522/13582 (92%)	8790 (70%)	2335 (19%)	1397 (11%)	0	2

5 of 1397 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	12	GLU
2	AB	15	VAL
2	AB	19	HIS
2	AB	20	GLU
2	AB	64	ARG

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%)	185 (92%)	17 (8%)	11	38
2	CB	202/220 (92%)	185 (92%)	17 (8%)	11	38
3	AC	160/188 (85%)	146 (91%)	14 (9%)	10	36
3	CC	160/188 (85%)	146 (91%)	14 (9%)	10	36
4	AD	180/181 (99%)	160 (89%)	20 (11%)	6	24
4	CD	180/181 (99%)	159 (88%)	21 (12%)	5	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	AE	115/123 (94%)	110 (96%)	5 (4%)	29	62
5	CE	115/123 (94%)	110 (96%)	5 (4%)	29	62
6	AF	90/90 (100%)	87 (97%)	3 (3%)	38	69
6	CF	90/90 (100%)	87 (97%)	3 (3%)	38	69
7	AG	126/127 (99%)	121 (96%)	5 (4%)	31	65
7	CG	126/127 (99%)	121 (96%)	5 (4%)	31	65
8	AH	119/119 (100%)	115 (97%)	4 (3%)	37	69
8	CH	119/119 (100%)	114 (96%)	5 (4%)	30	62
9	AI	98/99 (99%)	89 (91%)	9 (9%)	9	33
9	CI	98/99 (99%)	89 (91%)	9 (9%)	9	33
10	AJ	88/92 (96%)	82 (93%)	6 (7%)	16	45
10	CJ	88/92 (96%)	82 (93%)	6 (7%)	16	45
11	AK	90/99 (91%)	86 (96%)	4 (4%)	28	61
11	CK	90/99 (91%)	86 (96%)	4 (4%)	28	61
12	AL	104/109 (95%)	90 (86%)	14 (14%)	4	16
12	CL	104/109 (95%)	90 (86%)	14 (14%)	4	16
13	AM	99/101 (98%)	92 (93%)	7 (7%)	14	44
13	CM	99/101 (98%)	91 (92%)	8 (8%)	11	39
14	AN	49/50 (98%)	45 (92%)	4 (8%)	11	38
14	CN	49/50 (98%)	45 (92%)	4 (8%)	11	38
15	AO	79/80 (99%)	73 (92%)	6 (8%)	13	41
15	CO	79/80 (99%)	73 (92%)	6 (8%)	13	41
16	AP	72/74 (97%)	68 (94%)	4 (6%)	21	52
16	CP	72/74 (97%)	68 (94%)	4 (6%)	21	52
17	AQ	94/97 (97%)	92 (98%)	2 (2%)	53	79
17	CQ	94/97 (97%)	92 (98%)	2 (2%)	53	79
18	AR	61/77 (79%)	59 (97%)	2 (3%)	38	69
18	CR	61/77 (79%)	59 (97%)	2 (3%)	38	69
19	AS	69/80 (86%)	60 (87%)	9 (13%)	4	18
19	CS	69/80 (86%)	59 (86%)	10 (14%)	3	13
20	AT	76/82 (93%)	70 (92%)	6 (8%)	12	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	CT	76/82 (93%)	69 (91%)	7 (9%)	9	33
21	AU	19/22 (86%)	17 (90%)	2 (10%)	7	26
21	CU	19/22 (86%)	17 (90%)	2 (10%)	7	26
24	AY	298/298 (100%)	267 (90%)	31 (10%)	7	27
24	CY	298/298 (100%)	265 (89%)	33 (11%)	6	24
25	B0	66/67 (98%)	61 (92%)	5 (8%)	13	41
25	D0	66/67 (98%)	61 (92%)	5 (8%)	13	41
26	B1	78/83 (94%)	69 (88%)	9 (12%)	5	22
26	D1	78/83 (94%)	68 (87%)	10 (13%)	4	18
27	B2	66/67 (98%)	64 (97%)	2 (3%)	41	71
27	D2	66/67 (98%)	56 (85%)	10 (15%)	3	12
28	B3	51/52 (98%)	49 (96%)	2 (4%)	32	65
28	D3	51/52 (98%)	49 (96%)	2 (4%)	32	65
29	B4	27/63 (43%)	25 (93%)	2 (7%)	13	42
29	D4	27/63 (43%)	25 (93%)	2 (7%)	13	42
30	B5	51/52 (98%)	43 (84%)	8 (16%)	2	11
30	D5	51/52 (98%)	43 (84%)	8 (16%)	2	11
31	B6	43/52 (83%)	34 (79%)	9 (21%)	1	5
31	D6	43/52 (83%)	33 (77%)	10 (23%)	1	3
32	B7	41/42 (98%)	39 (95%)	2 (5%)	25	57
32	D7	41/42 (98%)	39 (95%)	2 (5%)	25	57
33	B8	53/55 (96%)	43 (81%)	10 (19%)	1	6
33	D8	53/55 (96%)	43 (81%)	10 (19%)	1	6
34	B9	33/34 (97%)	32 (97%)	1 (3%)	41	71
34	D9	33/34 (97%)	32 (97%)	1 (3%)	41	71
37	BC	99/181 (55%)	96 (97%)	3 (3%)	41	71
37	DC	99/181 (55%)	96 (97%)	3 (3%)	41	71
38	BD	213/218 (98%)	183 (86%)	30 (14%)	3	15
38	DD	213/218 (98%)	184 (86%)	29 (14%)	3	16
39	BE	165/166 (99%)	140 (85%)	25 (15%)	3	12
39	DE	165/166 (99%)	141 (86%)	24 (14%)	3	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	BF	165/166 (99%)	149 (90%)	16 (10%)	8	30
40	DF	165/166 (99%)	149 (90%)	16 (10%)	8	30
41	BG	155/156 (99%)	138 (89%)	17 (11%)	6	25
41	DG	155/156 (99%)	133 (86%)	22 (14%)	3	14
42	BH	132/148 (89%)	116 (88%)	16 (12%)	5	20
42	DH	132/148 (89%)	116 (88%)	16 (12%)	5	20
43	BI	122/124 (98%)	112 (92%)	10 (8%)	11	38
43	DI	122/124 (98%)	101 (83%)	21 (17%)	2	9
45	BK	106/111 (96%)	91 (86%)	15 (14%)	3	14
45	DK	106/111 (96%)	92 (87%)	14 (13%)	4	17
46	BN	117/119 (98%)	107 (92%)	10 (8%)	10	37
46	DN	117/119 (98%)	107 (92%)	10 (8%)	10	37
47	BO	100/100 (100%)	94 (94%)	6 (6%)	19	49
47	DO	100/100 (100%)	94 (94%)	6 (6%)	19	49
48	BP	112/116 (97%)	89 (80%)	23 (20%)	1	5
48	DP	112/116 (97%)	89 (80%)	23 (20%)	1	5
49	BQ	111/111 (100%)	101 (91%)	10 (9%)	9	34
49	DQ	111/111 (100%)	100 (90%)	11 (10%)	8	29
50	BR	100/101 (99%)	84 (84%)	16 (16%)	2	11
50	DR	100/101 (99%)	84 (84%)	16 (16%)	2	11
51	BS	77/88 (88%)	66 (86%)	11 (14%)	3	14
51	DS	77/88 (88%)	66 (86%)	11 (14%)	3	14
52	BT	120/127 (94%)	97 (81%)	23 (19%)	1	6
52	DT	120/127 (94%)	98 (82%)	22 (18%)	1	7
53	BU	92/94 (98%)	84 (91%)	8 (9%)	10	36
53	DU	92/94 (98%)	84 (91%)	8 (9%)	10	36
54	BV	82/82 (100%)	64 (78%)	18 (22%)	1	4
54	DV	82/82 (100%)	64 (78%)	18 (22%)	1	4
55	BW	91/92 (99%)	81 (89%)	10 (11%)	6	25
55	DW	91/92 (99%)	81 (89%)	10 (11%)	6	25
56	BX	74/78 (95%)	63 (85%)	11 (15%)	3	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
56	DX	74/78 (95%)	63 (85%)	11 (15%)	3	13
57	BY	84/91 (92%)	70 (83%)	14 (17%)	2	9
57	DY	84/91 (92%)	70 (83%)	14 (17%)	2	9
58	BZ	162/179 (90%)	152 (94%)	10 (6%)	18	49
58	DZ	162/179 (90%)	140 (86%)	22 (14%)	3	16
All	All	10552/11246 (94%)	9458 (90%)	1094 (10%)	7	27

5 of 1094 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
56	BX	53	LYS
11	CK	117	ASN
53	DU	16	LYS
57	BY	40	GLU
3	CC	193	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 365 such sidechains are listed below:

Mol	Chain	Res	Type
55	BW	34	ASN
6	CF	27	GLN
50	DR	23	ASN
55	BW	62	HIS
2	CB	204	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1503/1522 (98%)	203 (13%)	32 (2%)
1	CA	1503/1522 (98%)	207 (13%)	31 (2%)
22	AV	74/77 (96%)	18 (24%)	0
22	AW	74/77 (96%)	17 (22%)	0
22	CV	74/77 (96%)	19 (25%)	0
22	CW	74/77 (96%)	17 (22%)	1 (1%)
23	AX	7/8 (87%)	3 (42%)	0
23	CX	7/8 (87%)	2 (28%)	1 (14%)
35	BA	2900/2915 (99%)	503 (17%)	54 (1%)
35	DA	2900/2915 (99%)	509 (17%)	56 (1%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
36	BB	118/122 (96%)	13 (11%)	1 (0%)
36	DB	118/122 (96%)	13 (11%)	1 (0%)
All	All	9352/9442 (99%)	1524 (16%)	177 (1%)

5 of 1524 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 177 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
35	BA	2464	C
1	CA	484	G
35	DA	2126	A
35	BA	2611	U
1	CA	115	G

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
22	8AN	AW	76	35,22	19,24,25	0.89	1 (5%)	13,35,38	0.96	1 (7%)
22	PHA	CV	77	22	10,11,11	0.92	0	10,13,13	0.56	0
22	8AN	AV	76	59,35,22	19,24,25	0.78	1 (5%)	13,35,38	1.01	1 (7%)
22	8AN	CV	76	59,35,22	19,24,25	0.76	1 (5%)	13,35,38	0.98	1 (7%)
22	PHA	CW	77	22	10,11,11	1.00	0	10,13,13	0.22	0
22	PHA	AV	77	22	10,11,11	1.01	0	10,13,13	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	8AN	CW	76	35,22	19,24,25	0.74	0	13,35,38	1.08	1 (7%)
22	PHA	AW	77	22	10,11,11	1.14	0	10,13,13	0.38	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	8AN	AW	76	35,22	-	1/3/25/26	0/3/3/3
22	PHA	CV	77	22	-	4/5/6/6	0/1/1/1
22	8AN	AV	76	59,35,22	-	1/3/25/26	0/3/3/3
22	8AN	CV	76	59,35,22	-	1/3/25/26	0/3/3/3
22	PHA	CW	77	22	-	3/5/6/6	0/1/1/1
22	PHA	AV	77	22	-	3/5/6/6	0/1/1/1
22	8AN	CW	76	35,22	-	0/3/25/26	0/3/3/3
22	PHA	AW	77	22	-	2/5/6/6	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	AV	76	8AN	C3'-N3'	-2.27	1.43	1.47
22	AW	76	8AN	C3'-N3'	-2.15	1.44	1.47
22	CV	76	8AN	C3'-N3'	-2.13	1.44	1.47

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	AV	76	8AN	O4'-C4'-C3'	2.24	107.36	104.15
22	AW	76	8AN	C5-C6-N6	2.18	123.67	120.35
22	CV	76	8AN	O4'-C4'-C3'	2.08	107.13	104.15
22	CW	76	8AN	C5-C6-N6	2.05	123.46	120.35

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	CV	77	PHA	C-CA-CB-CG
22	AV	76	8AN	C4'-C5'-O5'-P
22	CV	76	8AN	C4'-C5'-O5'-P

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Mol	Chain	Res	Type	Atoms
22	CW	77	PHA	O-C-CA-CB
22	CW	77	PHA	N-CA-CB-CG

There are no ring outliers.

8 monomers are involved in 36 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	AW	76	8AN	2	0
22	CV	77	PHA	4	0
22	AV	76	8AN	7	0
22	CV	76	8AN	2	0
22	CW	77	PHA	7	0
22	AV	77	PHA	3	0
22	CW	76	8AN	3	0
22	AW	77	PHA	12	0

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 1100 ligands modelled in this entry, 1100 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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
13	CM	5
13	AM	5
9	AI	2
9	CI	2
41	BG	1
31	B6	1

The worst 5 of 16 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B6	46:HIS	C	47:THR	N	7.42
1	AI	104:ARG	C	105:ASP	N	4.76
1	CI	104:ARG	C	105:ASP	N	4.74
1	AM	112:GLY	C	113:PRO	N	4.66
1	CM	112:GLY	C	113:PRO	N	4.66

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%)	0.05	41 (2%) 54 31	44, 101, 185, 201	0
1	CA	1504/1522 (98%)	-0.00	37 (2%) 57 34	34, 96, 178, 201	0
2	AB	235/256 (91%)	0.69	24 (10%) 6 2	81, 138, 188, 201	0
2	CB	235/256 (91%)	0.39	18 (7%) 13 5	34, 118, 174, 201	0
3	AC	207/239 (86%)	0.64	20 (9%) 7 2	73, 133, 173, 201	0
3	CC	207/239 (86%)	0.17	6 (2%) 51 28	62, 113, 157, 198	0
4	AD	208/209 (99%)	-0.07	3 (1%) 75 56	50, 93, 140, 190	0
4	CD	208/209 (99%)	0.17	1 (0%) 91 81	63, 108, 157, 201	0
5	AE	151/162 (93%)	0.21	3 (1%) 65 44	51, 97, 147, 177	0
5	CE	151/162 (93%)	0.01	2 (1%) 77 59	52, 84, 132, 163	0
6	AF	101/101 (100%)	0.04	2 (1%) 65 44	63, 105, 149, 201	0
6	CF	101/101 (100%)	-0.20	0 100 100	51, 88, 141, 168	0
7	AG	155/156 (99%)	0.67	20 (12%) 3 1	65, 130, 177, 191	0
7	CG	155/156 (99%)	0.35	11 (7%) 16 6	60, 106, 163, 201	0
8	AH	138/138 (100%)	0.14	2 (1%) 75 56	53, 105, 151, 172	0
8	CH	138/138 (100%)	0.02	0 100 100	48, 83, 125, 157	0
9	AI	127/128 (99%)	1.46	33 (25%) 0 0	82, 148, 193, 201	0
9	CI	127/128 (99%)	0.80	15 (11%) 4 2	57, 123, 185, 200	0
10	AJ	99/105 (94%)	1.45	32 (32%) 0 0	62, 148, 189, 201	0
10	CJ	99/105 (94%)	1.17	20 (20%) 1 0	66, 133, 186, 201	0
11	AK	119/129 (92%)	0.45	7 (5%) 22 10	50, 109, 158, 185	0
11	CK	119/129 (92%)	0.05	5 (4%) 36 18	38, 81, 138, 181	0
12	AL	125/132 (94%)	0.13	5 (4%) 38 19	46, 86, 126, 188	0
12	CL	125/132 (94%)	0.26	5 (4%) 38 19	40, 90, 142, 200	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AM	125/126 (99%)	1.34	30 (24%) 0 0	83, 152, 196, 201	0
13	CM	125/126 (99%)	0.65	16 (12%) 3 1	40, 112, 176, 201	0
14	AN	60/61 (98%)	1.20	10 (16%) 1 1	72, 143, 178, 201	0
14	CN	60/61 (98%)	0.18	1 (1%) 70 49	63, 102, 144, 167	0
15	AO	88/89 (98%)	0.22	3 (3%) 45 24	59, 101, 135, 182	0
15	CO	88/89 (98%)	-0.04	0 100 100	45, 82, 126, 162	0
16	AP	84/88 (95%)	0.13	3 (3%) 42 22	45, 83, 143, 196	0
16	CP	84/88 (95%)	0.57	7 (8%) 11 4	63, 105, 145, 168	0
17	AQ	100/105 (95%)	-0.02	1 (1%) 82 67	43, 89, 133, 153	0
17	CQ	100/105 (95%)	0.07	1 (1%) 82 67	49, 86, 121, 161	0
18	AR	70/88 (79%)	0.80	12 (17%) 1 0	74, 104, 159, 191	0
18	CR	70/88 (79%)	0.22	3 (4%) 35 17	61, 85, 129, 150	0
19	AS	79/93 (84%)	1.66	23 (29%) 0 0	102, 156, 194, 200	0
19	CS	79/93 (84%)	1.16	15 (18%) 1 0	69, 126, 187, 201	0
20	AT	99/106 (93%)	0.43	8 (8%) 12 5	54, 96, 158, 201	0
20	CT	99/106 (93%)	0.37	6 (6%) 21 9	49, 101, 152, 192	0
21	AU	25/27 (92%)	3.20	17 (68%) 0 0	92, 133, 184, 200	0
21	CU	25/27 (92%)	1.16	3 (12%) 4 2	77, 106, 145, 200	0
22	AV	75/77 (97%)	0.45	4 (5%) 26 12	82, 133, 176, 185	0
22	AW	75/77 (97%)	0.76	9 (12%) 4 2	91, 175, 200, 201	0
22	CV	75/77 (97%)	0.29	4 (5%) 26 12	61, 107, 152, 192	0
22	CW	75/77 (97%)	0.76	12 (16%) 1 1	64, 165, 200, 201	0
23	AX	8/8 (100%)	0.16	0 100 100	77, 106, 136, 153	0
23	CX	8/8 (100%)	0.43	1 (12%) 3 1	46, 77, 146, 167	0
24	AY	351/351 (100%)	1.50	94 (26%) 0 0	68, 137, 194, 201	0
24	CY	351/351 (100%)	1.61	115 (32%) 0 0	66, 142, 191, 201	0
25	B0	83/85 (97%)	0.53	7 (8%) 11 4	55, 90, 160, 185	0
25	D0	83/85 (97%)	-0.11	4 (4%) 30 14	17, 43, 119, 176	0
26	B1	94/98 (95%)	-0.07	0 100 100	32, 69, 121, 148	0
26	D1	94/98 (95%)	-0.31	1 (1%) 80 64	18, 50, 99, 171	0
27	B2	71/72 (98%)	0.26	4 (5%) 24 11	53, 93, 147, 185	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
27	D2	71/72 (98%)	-0.38	2 (2%) 53 30	23, 48, 119, 154	0
28	B3	60/60 (100%)	0.71	4 (6%) 17 7	53, 82, 125, 183	0
28	D3	60/60 (100%)	-0.39	1 (1%) 70 49	13, 40, 82, 179	0
29	B4	31/71 (43%)	0.71	4 (12%) 3 1	86, 154, 187, 200	0
29	D4	31/71 (43%)	-0.02	1 (3%) 47 25	77, 111, 160, 187	0
30	B5	59/60 (98%)	0.26	7 (11%) 4 2	30, 69, 181, 201	0
30	D5	59/60 (98%)	0.04	4 (6%) 17 7	10, 35, 157, 163	0
31	B6	45/54 (83%)	1.91	20 (44%) 0 0	71, 128, 178, 200	0
31	D6	45/54 (83%)	1.05	10 (22%) 0 0	40, 83, 144, 186	0
32	B7	49/49 (100%)	0.09	3 (6%) 21 9	25, 52, 117, 184	0
32	D7	49/49 (100%)	-0.19	3 (6%) 21 9	12, 26, 103, 200	0
33	B8	64/65 (98%)	0.38	3 (4%) 31 15	38, 78, 141, 201	0
33	D8	64/65 (98%)	-0.23	0 100 100	14, 45, 102, 180	0
34	B9	36/37 (97%)	1.36	6 (16%) 1 1	61, 94, 137, 149	0
34	D9	36/37 (97%)	0.17	0 100 100	29, 48, 106, 125	0
35	BA	2901/2915 (99%)	-0.06	81 (2%) 53 30	31, 70, 183, 201	0
35	DA	2901/2915 (99%)	-0.21	68 (2%) 60 39	10, 41, 178, 201	0
36	BB	119/122 (97%)	0.22	0 100 100	76, 144, 190, 200	0
36	DB	119/122 (97%)	-0.36	0 100 100	29, 59, 101, 171	0
37	BC	120/229 (52%)	2.98	77 (64%) 0 0	107, 177, 201, 201	0
37	DC	120/229 (52%)	2.64	60 (50%) 0 0	91, 170, 200, 201	0
38	BD	272/276 (98%)	-0.24	0 100 100	24, 63, 111, 158	0
38	DD	272/276 (98%)	-0.47	1 (0%) 92 84	15, 40, 84, 154	0
39	BE	205/206 (99%)	0.07	8 (3%) 39 20	29, 67, 136, 201	0
39	DE	205/206 (99%)	-0.24	5 (2%) 59 37	10, 41, 138, 200	0
40	BF	208/210 (99%)	-0.02	6 (2%) 51 28	33, 77, 161, 201	0
40	DF	208/210 (99%)	-0.30	8 (3%) 40 20	9, 44, 158, 196	0
41	BG	181/182 (99%)	0.70	29 (16%) 1 1	67, 137, 182, 201	0
41	DG	181/182 (99%)	-0.06	6 (3%) 46 24	34, 79, 147, 181	0
42	BH	160/180 (88%)	1.32	47 (29%) 0 0	70, 132, 180, 201	0
42	DH	160/180 (88%)	0.02	6 (3%) 40 20	29, 69, 139, 201	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
43	BI	146/148 (98%)	0.43	10 (6%) 17 7	53, 112, 152, 186	0
43	DI	146/148 (98%)	0.16	5 (3%) 45 24	36, 94, 142, 187	0
44	BJ	0/130	-	-	-	-
44	DJ	0/130	-	-	-	-
45	BK	141/147 (95%)	2.99	80 (56%) 0 0	122, 170, 201, 201	0
45	DK	141/147 (95%)	3.43	103 (73%) 0 0	117, 178, 201, 201	0
46	BN	139/140 (99%)	0.18	3 (2%) 62 41	43, 85, 141, 201	0
46	DN	139/140 (99%)	-0.45	1 (0%) 87 75	18, 42, 104, 201	0
47	BO	122/122 (100%)	-0.43	0 100 100	36, 62, 91, 112	0
47	DO	122/122 (100%)	-0.53	0 100 100	20, 43, 81, 130	0
48	BP	146/150 (97%)	0.60	17 (11%) 4 2	37, 100, 161, 198	0
48	DP	146/150 (97%)	0.05	2 (1%) 75 56	16, 58, 135, 188	0
49	BQ	141/141 (100%)	0.20	4 (2%) 53 30	46, 91, 143, 179	0
49	DQ	141/141 (100%)	-0.38	2 (1%) 75 56	21, 46, 101, 181	0
50	BR	117/118 (99%)	-0.09	0 100 100	36, 66, 109, 152	0
50	DR	117/118 (99%)	-0.42	0 100 100	14, 39, 82, 142	0
51	BS	99/112 (88%)	1.22	25 (25%) 0 0	64, 131, 182, 191	0
51	DS	99/112 (88%)	0.15	4 (4%) 38 19	31, 67, 128, 181	0
52	BT	138/146 (94%)	0.25	11 (7%) 12 5	40, 81, 169, 201	0
52	DT	138/146 (94%)	-0.16	4 (2%) 51 28	22, 61, 150, 201	0
53	BU	117/118 (99%)	-0.10	3 (2%) 56 33	33, 73, 134, 191	0
53	DU	117/118 (99%)	-0.51	0 100 100	11, 32, 85, 147	0
54	BV	101/101 (100%)	0.22	3 (2%) 50 27	33, 96, 143, 201	0
54	DV	101/101 (100%)	-0.41	3 (2%) 50 27	7, 45, 101, 201	0
55	BW	113/113 (100%)	-0.18	0 100 100	31, 62, 117, 193	0
55	DW	113/113 (100%)	-0.46	2 (1%) 68 47	9, 32, 68, 201	0
56	BX	93/96 (96%)	-0.04	1 (1%) 80 64	45, 79, 118, 158	0
56	DX	93/96 (96%)	-0.45	0 100 100	12, 43, 80, 121	0
57	BY	101/110 (91%)	0.91	19 (18%) 1 0	52, 102, 172, 201	0
57	DY	101/110 (91%)	0.20	4 (3%) 38 19	18, 73, 156, 191	0
58	BZ	185/206 (89%)	0.51	17 (9%) 9 3	64, 120, 168, 201	0
58	DZ	185/206 (89%)	-0.14	5 (2%) 54 31	36, 75, 154, 201	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	22130/23284 (95%)	0.21	1524 (6%) 16 7	7, 85, 180, 201	0

The worst 5 of 1524 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
45	BK	3	LYS	14.1
13	CM	123	ALA	13.6
1	AA	82	U	13.5
52	BT	138	ALA	13.2
13	CM	126	LYS	13.0

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

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
22	PHA	AW	77	11/11	0.65	0.84	77,77,79,80	0
22	PHA	CW	77	11/11	0.83	0.57	77,77,79,80	0
22	PHA	CV	77	11/11	0.84	0.45	70,70,72,73	0
22	PHA	AV	77	11/11	0.89	0.43	70,70,72,73	0
22	8AN	AW	76	22/23	0.93	0.17	71,74,82,82	0
22	8AN	CW	76	22/23	0.94	0.22	71,74,82,82	0
22	8AN	AV	76	22/23	0.94	0.21	59,59,59,104	0
22	8AN	CV	76	22/23	0.95	0.25	59,59,59,104	0

6.3 Carbohydrates ⓘ

There are no carbohydrates 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(\AA^2)	Q<0.9
59	MG	BA	3335	1/1	-0.17	0.24	173,173,173,173	0
59	MG	DA	3153	1/1	0.12	0.45	94,94,94,94	0
59	MG	CA	1603	1/1	0.25	0.78	130,130,130,130	0
59	MG	DP	201	1/1	0.28	1.05	1,1,1,1	1
59	MG	CA	1601	1/1	0.32	0.28	59,59,59,59	0
59	MG	DA	3339	1/1	0.36	0.64	89,89,89,89	0
59	MG	CA	1638	1/1	0.39	0.50	77,77,77,77	0
59	MG	CA	1632	1/1	0.41	0.73	88,88,88,88	0
59	MG	CW	101	1/1	0.46	0.21	46,46,46,46	1
59	MG	AA	1699	1/1	0.48	0.29	83,83,83,83	0
59	MG	AA	1758	1/1	0.48	0.22	99,99,99,99	0
59	MG	BA	3331	1/1	0.49	0.29	47,47,47,47	0
59	MG	CA	1713	1/1	0.50	0.29	94,94,94,94	0
59	MG	DA	3214	1/1	0.52	0.39	117,117,117,117	0
59	MG	DA	3240	1/1	0.52	0.36	50,50,50,50	1
59	MG	CA	1675	1/1	0.53	0.42	64,64,64,64	0
59	MG	AA	1614	1/1	0.54	0.19	68,68,68,68	0
59	MG	CA	1724	1/1	0.55	0.31	58,58,58,58	0
59	MG	DA	3204	1/1	0.55	0.27	59,59,59,59	0
59	MG	BA	3163	1/1	0.55	0.36	67,67,67,67	0
59	MG	CD	301	1/1	0.55	0.13	84,84,84,84	0
59	MG	BA	3039	1/1	0.57	0.47	111,111,111,111	0
59	MG	AA	1735	1/1	0.57	0.32	74,74,74,74	0
59	MG	BA	3313	1/1	0.57	0.46	86,86,86,86	0
59	MG	BA	3180	1/1	0.58	0.34	46,46,46,46	1
59	MG	BA	3131	1/1	0.58	0.60	67,67,67,67	0
59	MG	CA	1730	1/1	0.59	0.25	72,72,72,72	0
59	MG	AA	1727	1/1	0.59	0.84	20,20,20,20	1
59	MG	BA	3143	1/1	0.59	0.32	90,90,90,90	0
59	MG	BA	3357	1/1	0.59	0.46	68,68,68,68	1
59	MG	DA	3095	1/1	0.59	0.65	111,111,111,111	0
59	MG	BA	3111	1/1	0.60	0.41	65,65,65,65	0
59	MG	DA	3210	1/1	0.60	0.60	95,95,95,95	0
59	MG	AA	1721	1/1	0.60	0.41	87,87,87,87	0
59	MG	CA	1734	1/1	0.61	0.33	72,72,72,72	1
59	MG	AA	1601	1/1	0.61	0.38	58,58,58,58	1
59	MG	DA	3338	1/1	0.61	0.34	58,58,58,58	0
59	MG	CL	202	1/1	0.61	0.60	80,80,80,80	0
59	MG	BA	3161	1/1	0.61	0.20	54,54,54,54	0
59	MG	CA	1612	1/1	0.62	0.18	65,65,65,65	0
59	MG	DA	3197	1/1	0.62	0.40	94,94,94,94	0
59	MG	DA	3356	1/1	0.62	0.60	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	AA	1630	1/1	0.63	0.42	72,72,72,72	0
59	MG	AV	105	1/1	0.63	0.55	88,88,88,88	0
59	MG	BA	3127	1/1	0.64	0.56	75,75,75,75	0
59	MG	BA	3273	1/1	0.64	0.62	12,12,12,12	1
59	MG	CA	1648	1/1	0.64	0.42	72,72,72,72	0
59	MG	BA	3354	1/1	0.65	0.80	91,91,91,91	0
59	MG	CA	1753	1/1	0.65	0.11	67,67,67,67	0
59	MG	DA	3244	1/1	0.66	0.53	1,1,1,1	1
59	MG	AA	1728	1/1	0.66	0.34	69,69,69,69	0
59	MG	AA	1731	1/1	0.66	0.30	68,68,68,68	0
59	MG	BA	3208	1/1	0.67	0.56	100,100,100,100	0
59	MG	AA	1622	1/1	0.67	0.21	81,81,81,81	0
59	MG	CA	1722	1/1	0.67	0.28	74,74,74,74	1
59	MG	AX	101	1/1	0.67	0.44	27,27,27,27	1
59	MG	BA	3216	1/1	0.68	0.21	59,59,59,59	0
59	MG	CA	1680	1/1	0.68	0.56	67,67,67,67	0
59	MG	BA	3001	1/1	0.68	0.20	62,62,62,62	0
59	MG	CA	1699	1/1	0.68	0.56	84,84,84,84	0
59	MG	CA	1743	1/1	0.69	0.30	61,61,61,61	0
59	MG	BA	3305	1/1	0.69	0.34	54,54,54,54	0
59	MG	CA	1672	1/1	0.69	0.19	52,52,52,52	1
59	MG	DA	3044	1/1	0.69	0.71	62,62,62,62	0
59	MG	AA	1611	1/1	0.69	0.53	74,74,74,74	0
59	MG	BA	3246	1/1	0.69	0.37	60,60,60,60	0
59	MG	CA	1712	1/1	0.69	0.49	67,67,67,67	0
59	MG	BA	3140	1/1	0.69	0.32	77,77,77,77	0
59	MG	BA	3296	1/1	0.70	0.23	83,83,83,83	0
59	MG	DA	3130	1/1	0.70	0.36	45,45,45,45	0
59	MG	DA	3250	1/1	0.70	0.40	68,68,68,68	0
59	MG	AA	1718	1/1	0.70	0.27	71,71,71,71	0
59	MG	BA	3159	1/1	0.70	0.40	55,55,55,55	0
59	MG	DB	201	1/1	0.70	0.42	27,27,27,27	1
59	MG	CA	1715	1/1	0.70	0.41	50,50,50,50	1
59	MG	AA	1746	1/1	0.70	0.37	54,54,54,54	0
59	MG	AA	1723	1/1	0.70	0.25	54,54,54,54	1
59	MG	CA	1633	1/1	0.71	0.21	69,69,69,69	0
59	MG	AA	1748	1/1	0.71	0.69	81,81,81,81	0
59	MG	BA	3218	1/1	0.71	0.49	89,89,89,89	0
59	MG	CA	1637	1/1	0.71	0.43	65,65,65,65	0
59	MG	AA	1649	1/1	0.71	0.27	67,67,67,67	0
59	MG	CA	1660	1/1	0.71	0.26	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	BA	3099	1/1	0.71	0.26	43,43,43,43	0
59	MG	BA	3149	1/1	0.72	0.79	75,75,75,75	0
59	MG	CA	1678	1/1	0.72	0.19	101,101,101,101	0
59	MG	BA	3309	1/1	0.72	0.18	51,51,51,51	0
59	MG	BA	3277	1/1	0.72	0.60	68,68,68,68	0
59	MG	AA	1621	1/1	0.72	0.17	93,93,93,93	0
59	MG	CA	1719	1/1	0.72	0.27	98,98,98,98	0
59	MG	CX	101	1/1	0.72	0.36	79,79,79,79	0
59	MG	DA	3221	1/1	0.72	0.26	63,63,63,63	0
59	MG	DA	3253	1/1	0.72	0.47	18,18,18,18	1
59	MG	BA	3333	1/1	0.73	0.34	23,23,23,23	1
59	MG	CA	1682	1/1	0.73	0.23	60,60,60,60	0
59	MG	CA	1714	1/1	0.73	0.54	62,62,62,62	0
59	MG	BA	3286	1/1	0.73	0.31	71,71,71,71	0
59	MG	CA	1748	1/1	0.73	1.01	1,1,1,1	1
59	MG	DA	3211	1/1	0.73	0.36	69,69,69,69	0
59	MG	BA	3096	1/1	0.73	0.34	59,59,59,59	0
59	MG	DA	3258	1/1	0.74	0.42	58,58,58,58	0
59	MG	CA	1679	1/1	0.74	0.33	60,60,60,60	0
59	MG	AA	1732	1/1	0.74	0.49	72,72,72,72	0
59	MG	DA	3260	1/1	0.74	0.36	43,43,43,43	0
59	MG	BA	3290	1/1	0.74	0.52	11,11,11,11	1
59	MG	CA	1614	1/1	0.75	0.12	44,44,44,44	0
59	MG	AA	1707	1/1	0.75	0.15	58,58,58,58	0
59	MG	BA	3191	1/1	0.75	0.18	84,84,84,84	0
59	MG	BB	204	1/1	0.75	0.27	22,22,22,22	1
59	MG	AV	103	1/1	0.75	0.10	74,74,74,74	0
59	MG	CA	1739	1/1	0.75	0.20	94,94,94,94	1
59	MG	BG	201	1/1	0.75	0.53	1,1,1,1	1
59	MG	DA	3357	1/1	0.76	0.40	55,55,55,55	0
59	MG	BA	3192	1/1	0.76	0.33	65,65,65,65	0
59	MG	BA	3010	1/1	0.76	0.62	63,63,63,63	0
59	MG	AA	1706	1/1	0.76	0.33	69,69,69,69	0
59	MG	BA	3281	1/1	0.76	0.35	51,51,51,51	1
59	MG	BA	3176	1/1	0.76	0.19	59,59,59,59	0
59	MG	AS	101	1/1	0.76	0.08	115,115,115,115	0
59	MG	B5	102	1/1	0.76	0.49	78,78,78,78	0
59	MG	AA	1648	1/1	0.76	0.12	69,69,69,69	0
59	MG	AA	1680	1/1	0.76	0.19	91,91,91,91	0
59	MG	CV	106	1/1	0.77	0.18	96,96,96,96	0
59	MG	CA	1658	1/1	0.77	0.22	53,53,53,53	0
59	MG	BA	3241	1/1	0.77	0.20	1,1,1,1	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	DA	3226	1/1	0.77	0.63	64,64,64,64	0
59	MG	BA	3310	1/1	0.77	0.27	68,68,68,68	0
59	MG	BA	3151	1/1	0.77	0.16	52,52,52,52	0
59	MG	DA	3335	1/1	0.77	0.35	88,88,88,88	0
59	MG	DA	3141	1/1	0.77	0.32	56,56,56,56	0
59	MG	BA	3209	1/1	0.77	0.67	66,66,66,66	0
59	MG	BA	3213	1/1	0.77	0.20	80,80,80,80	1
59	MG	BA	3031	1/1	0.77	0.29	37,37,37,37	0
59	MG	DA	3308	1/1	0.77	0.18	41,41,41,41	0
59	MG	BA	3280	1/1	0.77	0.15	56,56,56,56	0
59	MG	DA	3215	1/1	0.77	0.48	129,129,129,129	0
59	MG	AA	1752	1/1	0.77	0.73	57,57,57,57	1
59	MG	DA	3355	1/1	0.78	0.39	68,68,68,68	0
59	MG	AA	1703	1/1	0.78	0.35	71,71,71,71	0
59	MG	DA	3138	1/1	0.78	0.29	58,58,58,58	0
59	MG	BA	3351	1/1	0.78	0.40	82,82,82,82	0
59	MG	BA	3311	1/1	0.78	0.25	75,75,75,75	0
59	MG	AA	1659	1/1	0.78	0.18	78,78,78,78	0
59	MG	BA	3002	1/1	0.78	0.39	80,80,80,80	0
59	MG	BA	3303	1/1	0.78	0.40	57,57,57,57	0
59	MG	BA	3322	1/1	0.78	0.30	52,52,52,52	0
59	MG	BA	3344	1/1	0.78	0.55	63,63,63,63	0
59	MG	BA	3029	1/1	0.78	0.50	66,66,66,66	0
59	MG	BA	3212	1/1	0.78	0.50	74,74,74,74	0
59	MG	DA	3282	1/1	0.78	0.16	41,41,41,41	0
59	MG	BA	3319	1/1	0.78	0.59	77,77,77,77	0
59	MG	CA	1700	1/1	0.79	0.33	58,58,58,58	0
59	MG	BA	3007	1/1	0.79	0.29	39,39,39,39	0
59	MG	BA	3353	1/1	0.79	0.27	61,61,61,61	0
59	MG	AA	1664	1/1	0.79	0.28	65,65,65,65	0
59	MG	BA	3268	1/1	0.79	0.31	66,66,66,66	0
59	MG	DA	3349	1/1	0.79	0.32	18,18,18,18	1
59	MG	AA	1691	1/1	0.79	0.15	69,69,69,69	0
59	MG	CA	1710	1/1	0.79	0.11	120,120,120,120	0
59	MG	DA	3320	1/1	0.79	0.28	56,56,56,56	0
59	MG	CA	1702	1/1	0.79	0.27	57,57,57,57	0
59	MG	BA	3312	1/1	0.79	0.12	93,93,93,93	0
59	MG	BA	3288	1/1	0.79	0.17	52,52,52,52	0
59	MG	DA	3219	1/1	0.79	0.17	32,32,32,32	0
59	MG	BA	3254	1/1	0.79	0.29	62,62,62,62	0
59	MG	BA	3261	1/1	0.79	0.27	60,60,60,60	0
59	MG	CA	1645	1/1	0.80	0.17	45,45,45,45	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	AA	1647	1/1	0.80	0.16	66,66,66,66	0
59	MG	BA	3352	1/1	0.80	0.43	62,62,62,62	0
59	MG	DA	3237	1/1	0.80	0.36	39,39,39,39	0
59	MG	AA	1658	1/1	0.80	0.28	66,66,66,66	0
59	MG	AA	1702	1/1	0.80	0.21	51,51,51,51	0
59	MG	BA	3082	1/1	0.80	0.24	60,60,60,60	0
59	MG	BA	3276	1/1	0.80	0.41	60,60,60,60	0
59	MG	BA	3217	1/1	0.80	0.46	54,54,54,54	0
59	MG	CA	1663	1/1	0.80	0.21	57,57,57,57	0
59	MG	AA	1681	1/1	0.80	0.19	60,60,60,60	0
59	MG	DG	201	1/1	0.80	0.37	1,1,1,1	1
59	MG	BA	3298	1/1	0.80	0.26	68,68,68,68	0
59	MG	BA	3152	1/1	0.80	0.21	104,104,104,104	0
59	MG	BA	3226	1/1	0.81	0.57	58,58,58,58	0
59	MG	BA	3117	1/1	0.81	0.23	30,30,30,30	0
59	MG	DA	3256	1/1	0.81	0.20	49,49,49,49	0
59	MG	BB	203	1/1	0.81	0.15	69,69,69,69	0
59	MG	BA	3198	1/1	0.81	0.27	38,38,38,38	0
59	MG	AA	1690	1/1	0.81	0.10	64,64,64,64	0
59	MG	BA	3220	1/1	0.81	0.20	79,79,79,79	0
59	MG	AA	1682	1/1	0.81	0.70	77,77,77,77	0
59	MG	BA	3095	1/1	0.81	0.31	73,73,73,73	0
59	MG	AA	1604	1/1	0.81	0.15	57,57,57,57	0
59	MG	BA	3167	1/1	0.81	0.31	70,70,70,70	0
59	MG	AA	1704	1/1	0.81	0.29	56,56,56,56	0
59	MG	AA	1607	1/1	0.81	0.32	57,57,57,57	0
59	MG	DA	3274	1/1	0.81	0.36	69,69,69,69	0
59	MG	BA	3356	1/1	0.81	0.23	68,68,68,68	0
59	MG	AA	1645	1/1	0.81	0.35	88,88,88,88	0
59	MG	CA	1613	1/1	0.81	0.32	58,58,58,58	0
59	MG	DA	3337	1/1	0.82	0.42	102,102,102,102	0
59	MG	DA	3006	1/1	0.82	0.67	52,52,52,52	0
59	MG	DA	3350	1/1	0.82	0.37	37,37,37,37	0
59	MG	DA	3303	1/1	0.82	0.27	25,25,25,25	0
59	MG	CA	1720	1/1	0.82	0.36	93,93,93,93	1
59	MG	CA	1716	1/1	0.82	0.31	50,50,50,50	0
59	MG	AA	1660	1/1	0.82	0.10	69,69,69,69	0
59	MG	BA	3203	1/1	0.82	0.29	43,43,43,43	0
59	MG	BA	3121	1/1	0.82	0.71	92,92,92,92	0
59	MG	AA	1724	1/1	0.82	0.49	1,1,1,1	1
59	MG	DA	3312	1/1	0.82	0.14	65,65,65,65	0
59	MG	BA	3080	1/1	0.82	0.30	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	BF	302	1/1	0.82	0.30	63,63,63,63	0
59	MG	DA	3159	1/1	0.82	0.33	68,68,68,68	0
59	MG	BA	3204	1/1	0.82	0.43	35,35,35,35	1
59	MG	DX	101	1/1	0.82	0.62	58,58,58,58	0
59	MG	BA	3336	1/1	0.82	0.34	40,40,40,40	0
59	MG	AW	103	1/1	0.82	0.15	84,84,84,84	0
59	MG	AV	104	1/1	0.82	0.08	109,109,109,109	0
59	MG	BA	3260	1/1	0.82	0.33	53,53,53,53	0
59	MG	AA	1740	1/1	0.82	0.56	75,75,75,75	0
59	MG	AA	1759	1/1	0.82	0.09	139,139,139,139	0
59	MG	DA	3228	1/1	0.82	0.34	41,41,41,41	0
59	MG	AW	101	1/1	0.82	0.14	58,58,58,58	1
59	MG	CA	1728	1/1	0.83	0.29	53,53,53,53	0
59	MG	CA	1640	1/1	0.83	0.29	37,37,37,37	0
59	MG	AA	1694	1/1	0.83	0.35	54,54,54,54	0
59	MG	BA	3145	1/1	0.83	0.12	60,60,60,60	0
59	MG	AA	1760	1/1	0.83	0.21	27,27,27,27	1
59	MG	AA	1697	1/1	0.83	0.21	60,60,60,60	0
59	MG	AA	1667	1/1	0.83	0.29	85,85,85,85	0
59	MG	AA	1677	1/1	0.83	0.57	68,68,68,68	0
59	MG	BA	3289	1/1	0.83	0.22	59,59,59,59	0
59	MG	BA	3139	1/1	0.83	0.70	84,84,84,84	0
59	MG	BA	3194	1/1	0.83	0.43	70,70,70,70	0
59	MG	DA	3298	1/1	0.83	0.30	78,78,78,78	0
59	MG	AA	1717	1/1	0.83	0.58	110,110,110,110	0
59	MG	BA	3172	1/1	0.83	0.21	58,58,58,58	0
59	MG	CA	1690	1/1	0.83	0.28	54,54,54,54	0
59	MG	AA	1709	1/1	0.83	0.21	50,50,50,50	0
59	MG	CA	1695	1/1	0.83	0.37	46,46,46,46	1
59	MG	CA	1689	1/1	0.83	0.13	57,57,57,57	0
59	MG	BA	3250	1/1	0.83	0.22	50,50,50,50	1
59	MG	AA	1749	1/1	0.83	0.25	48,48,48,48	0
59	MG	DA	3276	1/1	0.83	0.49	57,57,57,57	0
59	MG	BA	3262	1/1	0.83	0.08	49,49,49,49	0
59	MG	BA	3195	1/1	0.83	0.12	62,62,62,62	0
59	MG	AA	1640	1/1	0.83	0.27	47,47,47,47	0
59	MG	DA	3285	1/1	0.84	0.32	48,48,48,48	0
59	MG	BA	3065	1/1	0.84	0.35	67,67,67,67	0
59	MG	AA	1633	1/1	0.84	0.24	73,73,73,73	0
59	MG	CA	1670	1/1	0.84	0.35	77,77,77,77	0
59	MG	BA	3320	1/1	0.84	0.28	57,57,57,57	0
59	MG	CA	1659	1/1	0.84	0.29	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	BA	3166	1/1	0.84	0.14	42,42,42,42	0
59	MG	AA	1606	1/1	0.84	0.39	65,65,65,65	0
59	MG	CA	1708	1/1	0.84	0.35	104,104,104,104	0
59	MG	CA	1607	1/1	0.84	0.28	32,32,32,32	0
59	MG	AA	1742	1/1	0.84	0.85	72,72,72,72	0
59	MG	AA	1734	1/1	0.84	0.31	51,51,51,51	0
59	MG	AA	1652	1/1	0.84	0.38	50,50,50,50	0
59	MG	BA	3132	1/1	0.84	0.19	80,80,80,80	0
59	MG	BA	3348	1/1	0.84	0.50	48,48,48,48	1
59	MG	AA	1741	1/1	0.84	0.33	44,44,44,44	0
59	MG	AA	1639	1/1	0.84	0.36	73,73,73,73	0
59	MG	BA	3223	1/1	0.84	0.34	38,38,38,38	0
59	MG	AA	1687	1/1	0.84	0.28	51,51,51,51	0
59	MG	AY	401	1/1	0.84	0.27	74,74,74,74	0
59	MG	CA	1641	1/1	0.84	0.48	43,43,43,43	0
59	MG	DH	201	1/1	0.84	0.19	44,44,44,44	0
59	MG	AA	1674	1/1	0.84	0.17	69,69,69,69	0
59	MG	BA	3227	1/1	0.84	0.31	56,56,56,56	0
59	MG	CA	1617	1/1	0.84	0.31	61,61,61,61	0
59	MG	CA	1696	1/1	0.84	0.53	17,17,17,17	1
59	MG	AA	1711	1/1	0.85	0.19	63,63,63,63	0
59	MG	DA	3045	1/1	0.85	0.45	34,34,34,34	0
59	MG	DA	3078	1/1	0.85	0.26	33,33,33,33	0
59	MG	DA	3144	1/1	0.85	0.20	56,56,56,56	0
59	MG	AA	1730	1/1	0.85	1.01	78,78,78,78	0
59	MG	CA	1688	1/1	0.85	0.12	56,56,56,56	0
59	MG	DA	3053	1/1	0.85	0.31	50,50,50,50	0
59	MG	BA	3297	1/1	0.85	0.34	75,75,75,75	1
59	MG	BA	3036	1/1	0.85	0.13	44,44,44,44	0
59	MG	BA	3146	1/1	0.85	0.20	58,58,58,58	0
59	MG	BA	3205	1/1	0.85	0.22	75,75,75,75	0
59	MG	CA	1639	1/1	0.85	0.24	51,51,51,51	0
59	MG	BA	3232	1/1	0.85	0.49	59,59,59,59	0
59	MG	BA	3240	1/1	0.85	0.15	73,73,73,73	0
59	MG	BA	3214	1/1	0.85	0.19	55,55,55,55	0
59	MG	CA	1646	1/1	0.85	0.18	37,37,37,37	0
59	MG	BT	201	1/1	0.85	0.22	49,49,49,49	0
59	MG	AA	1716	1/1	0.85	0.20	66,66,66,66	1
59	MG	AA	1712	1/1	0.85	0.22	47,47,47,47	0
59	MG	AA	1646	1/1	0.85	0.39	48,48,48,48	0
59	MG	AA	1617	1/1	0.85	0.09	44,44,44,44	0
59	MG	CA	1707	1/1	0.85	0.18	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	BA	3293	1/1	0.85	0.63	83,83,83,83	0
59	MG	AA	1651	1/1	0.85	0.33	49,49,49,49	0
59	MG	CA	1738	1/1	0.85	0.26	15,15,15,15	1
59	MG	CW	102	1/1	0.86	0.21	51,51,51,51	1
59	MG	BA	3283	1/1	0.86	0.17	49,49,49,49	0
59	MG	DA	3277	1/1	0.86	0.31	37,37,37,37	0
59	MG	CA	1661	1/1	0.86	0.52	83,83,83,83	0
59	MG	AV	101	1/1	0.86	0.18	72,72,72,72	0
59	MG	BA	3069	1/1	0.86	0.28	32,32,32,32	0
59	MG	BA	3119	1/1	0.86	0.61	39,39,39,39	0
59	MG	AA	1653	1/1	0.86	0.33	44,44,44,44	0
59	MG	CS	101	1/1	0.86	0.19	52,52,52,52	1
59	MG	AA	1637	1/1	0.86	0.21	63,63,63,63	0
59	MG	BA	3342	1/1	0.86	0.38	64,64,64,64	0
59	MG	DA	3123	1/1	0.86	0.56	76,76,76,76	0
59	MG	DA	3318	1/1	0.86	0.36	49,49,49,49	0
59	MG	CA	1732	1/1	0.86	0.33	70,70,70,70	0
59	MG	DA	3107	1/1	0.86	0.27	31,31,31,31	0
59	MG	AA	1644	1/1	0.86	0.15	54,54,54,54	0
59	MG	DA	3281	1/1	0.86	0.34	59,59,59,59	0
59	MG	CA	1723	1/1	0.86	0.31	45,45,45,45	1
59	MG	DA	3290	1/1	0.86	0.40	1,1,1,1	1
59	MG	DA	3031	1/1	0.86	0.28	52,52,52,52	0
59	MG	BA	3173	1/1	0.86	0.38	51,51,51,51	0
59	MG	CA	1704	1/1	0.86	0.45	75,75,75,75	0
59	MG	AA	1737	1/1	0.86	0.22	42,42,42,42	0
59	MG	AA	1669	1/1	0.86	0.29	34,34,34,34	0
59	MG	AA	1745	1/1	0.86	0.33	62,62,62,62	0
59	MG	AA	1714	1/1	0.86	0.21	21,21,21,21	1
59	MG	BA	3329	1/1	0.86	0.51	58,58,58,58	0
59	MG	CA	1621	1/1	0.86	0.14	77,77,77,77	0
59	MG	DA	3161	1/1	0.86	0.30	44,44,44,44	0
59	MG	DA	3317	1/1	0.86	0.32	63,63,63,63	0
59	MG	DA	3243	1/1	0.86	0.30	54,54,54,54	1
59	MG	DB	204	1/1	0.87	0.27	1,1,1,1	1
59	MG	DA	3064	1/1	0.87	0.28	18,18,18,18	0
59	MG	BB	202	1/1	0.87	0.21	51,51,51,51	0
59	MG	DA	3323	1/1	0.87	0.47	45,45,45,45	0
59	MG	DA	3065	1/1	0.87	0.59	65,65,65,65	0
59	MG	DA	3158	1/1	0.87	0.32	37,37,37,37	0
59	MG	BA	3346	1/1	0.87	0.21	69,69,69,69	0
59	MG	BA	3243	1/1	0.87	0.23	10,10,10,10	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	BA	3202	1/1	0.87	0.17	42,42,42,42	0
59	MG	AA	1733	1/1	0.87	0.41	79,79,79,79	0
59	MG	BA	3323	1/1	0.87	0.30	49,49,49,49	1
59	MG	BA	3003	1/1	0.87	0.24	56,56,56,56	0
59	MG	CA	1650	1/1	0.87	0.25	46,46,46,46	0
59	MG	BA	3182	1/1	0.87	0.23	70,70,70,70	0
59	MG	DA	3212	1/1	0.87	0.21	59,59,59,59	0
59	MG	AA	1739	1/1	0.87	0.14	54,54,54,54	0
59	MG	BA	3249	1/1	0.87	0.47	103,103,103,103	0
59	MG	BA	3199	1/1	0.87	0.32	60,60,60,60	0
59	MG	DA	3331	1/1	0.87	0.14	30,30,30,30	0
59	MG	DA	3273	1/1	0.87	0.26	1,1,1,1	1
59	MG	DA	3039	1/1	0.87	0.36	97,97,97,97	0
59	MG	DA	3080	1/1	0.87	0.34	32,32,32,32	0
59	MG	BA	3179	1/1	0.87	0.49	43,43,43,43	0
59	MG	AA	1747	1/1	0.87	0.36	81,81,81,81	0
59	MG	CA	1749	1/1	0.87	0.26	65,65,65,65	0
59	MG	BA	3355	1/1	0.87	0.18	9,9,9,9	1
59	MG	BA	3077	1/1	0.87	0.25	74,74,74,74	0
59	MG	DA	3170	1/1	0.88	0.20	25,25,25,25	0
59	MG	BA	3185	1/1	0.88	0.32	46,46,46,46	0
59	MG	BA	3004	1/1	0.88	0.36	118,118,118,118	1
59	MG	AA	1692	1/1	0.88	0.35	50,50,50,50	0
59	MG	BA	3183	1/1	0.88	0.25	59,59,59,59	1
59	MG	BA	3278	1/1	0.88	0.28	59,59,59,59	0
59	MG	DA	3322	1/1	0.88	0.18	38,38,38,38	0
59	MG	AA	1679	1/1	0.88	0.24	82,82,82,82	0
59	MG	CA	1706	1/1	0.88	0.20	53,53,53,53	0
59	MG	BA	3078	1/1	0.88	0.30	58,58,58,58	0
59	MG	BA	3219	1/1	0.88	0.33	46,46,46,46	0
59	MG	CV	105	1/1	0.88	0.31	66,66,66,66	0
59	MG	AV	106	1/1	0.88	0.09	77,77,77,77	0
59	MG	AA	1657	1/1	0.88	0.45	46,46,46,46	0
59	MG	BA	3245	1/1	0.88	0.25	43,43,43,43	0
59	MG	DA	3319	1/1	0.88	0.39	71,71,71,71	0
59	MG	AA	1642	1/1	0.88	0.31	55,55,55,55	0
59	MG	DA	3342	1/1	0.88	0.51	61,61,61,61	0
59	MG	BA	3252	1/1	0.88	0.20	32,32,32,32	1
59	MG	BA	3154	1/1	0.88	0.23	44,44,44,44	0
59	MG	CA	1742	1/1	0.88	0.23	32,32,32,32	1
59	MG	CA	1622	1/1	0.88	0.16	53,53,53,53	0
59	MG	AV	107	1/1	0.88	0.22	65,65,65,65	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	DA	3311	1/1	0.88	0.18	75,75,75,75	0
59	MG	DA	3193	1/1	0.88	0.23	61,61,61,61	0
59	MG	CA	1642	1/1	0.88	0.29	67,67,67,67	1
59	MG	BA	3292	1/1	0.88	0.35	55,55,55,55	0
59	MG	DA	3229	1/1	0.88	0.22	56,56,56,56	0
59	MG	CA	1691	1/1	0.88	0.35	33,33,33,33	0
59	MG	AA	1719	1/1	0.88	0.21	63,63,63,63	0
59	MG	CA	1654	1/1	0.88	0.42	48,48,48,48	0
59	MG	BA	3338	1/1	0.89	0.43	54,54,54,54	0
59	MG	DA	3178	1/1	0.89	0.17	51,51,51,51	0
59	MG	AA	1736	1/1	0.89	0.14	43,43,43,43	1
59	MG	BA	3255	1/1	0.89	0.35	73,73,73,73	0
59	MG	BA	3274	1/1	0.89	0.10	57,57,57,57	0
59	MG	BA	3318	1/1	0.89	0.24	42,42,42,42	0
59	MG	BA	3200	1/1	0.89	0.31	36,36,36,36	0
59	MG	AA	1666	1/1	0.89	0.81	70,70,70,70	0
59	MG	AA	1726	1/1	0.89	0.19	2,2,2,2	1
59	MG	BB	201	1/1	0.89	0.63	38,38,38,38	1
59	MG	AA	1729	1/1	0.89	0.36	88,88,88,88	0
59	MG	DA	3279	1/1	0.89	0.23	16,16,16,16	0
59	MG	AA	1701	1/1	0.89	0.19	61,61,61,61	0
59	MG	DA	3184	1/1	0.89	0.21	46,46,46,46	0
59	MG	DA	3270	1/1	0.89	0.22	30,30,30,30	0
59	MG	CA	1698	1/1	0.89	0.40	20,20,20,20	1
59	MG	CA	1731	1/1	0.89	0.21	69,69,69,69	0
59	MG	DA	3119	1/1	0.89	0.59	40,40,40,40	0
59	MG	DA	3304	1/1	0.89	0.26	18,18,18,18	1
59	MG	BA	3287	1/1	0.89	0.14	65,65,65,65	0
59	MG	CA	1727	1/1	0.89	0.27	44,44,44,44	0
59	MG	DA	3165	1/1	0.89	0.33	45,45,45,45	0
59	MG	CA	1674	1/1	0.89	0.11	35,35,35,35	1
59	MG	BA	3259	1/1	0.89	0.17	80,80,80,80	0
59	MG	DA	3333	1/1	0.89	0.15	55,55,55,55	0
59	MG	AA	1722	1/1	0.89	0.18	46,46,46,46	1
59	MG	BA	3327	1/1	0.89	0.25	52,52,52,52	0
59	MG	BA	3113	1/1	0.89	0.32	33,33,33,33	0
59	MG	DA	3292	1/1	0.89	0.24	40,40,40,40	0
59	MG	BA	3302	1/1	0.89	0.20	20,20,20,20	0
59	MG	AA	1616	1/1	0.89	0.21	36,36,36,36	1
59	MG	BA	3067	1/1	0.89	0.12	30,30,30,30	0
59	MG	DA	3336	1/1	0.89	0.37	48,48,48,48	0
59	MG	CA	1619	1/1	0.89	0.27	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	DA	3198	1/1	0.89	0.35	52,52,52,52	0
59	MG	CA	1747	1/1	0.89	0.19	21,21,21,21	1
59	MG	CA	1667	1/1	0.89	0.13	57,57,57,57	0
59	MG	AA	1671	1/1	0.89	0.31	66,66,66,66	0
59	MG	BA	3160	1/1	0.89	0.12	36,36,36,36	0
59	MG	BA	3048	1/1	0.89	0.24	32,32,32,32	0
59	MG	BA	3324	1/1	0.89	0.43	19,19,19,19	1
59	MG	BA	3196	1/1	0.89	0.31	52,52,52,52	0
59	MG	BA	3304	1/1	0.89	0.77	64,64,64,64	0
59	MG	BA	3129	1/1	0.89	0.44	59,59,59,59	0
59	MG	BA	3122	1/1	0.90	0.63	62,62,62,62	0
59	MG	BA	3332	1/1	0.90	0.20	54,54,54,54	0
59	MG	DA	3242	1/1	0.90	0.16	11,11,11,11	1
59	MG	AA	1710	1/1	0.90	0.29	61,61,61,61	0
59	MG	BA	3097	1/1	0.90	0.12	45,45,45,45	0
59	MG	AA	1641	1/1	0.90	0.16	38,38,38,38	0
59	MG	BA	3334	1/1	0.90	0.12	55,55,55,55	0
59	MG	DA	3280	1/1	0.90	0.37	54,54,54,54	0
59	MG	AA	1743	1/1	0.90	0.09	49,49,49,49	1
59	MG	AA	1751	1/1	0.90	0.23	11,11,11,11	1
59	MG	DA	3262	1/1	0.90	0.10	32,32,32,32	0
59	MG	CA	1611	1/1	0.90	0.35	51,51,51,51	0
59	MG	DA	3325	1/1	0.90	0.26	48,48,48,48	0
59	MG	BA	3033	1/1	0.90	0.31	35,35,35,35	0
59	MG	AA	1662	1/1	0.90	0.33	56,56,56,56	0
59	MG	CA	1677	1/1	0.90	0.12	46,46,46,46	1
59	MG	CA	1701	1/1	0.90	0.53	55,55,55,55	1
59	MG	AA	1650	1/1	0.90	0.22	40,40,40,40	0
59	MG	BA	3114	1/1	0.90	0.28	37,37,37,37	0
59	MG	BA	3247	1/1	0.90	0.14	66,66,66,66	0
59	MG	BA	3236	1/1	0.90	0.24	54,54,54,54	0
59	MG	AW	102	1/1	0.90	0.15	25,25,25,25	1
59	MG	BA	3349	1/1	0.90	0.36	45,45,45,45	0
59	MG	BA	3124	1/1	0.90	0.50	65,65,65,65	0
59	MG	BA	3049	1/1	0.90	0.51	46,46,46,46	0
59	MG	DA	3289	1/1	0.90	0.12	17,17,17,17	0
59	MG	BF	301	1/1	0.90	0.14	33,33,33,33	0
59	MG	AA	1757	1/1	0.90	0.14	49,49,49,49	0
59	MG	CA	1662	1/1	0.90	0.12	49,49,49,49	0
59	MG	AA	1676	1/1	0.90	0.11	21,21,21,21	1
59	MG	BA	3044	1/1	0.90	0.41	49,49,49,49	0
59	MG	BA	3093	1/1	0.90	0.29	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	BA	3210	1/1	0.90	0.49	70,70,70,70	0
59	MG	CA	1626	1/1	0.90	0.18	75,75,75,75	0
59	MG	DA	3309	1/1	0.90	0.11	61,61,61,61	0
59	MG	DA	3313	1/1	0.90	0.27	74,74,74,74	0
59	MG	DA	3156	1/1	0.90	0.24	31,31,31,31	0
59	MG	DA	3340	1/1	0.91	0.15	25,25,25,25	0
59	MG	BA	3020	1/1	0.91	0.42	37,37,37,37	0
59	MG	BA	3045	1/1	0.91	0.54	44,44,44,44	0
59	MG	DA	3236	1/1	0.91	0.31	43,43,43,43	0
59	MG	CA	1673	1/1	0.91	0.09	15,15,15,15	0
59	MG	AA	1661	1/1	0.91	0.13	52,52,52,52	0
59	MG	DA	3071	1/1	0.91	0.20	18,18,18,18	0
59	MG	CA	1736	1/1	0.91	0.41	55,55,55,55	0
59	MG	BA	3023	1/1	0.91	0.43	52,52,52,52	0
59	MG	DA	3245	1/1	0.91	0.18	38,38,38,38	0
59	MG	DA	3179	1/1	0.91	0.20	49,49,49,49	0
59	MG	BA	3032	1/1	0.91	0.14	49,49,49,49	0
59	MG	AA	1613	1/1	0.91	0.15	60,60,60,60	0
59	MG	BA	3308	1/1	0.91	0.12	39,39,39,39	0
59	MG	AL	201	1/1	0.91	0.09	15,15,15,15	1
59	MG	BA	3317	1/1	0.91	0.26	1,1,1,1	1
59	MG	BA	3144	1/1	0.91	0.16	46,46,46,46	0
59	MG	BA	3028	1/1	0.91	0.29	40,40,40,40	0
59	MG	BA	3181	1/1	0.91	0.26	60,60,60,60	0
59	MG	CA	1692	1/1	0.91	0.66	73,73,73,73	0
59	MG	DA	3132	1/1	0.91	0.15	62,62,62,62	0
59	MG	DA	3332	1/1	0.91	0.24	26,26,26,26	1
59	MG	BA	3215	1/1	0.91	0.10	26,26,26,26	0
59	MG	AA	1623	1/1	0.91	0.23	60,60,60,60	0
59	MG	CA	1616	1/1	0.91	0.50	65,65,65,65	0
59	MG	DA	3052	1/1	0.91	0.26	25,25,25,25	0
59	MG	DA	3111	1/1	0.91	0.32	33,33,33,33	0
59	MG	CN	101	1/1	0.91	0.09	69,69,69,69	0
59	MG	BA	3162	1/1	0.91	0.34	96,96,96,96	0
59	MG	DA	3359	1/1	0.91	0.17	1,1,1,1	1
59	MG	BA	3326	1/1	0.91	0.34	42,42,42,42	0
59	MG	BA	3242	1/1	0.91	0.14	106,106,106,106	0
59	MG	CA	1652	1/1	0.91	0.47	71,71,71,71	0
59	MG	BA	3239	1/1	0.91	0.30	4,4,4,4	1
59	MG	DA	3121	1/1	0.91	0.38	14,14,14,14	1
59	MG	DA	3267	1/1	0.91	0.21	13,13,13,13	0
59	MG	DA	3192	1/1	0.91	0.12	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	BA	3325	1/1	0.91	0.08	62,62,62,62	0
59	MG	BA	3258	1/1	0.91	0.35	48,48,48,48	0
59	MG	DA	3146	1/1	0.91	0.11	27,27,27,27	0
59	MG	DA	3205	1/1	0.91	0.31	46,46,46,46	0
59	MG	BA	3169	1/1	0.91	0.22	45,45,45,45	0
59	MG	BA	3142	1/1	0.91	0.28	97,97,97,97	0
59	MG	CA	1636	1/1	0.91	0.31	52,52,52,52	0
59	MG	BA	3341	1/1	0.91	0.34	61,61,61,61	0
59	MG	BA	3225	1/1	0.91	0.50	73,73,73,73	0
59	MG	CA	1671	1/1	0.91	0.16	44,44,44,44	0
59	MG	DA	3187	1/1	0.91	0.56	44,44,44,44	0
59	MG	CA	1628	1/1	0.91	0.25	49,49,49,49	0
59	MG	DA	3152	1/1	0.91	0.23	38,38,38,38	0
59	MG	DA	3099	1/1	0.92	0.28	12,12,12,12	0
59	MG	CA	1733	1/1	0.92	0.23	50,50,50,50	0
59	MG	DA	3143	1/1	0.92	0.26	48,48,48,48	0
59	MG	BA	3030	1/1	0.92	0.32	59,59,59,59	0
59	MG	AA	1675	1/1	0.92	0.13	35,35,35,35	0
59	MG	BA	3006	1/1	0.92	0.50	73,73,73,73	0
59	MG	BA	3190	1/1	0.92	0.13	47,47,47,47	0
59	MG	DA	3220	1/1	0.92	0.56	51,51,51,51	0
59	MG	DA	3110	1/1	0.92	0.30	46,46,46,46	0
59	MG	DA	3327	1/1	0.92	0.24	38,38,38,38	0
59	MG	AA	1753	1/1	0.92	0.36	16,16,16,16	1
59	MG	CA	1602	1/1	0.92	0.30	16,16,16,16	1
59	MG	DA	3135	1/1	0.92	0.16	33,33,33,33	0
59	MG	CW	104	1/1	0.92	0.14	37,37,37,37	1
59	MG	DA	3263	1/1	0.92	0.42	53,53,53,53	0
59	MG	BA	3091	1/1	0.92	0.18	58,58,58,58	0
59	MG	DA	3351	1/1	0.92	0.74	70,70,70,70	0
59	MG	CA	1615	1/1	0.92	0.34	26,26,26,26	0
59	MG	BA	3170	1/1	0.92	0.28	38,38,38,38	0
59	MG	BA	3046	1/1	0.92	0.23	22,22,22,22	0
59	MG	DA	3194	1/1	0.92	0.27	32,32,32,32	0
59	MG	AA	1619	1/1	0.92	0.31	39,39,39,39	0
59	MG	AA	1665	1/1	0.92	0.25	61,61,61,61	0
59	MG	BA	3073	1/1	0.92	0.39	46,46,46,46	0
59	MG	CL	201	1/1	0.92	0.12	8,8,8,8	1
59	MG	BA	3221	1/1	0.92	0.42	53,53,53,53	0
59	MG	DA	3299	1/1	0.92	0.36	49,49,49,49	0
59	MG	DA	3241	1/1	0.92	0.12	69,69,69,69	0
59	MG	BA	3123	1/1	0.92	0.58	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	BA	3120	1/1	0.92	0.20	25,25,25,25	0
59	MG	DA	3175	1/1	0.92	0.38	59,59,59,59	0
59	MG	BA	3137	1/1	0.92	0.15	38,38,38,38	0
59	MG	AA	1673	1/1	0.92	0.25	72,72,72,72	0
59	MG	BA	3110	1/1	0.92	0.16	51,51,51,51	0
59	MG	DA	3278	1/1	0.92	0.41	40,40,40,40	0
59	MG	AA	1654	1/1	0.92	0.13	78,78,78,78	0
59	MG	CA	1685	1/1	0.92	0.40	53,53,53,53	0
59	MG	DA	3288	1/1	0.92	0.23	61,61,61,61	0
59	MG	DA	3305	1/1	0.92	0.17	39,39,39,39	0
59	MG	DA	3122	1/1	0.92	0.61	73,73,73,73	0
59	MG	CA	1687	1/1	0.92	0.14	64,64,64,64	0
59	MG	DA	3347	1/1	0.92	0.35	24,24,24,24	1
59	MG	DA	3321	1/1	0.92	0.45	85,85,85,85	0
59	MG	BA	3271	1/1	0.92	0.45	55,55,55,55	0
59	MG	CA	1725	1/1	0.92	0.22	72,72,72,72	0
59	MG	AA	1713	1/1	0.92	0.22	49,49,49,49	1
59	MG	AA	1720	1/1	0.92	0.56	55,55,55,55	0
59	MG	CA	1644	1/1	0.92	0.10	64,64,64,64	0
59	MG	BA	3107	1/1	0.92	0.22	25,25,25,25	1
59	MG	DD	301	1/1	0.92	0.28	37,37,37,37	0
59	MG	CA	1657	1/1	0.92	0.17	52,52,52,52	0
59	MG	CA	1744	1/1	0.92	0.31	38,38,38,38	0
59	MG	DA	3343	1/1	0.92	0.29	48,48,48,48	0
59	MG	DA	3352	1/1	0.92	0.22	46,46,46,46	0
59	MG	CA	1624	1/1	0.92	0.36	52,52,52,52	0
59	MG	DA	3155	1/1	0.92	0.21	50,50,50,50	0
59	MG	AA	1689	1/1	0.92	0.20	37,37,37,37	0
59	MG	CA	1631	1/1	0.92	0.12	24,24,24,24	0
59	MG	DA	3058	1/1	0.92	0.35	23,23,23,23	0
59	MG	BA	3092	1/1	0.92	0.28	40,40,40,40	0
59	MG	DA	3315	1/1	0.93	0.18	15,15,15,15	0
59	MG	CA	1651	1/1	0.93	0.36	40,40,40,40	0
59	MG	BA	3264	1/1	0.93	0.13	64,64,64,64	0
59	MG	CA	1717	1/1	0.93	0.20	63,63,63,63	1
59	MG	BA	3115	1/1	0.93	0.46	43,43,43,43	0
59	MG	B1	101	1/1	0.93	0.27	6,6,6,6	1
59	MG	DA	3209	1/1	0.93	0.23	47,47,47,47	0
59	MG	CA	1655	1/1	0.93	0.32	37,37,37,37	0
59	MG	BA	3235	1/1	0.93	0.22	42,42,42,42	0
59	MG	AA	1668	1/1	0.93	0.23	40,40,40,40	0
59	MG	BA	3128	1/1	0.93	0.18	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	AA	1738	1/1	0.93	0.11	85,85,85,85	0
59	MG	DA	3109	1/1	0.93	0.20	6,6,6,6	1
59	MG	CA	1634	1/1	0.93	0.44	35,35,35,35	0
59	MG	AA	1670	1/1	0.93	0.19	34,34,34,34	0
59	MG	DA	3275	1/1	0.93	0.41	28,28,28,28	1
59	MG	AA	1615	1/1	0.93	0.50	50,50,50,50	0
59	MG	DA	3238	1/1	0.93	0.38	47,47,47,47	0
59	MG	DA	3207	1/1	0.93	0.19	40,40,40,40	0
59	MG	AA	1663	1/1	0.93	0.17	50,50,50,50	0
59	MG	BA	3233	1/1	0.93	0.24	50,50,50,50	0
59	MG	DA	3001	1/1	0.93	0.20	29,29,29,29	1
59	MG	DA	3056	1/1	0.93	0.40	26,26,26,26	0
59	MG	BA	3086	1/1	0.93	0.35	25,25,25,25	0
59	MG	BA	3316	1/1	0.93	0.26	74,74,74,74	0
59	MG	DA	3167	1/1	0.93	0.45	46,46,46,46	0
59	MG	BA	3306	1/1	0.93	0.36	29,29,29,29	0
59	MG	AA	1708	1/1	0.93	0.11	76,76,76,76	1
59	MG	DA	3224	1/1	0.93	0.48	44,44,44,44	0
59	MG	BA	3189	1/1	0.93	0.19	41,41,41,41	0
59	MG	DA	3316	1/1	0.93	0.18	33,33,33,33	1
59	MG	DA	3085	1/1	0.93	0.14	5,5,5,5	0
59	MG	DA	3091	1/1	0.93	0.28	21,21,21,21	1
59	MG	BA	3231	1/1	0.93	0.25	25,25,25,25	1
59	MG	DA	3271	1/1	0.93	0.46	58,58,58,58	0
59	MG	BA	3343	1/1	0.93	0.12	75,75,75,75	0
59	MG	DA	3341	1/1	0.93	0.24	36,36,36,36	1
59	MG	BA	3112	1/1	0.93	0.16	44,44,44,44	0
59	MG	DA	3314	1/1	0.93	0.54	31,31,31,31	0
59	MG	CA	1665	1/1	0.93	0.49	46,46,46,46	0
59	MG	BA	3134	1/1	0.93	0.19	52,52,52,52	0
59	MG	DA	3029	1/1	0.93	0.28	49,49,49,49	0
59	MG	BA	3059	1/1	0.93	0.21	30,30,30,30	0
59	MG	AA	1685	1/1	0.93	0.12	57,57,57,57	0
59	MG	AA	1756	1/1	0.93	0.09	64,64,64,64	0
59	MG	AV	102	1/1	0.93	0.12	61,61,61,61	0
59	MG	BA	3075	1/1	0.93	0.30	32,32,32,32	0
59	MG	DA	3202	1/1	0.93	0.32	35,35,35,35	0
59	MG	DA	3139	1/1	0.93	0.28	23,23,23,23	0
59	MG	CW	103	1/1	0.93	0.29	15,15,15,15	1
59	MG	DA	3096	1/1	0.93	0.40	50,50,50,50	0
59	MG	DA	3010	1/1	0.93	0.33	54,54,54,54	0
59	MG	CA	1755	1/1	0.93	0.19	97,97,97,97	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	BA	3168	1/1	0.93	0.15	37,37,37,37	0
59	MG	CA	1618	1/1	0.93	0.14	38,38,38,38	0
59	MG	BA	3237	1/1	0.93	0.39	64,64,64,64	0
59	MG	DA	3334	1/1	0.93	0.12	63,63,63,63	0
59	MG	AA	1605	1/1	0.93	0.10	58,58,58,58	0
59	MG	DA	3283	1/1	0.93	0.11	35,35,35,35	0
59	MG	DA	3181	1/1	0.94	0.31	26,26,26,26	0
59	MG	AA	1754	1/1	0.94	0.10	51,51,51,51	0
59	MG	CA	1750	1/1	0.94	0.16	76,76,76,76	0
59	MG	BA	3068	1/1	0.94	0.26	30,30,30,30	0
59	MG	AA	1638	1/1	0.94	0.11	43,43,43,43	0
59	MG	DA	3164	1/1	0.94	0.49	44,44,44,44	0
59	MG	AA	1684	1/1	0.94	0.30	59,59,59,59	0
59	MG	BA	3175	1/1	0.94	0.12	65,65,65,65	0
59	MG	DA	3345	1/1	0.94	0.26	46,46,46,46	0
59	MG	DA	3328	1/1	0.94	0.15	32,32,32,32	0
59	MG	BA	3263	1/1	0.94	0.36	54,54,54,54	0
59	MG	BA	3266	1/1	0.94	0.36	35,35,35,35	0
59	MG	CA	1711	1/1	0.94	0.22	40,40,40,40	0
59	MG	DA	3069	1/1	0.94	0.26	19,19,19,19	0
59	MG	AA	1750	1/1	0.94	0.31	54,54,54,54	0
59	MG	DA	3051	1/1	0.94	0.34	23,23,23,23	0
59	MG	B5	101	1/1	0.94	0.25	38,38,38,38	0
59	MG	BA	3072	1/1	0.94	0.41	41,41,41,41	0
59	MG	DA	3117	1/1	0.94	0.13	16,16,16,16	0
59	MG	DA	3261	1/1	0.94	0.20	33,33,33,33	0
59	MG	BA	3089	1/1	0.94	0.27	28,28,28,28	0
59	MG	DA	3036	1/1	0.94	0.15	39,39,39,39	0
59	MG	BA	3136	1/1	0.94	0.23	42,42,42,42	0
59	MG	DA	3326	1/1	0.94	0.61	35,35,35,35	0
59	MG	AA	1688	1/1	0.94	0.25	52,52,52,52	0
59	MG	BA	3108	1/1	0.94	0.40	15,15,15,15	0
59	MG	AA	1610	1/1	0.94	0.14	80,80,80,80	1
59	MG	DA	3028	1/1	0.94	0.28	24,24,24,24	0
59	MG	DA	3002	1/1	0.94	0.17	39,39,39,39	1
59	MG	CA	1697	1/1	0.94	0.09	58,58,58,58	0
59	MG	BA	3339	1/1	0.94	0.09	21,21,21,21	1
59	MG	CA	1605	1/1	0.94	0.12	44,44,44,44	0
59	MG	CA	1623	1/1	0.94	0.25	51,51,51,51	0
59	MG	AA	1700	1/1	0.94	0.37	77,77,77,77	0
59	MG	DA	3128	1/1	0.94	0.38	56,56,56,56	0
59	MG	BA	3330	1/1	0.94	0.42	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	AA	1744	1/1	0.94	0.24	1,1,1,1	1
59	MG	DA	3030	1/1	0.94	0.35	34,34,34,34	0
59	MG	BA	3064	1/1	0.94	0.63	61,61,61,61	0
59	MG	DA	3216	1/1	0.94	0.16	11,11,11,11	1
59	MG	BA	3022	1/1	0.94	0.41	22,22,22,22	0
59	MG	BA	3109	1/1	0.94	0.26	37,37,37,37	1
59	MG	BA	3138	1/1	0.94	0.12	31,31,31,31	0
59	MG	AA	1655	1/1	0.94	0.18	57,57,57,57	0
59	MG	BA	3125	1/1	0.94	0.34	19,19,19,19	0
59	MG	BA	3088	1/1	0.94	0.51	38,38,38,38	0
59	MG	AW	104	1/1	0.94	0.22	67,67,67,67	1
59	MG	DA	3218	1/1	0.94	0.32	29,29,29,29	0
59	MG	DA	3166	1/1	0.94	0.15	29,29,29,29	0
59	MG	DA	3032	1/1	0.94	0.16	32,32,32,32	0
59	MG	AA	1698	1/1	0.94	0.33	25,25,25,25	1
59	MG	DA	3201	1/1	0.94	0.42	29,29,29,29	0
59	MG	BA	3016	1/1	0.94	0.39	18,18,18,18	0
59	MG	BA	3291	1/1	0.94	0.16	42,42,42,42	0
59	MG	AA	1678	1/1	0.94	0.38	56,56,56,56	0
59	MG	DA	3251	1/1	0.94	0.16	18,18,18,18	1
59	MG	AA	1656	1/1	0.94	0.07	30,30,30,30	0
59	MG	DA	3291	1/1	0.94	0.11	49,49,49,49	0
59	MG	CA	1649	1/1	0.94	0.19	22,22,22,22	0
59	MG	BA	3257	1/1	0.94	0.18	45,45,45,45	0
59	MG	DA	3264	1/1	0.94	0.28	58,58,58,58	1
59	MG	AA	1696	1/1	0.94	0.09	57,57,57,57	1
59	MG	CA	1737	1/1	0.94	0.59	59,59,59,59	0
59	MG	BA	3177	1/1	0.94	0.22	77,77,77,77	0
59	MG	DA	3358	1/1	0.94	0.42	50,50,50,50	0
59	MG	BA	3272	1/1	0.94	0.50	44,44,44,44	0
59	MG	AA	1603	1/1	0.94	0.16	60,60,60,60	0
59	MG	DA	3182	1/1	0.94	0.23	42,42,42,42	0
59	MG	BX	101	1/1	0.94	0.32	47,47,47,47	0
59	MG	DA	3239	1/1	0.94	0.12	29,29,29,29	0
59	MG	DA	3195	1/1	0.94	0.14	102,102,102,102	0
59	MG	CA	1627	1/1	0.94	0.08	51,51,51,51	0
59	MG	BA	3282	1/1	0.94	0.09	68,68,68,68	0
59	MG	DA	3160	1/1	0.94	0.34	18,18,18,18	0
59	MG	DA	3196	1/1	0.94	0.20	41,41,41,41	0
59	MG	BA	3094	1/1	0.94	0.25	36,36,36,36	0
59	MG	BA	3299	1/1	0.94	0.30	55,55,55,55	0
59	MG	BA	3135	1/1	0.94	0.41	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	AA	1625	1/1	0.94	0.28	53,53,53,53	0
59	MG	DA	3235	1/1	0.94	0.29	18,18,18,18	0
59	MG	BA	3100	1/1	0.94	0.29	29,29,29,29	0
59	MG	BA	3207	1/1	0.94	0.22	68,68,68,68	0
59	MG	DA	3169	1/1	0.94	0.15	47,47,47,47	0
59	MG	CA	1752	1/1	0.94	0.08	84,84,84,84	0
59	MG	DA	3252	1/1	0.94	0.31	51,51,51,51	0
59	MG	DA	3286	1/1	0.94	0.34	41,41,41,41	0
59	MG	DA	3225	1/1	0.95	0.10	34,34,34,34	0
59	MG	BA	3206	1/1	0.95	0.12	85,85,85,85	0
59	MG	BA	3104	1/1	0.95	0.38	57,57,57,57	0
59	MG	D5	101	1/1	0.95	0.26	25,25,25,25	0
59	MG	DA	3268	1/1	0.95	0.17	30,30,30,30	0
59	MG	DA	3040	1/1	0.95	0.25	27,27,27,27	0
59	MG	BA	3340	1/1	0.95	0.08	73,73,73,73	0
59	MG	BA	3321	1/1	0.95	0.15	73,73,73,73	0
59	MG	BA	3229	1/1	0.95	0.13	37,37,37,37	0
59	MG	CA	1693	1/1	0.95	0.45	56,56,56,56	0
59	MG	DA	3227	1/1	0.95	0.24	22,22,22,22	0
59	MG	DA	3191	1/1	0.95	0.28	34,34,34,34	0
59	MG	DA	3093	1/1	0.95	0.27	11,11,11,11	0
59	MG	BA	3034	1/1	0.95	0.19	39,39,39,39	0
59	MG	DA	3163	1/1	0.95	0.17	27,27,27,27	0
59	MG	BA	3285	1/1	0.95	0.22	37,37,37,37	1
59	MG	BA	3024	1/1	0.95	0.34	36,36,36,36	0
59	MG	BA	3021	1/1	0.95	0.22	32,32,32,32	0
59	MG	DA	3137	1/1	0.95	0.28	11,11,11,11	0
59	MG	DA	3329	1/1	0.95	0.53	47,47,47,47	0
59	MG	BA	3017	1/1	0.95	0.29	45,45,45,45	0
59	MG	DA	3115	1/1	0.95	0.26	44,44,44,44	0
59	MG	BA	3008	1/1	0.95	0.29	58,58,58,58	0
59	MG	BA	3279	1/1	0.95	0.30	39,39,39,39	0
59	MG	DA	3025	1/1	0.95	0.27	29,29,29,29	0
59	MG	AA	1761	1/1	0.95	0.16	88,88,88,88	0
59	MG	DB	202	1/1	0.95	0.26	23,23,23,23	0
59	MG	DA	3255	1/1	0.95	0.17	13,13,13,13	0
59	MG	CA	1681	1/1	0.95	0.09	58,58,58,58	0
59	MG	DA	3134	1/1	0.95	0.20	28,28,28,28	0
59	MG	CA	1610	1/1	0.95	0.21	60,60,60,60	0
59	MG	DA	3259	1/1	0.95	0.34	31,31,31,31	0
59	MG	BA	3174	1/1	0.95	0.28	29,29,29,29	0
59	MG	DA	3307	1/1	0.95	0.31	14,14,14,14	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	DA	3104	1/1	0.95	0.35	35,35,35,35	0
59	MG	BA	3315	1/1	0.95	0.12	45,45,45,45	0
59	MG	DA	3129	1/1	0.95	0.20	46,46,46,46	0
59	MG	DA	3021	1/1	0.95	0.23	20,20,20,20	0
59	MG	BA	3222	1/1	0.95	0.41	29,29,29,29	0
59	MG	BA	3060	1/1	0.95	0.26	14,14,14,14	0
59	MG	DA	3150	1/1	0.95	0.25	48,48,48,48	0
59	MG	DA	3147	1/1	0.95	0.20	52,52,52,52	0
59	MG	BA	3150	1/1	0.95	0.15	44,44,44,44	0
59	MG	DA	3203	1/1	0.95	0.21	37,37,37,37	0
59	MG	BA	3102	1/1	0.95	0.14	20,20,20,20	0
59	MG	DA	3004	1/1	0.95	0.25	25,25,25,25	0
59	MG	BA	3267	1/1	0.95	0.23	25,25,25,25	0
59	MG	BA	3156	1/1	0.95	0.14	58,58,58,58	0
59	MG	DA	3287	1/1	0.95	0.15	28,28,28,28	0
59	MG	BA	3019	1/1	0.95	0.36	26,26,26,26	0
59	MG	CA	1653	1/1	0.95	0.07	44,44,44,44	0
59	MG	DA	3054	1/1	0.95	0.42	22,22,22,22	0
59	MG	BA	3284	1/1	0.95	0.19	31,31,31,31	0
59	MG	CA	1635	1/1	0.95	0.09	31,31,31,31	0
59	MG	DA	3233	1/1	0.95	0.30	37,37,37,37	0
59	MG	D5	102	1/1	0.95	0.44	28,28,28,28	0
59	MG	AA	1609	1/1	0.95	0.13	38,38,38,38	1
59	MG	DA	3024	1/1	0.95	0.35	10,10,10,10	0
59	MG	AA	1643	1/1	0.95	0.21	93,93,93,93	0
59	MG	DA	3208	1/1	0.95	0.15	26,26,26,26	0
59	MG	DE	301	1/1	0.95	0.24	41,41,41,41	0
59	MG	DA	3297	1/1	0.95	0.31	42,42,42,42	1
59	MG	DA	3232	1/1	0.95	0.29	37,37,37,37	1
59	MG	DA	3118	1/1	0.95	0.27	15,15,15,15	0
59	MG	BA	3251	1/1	0.95	0.28	55,55,55,55	0
59	MG	DA	3330	1/1	0.95	0.23	23,23,23,23	0
59	MG	DA	3151	1/1	0.96	0.27	25,25,25,25	0
59	MG	DA	3171	1/1	0.96	0.16	3,3,3,3	0
59	MG	DA	3124	1/1	0.96	0.38	20,20,20,20	1
59	MG	BA	3090	1/1	0.96	0.27	33,33,33,33	0
59	MG	CA	1751	1/1	0.96	0.14	62,62,62,62	0
59	MG	BA	3337	1/1	0.96	0.28	55,55,55,55	0
59	MG	CV	103	1/1	0.96	0.08	57,57,57,57	0
59	MG	DA	3011	1/1	0.96	0.25	10,10,10,10	0
59	MG	AA	1629	1/1	0.96	0.20	61,61,61,61	0
59	MG	BA	3018	1/1	0.96	0.22	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	DS	201	1/1	0.96	0.26	30,30,30,30	0
59	MG	CA	1608	1/1	0.96	0.14	35,35,35,35	0
59	MG	CA	1620	1/1	0.96	0.19	48,48,48,48	0
59	MG	BA	3350	1/1	0.96	0.69	69,69,69,69	0
59	MG	DA	3310	1/1	0.96	0.23	51,51,51,51	0
59	MG	BA	3063	1/1	0.96	0.14	56,56,56,56	0
59	MG	DA	3007	1/1	0.96	0.24	4,4,4,4	0
59	MG	DA	3213	1/1	0.96	0.24	17,17,17,17	0
59	MG	DA	3200	1/1	0.96	0.31	18,18,18,18	0
59	MG	DA	3034	1/1	0.96	0.33	32,32,32,32	0
59	MG	DA	3206	1/1	0.96	0.21	57,57,57,57	0
59	MG	DA	3101	1/1	0.96	0.39	16,16,16,16	0
59	MG	CV	104	1/1	0.96	0.07	2,2,2,2	1
59	MG	BA	3347	1/1	0.96	0.19	30,30,30,30	0
59	MG	DA	3217	1/1	0.96	0.19	7,7,7,7	0
59	MG	BA	3164	1/1	0.96	0.30	52,52,52,52	0
59	MG	DA	3293	1/1	0.96	0.84	63,63,63,63	0
59	MG	BA	3275	1/1	0.96	0.36	27,27,27,27	1
59	MG	BA	3234	1/1	0.96	0.35	26,26,26,26	0
59	MG	DA	3183	1/1	0.96	0.15	45,45,45,45	0
59	MG	BY	201	1/1	0.96	0.12	42,42,42,42	0
59	MG	CA	1741	1/1	0.96	0.36	34,34,34,34	0
59	MG	AA	1715	1/1	0.96	0.30	59,59,59,59	0
59	MG	CA	1745	1/1	0.96	0.26	37,37,37,37	0
59	MG	CA	1630	1/1	0.96	0.29	68,68,68,68	0
59	MG	DA	3086	1/1	0.96	0.25	18,18,18,18	0
59	MG	AA	1620	1/1	0.96	0.24	54,54,54,54	0
59	MG	DA	3075	1/1	0.96	0.29	26,26,26,26	0
59	MG	CA	1609	1/1	0.96	0.25	58,58,58,58	0
59	MG	DA	3168	1/1	0.96	0.09	18,18,18,18	0
59	MG	CA	1647	1/1	0.96	0.32	44,44,44,44	0
59	MG	BA	3270	1/1	0.96	0.30	49,49,49,49	0
59	MG	CA	1703	1/1	0.96	0.11	62,62,62,62	0
59	MG	DA	3113	1/1	0.96	0.23	16,16,16,16	0
59	MG	DA	3348	1/1	0.96	0.16	18,18,18,18	0
59	MG	DA	3014	1/1	0.96	0.29	20,20,20,20	0
59	MG	DA	3231	1/1	0.96	0.22	27,27,27,27	0
59	MG	CA	1643	1/1	0.96	0.13	10,10,10,10	1
59	MG	DA	3088	1/1	0.96	0.43	8,8,8,8	0
59	MG	AA	1618	1/1	0.96	0.09	30,30,30,30	1
59	MG	BA	3013	1/1	0.96	0.21	54,54,54,54	0
59	MG	DA	3063	1/1	0.96	0.19	17,17,17,17	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	DA	3003	1/1	0.96	0.31	35,35,35,35	0
59	MG	BA	3193	1/1	0.96	0.39	5,5,5,5	1
59	MG	DA	3026	1/1	0.96	0.22	21,21,21,21	0
59	MG	BD	302	1/1	0.96	0.21	29,29,29,29	0
59	MG	BA	3040	1/1	0.96	0.27	36,36,36,36	0
59	MG	BA	3035	1/1	0.96	0.19	21,21,21,21	0
59	MG	BA	3148	1/1	0.96	0.09	44,44,44,44	0
59	MG	BA	3230	1/1	0.96	0.21	40,40,40,40	0
59	MG	CA	1676	1/1	0.96	0.15	46,46,46,46	1
59	MG	BA	3038	1/1	0.96	0.26	44,44,44,44	0
59	MG	DA	3246	1/1	0.96	0.26	45,45,45,45	0
59	MG	BA	3211	1/1	0.96	0.22	44,44,44,44	0
59	MG	DA	3068	1/1	0.96	0.22	6,6,6,6	0
59	MG	BA	3101	1/1	0.96	0.40	27,27,27,27	0
59	MG	DA	3306	1/1	0.96	0.39	15,15,15,15	0
59	MG	DA	3108	1/1	0.96	0.38	16,16,16,16	0
59	MG	DA	3017	1/1	0.96	0.22	22,22,22,22	0
59	MG	AA	1631	1/1	0.96	0.06	45,45,45,45	0
59	MG	CA	1729	1/1	0.96	0.30	33,33,33,33	1
59	MG	BA	3307	1/1	0.96	0.29	14,14,14,14	0
59	MG	DA	3009	1/1	0.96	0.29	15,15,15,15	0
59	MG	DA	3234	1/1	0.96	0.46	69,69,69,69	0
59	MG	CV	102	1/1	0.96	0.11	43,43,43,43	0
59	MG	BA	3328	1/1	0.96	0.22	32,32,32,32	0
59	MG	DA	3074	1/1	0.96	0.26	24,24,24,24	0
59	MG	DA	3180	1/1	0.96	0.32	11,11,11,11	0
59	MG	BA	3074	1/1	0.96	0.28	37,37,37,37	0
59	MG	AA	1725	1/1	0.96	0.11	94,94,94,94	0
59	MG	BA	3042	1/1	0.96	0.45	43,43,43,43	0
59	MG	CA	1625	1/1	0.96	0.17	36,36,36,36	0
59	MG	DF	301	1/1	0.96	0.11	9,9,9,9	0
59	MG	DA	3149	1/1	0.96	0.16	43,43,43,43	0
59	MG	DA	3176	1/1	0.96	0.28	7,7,7,7	0
59	MG	AA	1636	1/1	0.96	0.14	21,21,21,21	0
59	MG	DA	3097	1/1	0.96	0.14	15,15,15,15	0
59	MG	CA	1718	1/1	0.96	0.14	44,44,44,44	1
59	MG	CA	1705	1/1	0.96	0.24	47,47,47,47	0
59	MG	DA	3082	1/1	0.96	0.24	56,56,56,56	0
59	MG	DA	3172	1/1	0.96	0.20	3,3,3,3	0
59	MG	DA	3035	1/1	0.96	0.25	19,19,19,19	0
59	MG	DA	3131	1/1	0.96	0.12	18,18,18,18	0
59	MG	BA	3012	1/1	0.97	0.24	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	BA	3083	1/1	0.97	0.25	25,25,25,25	0
59	MG	AA	1634	1/1	0.97	0.49	39,39,39,39	0
59	MG	DA	3027	1/1	0.97	0.17	1,1,1,1	0
59	MG	BA	3201	1/1	0.97	0.19	37,37,37,37	0
59	MG	AA	1686	1/1	0.97	0.34	64,64,64,64	0
59	MG	BA	3301	1/1	0.97	0.23	36,36,36,36	0
59	MG	DA	3019	1/1	0.97	0.31	17,17,17,17	0
59	MG	DA	3022	1/1	0.97	0.41	16,16,16,16	0
59	MG	BA	3053	1/1	0.97	0.17	45,45,45,45	1
59	MG	DA	3067	1/1	0.97	0.11	13,13,13,13	0
59	MG	BA	3014	1/1	0.97	0.33	45,45,45,45	0
59	MG	DA	3012	1/1	0.97	0.35	19,19,19,19	0
59	MG	DA	3106	1/1	0.97	0.39	23,23,23,23	0
59	MG	AA	1624	1/1	0.97	0.37	62,62,62,62	0
60	ZN	B9	101	1/1	0.97	0.06	77,77,77,77	1
59	MG	DA	3126	1/1	0.97	0.29	6,6,6,6	0
59	MG	BA	3224	1/1	0.97	0.08	37,37,37,37	0
59	MG	DA	3269	1/1	0.97	0.21	7,7,7,7	0
59	MG	BA	3244	1/1	0.97	0.26	51,51,51,51	0
59	MG	DA	3346	1/1	0.97	0.26	42,42,42,42	0
59	MG	DA	3105	1/1	0.97	0.10	1,1,1,1	0
59	MG	DA	3302	1/1	0.97	0.13	1,1,1,1	0
59	MG	BA	3314	1/1	0.97	0.47	45,45,45,45	0
59	MG	DA	3140	1/1	0.97	0.27	57,57,57,57	0
59	MG	DA	3043	1/1	0.97	0.29	2,2,2,2	0
59	MG	BA	3186	1/1	0.97	0.31	28,28,28,28	0
59	MG	DA	3353	1/1	0.97	0.21	43,43,43,43	0
59	MG	BA	3106	1/1	0.97	0.23	34,34,34,34	0
59	MG	DA	3354	1/1	0.97	0.21	21,21,21,21	0
59	MG	DA	3324	1/1	0.97	0.28	25,25,25,25	1
59	MG	CA	1606	1/1	0.97	0.42	58,58,58,58	0
59	MG	DA	3136	1/1	0.97	0.34	38,38,38,38	0
59	MG	BA	3238	1/1	0.97	0.09	17,17,17,17	0
59	MG	CA	1684	1/1	0.97	0.53	50,50,50,50	0
59	MG	DA	3081	1/1	0.97	0.23	16,16,16,16	0
59	MG	AA	1632	1/1	0.97	0.57	56,56,56,56	0
59	MG	BA	3005	1/1	0.97	0.37	27,27,27,27	0
59	MG	DA	3060	1/1	0.97	0.24	17,17,17,17	0
59	MG	CV	101	1/1	0.97	0.16	29,29,29,29	0
59	MG	BA	3228	1/1	0.97	0.12	48,48,48,48	1
59	MG	CA	1668	1/1	0.97	0.43	50,50,50,50	0
59	MG	BA	3265	1/1	0.97	0.08	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	BA	3345	1/1	0.97	0.43	63,63,63,63	0
59	MG	DA	3142	1/1	0.97	0.43	17,17,17,17	0
59	MG	BA	3294	1/1	0.97	0.28	32,32,32,32	0
59	MG	DA	3247	1/1	0.97	0.14	44,44,44,44	0
59	MG	DA	3254	1/1	0.97	0.15	50,50,50,50	1
59	MG	AA	1627	1/1	0.97	0.13	40,40,40,40	0
59	MG	DA	3103	1/1	0.97	0.28	12,12,12,12	0
59	MG	BA	3054	1/1	0.97	0.32	19,19,19,19	0
59	MG	DA	3127	1/1	0.97	0.10	6,6,6,6	0
59	MG	DA	3185	1/1	0.97	0.13	39,39,39,39	0
59	MG	AA	1628	1/1	0.97	0.20	50,50,50,50	0
59	MG	DA	3296	1/1	0.97	0.07	34,34,34,34	0
59	MG	DA	3087	1/1	0.97	0.20	1,1,1,1	0
59	MG	DA	3038	1/1	0.97	0.26	20,20,20,20	0
59	MG	BA	3055	1/1	0.97	0.33	25,25,25,25	0
59	MG	AA	1695	1/1	0.97	0.18	56,56,56,56	0
59	MG	CA	1683	1/1	0.97	0.12	35,35,35,35	0
59	MG	DA	3072	1/1	0.97	0.23	20,20,20,20	0
59	MG	AA	1626	1/1	0.97	0.56	61,61,61,61	0
59	MG	CA	1664	1/1	0.97	0.20	28,28,28,28	0
59	MG	DB	203	1/1	0.97	0.25	20,20,20,20	0
59	MG	DA	3049	1/1	0.97	0.29	15,15,15,15	0
59	MG	BA	3295	1/1	0.97	0.20	81,81,81,81	1
59	MG	DA	3162	1/1	0.97	0.19	1,1,1,1	0
59	MG	DA	3300	1/1	0.97	0.19	10,10,10,10	0
59	MG	DA	3284	1/1	0.97	0.22	1,1,1,1	0
59	MG	AA	1602	1/1	0.97	0.29	53,53,53,53	1
59	MG	DA	3133	1/1	0.97	0.19	13,13,13,13	1
59	MG	BA	3084	1/1	0.97	0.16	27,27,27,27	0
59	MG	DA	3266	1/1	0.97	0.23	27,27,27,27	0
59	MG	DA	3023	1/1	0.97	0.48	20,20,20,20	0
59	MG	CA	1754	1/1	0.97	0.52	68,68,68,68	1
59	MG	DA	3257	1/1	0.97	0.11	35,35,35,35	0
59	MG	AA	1672	1/1	0.97	0.06	55,55,55,55	0
59	MG	BA	3253	1/1	0.97	0.11	65,65,65,65	1
59	MG	BA	3047	1/1	0.97	0.17	18,18,18,18	0
59	MG	CA	1666	1/1	0.97	0.45	59,59,59,59	0
59	MG	DA	3076	1/1	0.97	0.21	11,11,11,11	0
59	MG	AA	1693	1/1	0.97	0.20	41,41,41,41	0
59	MG	DA	3294	1/1	0.97	0.34	33,33,33,33	0
59	MG	CA	1735	1/1	0.97	0.10	21,21,21,21	0
59	MG	BA	3052	1/1	0.97	0.15	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	DA	3090	1/1	0.97	0.26	20,20,20,20	0
59	MG	BA	3058	1/1	0.97	0.36	30,30,30,30	0
59	MG	BA	3066	1/1	0.97	0.51	25,25,25,25	0
59	MG	DA	3077	1/1	0.98	0.31	9,9,9,9	0
59	MG	CA	1721	1/1	0.98	0.19	74,74,74,74	0
59	MG	BA	3300	1/1	0.98	0.25	17,17,17,17	0
59	MG	BA	3098	1/1	0.98	0.11	15,15,15,15	0
59	MG	DA	3042	1/1	0.98	0.30	12,12,12,12	0
59	MG	BA	3057	1/1	0.98	0.30	21,21,21,21	0
59	MG	DA	3272	1/1	0.98	0.25	19,19,19,19	0
59	MG	AA	1683	1/1	0.98	0.13	63,63,63,63	0
59	MG	BA	3197	1/1	0.98	0.35	12,12,12,12	0
59	MG	BA	3248	1/1	0.98	0.07	62,62,62,62	0
59	MG	BA	3009	1/1	0.98	0.34	21,21,21,21	0
59	MG	DA	3061	1/1	0.98	0.26	10,10,10,10	0
59	MG	BA	3037	1/1	0.98	0.25	23,23,23,23	0
59	MG	BA	3116	1/1	0.98	0.30	45,45,45,45	0
59	MG	BA	3157	1/1	0.98	0.22	36,36,36,36	1
59	MG	DA	3157	1/1	0.98	0.23	26,26,26,26	0
59	MG	BA	3062	1/1	0.98	0.35	16,16,16,16	0
59	MG	DA	3102	1/1	0.98	0.12	1,1,1,1	0
59	MG	DA	3015	1/1	0.98	0.24	9,9,9,9	0
59	MG	BA	3076	1/1	0.98	0.18	28,28,28,28	0
59	MG	BA	3256	1/1	0.98	0.05	25,25,25,25	0
59	MG	BA	3061	1/1	0.98	0.43	21,21,21,21	0
59	MG	DA	3094	1/1	0.98	0.31	9,9,9,9	0
59	MG	BD	301	1/1	0.98	0.26	22,22,22,22	0
59	MG	BA	3130	1/1	0.98	0.09	29,29,29,29	0
59	MG	BA	3087	1/1	0.98	0.21	13,13,13,13	0
59	MG	BA	3165	1/1	0.98	0.41	40,40,40,40	0
59	MG	DA	3188	1/1	0.98	0.26	7,7,7,7	0
59	MG	BA	3011	1/1	0.98	0.38	43,43,43,43	0
59	MG	DA	3020	1/1	0.98	0.28	11,11,11,11	0
59	MG	DA	3173	1/1	0.98	0.24	12,12,12,12	0
59	MG	BA	3056	1/1	0.98	0.40	33,33,33,33	0
59	MG	BA	3147	1/1	0.98	0.27	35,35,35,35	0
59	MG	DA	3033	1/1	0.98	0.26	16,16,16,16	0
59	MG	BA	3269	1/1	0.98	0.41	34,34,34,34	0
59	MG	DA	3145	1/1	0.98	0.20	43,43,43,43	0
59	MG	DA	3073	1/1	0.98	0.30	15,15,15,15	0
59	MG	CA	1604	1/1	0.98	0.17	51,51,51,51	0
59	MG	BA	3133	1/1	0.98	0.26	118,118,118,118	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	CA	1746	1/1	0.98	0.12	10,10,10,10	1
59	MG	BA	3158	1/1	0.98	0.47	23,23,23,23	0
59	MG	DA	3120	1/1	0.98	0.27	9,9,9,9	0
59	MG	DA	3066	1/1	0.98	0.41	14,14,14,14	0
59	MG	AA	1635	1/1	0.98	0.07	50,50,50,50	0
59	MG	DA	3301	1/1	0.98	0.21	21,21,21,21	0
59	MG	DA	3265	1/1	0.98	0.08	27,27,27,27	0
59	MG	DA	3148	1/1	0.98	0.27	7,7,7,7	0
59	MG	BA	3079	1/1	0.98	0.32	36,36,36,36	0
59	MG	DA	3005	1/1	0.98	0.33	21,21,21,21	0
59	MG	DA	3116	1/1	0.98	0.16	7,7,7,7	0
59	MG	AA	1755	1/1	0.98	0.05	51,51,51,51	0
59	MG	BA	3103	1/1	0.98	0.42	28,28,28,28	0
59	MG	DA	3177	1/1	0.98	0.22	53,53,53,53	0
59	MG	DA	3083	1/1	0.98	0.26	11,11,11,11	0
59	MG	AA	1705	1/1	0.98	0.16	43,43,43,43	0
59	MG	D1	101	1/1	0.98	0.14	22,22,22,22	1
59	MG	DA	3344	1/1	0.98	0.14	43,43,43,43	0
59	MG	AA	1612	1/1	0.98	0.09	47,47,47,47	0
59	MG	BA	3071	1/1	0.98	0.11	28,28,28,28	0
59	MG	DA	3062	1/1	0.98	0.25	1,1,1,1	0
59	MG	AA	1608	1/1	0.98	0.15	48,48,48,48	0
59	MG	DA	3190	1/1	0.98	0.29	16,16,16,16	0
59	MG	DA	3222	1/1	0.98	0.30	15,15,15,15	0
59	MG	BA	3043	1/1	0.98	0.28	22,22,22,22	0
59	MG	DA	3047	1/1	0.98	0.20	20,20,20,20	0
59	MG	DA	3016	1/1	0.98	0.46	16,16,16,16	0
59	MG	DA	3223	1/1	0.98	0.41	32,32,32,32	0
60	ZN	AN	101	1/1	0.98	0.11	104,104,104,104	0
59	MG	DA	3186	1/1	0.98	0.30	17,17,17,17	0
59	MG	CA	1669	1/1	0.98	0.28	33,33,33,33	0
59	MG	DA	3037	1/1	0.98	0.25	7,7,7,7	0
59	MG	BA	3187	1/1	0.98	0.36	18,18,18,18	0
59	MG	BA	3178	1/1	0.98	0.33	22,22,22,22	0
59	MG	BA	3126	1/1	0.98	0.11	21,21,21,21	0
59	MG	DA	3114	1/1	0.98	0.18	15,15,15,15	0
59	MG	BA	3184	1/1	0.98	0.31	27,27,27,27	0
59	MG	BA	3141	1/1	0.98	0.26	42,42,42,42	0
59	MG	CA	1686	1/1	0.98	0.14	21,21,21,21	0
59	MG	BA	3085	1/1	0.98	0.17	38,38,38,38	0
59	MG	CA	1726	1/1	0.98	0.76	48,48,48,48	0
59	MG	CA	1709	1/1	0.98	0.08	40,40,40,40	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	DA	3070	1/1	0.98	0.22	11,11,11,11	0
59	MG	DA	3230	1/1	0.98	0.20	42,42,42,42	0
59	MG	DA	3098	1/1	0.98	0.15	6,6,6,6	0
59	MG	DA	3154	1/1	0.98	0.20	31,31,31,31	0
59	MG	BA	3105	1/1	0.99	0.15	9,9,9,9	0
59	MG	BA	3051	1/1	0.99	0.22	25,25,25,25	0
59	MG	CA	1694	1/1	0.99	0.14	37,37,37,37	1
59	MG	DA	3125	1/1	0.99	0.38	18,18,18,18	0
59	MG	DA	3008	1/1	0.99	0.25	10,10,10,10	0
59	MG	BA	3118	1/1	0.99	0.44	38,38,38,38	0
60	ZN	CN	102	1/1	0.99	0.12	101,101,101,101	0
59	MG	BA	3070	1/1	0.99	0.22	37,37,37,37	0
60	ZN	AD	301	1/1	0.99	0.21	67,67,67,67	0
59	MG	DA	3079	1/1	0.99	0.30	10,10,10,10	0
59	MG	BA	3041	1/1	0.99	0.35	17,17,17,17	0
59	MG	DA	3199	1/1	0.99	0.41	14,14,14,14	0
59	MG	DA	3048	1/1	0.99	0.28	22,22,22,22	0
59	MG	BA	3153	1/1	0.99	0.25	48,48,48,48	0
59	MG	BA	3025	1/1	0.99	0.26	40,40,40,40	0
59	MG	DA	3041	1/1	0.99	0.32	17,17,17,17	0
59	MG	BA	3026	1/1	0.99	0.22	8,8,8,8	0
59	MG	DA	3055	1/1	0.99	0.30	23,23,23,23	0
59	MG	DA	3092	1/1	0.99	0.28	18,18,18,18	0
59	MG	DA	3174	1/1	0.99	0.14	46,46,46,46	0
59	MG	DA	3018	1/1	0.99	0.24	16,16,16,16	0
59	MG	CA	1740	1/1	0.99	0.48	56,56,56,56	0
60	ZN	D9	101	1/1	0.99	0.10	59,59,59,59	0
59	MG	BA	3171	1/1	0.99	0.17	30,30,30,30	0
59	MG	DA	3100	1/1	0.99	0.34	3,3,3,3	0
59	MG	DA	3013	1/1	0.99	0.19	16,16,16,16	0
59	MG	BA	3155	1/1	0.99	0.19	53,53,53,53	0
59	MG	DA	3057	1/1	0.99	0.34	10,10,10,10	0
59	MG	CV	107	1/1	0.99	0.13	51,51,51,51	0
59	MG	DA	3112	1/1	0.99	0.16	42,42,42,42	0
59	MG	BA	3188	1/1	0.99	0.34	14,14,14,14	0
59	MG	DA	3189	1/1	0.99	0.51	21,21,21,21	0
59	MG	CA	1656	1/1	0.99	0.43	29,29,29,29	0
59	MG	BA	3027	1/1	0.99	0.21	19,19,19,19	0
59	MG	DA	3248	1/1	0.99	0.12	2,2,2,2	1
59	MG	CA	1629	1/1	0.99	0.47	55,55,55,55	0
59	MG	DA	3295	1/1	0.99	0.20	13,13,13,13	1
59	MG	BA	3015	1/1	0.99	0.26	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	BA	3081	1/1	0.99	0.29	21,21,21,21	0
59	MG	DA	3084	1/1	0.99	0.23	13,13,13,13	0
59	MG	DA	3050	1/1	0.99	0.15	13,13,13,13	0
59	MG	DA	3059	1/1	0.99	0.24	13,13,13,13	0
59	MG	DA	3046	1/1	0.99	0.27	11,11,11,11	0
59	MG	DA	3249	1/1	0.99	0.13	27,27,27,27	1
59	MG	BA	3050	1/1	0.99	0.20	36,36,36,36	0
59	MG	DA	3089	1/1	0.99	0.32	5,5,5,5	0
60	ZN	CD	302	1/1	0.99	0.23	80,80,80,80	0

6.5 Other polymers [i](#)

There are no such residues in this entry.