



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 02:48 PM UTC

PDB ID : 4V84 / pdb_00004v84
Title : Crystal structure of a complex containing domain 3 of CrPV IGR IRES RNA bound to the 70S ribosome.
Authors : Zhu, J.; Korostelev, A.; Costantino, D.; Noller, H.F.; Kieft, J.S.
Deposited on : 2010-12-13
Resolution : 3.40 Å(reported)

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

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A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

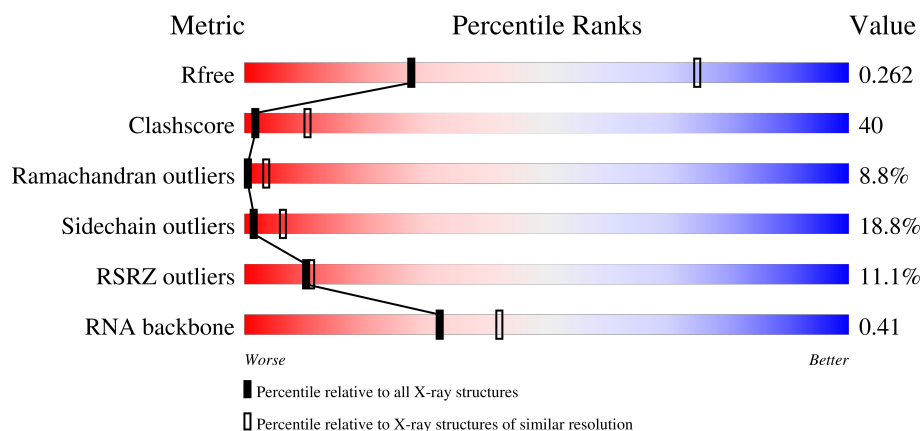
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)
RNA backbone	3983	1157 (3.80-3.00)

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

Mol	Chain	Length	Quality of chain
1	AA	1506	6% 20% 65% 15%
1	CA	1506	5% 19% 66% 15%
2	AB	234	15% 31% 55% 14%
2	CB	234	16% 30% 56% 13%

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Mol	Chain	Length	Quality of chain
3	AC	206	
3	CC	206	
4	AD	208	
4	CD	208	
5	AE	151	
5	CE	151	
6	AF	101	
6	CF	101	
7	AG	155	
7	CG	155	
8	AH	138	
8	CH	138	
9	AI	127	
9	CI	127	
10	AJ	98	
10	CJ	98	
11	AK	119	
11	CK	119	
12	AL	124	
12	CL	124	
13	AM	116	
13	CM	116	
14	AN	60	
14	CN	60	
15	AO	88	

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Mol	Chain	Length	Quality of chain
15	CO	88	
16	AP	83	
16	CP	83	
17	AQ	99	
17	CQ	99	
18	AR	70	
18	CR	70	
19	AS	78	
19	CS	78	
20	AT	99	
20	CT	99	
21	AU	24	
21	CU	24	
22	AV	43	
22	CV	43	
23	BA	2879	
23	DA	2879	
24	BB	119	
24	DB	119	
25	BC	271	
25	DC	271	
26	BD	204	
26	DD	204	
27	BE	202	
27	DE	202	

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Mol	Chain	Length	Quality of chain
28	BF	181	
28	DF	181	
29	BG	159	
29	DG	159	
30	BH	145	
30	DH	145	
31	BI	65	
31	DI	65	
32	BJ	137	
32	DJ	137	
33	BK	122	
33	DK	122	
34	BL	146	
34	DL	146	
35	BM	136	
35	DM	136	
36	BN	117	
36	DN	117	
37	BO	98	
37	DO	98	
38	BP	137	
38	DP	137	
39	BQ	116	
39	DQ	116	
40	BR	101	

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Mol	Chain	Length	Quality of chain
40	DR	101	
41	BS	112	
41	DS	112	
42	BT	92	
42	DT	92	
43	BU	100	
43	DU	100	
44	BV	188	
44	DV	188	
45	BW	76	
45	DW	76	
46	BX	88	
46	DX	88	
47	BY	62	
47	DY	62	
48	BZ	59	
48	DZ	59	
49	B1	30	
49	D1	30	
50	B2	52	
50	D2	52	
51	B3	44	
51	D3	44	
52	B4	48	
52	D4	48	

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Mol	Chain	Length	Quality of chain
53	B5	63	
53	D5	63	

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
54	MG	BA	3031	-	-	-	X
54	MG	CA	1685	-	-	-	X

2 Entry composition [i](#)

There are 55 unique types of molecules in this entry. The entry contains 282142 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 ribosomal RNA 16S.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1506	Total	C	N	O	P	0	0	0
			32372	14409	5999	10459	1505			
1	CA	1506	Total	C	N	O	P	0	0	0
			32372	14409	5999	10459	1505			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AB	234	Total	C	N	O	S	0	0	0
			1901	1213	341	342	5			
2	CB	234	Total	C	N	O	S	0	0	0
			1901	1213	341	342	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AC	206	Total	C	N	O	S	0	0	0
			1613	1016	314	282	1			
3	CC	206	Total	C	N	O	S	0	0	0
			1613	1016	314	282	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	0
			1156	729	218	205	4			
5	CE	151	Total	C	N	O	S	0	0	0
			1156	729	218	205	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	98	Total	C	N	O	S	0	0	0
			795	499	156	139	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	CJ	98	Total	C	N	O	S	0	0	0
			795	499	156	139	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	124	Total	C	N	O	S	0	0	0
			971	611	195	164	1			
12	CL	124	Total	C	N	O	S	0	0	0
			971	611	195	164	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AM	116	Total	C	N	O	S	0	0	0
			929	574	191	162	2			
13	CM	116	Total	C	N	O	S	0	0	0
			929	574	191	162	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	83	Total	C	N	O	S	0	0	0
			701	443	139	118	1			
16	CP	83	Total	C	N	O	S	0	0	0
			701	443	139	118	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AQ	99	Total	C	N	O	S	0	0	0
			824	528	152	142	2			
17	CQ	99	Total	C	N	O	S	0	0	0
			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	78	Total	C	N	O	S	0	0	0
			630	403	114	111	2			
19	CS	78	Total	C	N	O	S	0	0	0
			630	403	114	111	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
			762	469	162	129	2			
20	CT	99	Total	C	N	O	S	0	0	0
			762	469	162	129	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	AU	24	Total	C	N	O	0	0	0
			209	128	50	31			
21	CU	24	Total	C	N	O	0	0	0
			209	128	50	31			

- Molecule 22 is a RNA chain called RNA (34-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AV	34	Total	C	N	O	P	0	0	0
			719	323	125	238	33			
22	CV	34	Total	C	N	O	P	0	0	0
			719	323	125	238	33			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	BA	2760	Total	C	N	O	P	0	0	0
			59440	26455	11114	19112	2759			
23	DA	2760	Total	C	N	O	P	0	0	0
			59442	26456	11114	19113	2759			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BA	1142	U	C	conflict	GB 46197919
BA	2825	U	G	conflict	GB 46197919
DA	1142	U	C	conflict	GB 46197919
DA	2825	U	G	conflict	GB 46197919

- Molecule 24 is a RNA chain called 5S ribosomal RNA.

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

- Molecule 25 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	BC	271	Total	C	N	O	S	0	0	0
			2105	1329	416	357	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	DC	271	Total	C	N	O	S	0	0	0
			2105	1329	416	357	3			

- Molecule 26 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	BD	204	Total	C	N	O	S	0	0	0
			1564	988	299	271	6			
26	DD	204	Total	C	N	O	S	0	0	0
			1564	988	299	271	6			

- Molecule 27 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	BE	202	Total	C	N	O	S	0	0	0
			1587	1011	297	276	3			
27	DE	202	Total	C	N	O	S	0	0	0
			1587	1011	297	276	3			

- Molecule 28 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	BF	181	Total	C	N	O	S	0	0	0
			1475	943	268	260	4			
28	DF	181	Total	C	N	O	S	0	0	0
			1475	943	268	260	4			

- Molecule 29 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	BG	159	Total	C	N	O	S	0	0	0
			1223	773	228	221	1			
29	DG	159	Total	C	N	O	S	0	0	0
			1223	773	228	221	1			

- Molecule 30 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	BH	145	Total	C	N	O	S	0	0	0
			1133	724	200	208	1			
30	DH	145	Total	C	N	O	S	0	0	0
			1133	724	200	208	1			

- Molecule 31 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
31	BI	32	Total	C	N	O	0	0	0
			254	157	49	48			
31	DI	32	Total	C	N	O	0	0	0
			254	157	49	48			

- Molecule 32 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	BJ	137	Total	C	N	O	S	0	0	0
			1097	707	205	182	3			
32	DJ	137	Total	C	N	O	S	0	0	0
			1097	707	205	182	3			

- Molecule 33 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	BK	122	Total	C	N	O	S	0	0	0
			932	587	171	170	4			
33	DK	122	Total	C	N	O	S	0	0	0
			932	587	171	170	4			

- Molecule 34 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	BL	146	Total	C	N	O	S	0	0	0
			1114	692	227	193	2			
34	DL	146	Total	C	N	O	S	0	0	0
			1114	692	227	193	2			

- Molecule 35 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BM	136	Total	C	N	O	S	0	0	0
			1079	688	204	182	5			
35	DM	136	Total	C	N	O	S	0	0	0
			1079	688	204	182	5			

- Molecule 36 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
36	BN	117	Total	C	N	O	0	0	0
			960	599	202	159			
36	DN	117	Total	C	N	O	0	0	0
			960	599	202	159			

- Molecule 37 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
37	BO	98	Total	C	N	O	0	0	0
			771	486	154	131			
37	DO	98	Total	C	N	O	0	0	0
			771	486	154	131			

- Molecule 38 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	BP	137	Total	C	N	O	S	0	0	0
			1144	713	234	196	1			
38	DP	137	Total	C	N	O	S	0	0	0
			1144	713	234	196	1			

- Molecule 39 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BQ	116	Total	C	N	O	S	0	0	0
			953	601	201	150	1			
39	DQ	116	Total	C	N	O	S	0	0	0
			953	601	201	150	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BQ	?	-	PHE	deletion	UNP Q72L76
DQ	?	-	PHE	deletion	UNP Q72L76

- Molecule 40 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	BR	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			
40	DR	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			

- Molecule 41 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BS	112	Total	C	N	O	S	0	0	0
			891	560	175	154	2			
41	DS	112	Total	C	N	O	S	0	0	0
			891	560	175	154	2			

- Molecule 42 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
42	BT	92	Total	C	N	O	0	0	0
			726	471	131	124			
42	DT	92	Total	C	N	O	0	0	0
			726	471	131	124			

- Molecule 43 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BU	100	Total	C	N	O	S	0	0	0
			776	500	148	124	4			
43	DU	100	Total	C	N	O	S	0	0	0
			776	500	148	124	4			

- Molecule 44 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	BV	188	Total	C	N	O	S	0	0	0
			1492	950	265	275	2			
44	DV	188	Total	C	N	O	S	0	0	0
			1492	950	265	275	2			

- Molecule 45 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	BW	76	Total	C	N	O	S	0	0	0
			605	376	126	102	1			
45	DW	76	Total	C	N	O	S	0	0	0
			605	376	126	102	1			

- Molecule 46 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
46	BX	88	Total	C	N	O	0	0	0
			695	435	141	119			
46	DX	88	Total	C	N	O	0	0	0
			695	435	141	119			

- Molecule 47 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	BY	62	Total	C	N	O	S	0	0	0
			521	325	102	92	2			
47	DY	62	Total	C	N	O	S	0	0	0
			521	325	102	92	2			

- Molecule 48 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	BZ	59	Total	C	N	O	S	0	0	0
			468	298	90	79	1			
48	DZ	59	Total	C	N	O	S	0	0	0
			468	298	90	79	1			

- Molecule 49 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	B1	30	Total	C	N	O	S	0	0	0
			226	142	36	44	4			
49	D1	30	Total	C	N	O	S	0	0	0
			226	142	36	44	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	B2	52	Total	C	N	O	S	0	0	0
			405	255	79	66	5			
50	D2	52	Total	C	N	O	S	0	0	0
			405	255	79	66	5			

- Molecule 51 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	B3	44	Total	C	N	O	S	0	0	0
			381	235	77	65	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	D3	44	Total	C	N	O	S	0	0	0
			381	235	77	65	4			

- Molecule 52 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	B4	48	Total	C	N	O	S	0	0	0
			419	257	104	56	2			
52	D4	48	Total	C	N	O	S	0	0	0
			419	257	104	56	2			

- Molecule 53 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	B5	63	Total	C	N	O	S	0	0	0
			508	326	101	79	2			
53	D5	63	Total	C	N	O	S	0	0	0
			508	326	101	79	2			

- Molecule 54 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	AA	163	Total	Mg	0	0
			163	163		
54	AD	1	Total	Mg	0	0
			1	1		
54	AV	4	Total	Mg	0	0
			4	4		
54	BA	408	Total	Mg	0	0
			408	408		
54	BB	17	Total	Mg	0	0
			17	17		
54	BK	1	Total	Mg	0	0
			1	1		
54	B2	1	Total	Mg	0	0
			1	1		
54	CA	140	Total	Mg	0	0
			140	140		
54	CP	1	Total	Mg	0	0
			1	1		
54	CV	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	DA	436	Total 436	Mg 436	0	0
54	DB	17	Total 17	Mg 17	0	0
54	DE	1	Total 1	Mg 1	0	0
54	DG	1	Total 1	Mg 1	0	0
54	D2	1	Total 1	Mg 1	0	0
54	D4	1	Total 1	Mg 1	0	0

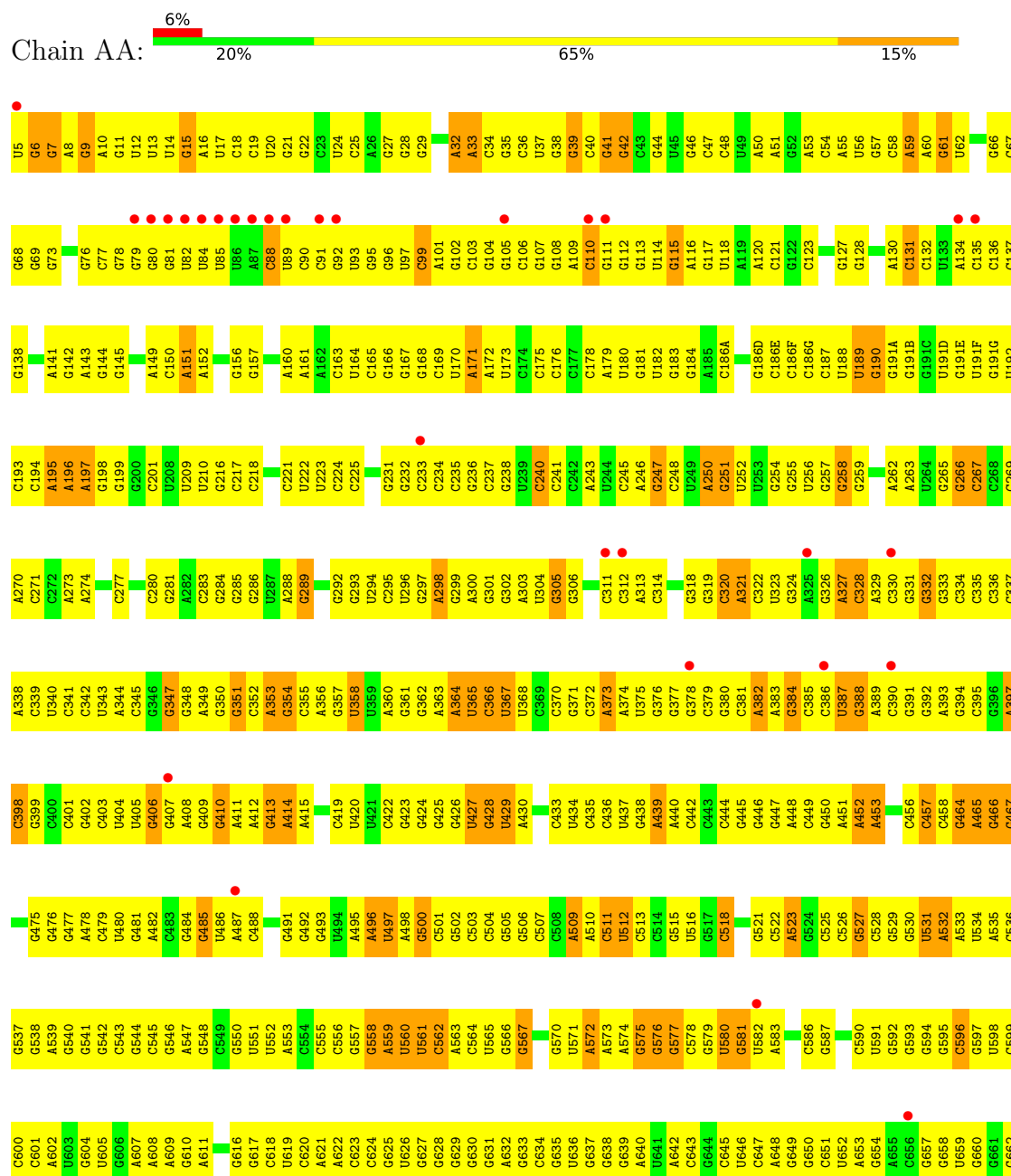
- Molecule 55 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

3 Residue-property plots

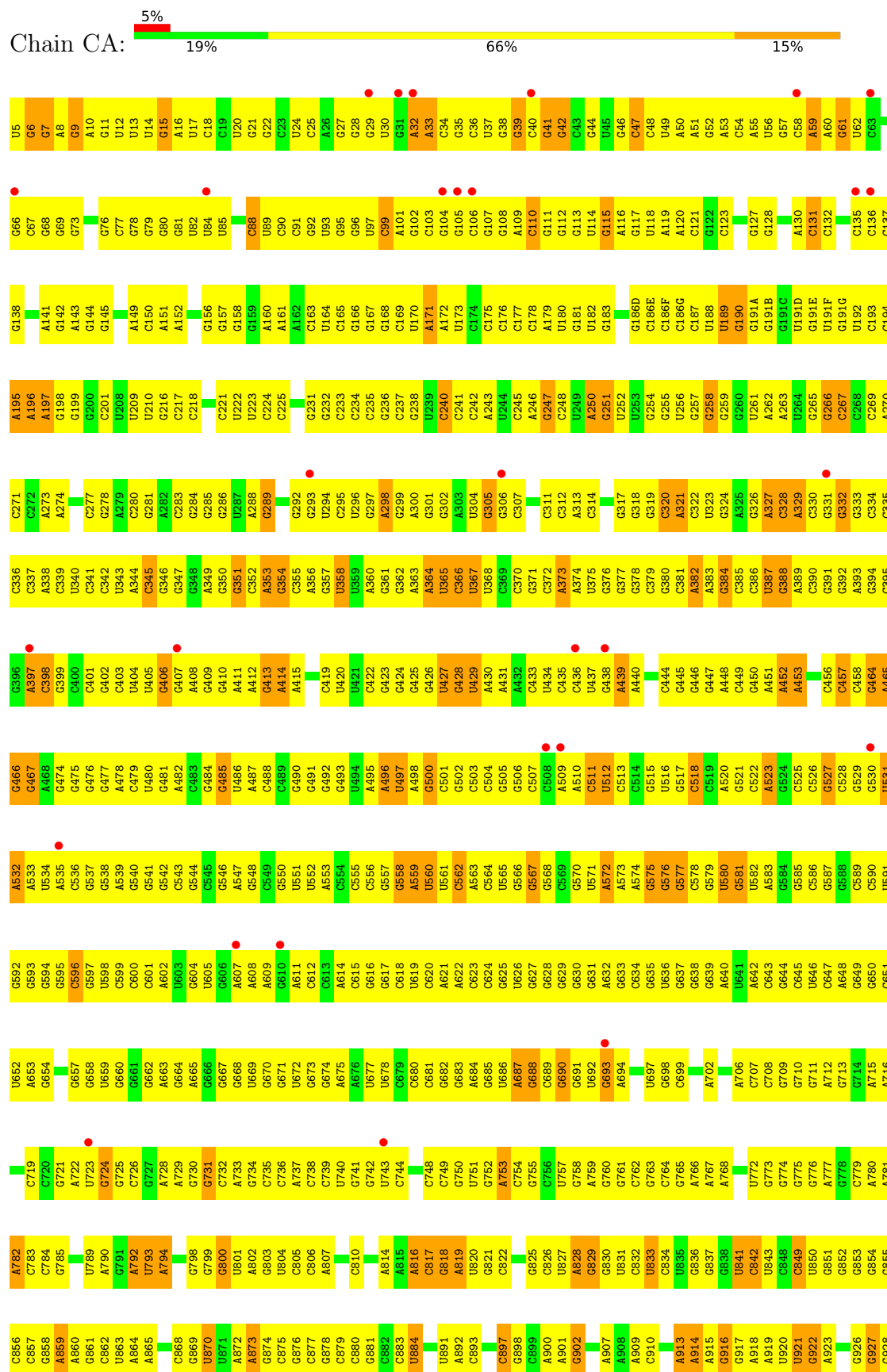
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

● Molecule 1: ribosomal RNA 16S



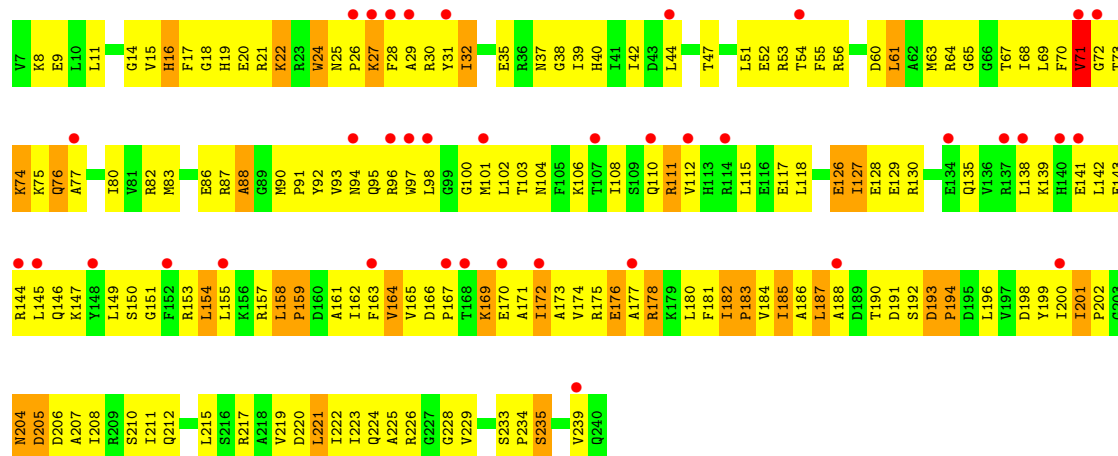
G1524	C1452	G1386	C1326	G1258	U1196	G1131	C1069	A1000	A938	G791	U863	G663	A663
G1525	G1453	G1387	C1327	C1259	G1197	U1135	U1070	G1001	G939	A792	U864	G664	A664
G1526	G1454	C1388	C1328	G1260	G1198	U1136	C1071	G1002	C940	A793	A865	G665	A665
C1527	G1455	C1389	A1329	A1261	U1199	C1137	U1072	G1003	G941	A794	C868	G666	
U1528	U1350	U1390	C1330	C1262	C1200	C1137	G1073	G1003	G942		G869	G667	
G1529	U1460	U1391	G1331	C1263	A1201	G1138	G1074	A1004	U943	C797	G870	G668	
G1530	G1461	G1392	A1332	A1332	G1202	G1139	C1075	A1005	G944	G798	U870	G669	
A1531	U1393	U1393	C1333	C1270	C1203	C1140	C1076	C1006	G945	G799	G873	G670	
U1532	G1464	G1394	G1334	G1271	A1204	G1141	G1077		A946	U800	A874	G671	
C1533	C1465	C1395	G1335	G1272	U1205	G1142		G1009	G947	G801	G874	G672	
	C1466	A1396	C1336	G1273	G1206	G1143		G1010	C948	A802	C875	G673	
	G1467	C1397	G1337		G1207	G1144		G1011	A949	G803	C876	G674	
	A1468	C1397	G1338	C1277	C1208	G1145	G1080		U950	U804	C877	G675	
	G1469	U1278	C1339	U1278	C1209	G1146	G1081	A1014	G851	C878	G877	G676	
	G1470	A1340	A1340	A1279	G1210	G1147	U1083	A1015	U952	C879	G878	A676	
	G1471	G1401	U1341	A1280	U1211	U1148	U1084	A1016	G953	C880	C879	U677	
		C1402	C1342	U1281	U1212	C1149	U1085	A1017	G954	A807	G881	U678	
		C1403	G1343	C1282	A1213	U1150	G1086	G1017	U955		G882		
	C1479		C1344	C1283	C1214	A1151	G1087		U956	C910	G883	G682	
	U1481	C1407	U1345	C1284		A1152	G1088	G1022	U957		U884	G683	
	A1482		C1346	C1285	C1217	G1153	U1089	G1023	U957	A814	C885	G684	
	A1483	G1410	G1347	A1285	C1218	G1154	U1090	G1024	A958	A815	A815	G685	
	C1484	C1411	U1348	A1287	U1219	G1155	G1154	U1091	A959	C917	C892	U686	
	U1485	C1412	A1349	A1288	G1220	G1156	G1155		U960	G818	C893	A687	
	G1486	C1413	A1350	A1289	G1221	A1157	U1095	C102A	U961	C917	C897	G688	
	G1487	U1414	U1351	G1290	G1222	C1158	C1096	G1031	G963	U820	G898	U689	
	G1488	C1415	C1352	G1291	C1223	U1159	C1097	A103A	G821	C922	G754	G690	
	G1489		G1353	U1292	G1224	G1160	C1098		A965		G902	U692	
	C1490	A1418		U1293	G1225	C1161	G1099	C1037	G966	C756	C897	G693	
	G1491	G1419	G1356	G1294	C1226	C1162	G1100	C1038	C967	C926	G906	A694	
	A1492	C1420	A1357	G1295	A1227	C1163	A1101	C1039	U968	U827	A907		
	A1493	G1421	C1358	C1296	C1228	G1164	A1102	U1040	A969	A828	A908	U697	
	G1494	G1422	C1359	C1297	A1229	C1165	G1103	A909	G829	G760	A909	G698	
		G1423	A1360	C1298	C1230	G1166	C1104	G1041	G971	G761	C910	C699	
	G1497	C1424	G1361	A1299	U1231	A1167	A1105	C1043	C972	G700	U831	G700	
		U1425	C1364	G1300	U1232	A1169	G1106	A1044	G973	C832	C832	G763	
	A1500	C1426	C1368	G1301	G1233	A1170	C1107	C1045	A974	U833	A913	G701	
	C1501	U1427	A1363	U1302	C1234	G1171	C1108	A1046	A975	C834	A914	A702	
	A1502	A1428	C1364	C1303	U1235	C1172	G1109	G1047	G976	G765	A915	A703	
	A1503	C1429	G1365	A1236	A1236	A1110	A1110	U1048	A977	A766	G916	A704	
	G1504	C1430	C1366	G1305	C1237	A1176	A1111	G1049	A978	G837	A917	U705	
	G1505	C1431	C1367	A1306	A1238	G1177	C1112	G1050	C979	G838	A918	A706	
	U1506	G1432	G1368	A1307	A1239	G1178	C1113	C980	C979		A919	C707	
	A1507	A1433	C1369	U1308	U1240	A1179	C1114	U921	U981	U841	U920		
	G1508	A1434	G1370	C1309	G1241	A1180	G1115	U1052	G981	C942	G922	G708	
	C1509	G1435	G1371	G1310	C1242	G1181	C1116	G1053	U982	U843	G923	G710	
	U1436	U1436	U1372	G1311	C1243	G1182	G1117	A1055	A983	C848	C924	G711	
	G1511	G1437	G1373		C1244	A1183	C1118	U1056	C865	U850	G925	A712	
	U1512	C1438	A1374	C1314	A1245	G1184	C1119	U1057	A986	U851	G926	G713	
	A1513	C1439	A1375	U1315	U1246	G1185	C1120	G1058	G981	G852	G927	G714	
	C1514	C1440	U1376	G1316	U1247	G1186	U1121	C1059	G988	G778	G928	A716	
	C1515	G1441	A1377	C1317	C1248	G1187	G1122	G1061	G984	A780	G929	G717	
	G1516	G1442	C1378	A1318	A1250	A1188	A1123	C1060	C930	G855	C930	G718	
	G1517	G1443	G1379	A1319	A1251	C1189	G1124	U1062	C931	C856	C931	C719	
	A1518	A1446	U1380	C1320	A1252	C1190	U1125	C1063	G993	C857	G932	C720	
	A1519	G1447	U1381	G1253	A1253	A1191	U1126	G1064	G984	C858	G933	G721	
	G1520	C1448	C1382	C1322	C1254	C1192	G1127	U1065	C995	G859	G934	G722	
	G1521	C1449	C1383	G1323	G1255	G1193	C1128	C1066	A859	G785	A935	A723	
		U1450	C1384	A1324	A1256	U1194	C1129	A1067	A996	A860	C936	G724	
	C1522	U1451	C1385	A1325	U1257	U1195	A1120	C1068	C994	C861	A937	G725	

● Molecule 1: ribosomal RNA 16S

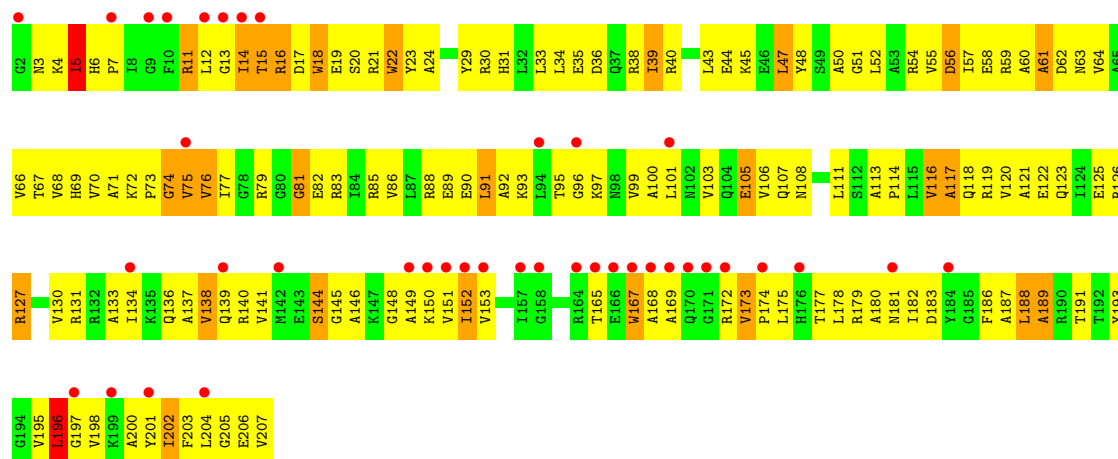




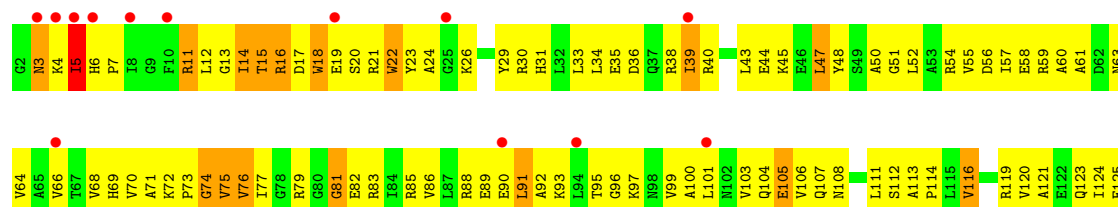
• Molecule 2: 30S ribosomal protein S2

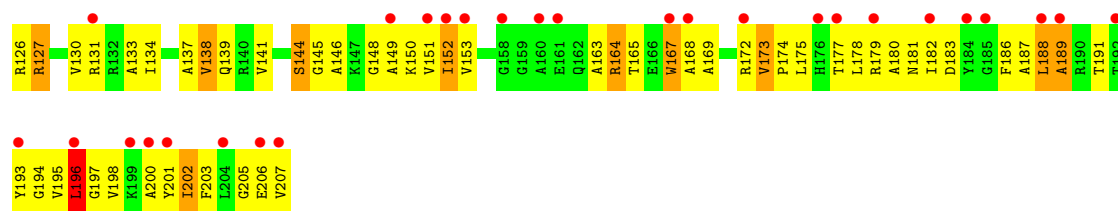


• Molecule 3: 30S ribosomal protein S3

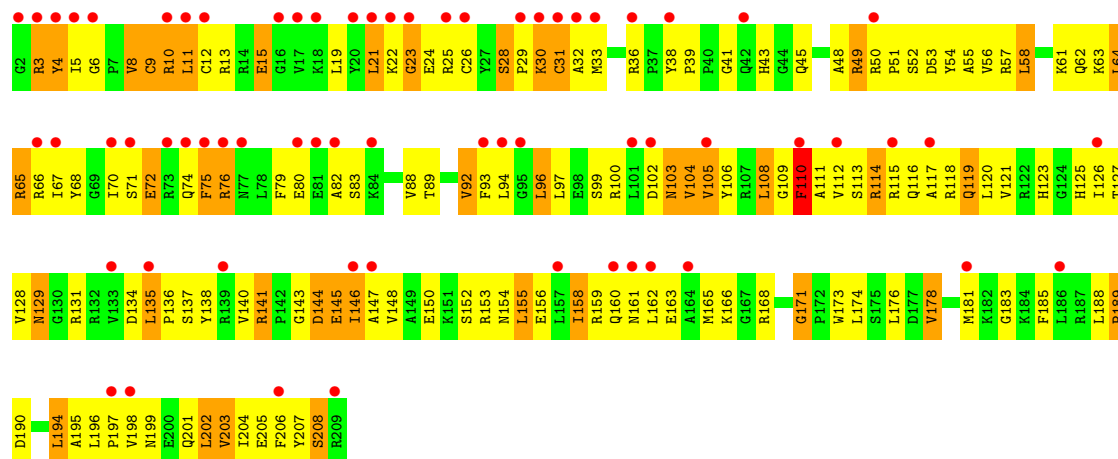


• Molecule 3: 30S ribosomal protein S3

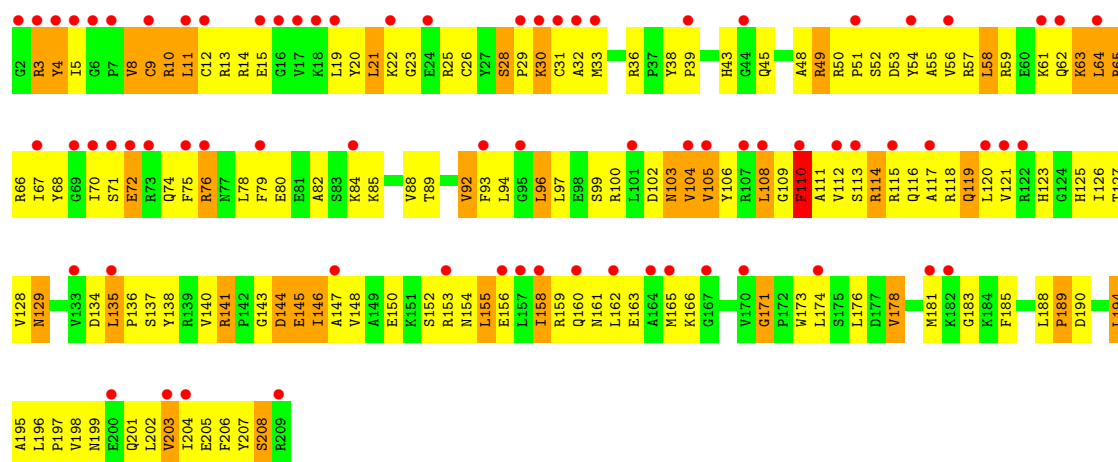




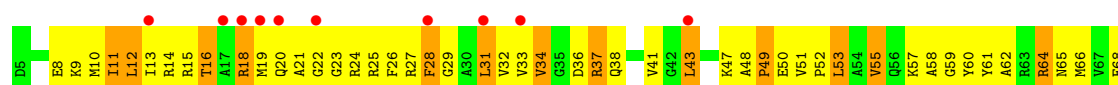
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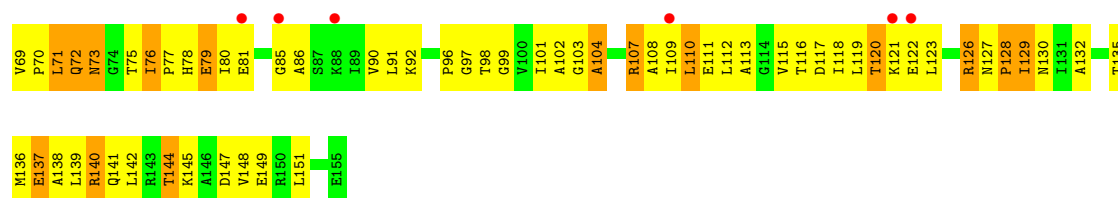


● Molecule 4: 30S ribosomal protein S4

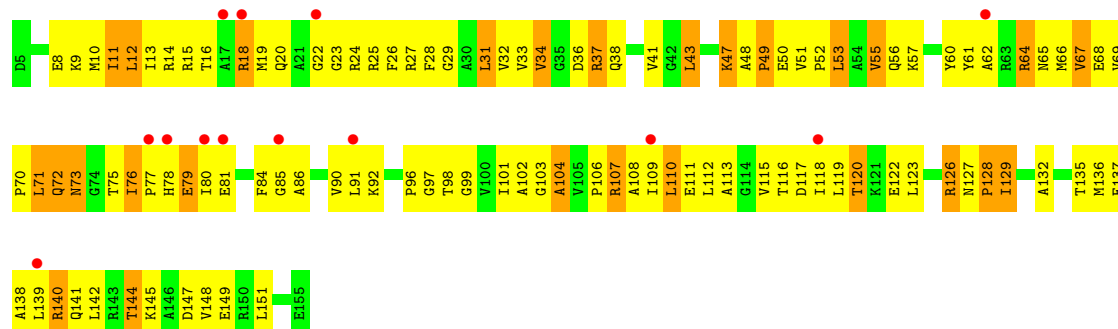


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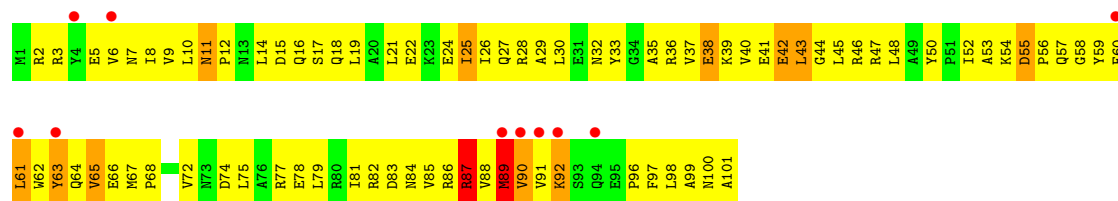




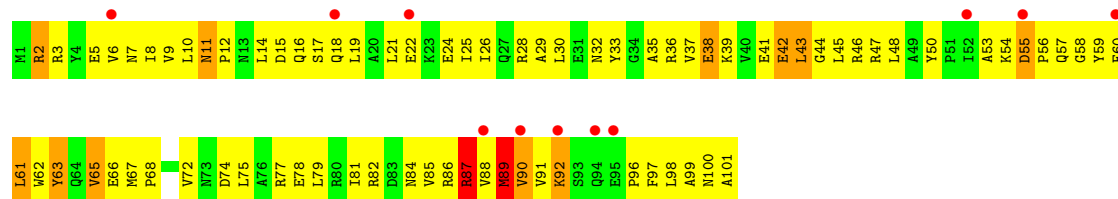
• Molecule 5: 30S ribosomal protein S5



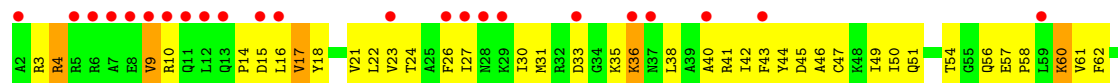
• Molecule 6: 30S ribosomal protein S6

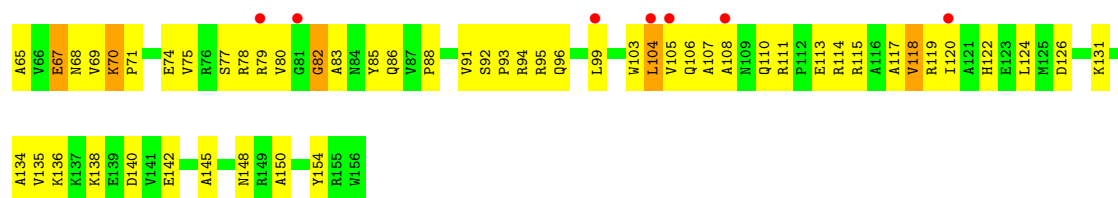


• Molecule 6: 30S ribosomal protein S6

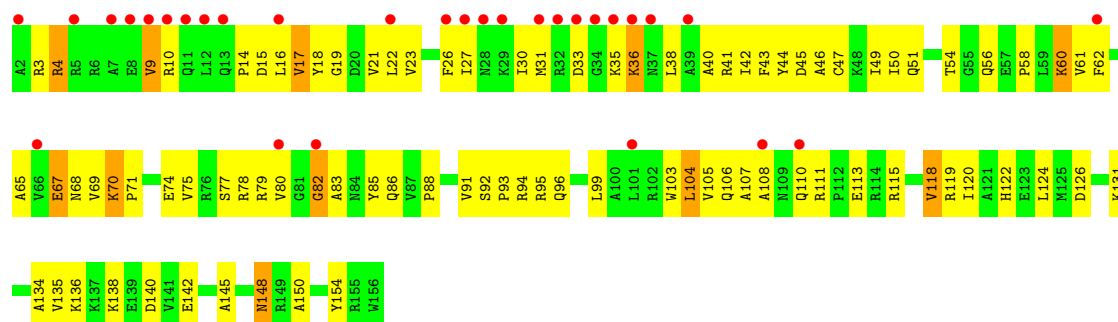
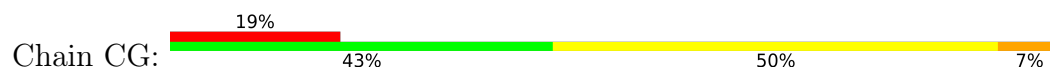


• Molecule 7: 30S ribosomal protein S7

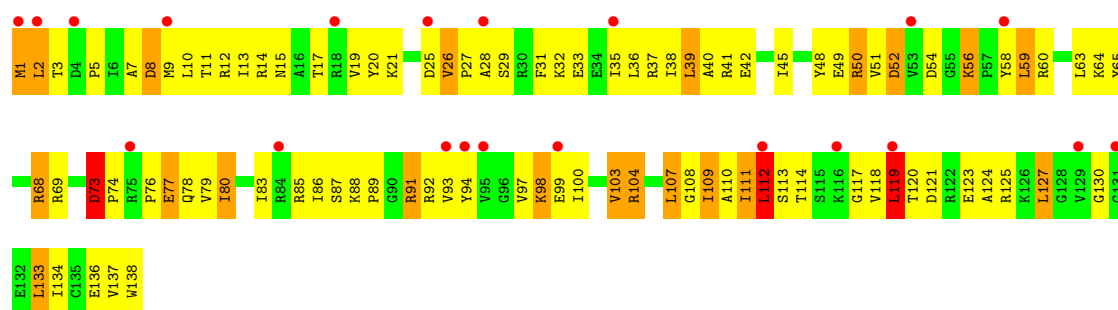




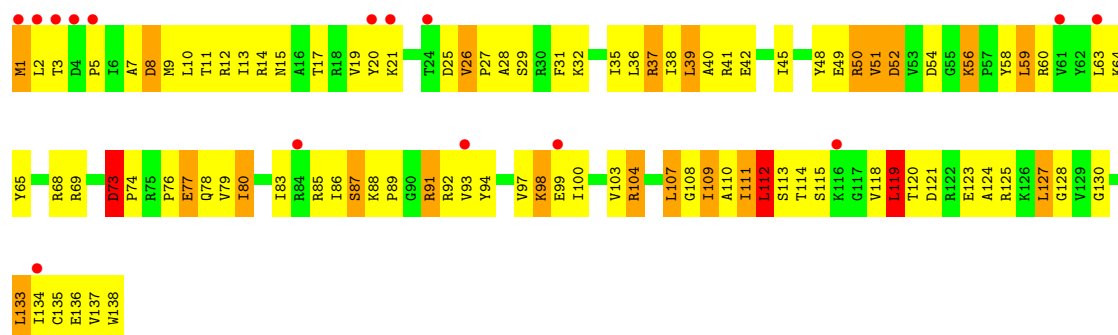
• Molecule 7: 30S ribosomal protein S7



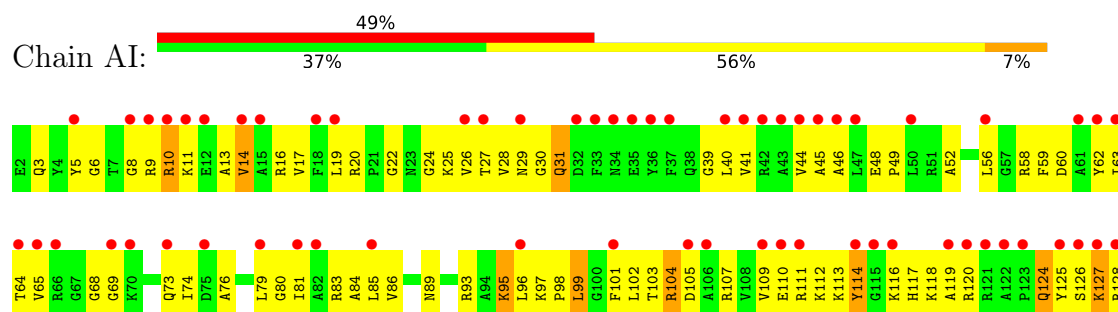
• Molecule 8: 30S ribosomal protein S8



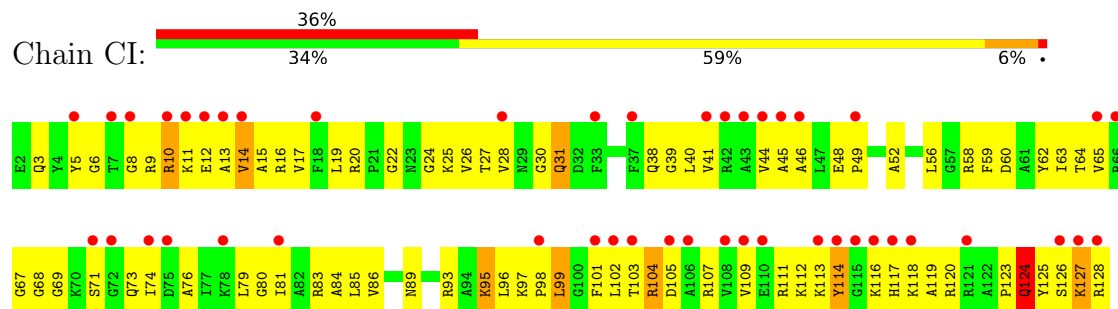
• Molecule 8: 30S ribosomal protein S8



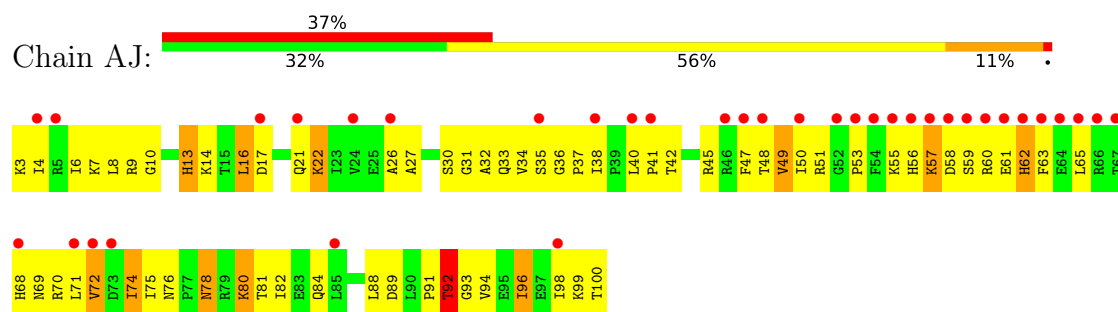
• Molecule 9: 30S ribosomal protein S9



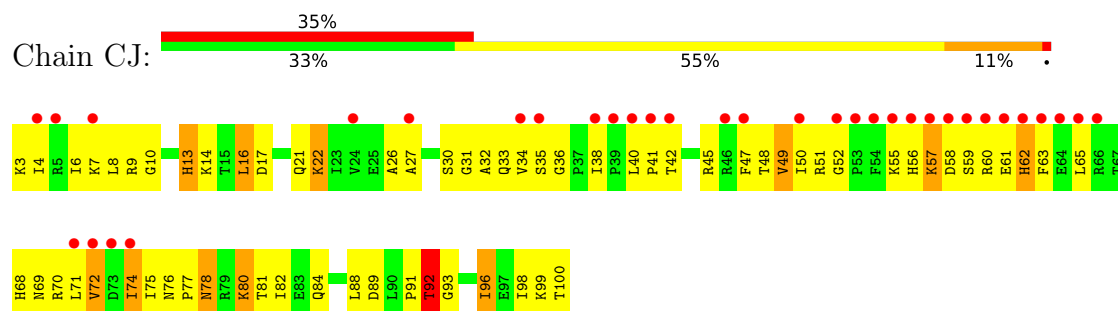
• Molecule 9: 30S ribosomal protein S9



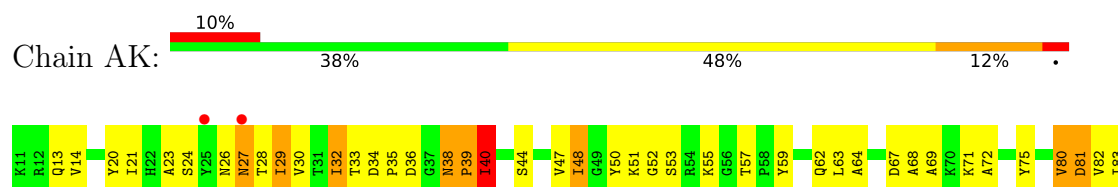
• Molecule 10: 30S ribosomal protein S10

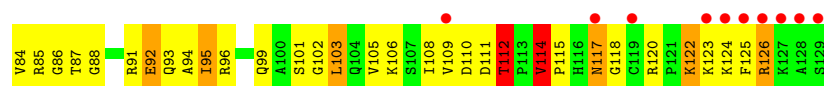


• Molecule 10: 30S ribosomal protein S10



• Molecule 11: 30S ribosomal protein S11

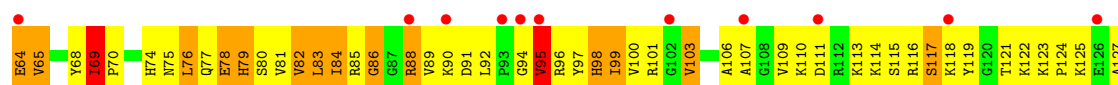
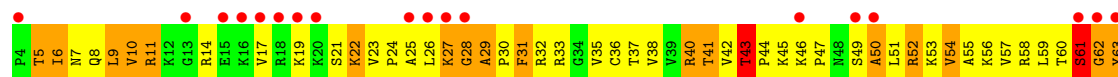
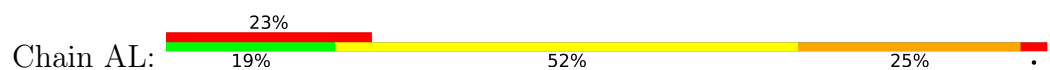




- Molecule 11: 30S ribosomal protein S11



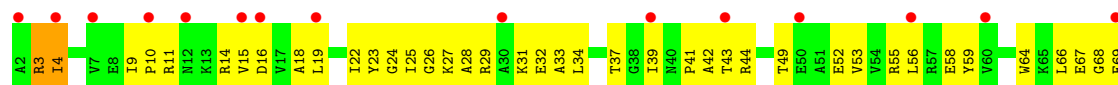
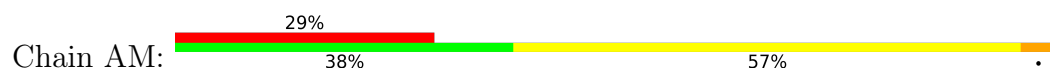
- Molecule 12: 30S ribosomal protein S12



- Molecule 12: 30S ribosomal protein S12

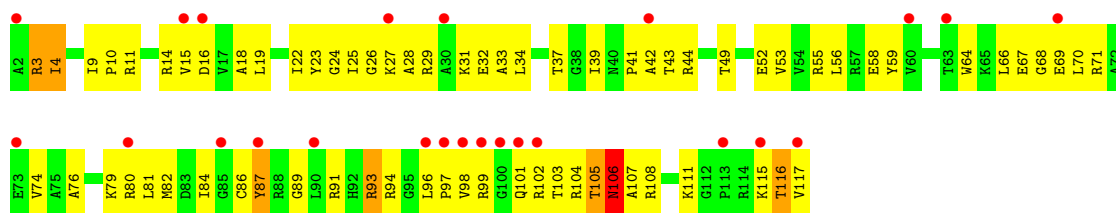


- Molecule 13: 30S ribosomal protein S13

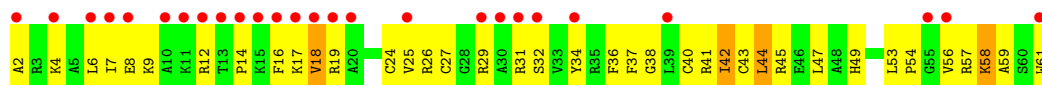
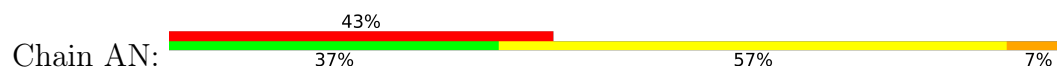


- Molecule 13: 30S ribosomal protein S13

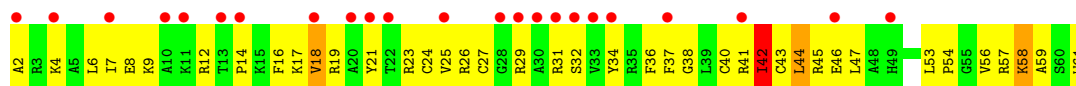




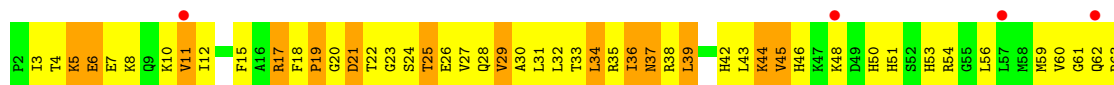
• Molecule 14: 30S ribosomal protein S14 type Z



• Molecule 14: 30S ribosomal protein S14 type Z



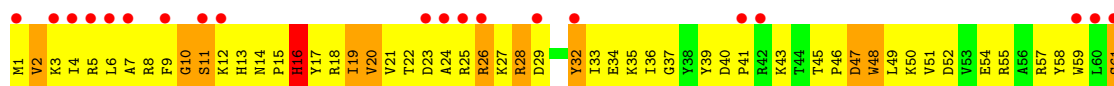
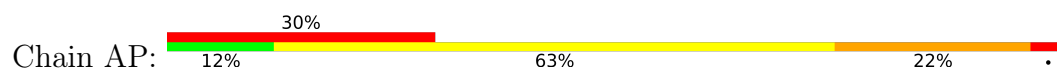
• Molecule 15: 30S ribosomal protein S15



• Molecule 15: 30S ribosomal protein S15

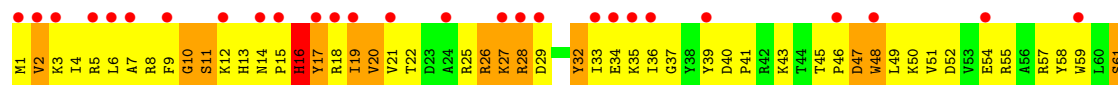
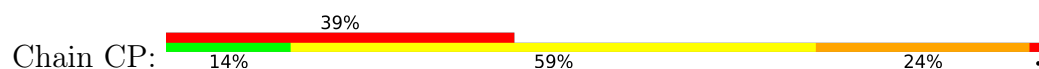


• Molecule 16: 30S ribosomal protein S16

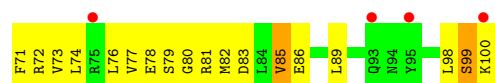
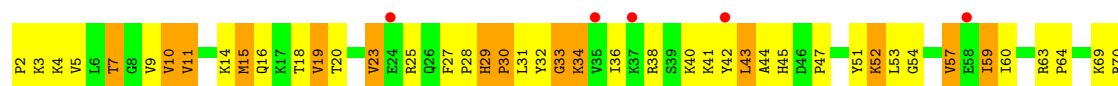




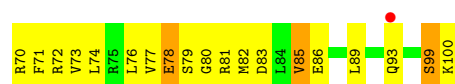
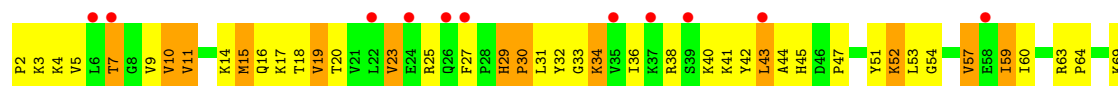
- Molecule 16: 30S ribosomal protein S16



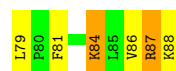
- Molecule 17: 30S ribosomal protein S17



- Molecule 17: 30S ribosomal protein S17

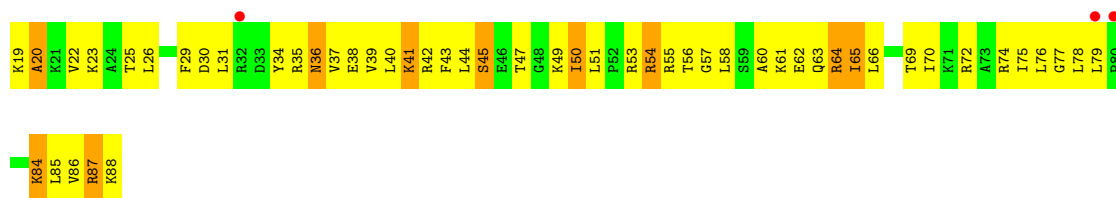


- Molecule 18: 30S ribosomal protein S18

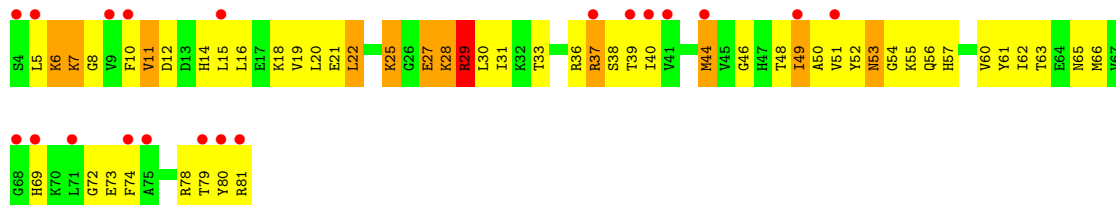


- Molecule 18: 30S ribosomal protein S18

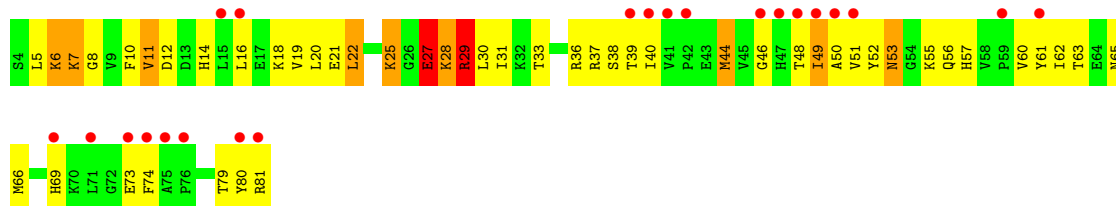




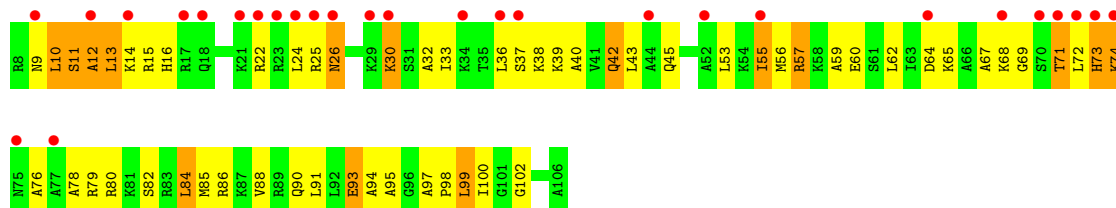
• Molecule 19: 30S ribosomal protein S19



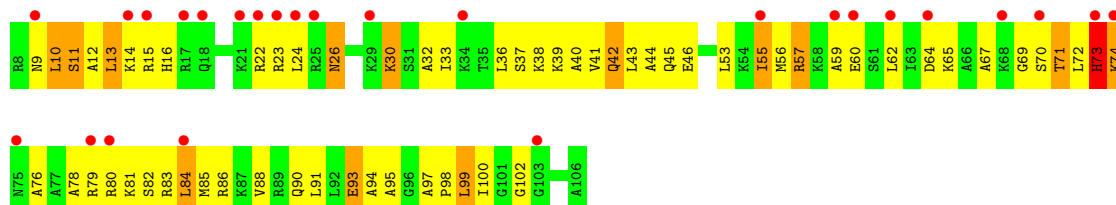
• Molecule 19: 30S ribosomal protein S19



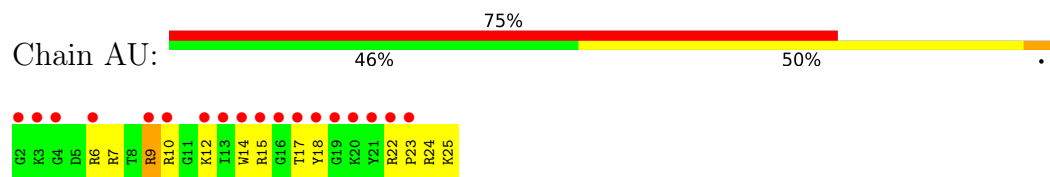
• Molecule 20: 30S ribosomal protein S20



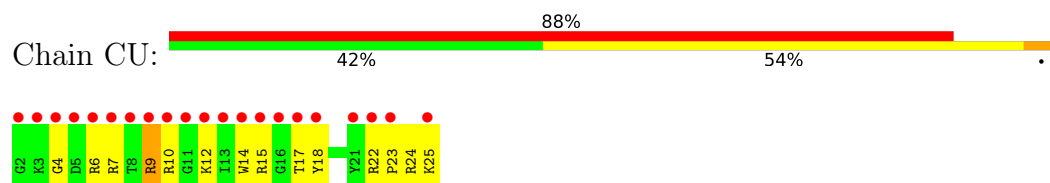
• Molecule 20: 30S ribosomal protein S20



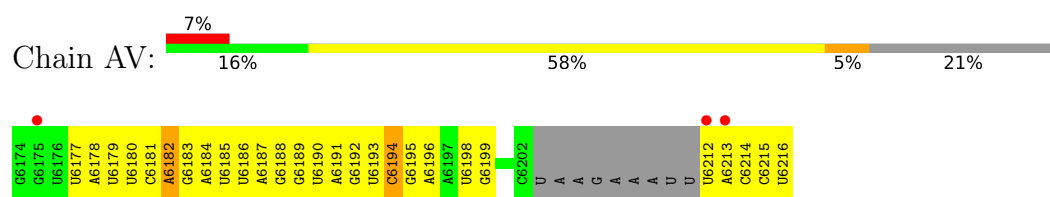
- Molecule 21: 30S ribosomal protein Thx



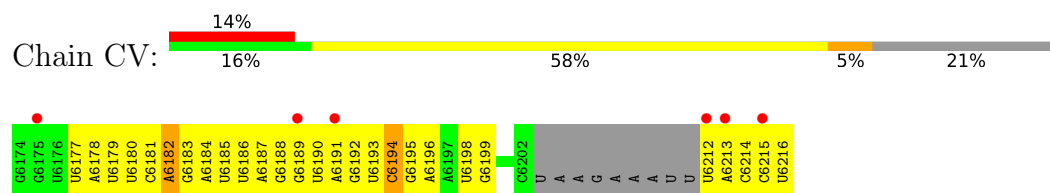
- Molecule 21: 30S ribosomal protein Thx



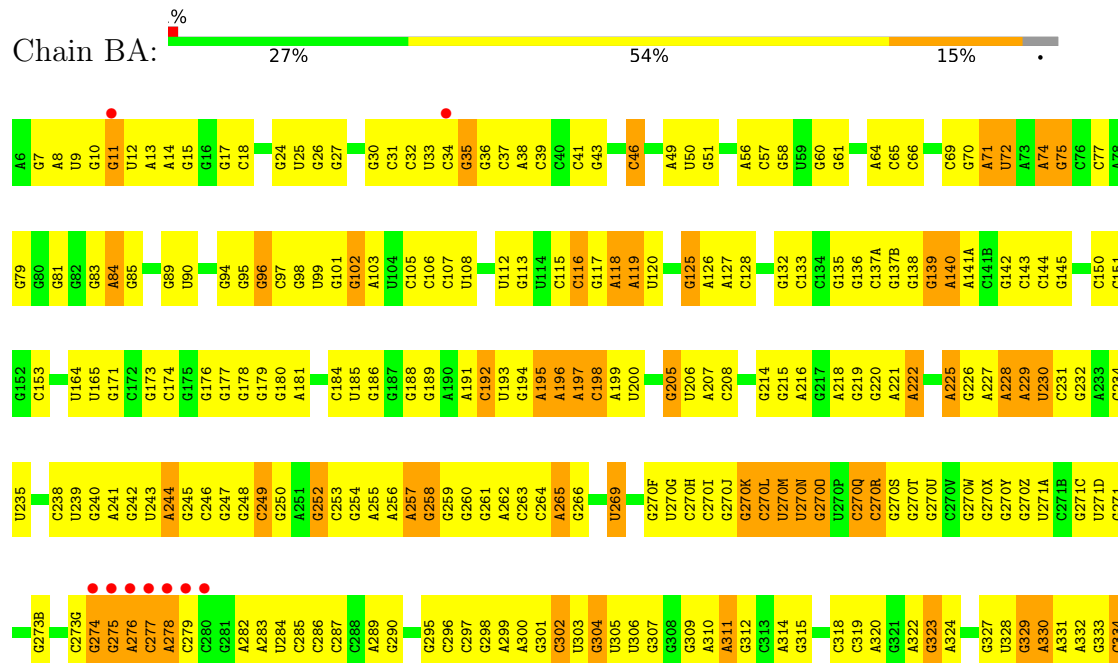
- Molecule 22: RNA (34-MER)



- Molecule 22: RNA (34-MER)

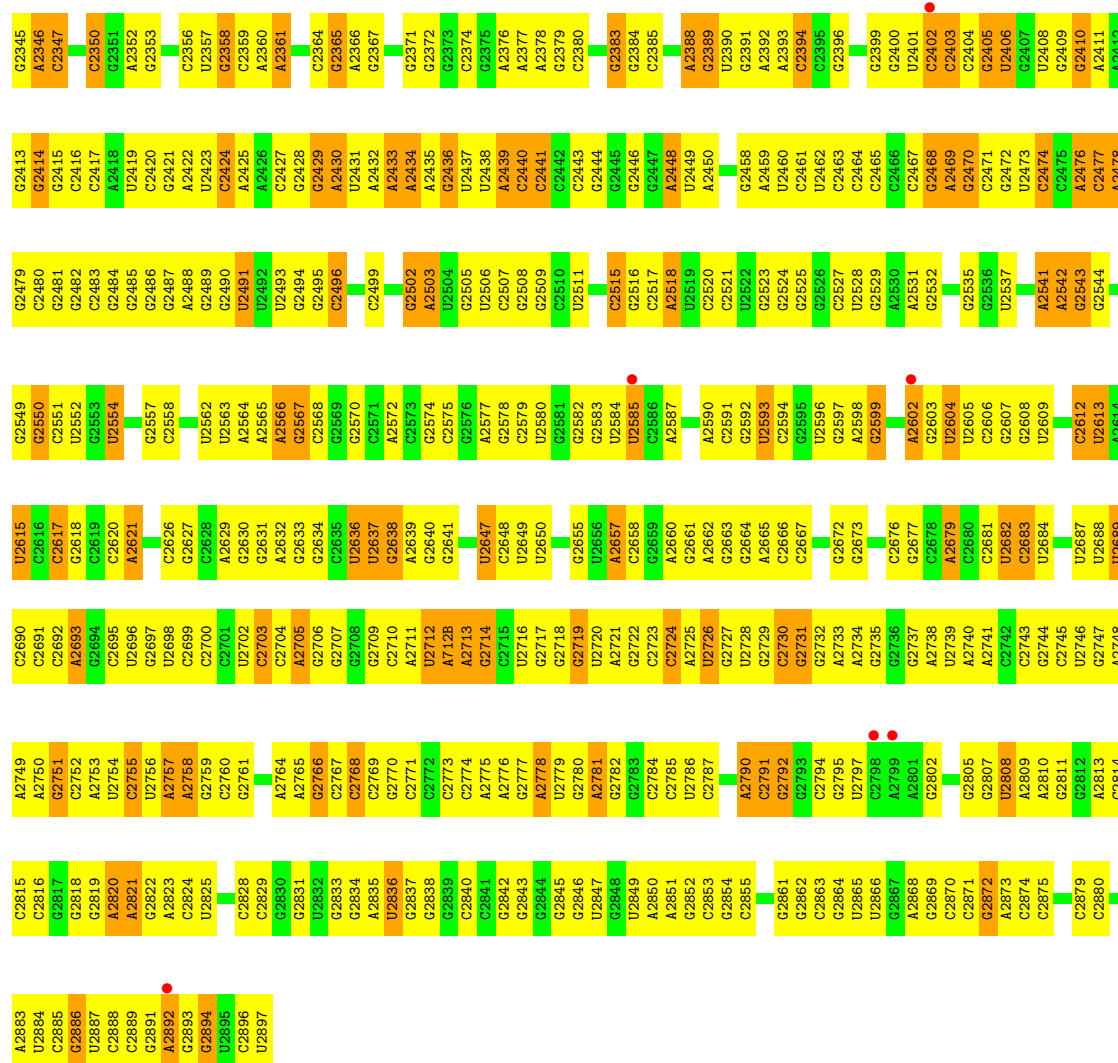


- Molecule 23: 23S ribosomal RNA

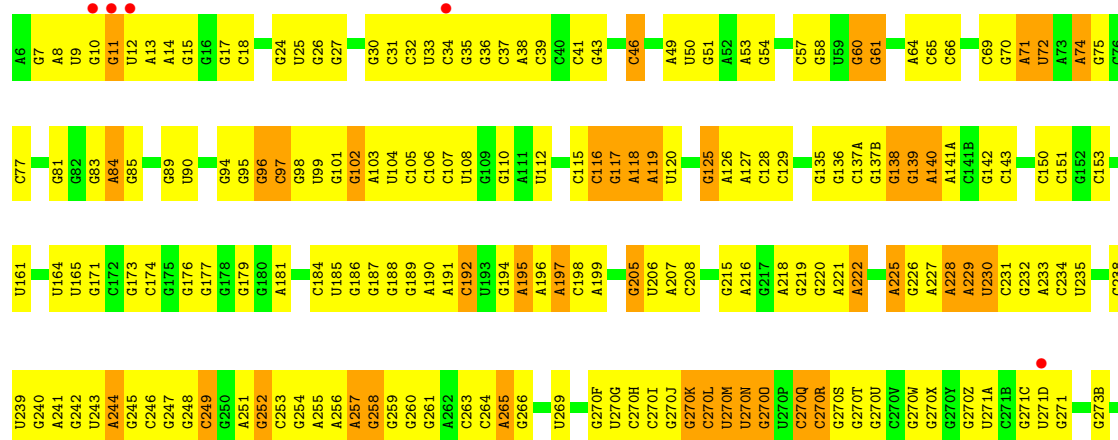


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C1313	G1236	G1171	G107	G1047	G979	A910	U839	U774	C697	G630	U566	G494	G411	C337
C1314		G1172	C1109	A1048	G980	A911		G775	C698	A631	A567	G495		G338
C1315	U1239	U1173	G1110	C1049	A980	C912	G844	G776	A699	A632	U568	G496	C414	U2339
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A1366	U1298	A1226	G1163	G	G1030	C970	C902	G831	G762	C617	U471			G399
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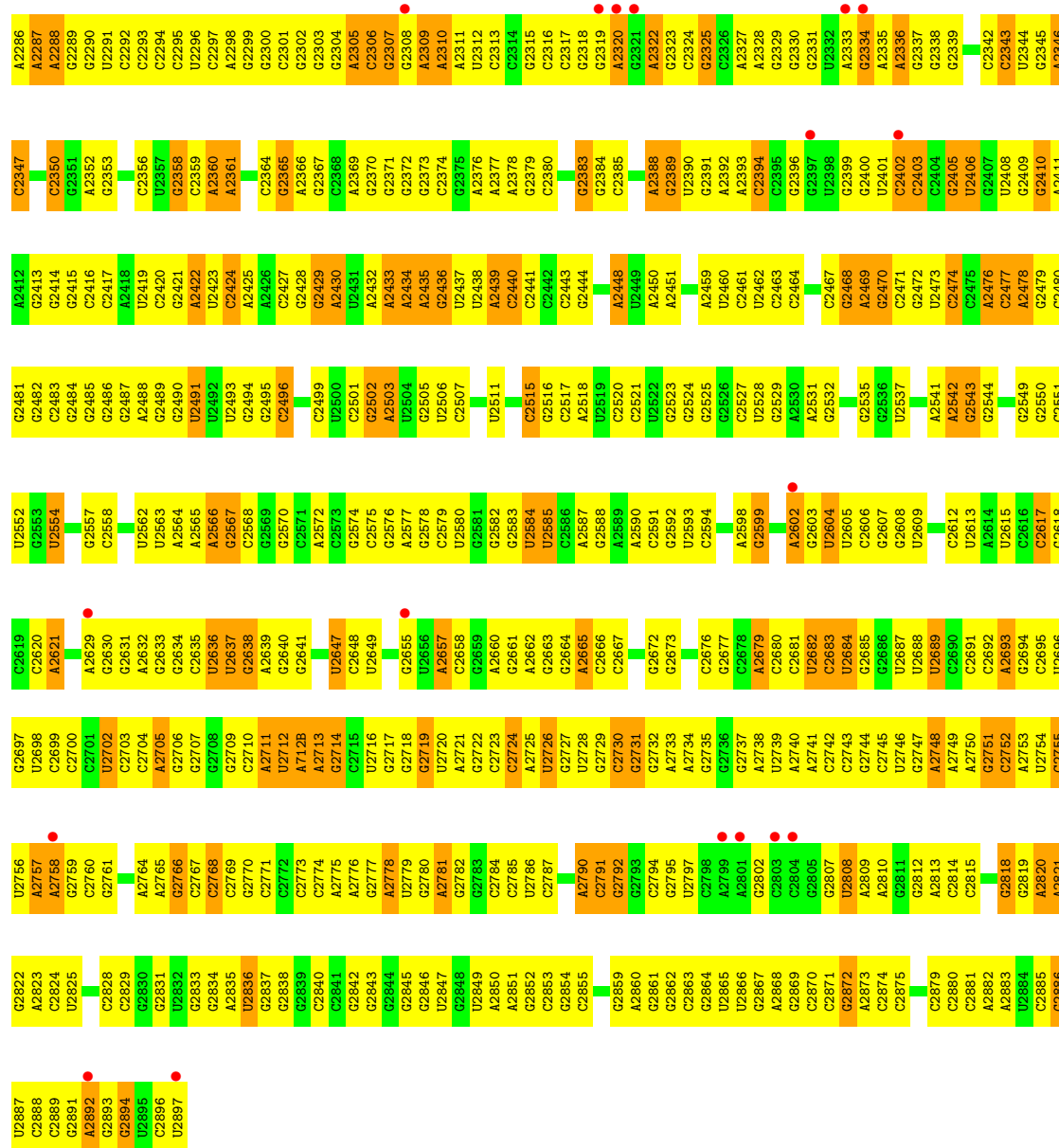


• Molecule 23: 23S ribosomal RNA

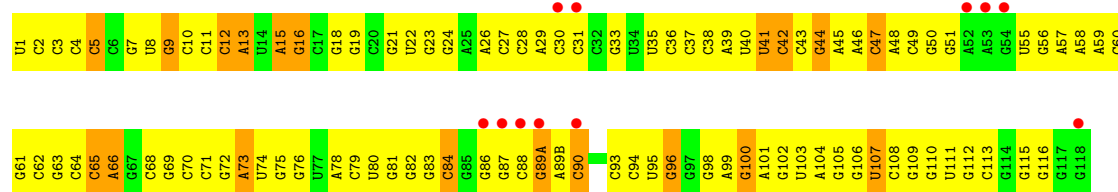




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G2215	G2088	A2020	A1952	U1805	C1806	G1647	U1578	A1511	G1448	C1386	C1320
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G2281	C	G2080	G2011	U1939	G1869	G1717	C1638	U1568	C1502	G1441	G1441
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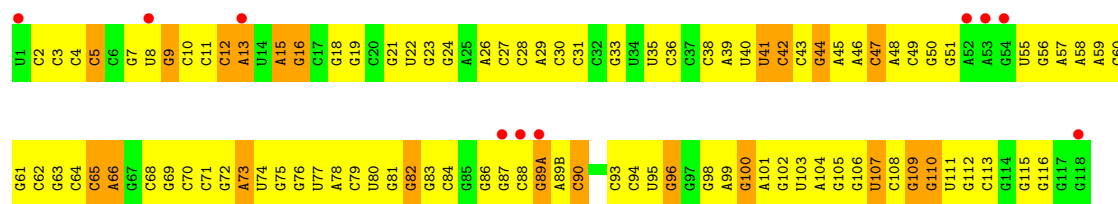


• Molecule 24: 5S ribosomal RNA

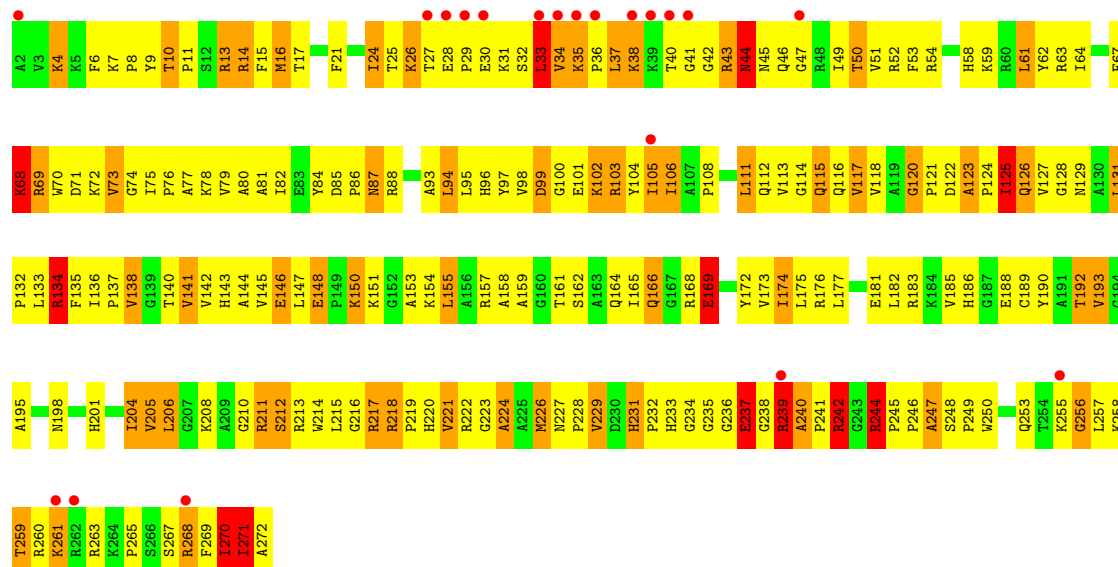


• Molecule 24: 5S ribosomal RNA

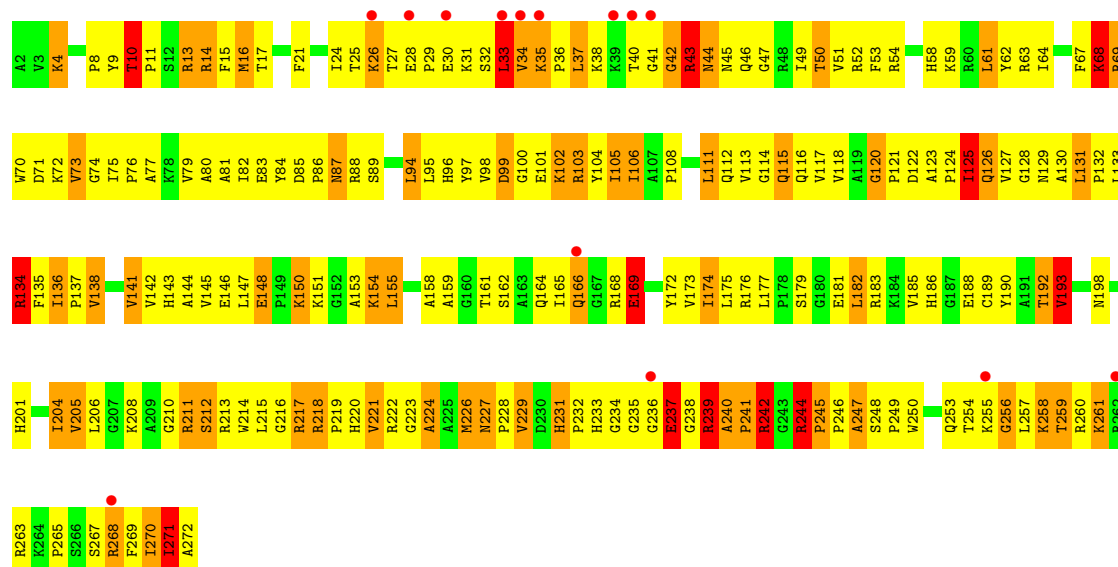




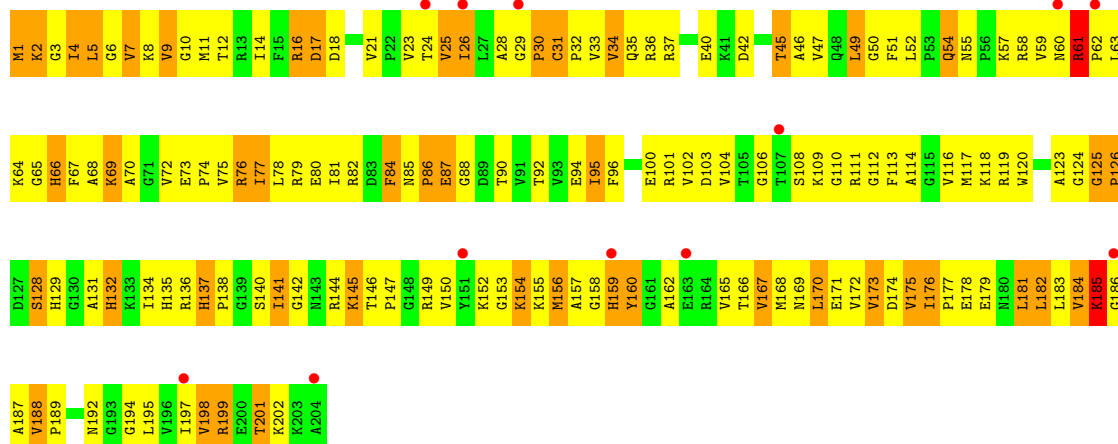
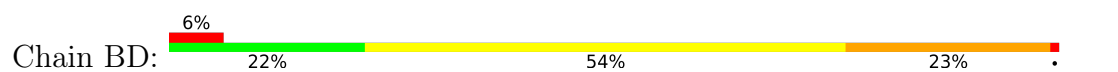
• Molecule 25: 50S ribosomal protein L2



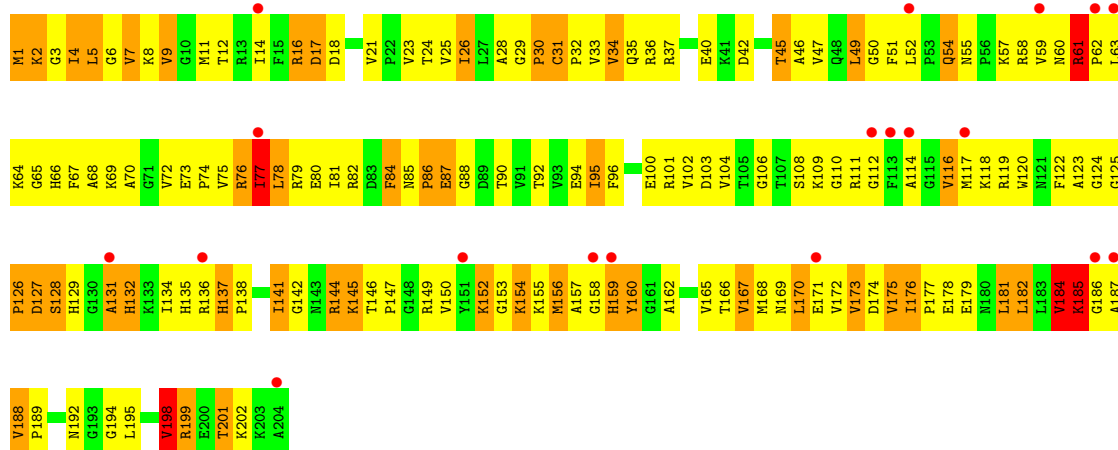
• Molecule 25: 50S ribosomal protein L2



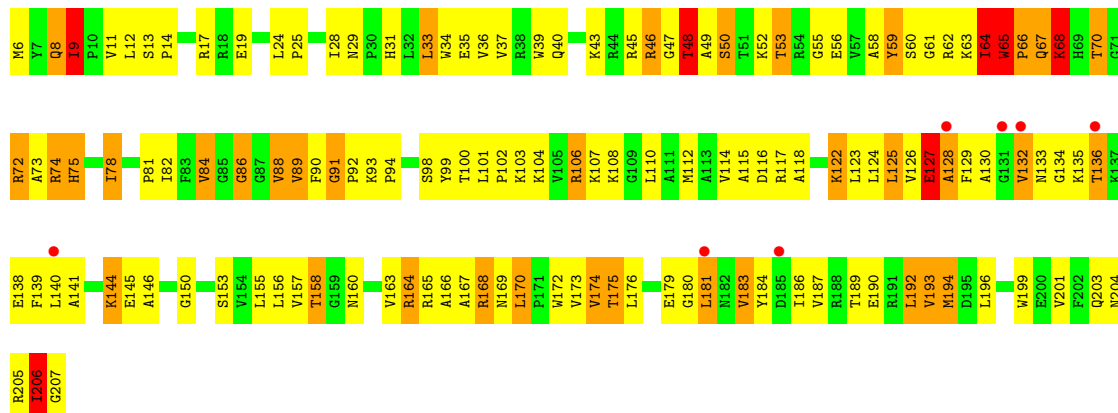
• Molecule 26: 50S ribosomal protein L3



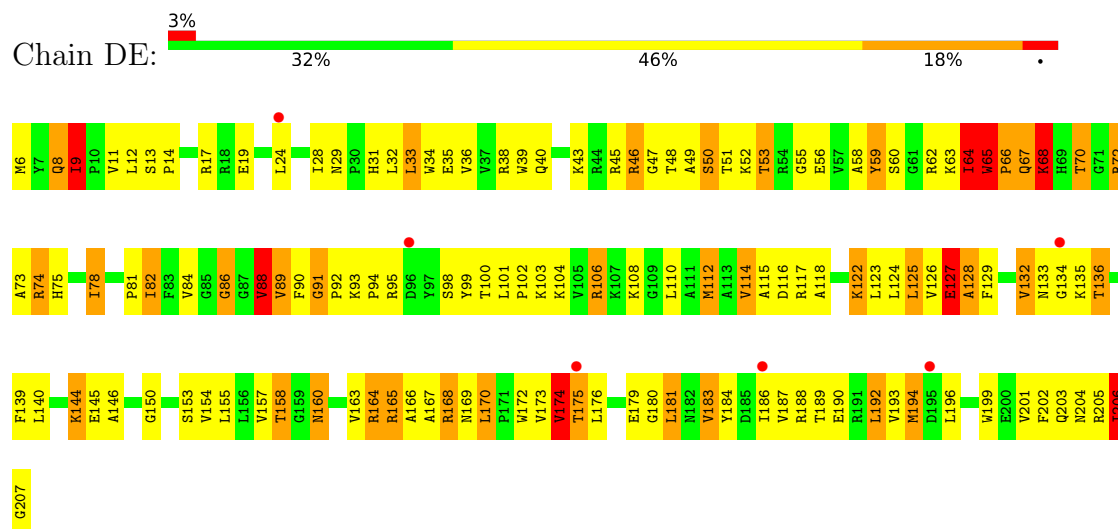
• Molecule 26: 50S ribosomal protein L3



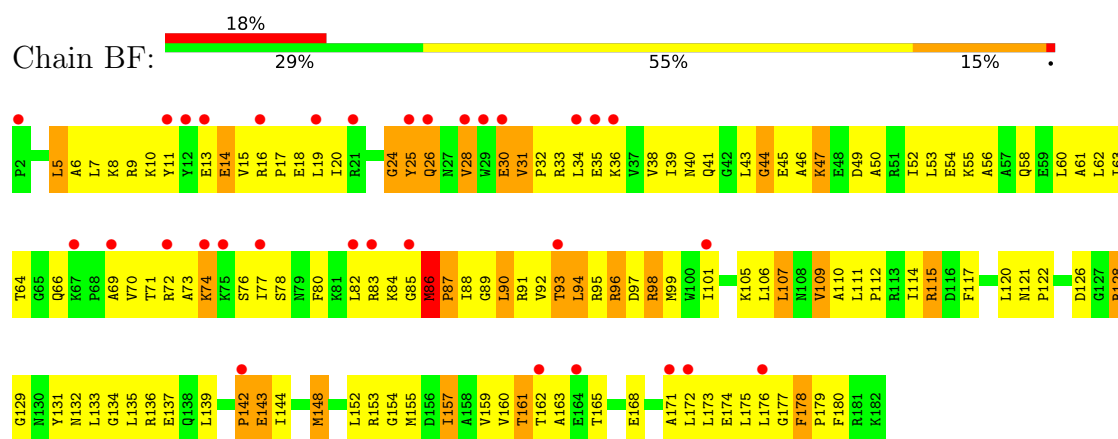
• Molecule 27: 50S ribosomal protein L4



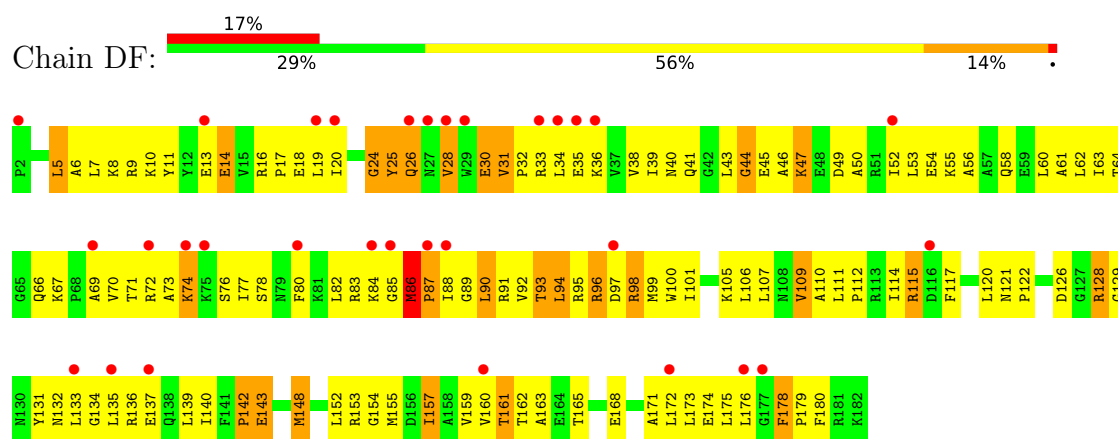
- Molecule 27: 50S ribosomal protein L4



- Molecule 28: 50S ribosomal protein L5

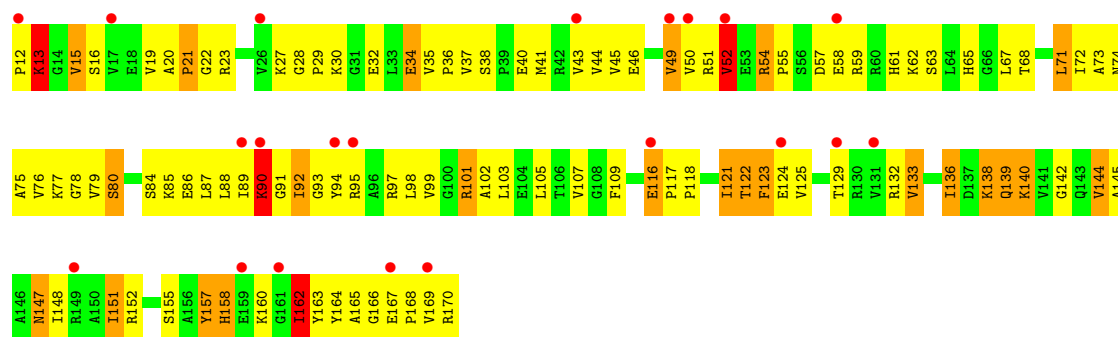


- Molecule 28: 50S ribosomal protein L5



- Molecule 29: 50S ribosomal protein L6

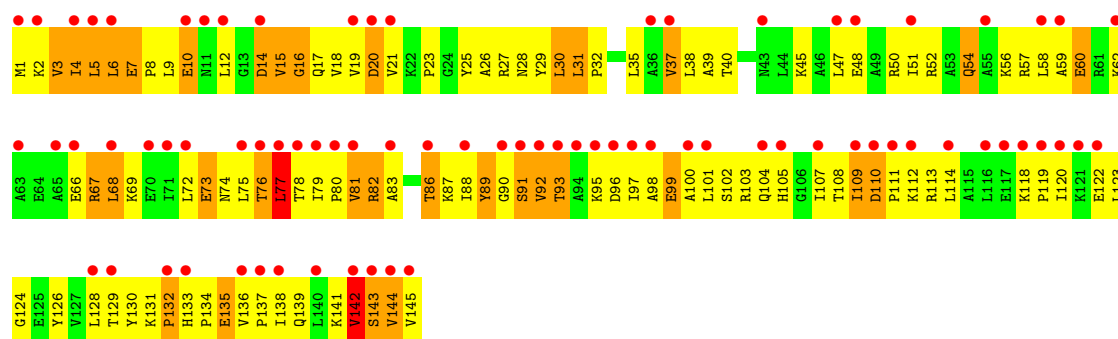




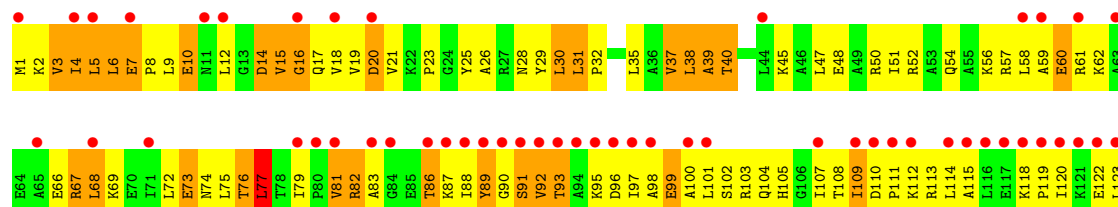
• Molecule 29: 50S ribosomal protein L6

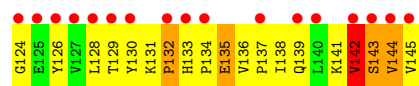


• Molecule 30: 50S ribosomal protein L9

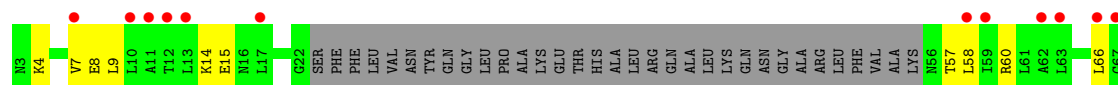
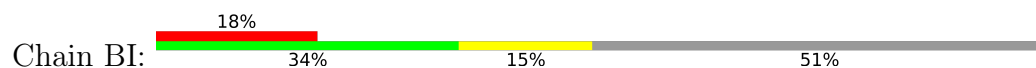


• Molecule 30: 50S ribosomal protein L9

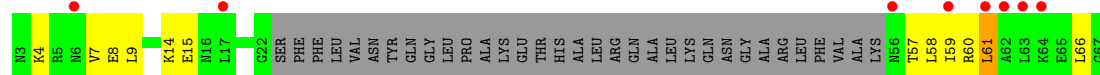
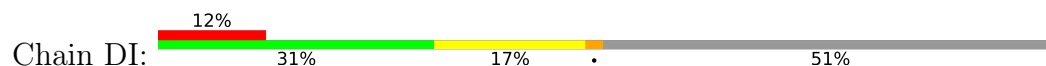




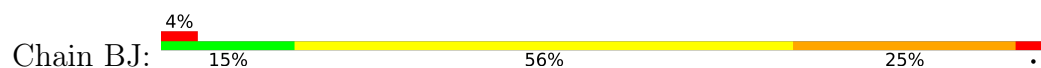
- Molecule 31: 50S ribosomal protein L10



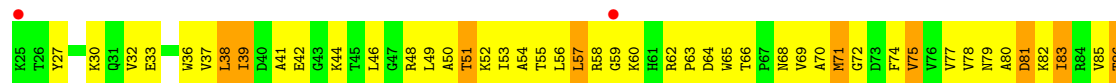
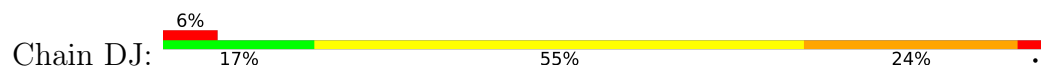
- Molecule 31: 50S ribosomal protein L10



- Molecule 32: 50S ribosomal protein L13

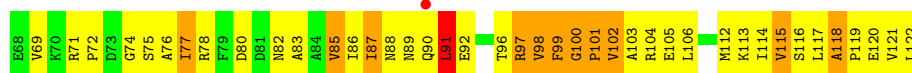


- Molecule 32: 50S ribosomal protein L13

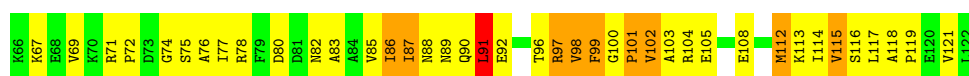
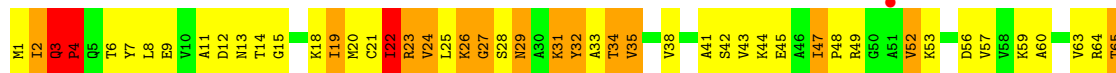


- Molecule 33: 50S ribosomal protein L14

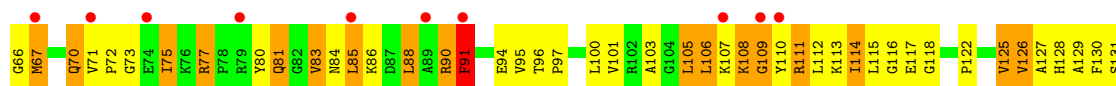
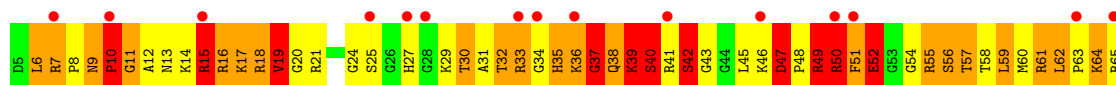
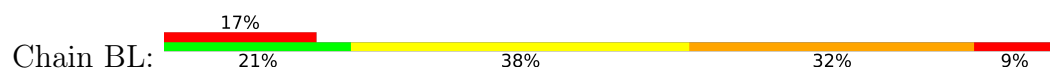




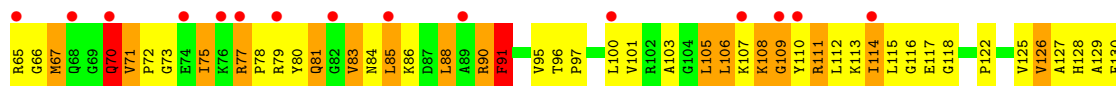
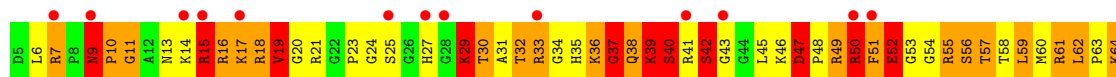
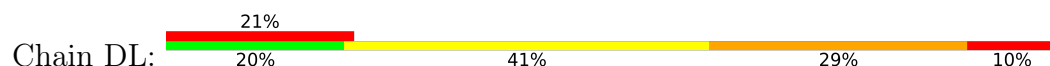
• Molecule 33: 50S ribosomal protein L14



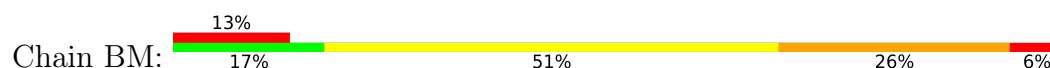
• Molecule 34: 50S ribosomal protein L15

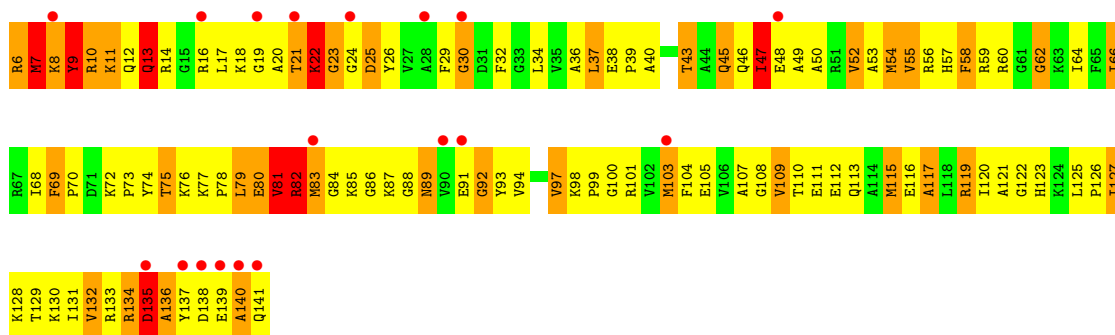


• Molecule 34: 50S ribosomal protein L15

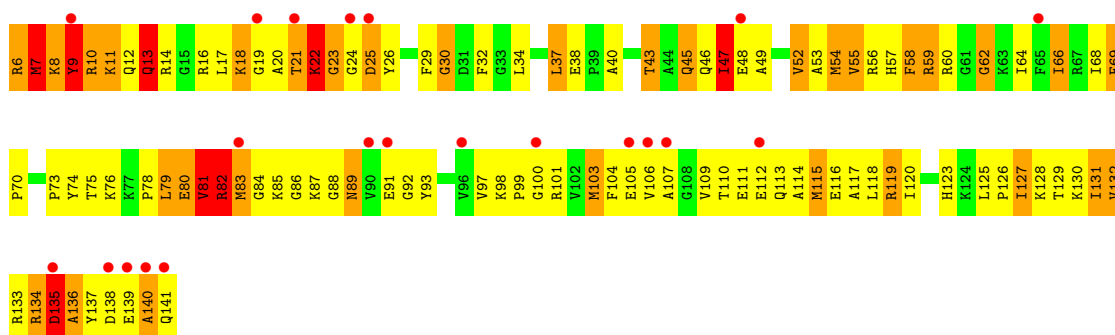


• Molecule 35: 50S ribosomal protein L16

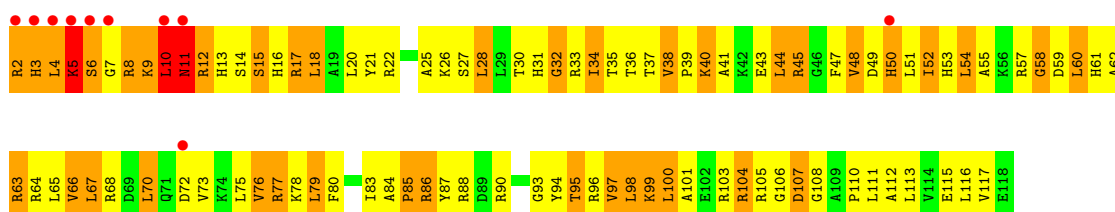
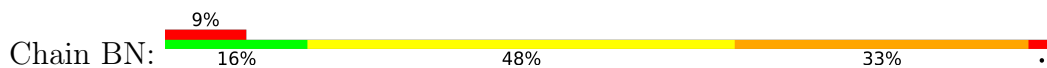




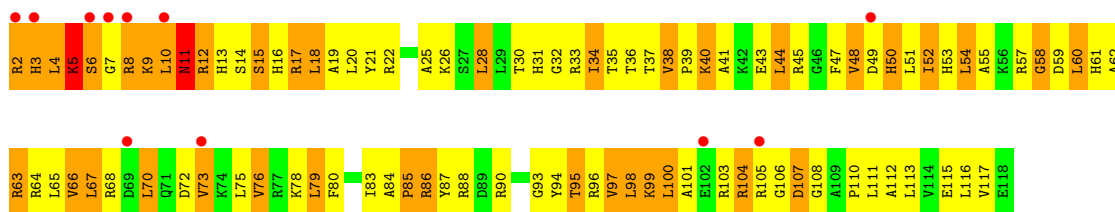
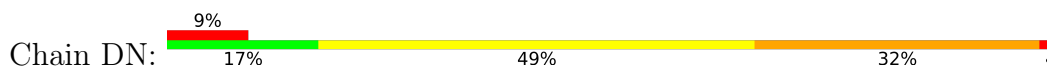
- Molecule 35: 50S ribosomal protein L16



- Molecule 36: 50S ribosomal protein L17

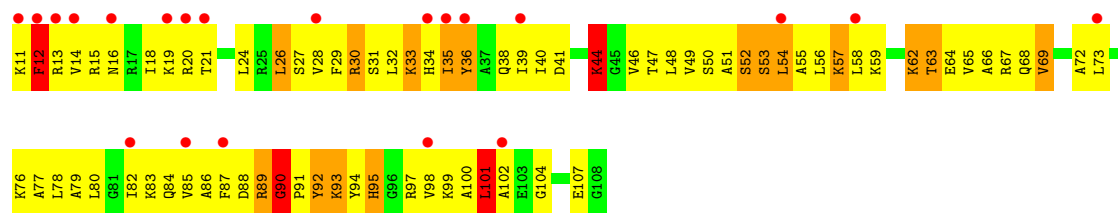


- Molecule 36: 50S ribosomal protein L17

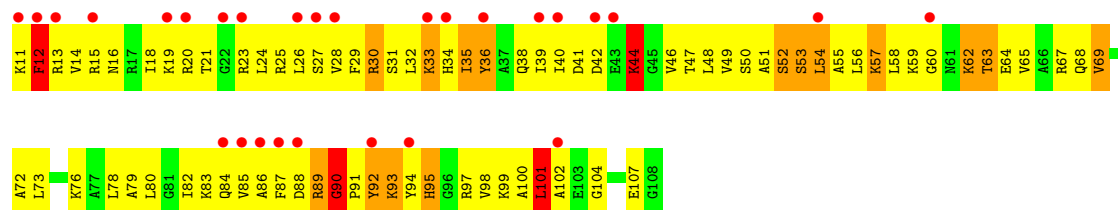


- Molecule 37: 50S ribosomal protein L18

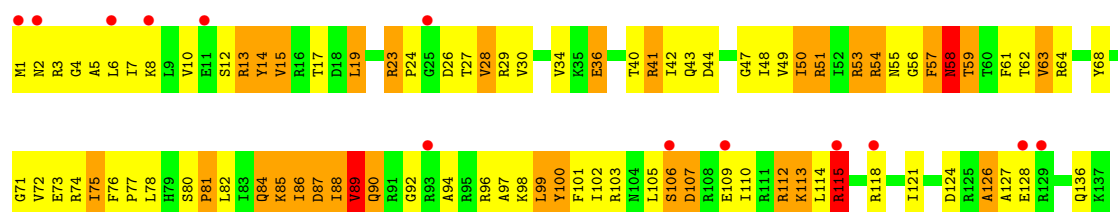




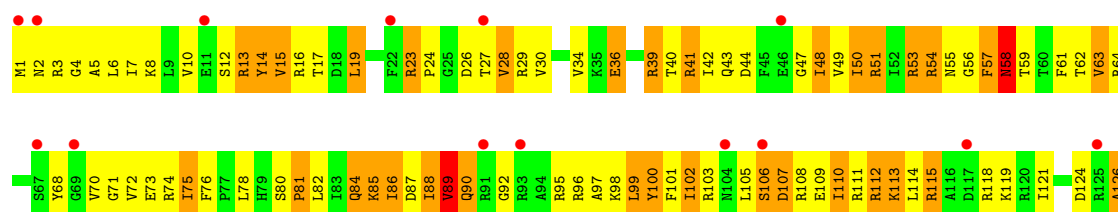
• Molecule 37: 50S ribosomal protein L18



• Molecule 38: 50S ribosomal protein L19

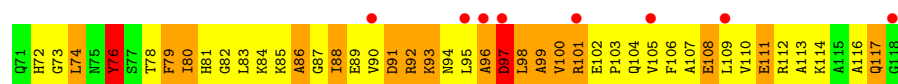


• Molecule 38: 50S ribosomal protein L19



• Molecule 39: 50S ribosomal protein L20





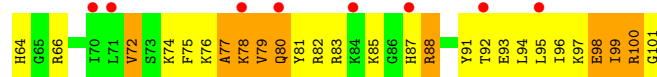
- Molecule 39: 50S ribosomal protein L20



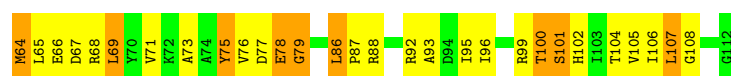
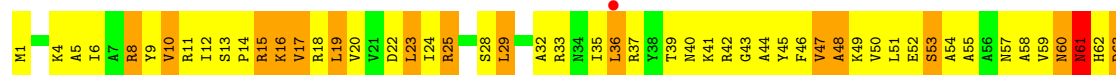
- Molecule 40: 50S ribosomal protein L21



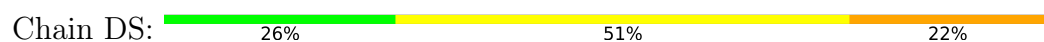
- Molecule 40: 50S ribosomal protein L21

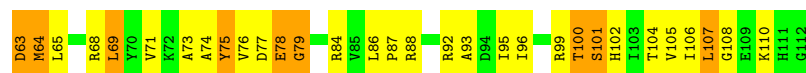


- Molecule 41: 50S ribosomal protein L22

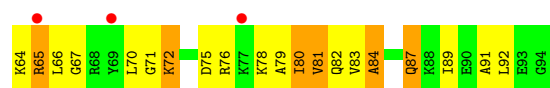
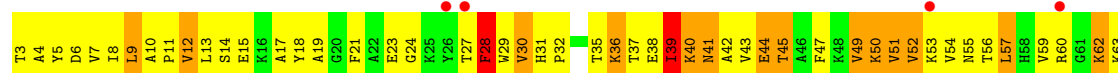


- Molecule 41: 50S ribosomal protein L22

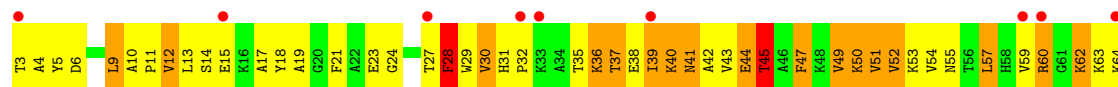




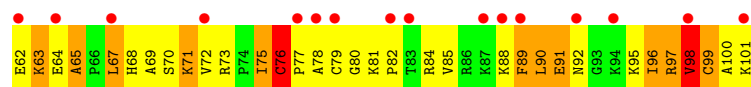
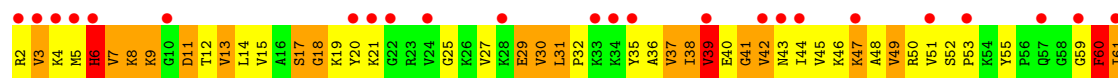
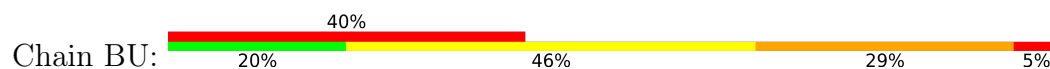
• Molecule 42: 50S ribosomal protein L23



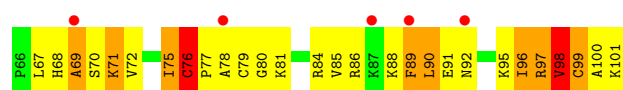
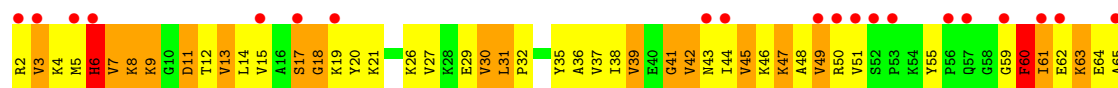
• Molecule 42: 50S ribosomal protein L23



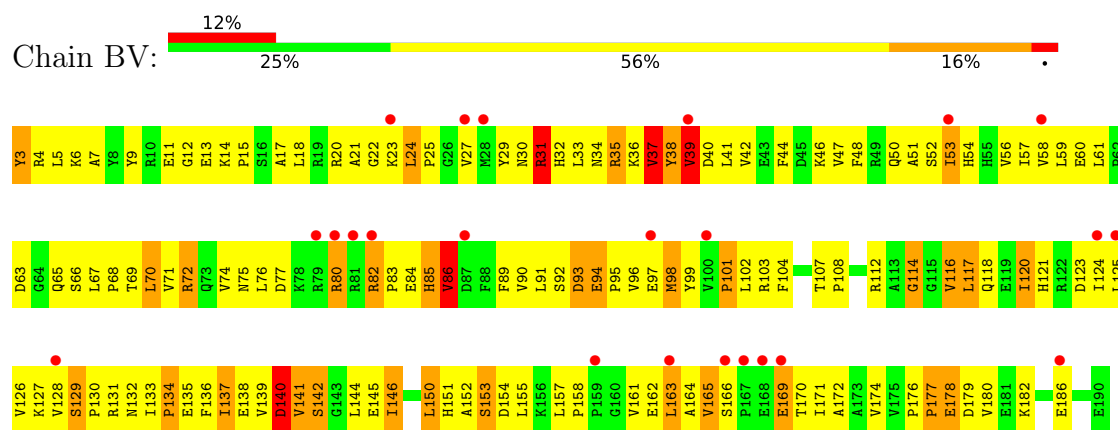
• Molecule 43: 50S ribosomal protein L24



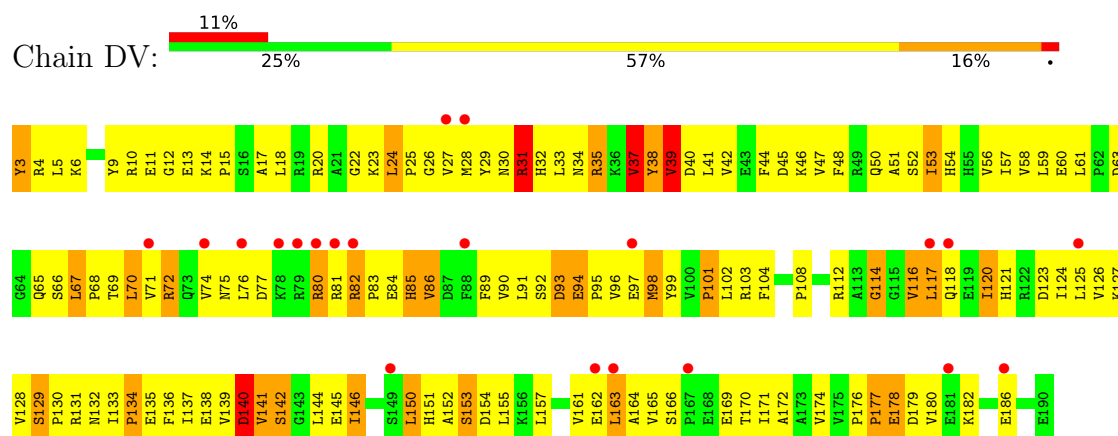
• Molecule 43: 50S ribosomal protein L24



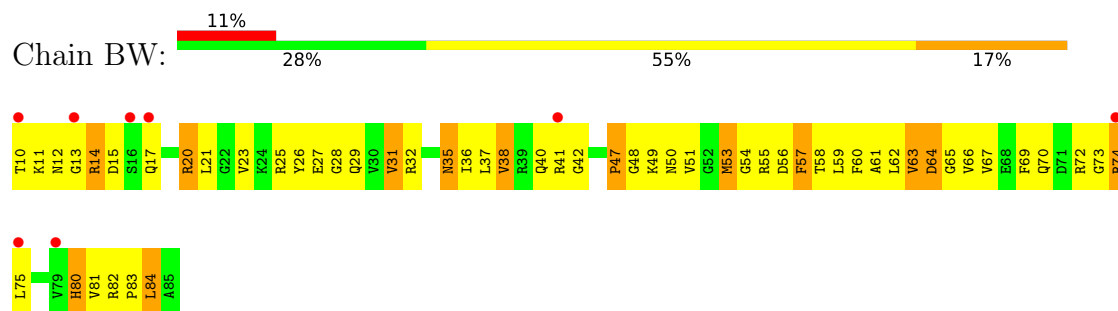
• Molecule 44: 50S ribosomal protein L25



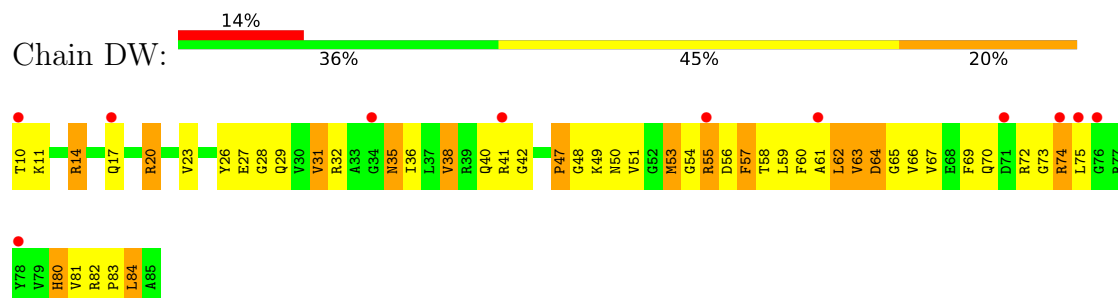
• Molecule 44: 50S ribosomal protein L25



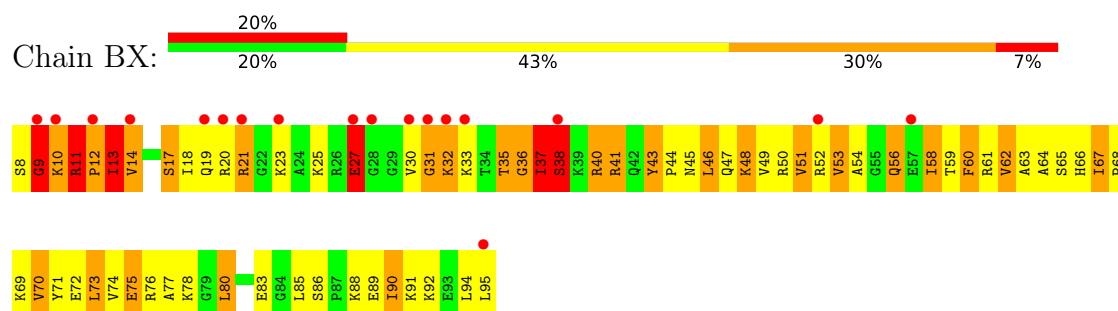
• Molecule 45: 50S ribosomal protein L27



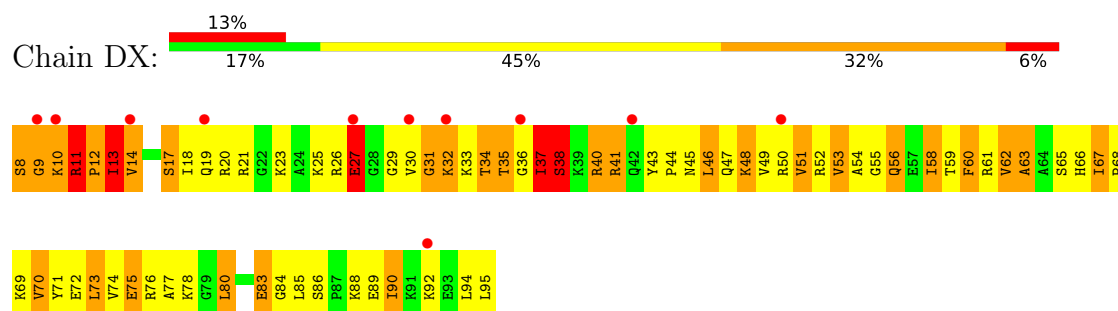
• Molecule 45: 50S ribosomal protein L27



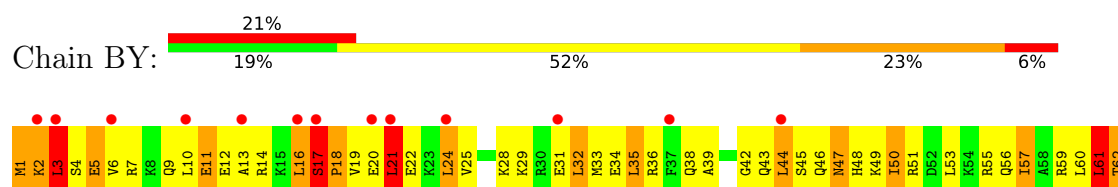
- Molecule 46: 50S ribosomal protein L28



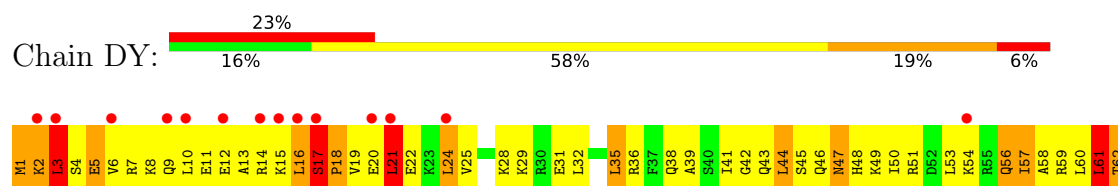
- Molecule 46: 50S ribosomal protein L28



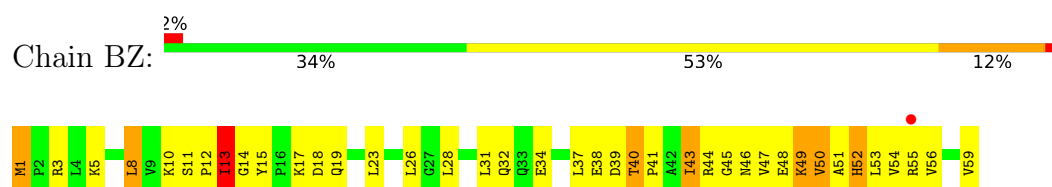
- Molecule 47: 50S ribosomal protein L29



- Molecule 47: 50S ribosomal protein L29



- Molecule 48: 50S ribosomal protein L30



- Molecule 48: 50S ribosomal protein L30

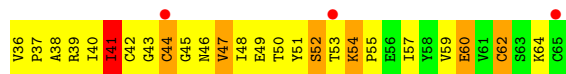




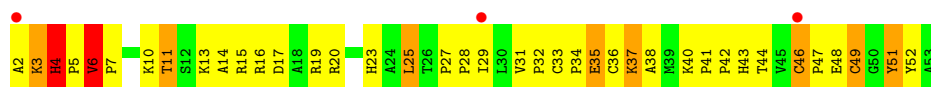
- Molecule 49: 50S ribosomal protein L31



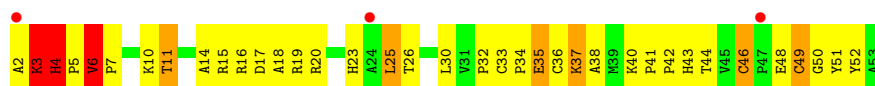
- Molecule 49: 50S ribosomal protein L31



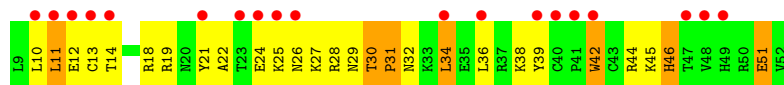
- Molecule 50: 50S ribosomal protein L32



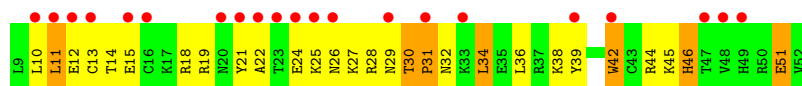
- Molecule 50: 50S ribosomal protein L32



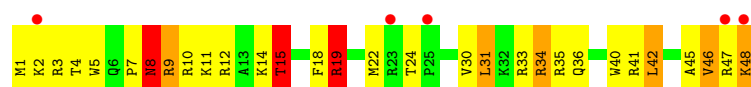
- Molecule 51: 50S ribosomal protein L33



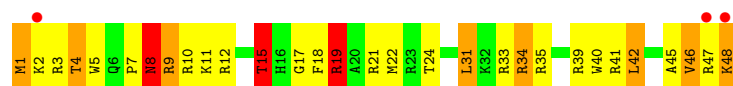
- Molecule 51: 50S ribosomal protein L33



- Molecule 52: 50S ribosomal protein L34



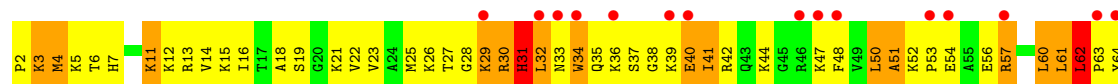
• Molecule 52: 50S ribosomal protein L34



• Molecule 53: 50S ribosomal protein L35



• Molecule 53: 50S ribosomal protein L35



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.69Å 451.66Å 614.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.52 – 3.40 49.52 – 3.40	Depositor EDS
% Data completeness (in resolution range)	97.5 (49.52-3.40) 97.5 (49.52-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.28 (at 3.40Å)	Xtriage
Refinement program	PHENIX 1.6.1_357, CNS	Depositor
R, R_{free}	0.228 , 0.266 0.224 , 0.262	Depositor DCC
R_{free} test set	7701 reflections (0.99%)	wwPDB-VP
Wilson B-factor (Å ²)	86.0	Xtriage
Anisotropy	0.391	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 95.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	282142	wwPDB-VP
Average B, all atoms (Å ²)	110.0	wwPDB-VP

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

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.36	0/36238	0.42	0/56561
1	CA	0.33	0/36238	0.41	0/56561
2	AB	0.39	0/1936	0.87	4/2609 (0.2%)
2	CB	0.37	0/1936	0.84	3/2609 (0.1%)
3	AC	0.41	0/1637	0.76	0/2205
3	CC	0.40	0/1637	0.76	0/2205
4	AD	0.51	0/1733	0.95	6/2318 (0.3%)
4	CD	0.43	0/1733	0.91	4/2318 (0.2%)
5	AE	0.54	0/1172	0.92	1/1576 (0.1%)
5	CE	0.48	0/1172	0.89	1/1576 (0.1%)
6	AF	0.41	0/856	0.85	2/1154 (0.2%)
6	CF	0.48	0/856	0.87	2/1154 (0.2%)
7	AG	0.36	0/1276	0.78	0/1709
7	CG	0.37	0/1276	0.78	0/1709
8	AH	0.50	0/1136	0.99	6/1527 (0.4%)
8	CH	0.44	0/1136	0.94	4/1527 (0.3%)
9	AI	0.35	0/1029	0.71	0/1378
9	CI	0.33	0/1029	0.72	0/1378
10	AJ	0.38	0/808	0.80	0/1085
10	CJ	0.38	0/808	0.79	0/1085
11	AK	0.52	0/900	1.04	6/1213 (0.5%)
11	CK	0.51	0/900	1.05	6/1213 (0.5%)
12	AL	0.63	0/987	1.12	8/1320 (0.6%)
12	CL	0.60	0/987	1.05	4/1320 (0.3%)
13	AM	0.35	0/939	0.77	0/1258
13	CM	0.33	0/939	0.77	0/1258
14	AN	0.36	0/501	0.74	0/664
14	CN	0.35	0/501	0.75	0/664
15	AO	0.52	0/745	0.86	1/992 (0.1%)
15	CO	0.48	0/745	0.86	1/992 (0.1%)
16	AP	0.53	0/717	0.95	2/963 (0.2%)
16	CP	0.43	0/717	0.90	2/963 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AQ	0.53	0/837	0.94	2/1117 (0.2%)
17	CQ	0.43	0/837	0.87	2/1117 (0.2%)
18	AR	0.44	0/579	0.86	0/768
18	CR	0.43	0/579	0.86	0/768
19	AS	0.35	0/643	0.71	0/865
19	CS	0.33	0/643	0.71	0/865
20	AT	0.48	0/764	0.89	1/1006 (0.1%)
20	CT	0.42	0/764	0.86	1/1006 (0.1%)
21	AU	0.31	0/213	0.75	0/277
21	CU	0.30	0/213	0.75	0/277
22	AV	0.25	0/802	0.34	0/1245
22	CV	0.25	0/802	0.37	0/1245
23	BA	0.58	0/66570	0.53	3/103918 (0.0%)
23	DA	0.65	2/66575 (0.0%)	0.55	4/103930 (0.0%)
24	BB	0.33	0/2853	0.43	0/4451
24	DB	0.34	0/2853	0.43	0/4451
25	BC	0.94	4/2155 (0.2%)	1.31	20/2905 (0.7%)
25	DC	0.96	3/2155 (0.1%)	1.31	23/2905 (0.8%)
26	BD	0.76	0/1597	1.24	18/2153 (0.8%)
26	DD	0.84	3/1597 (0.2%)	1.29	17/2153 (0.8%)
27	BE	0.76	0/1622	1.19	13/2194 (0.6%)
27	DE	0.80	0/1622	1.21	12/2194 (0.5%)
28	BF	0.35	0/1500	0.82	5/2017 (0.2%)
28	DF	0.35	0/1500	0.82	5/2017 (0.2%)
29	BG	0.43	0/1246	1.02	5/1682 (0.3%)
29	DG	0.58	0/1246	1.08	4/1682 (0.2%)
30	BH	0.47	0/1148	0.89	1/1552 (0.1%)
30	DH	0.50	0/1148	0.90	1/1552 (0.1%)
31	BI	0.34	0/252	0.73	0/333
31	DI	0.36	0/252	0.78	1/333 (0.3%)
32	BJ	0.68	0/1124	1.18	12/1515 (0.8%)
32	DJ	0.73	0/1124	1.16	9/1515 (0.6%)
33	BK	0.75	0/942	1.14	6/1268 (0.5%)
33	DK	0.82	0/942	1.18	6/1268 (0.5%)
34	BL	0.96	5/1131 (0.4%)	1.40	18/1504 (1.2%)
34	DL	0.95	3/1131 (0.3%)	1.41	19/1504 (1.3%)
35	BM	0.78	1/1099 (0.1%)	1.22	9/1468 (0.6%)
35	DM	0.80	0/1099	1.23	9/1468 (0.6%)
36	BN	0.80	1/974 (0.1%)	1.13	4/1302 (0.3%)
36	DN	0.78	1/974 (0.1%)	1.11	3/1302 (0.2%)
37	BO	0.48	0/779	0.88	2/1036 (0.2%)
37	DO	0.52	0/779	0.90	2/1036 (0.2%)
38	BP	0.64	0/1158	0.98	2/1544 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DP	0.69	0/1158	0.98	3/1544 (0.2%)
39	BQ	0.80	0/970	1.14	7/1290 (0.5%)
39	DQ	0.87	0/970	1.17	9/1290 (0.7%)
40	BR	0.70	0/790	1.04	2/1057 (0.2%)
40	DR	0.77	0/790	1.06	2/1057 (0.2%)
41	BS	0.82	0/902	1.09	3/1209 (0.2%)
41	DS	0.85	0/902	1.11	4/1209 (0.3%)
42	BT	0.79	1/740 (0.1%)	1.15	4/993 (0.4%)
42	DT	0.93	1/740 (0.1%)	1.22	7/993 (0.7%)
43	BU	0.73	1/789 (0.1%)	1.21	10/1051 (1.0%)
43	DU	0.77	0/789	1.17	4/1051 (0.4%)
44	BV	0.46	0/1524	0.90	4/2068 (0.2%)
44	DV	0.47	0/1524	0.91	3/2068 (0.1%)
45	BW	0.62	0/613	1.02	1/816 (0.1%)
45	DW	0.64	0/613	1.03	2/816 (0.2%)
46	BX	1.05	4/702 (0.6%)	1.52	15/932 (1.6%)
46	DX	1.14	5/702 (0.7%)	1.52	17/932 (1.8%)
47	BY	0.72	0/523	1.15	7/690 (1.0%)
47	DY	0.94	1/523 (0.2%)	1.27	7/690 (1.0%)
48	BZ	0.72	0/473	1.06	1/634 (0.2%)
48	DZ	0.66	0/473	1.01	1/634 (0.2%)
49	B1	0.34	0/229	0.67	0/309
49	D1	0.36	0/229	0.69	0/309
50	B2	0.81	0/419	1.38	8/567 (1.4%)
50	D2	0.79	0/419	1.41	8/567 (1.4%)
51	B3	0.39	0/388	0.79	0/518
51	D3	0.39	0/388	0.78	0/518
52	B4	0.95	0/427	1.25	3/561 (0.5%)
52	D4	1.05	0/427	1.35	6/561 (1.1%)
53	B5	0.83	0/516	1.25	5/679 (0.7%)
53	D5	0.85	0/516	1.25	5/679 (0.7%)
All	All	0.56	36/305211 (0.0%)	0.69	450/456064 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
25	DC	0	1
27	BE	0	1
27	DE	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
34	BL	0	5
34	DL	0	5
35	BM	0	1
35	DM	0	1
36	BN	0	1
36	DN	0	1
39	BQ	0	2
39	DQ	0	2
All	All	0	21

The worst 5 of 36 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	BX	35	THR	CA-C	9.63	1.65	1.52
46	DX	35	THR	CA-C	8.10	1.63	1.52
46	DX	67	ILE	CA-CB	-8.09	1.50	1.54
46	BX	67	ILE	CA-CB	-7.17	1.50	1.54
34	DL	39	LYS	CB-CG	6.99	1.73	1.52

The worst 5 of 450 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	DL	37	GLY	N-CA-C	11.75	130.35	115.42
25	BC	46	GLN	N-CA-C	-11.49	96.27	110.41
25	DC	46	GLN	N-CA-C	-10.87	96.50	110.53
46	BX	27	GLU	N-CA-C	10.67	124.91	107.73
34	DL	54	GLY	N-CA-C	-10.59	99.82	114.64

There are no chirality outliers.

5 of 21 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
27	BE	47	GLY	Peptide
34	BL	29	LYS	Peptide
34	BL	37	GLY	Peptide
34	BL	39	LYS	Peptide
34	BL	9	ASN	Peptide

5.2 Too-close contacts

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	32372	0	16339	1694	0
1	CA	32372	0	16339	1786	0
2	AB	1901	0	1951	189	0
2	CB	1901	0	1951	192	0
3	AC	1613	0	1677	185	0
3	CC	1613	0	1677	191	0
4	AD	1703	0	1764	200	0
4	CD	1703	0	1764	194	1
5	AE	1156	0	1213	148	0
5	CE	1156	0	1213	151	0
6	AF	843	0	857	103	1
6	CF	843	0	857	101	0
7	AG	1257	0	1296	99	0
7	CG	1257	0	1296	93	0
8	AH	1116	0	1177	139	0
8	CH	1116	0	1177	147	0
9	AI	1011	0	1043	107	0
9	CI	1011	0	1043	117	0
10	AJ	795	0	840	93	0
10	CJ	795	0	840	93	0
11	AK	885	0	904	79	0
11	CK	885	0	904	74	0
12	AL	971	0	1057	132	0
12	CL	971	0	1057	145	0
13	AM	929	0	987	85	0
13	CM	929	0	987	85	0
14	AN	492	0	530	51	0
14	CN	492	0	532	62	0
15	AO	734	0	771	71	0
15	CO	734	0	771	65	0
16	AP	701	0	720	101	0
16	CP	701	0	720	95	0
17	AQ	824	0	893	69	0
17	CQ	824	0	893	79	0
18	AR	574	0	644	76	0
18	CR	574	0	644	76	0
19	AS	630	0	652	74	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	CS	630	0	652	64	0
20	AT	762	0	859	70	0
20	CT	762	0	859	74	0
21	AU	209	0	221	16	0
21	CU	209	0	221	17	0
22	AV	719	0	366	58	0
22	CV	719	0	366	57	0
23	BA	59440	0	29964	2624	0
23	DA	59442	0	29965	2594	0
24	BB	2551	0	1295	147	0
24	DB	2551	0	1295	148	0
25	BC	2105	0	2182	374	0
25	DC	2105	0	2182	369	0
26	BD	1564	0	1629	231	0
26	DD	1564	0	1629	234	0
27	BE	1587	0	1632	154	0
27	DE	1587	0	1632	161	0
28	BF	1475	0	1537	158	0
28	DF	1475	0	1537	151	0
29	BG	1223	0	1282	117	0
29	DG	1223	0	1282	126	0
30	BH	1133	0	1220	137	0
30	DH	1133	0	1220	139	0
31	BI	254	0	275	8	0
31	DI	254	0	275	9	0
32	BJ	1097	0	1168	179	0
32	DJ	1097	0	1168	161	0
33	BK	932	0	994	104	0
33	DK	932	0	994	108	0
34	BL	1114	0	1187	276	0
34	DL	1114	0	1187	287	0
35	BM	1079	0	1127	180	0
35	DM	1079	0	1127	181	0
36	BN	960	0	1021	162	0
36	DN	960	0	1021	155	0
37	BO	771	0	832	98	0
37	DO	771	0	832	106	0
38	BP	1144	0	1211	138	0
38	DP	1144	0	1211	137	0
39	BQ	953	0	1013	159	0
39	DQ	953	0	1013	168	0
40	BR	779	0	852	140	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	DR	779	0	852	136	0
41	BS	891	0	951	111	0
41	DS	891	0	951	116	0
42	BT	726	0	778	91	0
42	DT	726	0	778	96	0
43	BU	776	0	870	142	0
43	DU	776	0	870	141	0
44	BV	1492	0	1513	186	0
44	DV	1492	0	1513	185	0
45	BW	605	0	628	74	0
45	DW	605	0	628	65	0
46	BX	695	0	764	116	0
46	DX	695	0	764	113	0
47	BY	521	0	575	84	0
47	DY	521	0	575	83	0
48	BZ	468	0	523	48	0
48	DZ	468	0	523	49	0
49	B1	226	0	225	23	0
49	D1	226	0	225	24	0
50	B2	405	0	420	62	0
50	D2	405	0	420	66	0
51	B3	381	0	391	25	0
51	D3	381	0	391	28	0
52	B4	419	0	467	54	0
52	D4	419	0	467	51	0
53	B5	508	0	576	117	0
53	D5	508	0	576	115	0
54	AA	163	0	0	0	0
54	AD	1	0	0	0	0
54	AV	4	0	0	0	0
54	B2	1	0	0	0	0
54	BA	408	0	0	0	0
54	BB	17	0	0	0	0
54	BK	1	0	0	0	0
54	CA	140	0	0	0	0
54	CP	1	0	0	0	0
54	CV	1	0	0	0	0
54	D2	1	0	0	0	0
54	D4	1	0	0	0	0
54	DA	436	0	0	0	0
54	DB	17	0	0	0	0
54	DE	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	DG	1	0	0	0	0
55	AD	1	0	0	0	0
55	AN	1	0	0	0	0
55	CD	1	0	0	0	0
55	CN	1	0	0	0	0
All	All	282142	0	191729	18883	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 40.

The worst 5 of 18883 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)
52:D4:8:ASN:HD22	52:D4:8:ASN:C	1.42	1.23
34:DL:57:THR:HG23	34:DL:59:LEU:HD22	1.22	1.20
34:DL:59:LEU:HA	34:DL:61:ARG:NE	1.55	1.20
35:BM:81:VAL:O	35:BM:82:ARG:HG2	1.39	1.19
34:BL:57:THR:HG23	34:BL:59:LEU:HD22	1.21	1.19

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:AF:15:ASP:OD1	4:CD:20:TYR:OH[4_555]	2.18	0.02

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	232/234 (99%)	172 (74%)	40 (17%)	20 (9%)	0 4
2	CB	232/234 (99%)	173 (75%)	38 (16%)	21 (9%)	0 3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	AC	204/206 (99%)	136 (67%)	43 (21%)	25 (12%)	0	1
3	CC	204/206 (99%)	134 (66%)	45 (22%)	25 (12%)	0	1
4	AD	206/208 (99%)	152 (74%)	38 (18%)	16 (8%)	1	4
4	CD	206/208 (99%)	151 (73%)	40 (19%)	15 (7%)	1	5
5	AE	149/151 (99%)	103 (69%)	34 (23%)	12 (8%)	1	4
5	CE	149/151 (99%)	104 (70%)	34 (23%)	11 (7%)	1	5
6	AF	99/101 (98%)	71 (72%)	17 (17%)	11 (11%)	0	2
6	CF	99/101 (98%)	71 (72%)	18 (18%)	10 (10%)	0	3
7	AG	153/155 (99%)	121 (79%)	27 (18%)	5 (3%)	3	17
7	CG	153/155 (99%)	121 (79%)	27 (18%)	5 (3%)	3	17
8	AH	136/138 (99%)	97 (71%)	29 (21%)	10 (7%)	1	5
8	CH	136/138 (99%)	98 (72%)	28 (21%)	10 (7%)	1	5
9	AI	125/127 (98%)	91 (73%)	31 (25%)	3 (2%)	4	22
9	CI	125/127 (98%)	89 (71%)	32 (26%)	4 (3%)	3	17
10	AJ	96/98 (98%)	72 (75%)	20 (21%)	4 (4%)	2	14
10	CJ	96/98 (98%)	74 (77%)	18 (19%)	4 (4%)	2	14
11	AK	117/119 (98%)	83 (71%)	29 (25%)	5 (4%)	2	13
11	CK	117/119 (98%)	82 (70%)	30 (26%)	5 (4%)	2	13
12	AL	122/124 (98%)	78 (64%)	28 (23%)	16 (13%)	0	1
12	CL	122/124 (98%)	80 (66%)	27 (22%)	15 (12%)	0	1
13	AM	114/116 (98%)	93 (82%)	17 (15%)	4 (4%)	3	16
13	CM	114/116 (98%)	93 (82%)	17 (15%)	4 (4%)	3	16
14	AN	58/60 (97%)	46 (79%)	9 (16%)	3 (5%)	1	10
14	CN	58/60 (97%)	46 (79%)	9 (16%)	3 (5%)	1	10
15	AO	86/88 (98%)	62 (72%)	17 (20%)	7 (8%)	1	4
15	CO	86/88 (98%)	61 (71%)	19 (22%)	6 (7%)	1	6
16	AP	81/83 (98%)	46 (57%)	24 (30%)	11 (14%)	0	1
16	CP	81/83 (98%)	46 (57%)	25 (31%)	10 (12%)	0	1
17	AQ	97/99 (98%)	74 (76%)	16 (16%)	7 (7%)	1	5
17	CQ	97/99 (98%)	75 (77%)	16 (16%)	6 (6%)	1	7
18	AR	68/70 (97%)	40 (59%)	19 (28%)	9 (13%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	CR	68/70 (97%)	41 (60%)	18 (26%)	9 (13%)	0	1
19	AS	76/78 (97%)	51 (67%)	21 (28%)	4 (5%)	1	10
19	CS	76/78 (97%)	50 (66%)	21 (28%)	5 (7%)	1	6
20	AT	97/99 (98%)	67 (69%)	23 (24%)	7 (7%)	1	5
20	CT	97/99 (98%)	67 (69%)	23 (24%)	7 (7%)	1	5
21	AU	22/24 (92%)	13 (59%)	8 (36%)	1 (4%)	2	12
21	CU	22/24 (92%)	13 (59%)	8 (36%)	1 (4%)	2	12
25	BC	269/271 (99%)	213 (79%)	36 (13%)	20 (7%)	1	5
25	DC	269/271 (99%)	210 (78%)	39 (14%)	20 (7%)	1	5
26	BD	202/204 (99%)	154 (76%)	34 (17%)	14 (7%)	1	6
26	DD	202/204 (99%)	155 (77%)	32 (16%)	15 (7%)	1	5
27	BE	200/202 (99%)	152 (76%)	32 (16%)	16 (8%)	1	4
27	DE	200/202 (99%)	155 (78%)	30 (15%)	15 (8%)	1	5
28	BF	179/181 (99%)	136 (76%)	31 (17%)	12 (7%)	1	6
28	DF	179/181 (99%)	136 (76%)	31 (17%)	12 (7%)	1	6
29	BG	157/159 (99%)	112 (71%)	35 (22%)	10 (6%)	1	7
29	DG	157/159 (99%)	111 (71%)	36 (23%)	10 (6%)	1	7
30	BH	143/145 (99%)	95 (66%)	29 (20%)	19 (13%)	0	1
30	DH	143/145 (99%)	91 (64%)	31 (22%)	21 (15%)	0	0
31	BI	28/65 (43%)	25 (89%)	3 (11%)	0	100	100
31	DI	28/65 (43%)	25 (89%)	3 (11%)	0	100	100
32	BJ	135/137 (98%)	97 (72%)	26 (19%)	12 (9%)	0	3
32	DJ	135/137 (98%)	97 (72%)	24 (18%)	14 (10%)	0	2
33	BK	120/122 (98%)	100 (83%)	11 (9%)	9 (8%)	1	5
33	DK	120/122 (98%)	98 (82%)	14 (12%)	8 (7%)	1	6
34	BL	144/146 (99%)	87 (60%)	31 (22%)	26 (18%)	0	0
34	DL	144/146 (99%)	86 (60%)	35 (24%)	23 (16%)	0	0
35	BM	134/136 (98%)	86 (64%)	28 (21%)	20 (15%)	0	0
35	DM	134/136 (98%)	86 (64%)	30 (22%)	18 (13%)	0	1
36	BN	115/117 (98%)	91 (79%)	13 (11%)	11 (10%)	0	3
36	DN	115/117 (98%)	90 (78%)	15 (13%)	10 (9%)	0	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	BO	96/98 (98%)	57 (59%)	23 (24%)	16 (17%)	0	0
37	DO	96/98 (98%)	54 (56%)	25 (26%)	17 (18%)	0	0
38	BP	135/137 (98%)	101 (75%)	18 (13%)	16 (12%)	0	2
38	DP	135/137 (98%)	100 (74%)	19 (14%)	16 (12%)	0	2
39	BQ	114/116 (98%)	78 (68%)	22 (19%)	14 (12%)	0	1
39	DQ	114/116 (98%)	82 (72%)	20 (18%)	12 (10%)	0	2
40	BR	99/101 (98%)	70 (71%)	20 (20%)	9 (9%)	0	3
40	DR	99/101 (98%)	70 (71%)	20 (20%)	9 (9%)	0	3
41	BS	110/112 (98%)	88 (80%)	17 (16%)	5 (4%)	2	12
41	DS	110/112 (98%)	87 (79%)	17 (16%)	6 (6%)	1	9
42	BT	90/92 (98%)	69 (77%)	16 (18%)	5 (6%)	1	9
42	DT	90/92 (98%)	67 (74%)	18 (20%)	5 (6%)	1	9
43	BU	98/100 (98%)	55 (56%)	24 (24%)	19 (19%)	0	0
43	DU	98/100 (98%)	58 (59%)	21 (21%)	19 (19%)	0	0
44	BV	186/188 (99%)	135 (73%)	34 (18%)	17 (9%)	0	3
44	DV	186/188 (99%)	135 (73%)	34 (18%)	17 (9%)	0	3
45	BW	74/76 (97%)	61 (82%)	10 (14%)	3 (4%)	2	15
45	DW	74/76 (97%)	60 (81%)	10 (14%)	4 (5%)	1	10
46	BX	86/88 (98%)	57 (66%)	16 (19%)	13 (15%)	0	0
46	DX	86/88 (98%)	54 (63%)	19 (22%)	13 (15%)	0	0
47	BY	60/62 (97%)	45 (75%)	8 (13%)	7 (12%)	0	2
47	DY	60/62 (97%)	41 (68%)	12 (20%)	7 (12%)	0	2
48	BZ	57/59 (97%)	49 (86%)	7 (12%)	1 (2%)	6	26
48	DZ	57/59 (97%)	50 (88%)	6 (10%)	1 (2%)	6	26
49	B1	28/30 (93%)	15 (54%)	7 (25%)	6 (21%)	0	0
49	D1	28/30 (93%)	15 (54%)	7 (25%)	6 (21%)	0	0
50	B2	50/52 (96%)	40 (80%)	6 (12%)	4 (8%)	1	4
50	D2	50/52 (96%)	39 (78%)	7 (14%)	4 (8%)	1	4
51	B3	42/44 (96%)	26 (62%)	11 (26%)	5 (12%)	0	2
51	D3	42/44 (96%)	26 (62%)	11 (26%)	5 (12%)	0	2
52	B4	46/48 (96%)	42 (91%)	3 (6%)	1 (2%)	5	24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
52	D4	46/48 (96%)	42 (91%)	3 (6%)	1 (2%)	5	24
53	B5	61/63 (97%)	43 (70%)	12 (20%)	6 (10%)	0	3
53	D5	61/63 (97%)	44 (72%)	10 (16%)	7 (12%)	0	2
All	All	11192/11458 (98%)	8080 (72%)	2125 (19%)	987 (9%)	0	3

5 of 987 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	204	ASN
3	AC	189	ALA
3	AC	196	LEU
4	AD	28	SER
4	AD	30	LYS

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	202/202 (100%)	178 (88%)	24 (12%)	5	19
2	CB	202/202 (100%)	177 (88%)	25 (12%)	4	18
3	AC	160/160 (100%)	146 (91%)	14 (9%)	9	31
3	CC	160/160 (100%)	146 (91%)	14 (9%)	9	31
4	AD	180/180 (100%)	146 (81%)	34 (19%)	1	6
4	CD	180/180 (100%)	149 (83%)	31 (17%)	2	8
5	AE	116/116 (100%)	95 (82%)	21 (18%)	2	7
5	CE	116/116 (100%)	95 (82%)	21 (18%)	2	7
6	AF	90/90 (100%)	80 (89%)	10 (11%)	6	21
6	CF	90/90 (100%)	80 (89%)	10 (11%)	6	21
7	AG	126/126 (100%)	119 (94%)	7 (6%)	19	46
7	CG	126/126 (100%)	118 (94%)	8 (6%)	16	42
8	AH	119/119 (100%)	101 (85%)	18 (15%)	3	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	CH	119/119 (100%)	101 (85%)	18 (15%)	3	11
9	AI	98/98 (100%)	91 (93%)	7 (7%)	13	39
9	CI	98/98 (100%)	91 (93%)	7 (7%)	13	39
10	AJ	88/88 (100%)	78 (89%)	10 (11%)	5	21
10	CJ	88/88 (100%)	78 (89%)	10 (11%)	5	21
11	AK	90/90 (100%)	70 (78%)	20 (22%)	1	3
11	CK	90/90 (100%)	69 (77%)	21 (23%)	1	2
12	AL	104/104 (100%)	78 (75%)	26 (25%)	0	1
12	CL	104/104 (100%)	78 (75%)	26 (25%)	0	1
13	AM	94/94 (100%)	88 (94%)	6 (6%)	16	42
13	CM	94/94 (100%)	88 (94%)	6 (6%)	16	42
14	AN	49/49 (100%)	46 (94%)	3 (6%)	17	43
14	CN	49/49 (100%)	46 (94%)	3 (6%)	17	43
15	AO	79/79 (100%)	67 (85%)	12 (15%)	3	10
15	CO	79/79 (100%)	68 (86%)	11 (14%)	3	14
16	AP	72/72 (100%)	57 (79%)	15 (21%)	1	4
16	CP	72/72 (100%)	56 (78%)	16 (22%)	1	3
17	AQ	94/94 (100%)	80 (85%)	14 (15%)	3	12
17	CQ	94/94 (100%)	80 (85%)	14 (15%)	3	12
18	AR	61/61 (100%)	59 (97%)	2 (3%)	33	57
18	CR	61/61 (100%)	59 (97%)	2 (3%)	33	57
19	AS	69/69 (100%)	60 (87%)	9 (13%)	4	16
19	CS	69/69 (100%)	60 (87%)	9 (13%)	4	16
20	AT	76/76 (100%)	65 (86%)	11 (14%)	3	13
20	CT	76/76 (100%)	65 (86%)	11 (14%)	3	13
21	AU	19/19 (100%)	19 (100%)	0	100	100
21	CU	19/19 (100%)	19 (100%)	0	100	100
25	BC	213/213 (100%)	161 (76%)	52 (24%)	1	2
25	DC	213/213 (100%)	159 (75%)	54 (25%)	0	1
26	BD	165/165 (100%)	128 (78%)	37 (22%)	1	3
26	DD	165/165 (100%)	127 (77%)	38 (23%)	1	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
27	BE	161/161 (100%)	122 (76%)	39 (24%)	1	2
27	DE	161/161 (100%)	120 (74%)	41 (26%)	0	1
28	BF	155/155 (100%)	132 (85%)	23 (15%)	3	12
28	DF	155/155 (100%)	132 (85%)	23 (15%)	3	12
29	BG	132/132 (100%)	107 (81%)	25 (19%)	1	6
29	DG	132/132 (100%)	108 (82%)	24 (18%)	2	7
30	BH	122/122 (100%)	98 (80%)	24 (20%)	1	5
30	DH	122/122 (100%)	99 (81%)	23 (19%)	1	6
31	BI	27/53 (51%)	26 (96%)	1 (4%)	30	55
31	DI	27/53 (51%)	26 (96%)	1 (4%)	30	55
32	BJ	116/116 (100%)	84 (72%)	32 (28%)	0	1
32	DJ	116/116 (100%)	85 (73%)	31 (27%)	0	1
33	BK	100/100 (100%)	75 (75%)	25 (25%)	0	1
33	DK	100/100 (100%)	74 (74%)	26 (26%)	0	1
34	BL	112/112 (100%)	75 (67%)	37 (33%)	0	0
34	DL	112/112 (100%)	73 (65%)	39 (35%)	0	0
35	BM	106/106 (100%)	78 (74%)	28 (26%)	0	1
35	DM	106/106 (100%)	77 (73%)	29 (27%)	0	1
36	BN	100/100 (100%)	68 (68%)	32 (32%)	0	0
36	DN	100/100 (100%)	68 (68%)	32 (32%)	0	0
37	BO	77/77 (100%)	63 (82%)	14 (18%)	2	7
37	DO	77/77 (100%)	63 (82%)	14 (18%)	2	7
38	BP	121/121 (100%)	93 (77%)	28 (23%)	1	2
38	DP	121/121 (100%)	91 (75%)	30 (25%)	1	2
39	BQ	92/92 (100%)	73 (79%)	19 (21%)	1	4
39	DQ	92/92 (100%)	71 (77%)	21 (23%)	1	3
40	BR	82/82 (100%)	60 (73%)	22 (27%)	0	1
40	DR	82/82 (100%)	59 (72%)	23 (28%)	0	1
41	BS	91/91 (100%)	61 (67%)	30 (33%)	0	0
41	DS	91/91 (100%)	63 (69%)	28 (31%)	0	0
42	BT	74/74 (100%)	58 (78%)	16 (22%)	1	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
42	DT	74/74 (100%)	58 (78%)	16 (22%)	1	3
43	BU	84/84 (100%)	66 (79%)	18 (21%)	1	3
43	DU	84/84 (100%)	67 (80%)	17 (20%)	1	4
44	BV	163/163 (100%)	134 (82%)	29 (18%)	2	7
44	DV	163/163 (100%)	135 (83%)	28 (17%)	2	8
45	BW	61/61 (100%)	49 (80%)	12 (20%)	1	5
45	DW	61/61 (100%)	50 (82%)	11 (18%)	2	7
46	BX	73/73 (100%)	50 (68%)	23 (32%)	0	0
46	DX	73/73 (100%)	52 (71%)	21 (29%)	0	1
47	BY	58/58 (100%)	46 (79%)	12 (21%)	1	4
47	DY	58/58 (100%)	45 (78%)	13 (22%)	1	3
48	BZ	51/51 (100%)	42 (82%)	9 (18%)	2	8
48	DZ	51/51 (100%)	43 (84%)	8 (16%)	2	10
49	B1	27/27 (100%)	24 (89%)	3 (11%)	6	21
49	D1	27/27 (100%)	24 (89%)	3 (11%)	6	21
50	B2	45/45 (100%)	40 (89%)	5 (11%)	6	21
50	D2	45/45 (100%)	40 (89%)	5 (11%)	6	21
51	B3	43/43 (100%)	36 (84%)	7 (16%)	2	10
51	D3	43/43 (100%)	36 (84%)	7 (16%)	2	10
52	B4	41/41 (100%)	29 (71%)	12 (29%)	0	1
52	D4	41/41 (100%)	28 (68%)	13 (32%)	0	0
53	B5	53/53 (100%)	43 (81%)	10 (19%)	1	6
53	D5	53/53 (100%)	44 (83%)	9 (17%)	2	9
All	All	9462/9514 (100%)	7684 (81%)	1778 (19%)	1	6

5 of 1778 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	CD	3	ARG
53	D5	31	HIS
20	CT	62	LEU
51	D3	34	LEU
41	DS	1	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 260 such sidechains are listed below:

Mol	Chain	Res	Type
41	DS	61	ASN
43	DU	6	HIS
40	BR	64	HIS
39	BQ	49	HIS
46	DX	45	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1505/1506 (99%)	293 (19%)	14 (0%)
1	CA	1505/1506 (99%)	294 (19%)	14 (0%)
22	AV	32/43 (74%)	3 (9%)	0
22	CV	32/43 (74%)	3 (9%)	0
23	BA	2755/2879 (95%)	587 (21%)	27 (0%)
23	DA	2757/2879 (95%)	593 (21%)	29 (1%)
24	BB	118/119 (99%)	26 (22%)	0
24	DB	118/119 (99%)	27 (22%)	0
All	All	8822/9094 (97%)	1826 (20%)	84 (0%)

5 of 1826 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	6	G
1	AA	7	G
1	AA	9	G
1	AA	13	U
1	AA	14	U

5 of 84 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
23	DA	257	A
23	DA	1609	A
23	DA	479	A
23	DA	1022	G
23	DA	2062	A

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1198 ligands modelled in this entry, 1198 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	AA	1506/1506 (100%)	0.53	90 (5%)	27	21	51, 122, 245, 498	0
1	CA	1506/1506 (100%)	0.55	81 (5%)	31	24	51, 126, 251, 414	0
2	AB	234/234 (100%)	1.07	34 (14%)	6	7	113, 174, 244, 298	0
2	CB	234/234 (100%)	1.12	38 (16%)	4	6	111, 177, 259, 325	0
3	AC	206/206 (100%)	1.08	39 (18%)	3	4	106, 160, 225, 263	0
3	CC	206/206 (100%)	1.06	41 (19%)	3	4	105, 161, 226, 271	0
4	AD	208/208 (100%)	1.62	66 (31%)	1	1	90, 142, 199, 247	0
4	CD	208/208 (100%)	1.77	74 (35%)	1	1	94, 146, 220, 300	0
5	AE	151/151 (100%)	0.78	16 (10%)	11	11	73, 114, 172, 272	0
5	CE	151/151 (100%)	0.69	13 (8%)	16	15	72, 117, 188, 252	0
6	AF	101/101 (100%)	0.96	10 (9%)	13	12	83, 135, 192, 270	0
6	CF	101/101 (100%)	0.80	11 (10%)	10	11	79, 131, 184, 246	0
7	AG	155/155 (100%)	1.11	30 (19%)	3	4	118, 187, 237, 333	0
7	CG	155/155 (100%)	1.20	30 (19%)	3	4	119, 187, 237, 286	0
8	AH	138/138 (100%)	1.12	21 (15%)	5	7	77, 121, 166, 199	0
8	CH	138/138 (100%)	0.91	15 (10%)	10	11	81, 123, 167, 219	0
9	AI	127/127 (100%)	2.14	62 (48%)	0	1	119, 225, 289, 345	0
9	CI	127/127 (100%)	1.83	46 (36%)	1	1	121, 225, 286, 354	0
10	AJ	98/98 (100%)	1.68	36 (36%)	1	1	118, 198, 278, 356	0
10	CJ	98/98 (100%)	1.73	34 (34%)	1	1	122, 197, 264, 351	0
11	AK	119/119 (100%)	0.72	12 (10%)	12	12	71, 111, 171, 263	0
11	CK	119/119 (100%)	0.78	15 (12%)	8	9	74, 111, 178, 264	0
12	AL	124/124 (100%)	1.30	29 (23%)	2	3	67, 107, 165, 268	0
12	CL	124/124 (100%)	1.60	33 (26%)	1	2	70, 109, 178, 252	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
13	AM	116/116 (100%)	1.68	34 (29%)	1 2	134, 213, 299, 335	0
13	CM	116/116 (100%)	1.21	24 (20%)	2 4	135, 214, 309, 362	0
14	AN	60/60 (100%)	1.88	26 (43%)	0 1	114, 166, 217, 235	0
14	CN	60/60 (100%)	2.03	23 (38%)	1 1	116, 167, 227, 281	0
15	AO	88/88 (100%)	0.51	6 (6%)	23 19	66, 108, 159, 227	0
15	CO	88/88 (100%)	0.63	5 (5%)	29 22	67, 110, 166, 241	0
16	AP	83/83 (100%)	1.69	25 (30%)	1 2	84, 118, 174, 214	0
16	CP	83/83 (100%)	1.76	32 (38%)	1 1	87, 123, 177, 210	0
17	AQ	99/99 (100%)	0.86	9 (9%)	15 14	78, 112, 169, 216	0
17	CQ	99/99 (100%)	1.10	12 (12%)	8 9	79, 116, 166, 215	0
18	AR	70/70 (100%)	0.77	6 (8%)	16 15	84, 128, 183, 284	0
18	CR	70/70 (100%)	0.67	3 (4%)	40 29	82, 128, 192, 232	0
19	AS	78/78 (100%)	1.48	20 (25%)	1 3	152, 210, 275, 321	0
19	CS	78/78 (100%)	1.54	22 (28%)	1 2	151, 216, 291, 350	0
20	AT	99/99 (100%)	1.62	28 (28%)	1 2	86, 134, 203, 241	0
20	CT	99/99 (100%)	1.79	26 (26%)	1 3	92, 136, 212, 269	0
21	AU	24/24 (100%)	3.24	18 (75%)	0 0	160, 225, 264, 322	0
21	CU	24/24 (100%)	3.83	21 (87%)	0 0	163, 218, 265, 364	0
22	AV	34/43 (79%)	0.82	3 (8%)	15 14	89, 196, 324, 362	0
22	CV	34/43 (79%)	1.07	6 (17%)	4 5	92, 198, 333, 339	0
23	BA	2760/2879 (95%)	-0.27	31 (1%)	78 65	27, 65, 180, 398	0
23	DA	2760/2879 (95%)	-0.21	40 (1%)	73 59	25, 63, 178, 410	0
24	BB	119/119 (100%)	0.48	11 (9%)	14 14	76, 129, 182, 232	0
24	DB	119/119 (100%)	0.51	10 (8%)	17 15	78, 129, 184, 236	0
25	BC	271/271 (100%)	0.30	20 (7%)	20 17	25, 58, 109, 175	0
25	DC	271/271 (100%)	0.25	14 (5%)	33 24	18, 57, 109, 177	0
26	BD	204/204 (100%)	0.44	12 (5%)	28 22	36, 73, 146, 341	0
26	DD	204/204 (100%)	0.45	19 (9%)	14 14	33, 71, 145, 347	0
27	BE	202/202 (100%)	0.35	7 (3%)	47 34	31, 73, 155, 246	0
27	DE	202/202 (100%)	0.30	6 (2%)	52 39	25, 73, 155, 192	0
28	BF	181/181 (100%)	1.15	32 (17%)	4 5	102, 182, 254, 314	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
28	DF	181/181 (100%)	1.12	31 (17%)	4 5	104, 185, 268, 331	0
29	BG	159/159 (100%)	1.04	21 (13%)	7 8	85, 143, 221, 343	0
29	DG	159/159 (100%)	1.92	60 (37%)	1 1	79, 136, 186, 235	0
30	BH	145/145 (100%)	2.46	77 (53%)	0 0	67, 243, 391, 482	0
30	DH	145/145 (100%)	2.47	69 (47%)	0 1	64, 236, 379, 480	0
31	BI	32/65 (49%)	1.66	12 (37%)	1 1	171, 246, 347, 355	0
31	DI	32/65 (49%)	1.52	8 (25%)	2 3	168, 253, 310, 334	0
32	BJ	137/137 (100%)	0.47	5 (3%)	46 33	51, 81, 142, 201	0
32	DJ	137/137 (100%)	0.51	8 (5%)	29 22	52, 81, 146, 194	0
33	BK	122/122 (100%)	0.14	1 (0%)	82 71	42, 70, 111, 150	0
33	DK	122/122 (100%)	0.13	1 (0%)	82 71	41, 69, 111, 162	0
34	BL	146/146 (100%)	1.07	25 (17%)	4 5	34, 97, 166, 309	0
34	DL	146/146 (100%)	1.26	31 (21%)	2 4	32, 97, 163, 293	0
35	BM	136/136 (100%)	0.80	18 (13%)	7 8	49, 89, 199, 370	0
35	DM	136/136 (100%)	0.94	21 (15%)	5 7	48, 88, 205, 406	0
36	BN	117/117 (100%)	0.62	10 (8%)	16 15	45, 73, 137, 249	0
36	DN	117/117 (100%)	0.62	11 (9%)	14 14	43, 73, 134, 235	0
37	BO	98/98 (100%)	1.34	21 (21%)	2 4	82, 137, 197, 223	0
37	DO	98/98 (100%)	1.44	28 (28%)	1 2	80, 136, 190, 215	0
38	BP	137/137 (100%)	0.64	13 (9%)	14 13	58, 93, 185, 250	0
38	DP	137/137 (100%)	0.90	16 (11%)	9 10	55, 92, 190, 272	0
39	BQ	116/116 (100%)	0.50	13 (11%)	10 11	35, 75, 124, 239	0
39	DQ	116/116 (100%)	0.75	12 (10%)	12 12	26, 74, 126, 248	0
40	BR	101/101 (100%)	0.88	10 (9%)	13 12	41, 105, 164, 264	0
40	DR	101/101 (100%)	1.09	16 (15%)	5 6	41, 110, 156, 259	0
41	BS	112/112 (100%)	0.18	1 (0%)	81 68	44, 59, 137, 254	0
41	DS	112/112 (100%)	0.04	0	100 100	43, 59, 134, 255	0
42	BT	92/92 (100%)	0.68	7 (7%)	20 17	45, 77, 129, 170	0
42	DT	92/92 (100%)	0.80	11 (11%)	9 9	36, 73, 127, 169	0
43	BU	100/100 (100%)	1.83	40 (40%)	1 1	62, 104, 257, 396	0
43	DU	100/100 (100%)	1.41	25 (25%)	2 3	61, 102, 251, 408	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	BV	188/188 (100%)	0.92	23 (12%) 8 9	83, 138, 195, 245	0
44	DV	188/188 (100%)	0.86	21 (11%) 10 11	83, 139, 194, 230	0
45	BW	76/76 (100%)	0.56	8 (10%) 11 12	58, 84, 138, 261	0
45	DW	76/76 (100%)	0.92	11 (14%) 6 7	59, 84, 135, 256	0
46	BX	88/88 (100%)	1.16	18 (20%) 2 4	37, 74, 153, 322	0
46	DX	88/88 (100%)	1.01	11 (12%) 8 9	39, 70, 153, 326	0
47	BY	62/62 (100%)	1.27	13 (20%) 2 4	57, 98, 209, 292	0
47	DY	62/62 (100%)	1.47	14 (22%) 2 4	51, 96, 212, 328	0
48	BZ	59/59 (100%)	0.56	1 (1%) 69 54	43, 81, 156, 299	0
48	DZ	59/59 (100%)	0.73	4 (6%) 23 19	45, 85, 157, 305	0
49	B1	30/30 (100%)	0.71	2 (6%) 24 19	184, 253, 295, 311	0
49	D1	30/30 (100%)	0.74	3 (10%) 12 12	183, 261, 306, 358	0
50	B2	52/52 (100%)	0.45	3 (5%) 29 22	26, 71, 187, 233	0
50	D2	52/52 (100%)	0.48	3 (5%) 29 22	21, 72, 197, 229	0
51	B3	44/44 (100%)	2.06	19 (43%) 0 1	139, 249, 299, 320	0
51	D3	44/44 (100%)	2.27	21 (47%) 0 1	141, 245, 312, 333	0
52	B4	48/48 (100%)	0.42	5 (10%) 11 12	33, 43, 93, 194	0
52	D4	48/48 (100%)	0.23	3 (6%) 26 20	21, 41, 91, 200	0
53	B5	63/63 (100%)	0.78	8 (12%) 8 9	45, 68, 131, 215	0
53	D5	63/63 (100%)	1.07	15 (23%) 2 3	45, 70, 132, 216	0
All	All	20230/20552 (98%)	0.60	2255 (11%) 10 11	18, 104, 241, 498	0

The worst 5 of 2255 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
12	CL	27	LYS	11.4
35	BM	140	ALA	11.1
13	AM	99	ARG	10.8
30	BH	72	LEU	10.8
1	AA	82	U	10.7

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	AA	1762	1/1	-0.03	0.24	155,155,155,155	0
54	MG	DA	3084	1/1	0.11	0.31	146,146,146,146	0
54	MG	BA	3236	1/1	0.25	0.32	119,119,119,119	0
54	MG	DA	3313	1/1	0.25	0.20	107,107,107,107	0
54	MG	CA	1668	1/1	0.30	0.25	116,116,116,116	0
54	MG	BA	3278	1/1	0.31	0.33	115,115,115,115	0
54	MG	CA	1658	1/1	0.33	0.32	110,110,110,110	0
54	MG	CA	1701	1/1	0.35	0.27	112,112,112,112	0
54	MG	DA	3184	1/1	0.36	0.14	117,117,117,117	0
54	MG	DA	3312	1/1	0.39	0.16	66,66,66,66	0
54	MG	AV	6302	1/1	0.44	0.27	121,121,121,121	0
54	MG	CA	1704	1/1	0.46	0.18	108,108,108,108	0
54	MG	AA	1682	1/1	0.48	0.17	85,85,85,85	0
54	MG	BA	3305	1/1	0.48	0.10	103,103,103,103	0
54	MG	BA	3217	1/1	0.49	0.22	111,111,111,111	0
54	MG	DA	3116	1/1	0.50	0.14	115,115,115,115	0
54	MG	DA	3276	1/1	0.51	0.20	128,128,128,128	0
54	MG	CA	1670	1/1	0.51	0.26	128,128,128,128	0
54	MG	DA	3234	1/1	0.51	0.19	130,130,130,130	0
54	MG	CA	1696	1/1	0.52	0.21	133,133,133,133	0
54	MG	CA	1698	1/1	0.55	0.12	117,117,117,117	0
54	MG	DA	3317	1/1	0.55	0.25	97,97,97,97	0
54	MG	CA	1648	1/1	0.56	0.11	64,64,64,64	0
54	MG	AA	1739	1/1	0.57	0.22	129,129,129,129	0
54	MG	CA	1637	1/1	0.58	0.18	112,112,112,112	0
54	MG	DA	3265	1/1	0.58	0.18	120,120,120,120	0
54	MG	BA	3275	1/1	0.58	0.25	87,87,87,87	0
54	MG	CA	1703	1/1	0.59	0.22	108,108,108,108	0
54	MG	BA	3083	1/1	0.60	0.10	87,87,87,87	0
54	MG	BA	3189	1/1	0.60	0.17	88,88,88,88	0
54	MG	DA	2983	1/1	0.60	0.17	70,70,70,70	0
54	MG	BA	3287	1/1	0.60	0.21	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	AA	1728	1/1	0.61	0.26	105,105,105,105	0
54	MG	AA	1754	1/1	0.61	0.18	110,110,110,110	0
54	MG	CA	1730	1/1	0.61	0.12	122,122,122,122	0
54	MG	BA	3271	1/1	0.61	0.20	91,91,91,91	0
54	MG	DA	3235	1/1	0.61	0.28	90,90,90,90	0
54	MG	DA	3212	1/1	0.62	0.36	78,78,78,78	0
54	MG	BA	3061	1/1	0.62	0.16	91,91,91,91	0
54	MG	BA	3272	1/1	0.62	0.10	119,119,119,119	0
54	MG	BA	3079	1/1	0.62	0.23	86,86,86,86	0
54	MG	DA	3278	1/1	0.63	0.25	75,75,75,75	0
54	MG	AA	1718	1/1	0.63	0.32	98,98,98,98	0
54	MG	CA	1650	1/1	0.63	0.11	108,108,108,108	0
54	MG	DA	3163	1/1	0.63	0.14	83,83,83,83	0
54	MG	AA	1706	1/1	0.64	0.07	103,103,103,103	0
54	MG	DA	3269	1/1	0.64	0.35	91,91,91,91	0
54	MG	DA	3284	1/1	0.64	0.23	134,134,134,134	0
54	MG	CA	1617	1/1	0.65	0.24	90,90,90,90	0
54	MG	BA	3006	1/1	0.66	0.28	77,77,77,77	0
54	MG	DA	3311	1/1	0.66	0.13	95,95,95,95	0
54	MG	CA	1688	1/1	0.66	0.23	99,99,99,99	0
54	MG	AA	1761	1/1	0.66	0.16	104,104,104,104	0
54	MG	BA	3157	1/1	0.66	0.15	68,68,68,68	0
54	MG	DB	215	1/1	0.66	0.23	103,103,103,103	0
54	MG	BA	3176	1/1	0.67	0.17	99,99,99,99	0
54	MG	CA	1710	1/1	0.67	0.18	119,119,119,119	0
54	MG	DA	3011	1/1	0.67	0.17	99,99,99,99	0
54	MG	CA	1725	1/1	0.67	0.17	105,105,105,105	0
54	MG	DA	3316	1/1	0.68	0.09	97,97,97,97	0
54	MG	DA	3152	1/1	0.68	0.16	77,77,77,77	0
54	MG	BA	3039	1/1	0.68	0.10	94,94,94,94	0
54	MG	DA	3110	1/1	0.69	0.12	86,86,86,86	0
54	MG	BA	3190	1/1	0.69	0.18	115,115,115,115	0
54	MG	AA	1696	1/1	0.69	0.19	132,132,132,132	0
54	MG	BA	3163	1/1	0.69	0.14	72,72,72,72	0
54	MG	DA	3169	1/1	0.69	0.17	112,112,112,112	0
54	MG	DA	2970	1/1	0.69	0.19	67,67,67,67	0
54	MG	AA	1623	1/1	0.69	0.21	93,93,93,93	0
54	MG	CA	1614	1/1	0.69	0.22	89,89,89,89	0
54	MG	DA	3047	1/1	0.69	0.16	66,66,66,66	0
54	MG	BA	3109	1/1	0.69	0.09	90,90,90,90	0
54	MG	DG	201	1/1	0.69	0.24	101,101,101,101	0
54	MG	DA	3033	1/1	0.70	0.18	101,101,101,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	AA	1669	1/1	0.70	0.21	110,110,110,110	0
54	MG	DA	2938	1/1	0.70	0.29	66,66,66,66	0
54	MG	AA	1643	1/1	0.70	0.14	70,70,70,70	0
54	MG	AA	1734	1/1	0.70	0.16	103,103,103,103	0
54	MG	BB	211	1/1	0.70	0.23	112,112,112,112	0
54	MG	BA	3070	1/1	0.71	0.11	75,75,75,75	0
54	MG	BA	3073	1/1	0.71	0.11	89,89,89,89	0
54	MG	BA	3129	1/1	0.71	0.06	75,75,75,75	0
54	MG	DA	3260	1/1	0.71	0.39	102,102,102,102	0
54	MG	BA	3303	1/1	0.71	0.16	98,98,98,98	0
54	MG	AA	1657	1/1	0.71	0.11	101,101,101,101	0
54	MG	DA	3318	1/1	0.71	0.11	101,101,101,101	0
54	MG	DA	3087	1/1	0.71	0.21	67,67,67,67	0
54	MG	DA	3186	1/1	0.71	0.14	90,90,90,90	0
54	MG	CA	1678	1/1	0.72	0.09	107,107,107,107	0
54	MG	DA	3291	1/1	0.72	0.19	78,78,78,78	0
54	MG	CA	1685	1/1	0.72	0.40	106,106,106,106	0
54	MG	BA	3172	1/1	0.72	0.11	102,102,102,102	0
54	MG	AA	1625	1/1	0.72	0.35	88,88,88,88	0
54	MG	BA	3240	1/1	0.72	0.18	114,114,114,114	0
54	MG	BK	201	1/1	0.72	0.20	91,91,91,91	0
54	MG	DA	2999	1/1	0.72	0.29	76,76,76,76	0
54	MG	BA	3248	1/1	0.72	0.12	77,77,77,77	0
54	MG	BA	3265	1/1	0.72	0.14	80,80,80,80	0
54	MG	AA	1679	1/1	0.73	0.09	78,78,78,78	0
54	MG	AV	6304	1/1	0.73	0.16	118,118,118,118	0
54	MG	DA	3109	1/1	0.73	0.13	54,54,54,54	0
54	MG	CV	6301	1/1	0.73	0.08	98,98,98,98	0
54	MG	AA	1699	1/1	0.73	0.07	91,91,91,91	0
54	MG	DA	3128	1/1	0.73	0.13	114,114,114,114	0
54	MG	DA	2968	1/1	0.73	0.14	56,56,56,56	0
54	MG	BA	3031	1/1	0.73	0.45	87,87,87,87	0
54	MG	DA	2972	1/1	0.73	0.21	47,47,47,47	0
54	MG	BA	3204	1/1	0.73	0.27	74,74,74,74	0
54	MG	BA	3118	1/1	0.73	0.21	109,109,109,109	0
54	MG	AA	1641	1/1	0.73	0.27	85,85,85,85	0
54	MG	AA	1684	1/1	0.73	0.26	95,95,95,95	0
54	MG	AA	1685	1/1	0.73	0.17	106,106,106,106	0
54	MG	DA	3238	1/1	0.73	0.08	58,58,58,58	0
54	MG	DA	3162	1/1	0.74	0.13	143,143,143,143	0
54	MG	DA	3014	1/1	0.74	0.23	69,69,69,69	0
54	MG	CA	1740	1/1	0.74	0.15	117,117,117,117	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	DA	3181	1/1	0.74	0.07	106,106,106,106	0
54	MG	AA	1691	1/1	0.74	0.10	78,78,78,78	0
54	MG	DA	3296	1/1	0.74	0.07	104,104,104,104	0
54	MG	BA	3212	1/1	0.74	0.09	69,69,69,69	0
54	MG	BA	3025	1/1	0.74	0.14	65,65,65,65	0
54	MG	AA	1694	1/1	0.74	0.21	129,129,129,129	0
54	MG	AA	1609	1/1	0.74	0.26	70,70,70,70	0
54	MG	AA	1648	1/1	0.74	0.24	76,76,76,76	0
54	MG	CA	1728	1/1	0.74	0.11	82,82,82,82	0
54	MG	AA	1701	1/1	0.74	0.20	83,83,83,83	0
54	MG	DB	216	1/1	0.74	0.14	88,88,88,88	0
54	MG	DA	3268	1/1	0.74	0.26	81,81,81,81	0
54	MG	AA	1729	1/1	0.75	0.16	75,75,75,75	0
54	MG	BA	3115	1/1	0.75	0.09	91,91,91,91	0
54	MG	BA	3116	1/1	0.75	0.13	85,85,85,85	0
54	MG	DA	3259	1/1	0.75	0.10	108,108,108,108	0
54	MG	BA	3255	1/1	0.75	0.21	57,57,57,57	0
54	MG	AA	1653	1/1	0.75	0.17	89,89,89,89	0
54	MG	BA	3192	1/1	0.75	0.29	52,52,52,52	0
54	MG	BA	3027	1/1	0.75	0.21	62,62,62,62	0
54	MG	DB	211	1/1	0.75	0.08	109,109,109,109	0
54	MG	AA	1700	1/1	0.75	0.08	98,98,98,98	0
54	MG	BA	3213	1/1	0.75	0.20	101,101,101,101	0
54	MG	AA	1650	1/1	0.75	0.25	103,103,103,103	0
54	MG	AA	1745	1/1	0.76	0.07	97,97,97,97	0
54	MG	AA	1665	1/1	0.76	0.17	82,82,82,82	0
54	MG	BA	3058	1/1	0.76	0.11	114,114,114,114	0
54	MG	AA	1646	1/1	0.76	0.23	99,99,99,99	0
54	MG	DA	3147	1/1	0.76	0.18	78,78,78,78	0
54	MG	DA	3253	1/1	0.76	0.11	92,92,92,92	0
54	MG	BA	3283	1/1	0.76	0.09	76,76,76,76	0
54	MG	DA	3042	1/1	0.76	0.31	79,79,79,79	0
54	MG	CA	1672	1/1	0.76	0.09	62,62,62,62	0
54	MG	DB	206	1/1	0.76	0.15	99,99,99,99	0
54	MG	BA	3218	1/1	0.76	0.24	75,75,75,75	0
54	MG	DA	3086	1/1	0.76	0.26	92,92,92,92	0
54	MG	BA	3300	1/1	0.76	0.15	83,83,83,83	0
54	MG	DA	3185	1/1	0.76	0.13	108,108,108,108	0
54	MG	BA	3198	1/1	0.77	0.34	81,81,81,81	0
54	MG	BA	3107	1/1	0.77	0.17	87,87,87,87	0
54	MG	AA	1737	1/1	0.77	0.08	86,86,86,86	0
54	MG	BA	3135	1/1	0.77	0.09	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	DA	3127	1/1	0.77	0.27	90,90,90,90	0
54	MG	AA	1722	1/1	0.77	0.22	83,83,83,83	0
54	MG	DA	3323	1/1	0.77	0.07	69,69,69,69	0
54	MG	BA	3266	1/1	0.77	0.27	98,98,98,98	0
54	MG	DA	3055	1/1	0.77	0.13	93,93,93,93	0
54	MG	CA	1639	1/1	0.77	0.20	66,66,66,66	0
54	MG	AA	1760	1/1	0.77	0.16	84,84,84,84	0
54	MG	DA	3300	1/1	0.77	0.11	68,68,68,68	0
54	MG	CA	1666	1/1	0.78	0.16	116,116,116,116	0
54	MG	DA	3175	1/1	0.78	0.13	81,81,81,81	0
54	MG	DA	3281	1/1	0.78	0.15	73,73,73,73	0
54	MG	DA	3052	1/1	0.78	0.20	107,107,107,107	0
54	MG	BA	2978	1/1	0.78	0.27	59,59,59,59	0
54	MG	BB	212	1/1	0.78	0.06	89,89,89,89	0
54	MG	BB	213	1/1	0.78	0.33	84,84,84,84	0
54	MG	BA	2986	1/1	0.78	0.10	67,67,67,67	0
54	MG	DA	3220	1/1	0.78	0.13	70,70,70,70	0
54	MG	AA	1652	1/1	0.78	0.18	89,89,89,89	0
54	MG	AA	1613	1/1	0.78	0.14	47,47,47,47	0
54	MG	CA	1633	1/1	0.78	0.26	102,102,102,102	0
54	MG	BA	3263	1/1	0.78	0.08	80,80,80,80	0
54	MG	DA	3257	1/1	0.78	0.13	94,94,94,94	0
54	MG	BA	3187	1/1	0.78	0.28	40,40,40,40	0
54	MG	AA	1726	1/1	0.78	0.14	108,108,108,108	0
54	MG	BA	3136	1/1	0.78	0.09	87,87,87,87	0
54	MG	BB	207	1/1	0.78	0.09	105,105,105,105	0
54	MG	CA	1661	1/1	0.78	0.25	92,92,92,92	0
54	MG	CA	1663	1/1	0.79	0.19	86,86,86,86	0
54	MG	BA	3225	1/1	0.79	0.18	74,74,74,74	0
54	MG	BA	3149	1/1	0.79	0.30	82,82,82,82	0
54	MG	DA	3069	1/1	0.79	0.11	81,81,81,81	0
54	MG	AA	1678	1/1	0.79	0.11	115,115,115,115	0
54	MG	BA	3243	1/1	0.79	0.14	82,82,82,82	0
54	MG	BA	3284	1/1	0.79	0.16	85,85,85,85	0
54	MG	DA	3224	1/1	0.79	0.26	72,72,72,72	0
54	MG	CA	1628	1/1	0.79	0.12	100,100,100,100	0
54	MG	BA	3158	1/1	0.79	0.12	105,105,105,105	0
54	MG	BA	3117	1/1	0.79	0.26	77,77,77,77	0
54	MG	DA	3244	1/1	0.79	0.14	87,87,87,87	0
54	MG	BA	3103	1/1	0.79	0.12	88,88,88,88	0
54	MG	BA	3036	1/1	0.79	0.12	92,92,92,92	0
54	MG	AD	302	1/1	0.79	0.11	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	BB	208	1/1	0.79	0.15	109,109,109,109	0
54	MG	DA	3017	1/1	0.79	0.17	93,93,93,93	0
54	MG	AA	1647	1/1	0.79	0.12	85,85,85,85	0
54	MG	CA	1723	1/1	0.79	0.19	141,141,141,141	0
54	MG	DA	3091	1/1	0.80	0.08	125,125,125,125	0
54	MG	DA	3094	1/1	0.80	0.09	76,76,76,76	0
54	MG	AA	1612	1/1	0.80	0.16	64,64,64,64	0
54	MG	BA	3009	1/1	0.80	0.12	87,87,87,87	0
54	MG	AA	1618	1/1	0.80	0.19	91,91,91,91	0
54	MG	AA	1622	1/1	0.80	0.32	88,88,88,88	0
54	MG	CA	1675	1/1	0.80	0.25	107,107,107,107	0
54	MG	DA	3271	1/1	0.80	0.07	97,97,97,97	0
54	MG	DA	3141	1/1	0.80	0.06	95,95,95,95	0
54	MG	BA	3080	1/1	0.80	0.10	73,73,73,73	0
54	MG	CA	1684	1/1	0.80	0.07	117,117,117,117	0
54	MG	BA	3150	1/1	0.80	0.06	79,79,79,79	0
54	MG	BA	3152	1/1	0.80	0.09	75,75,75,75	0
54	MG	CA	1689	1/1	0.80	0.21	83,83,83,83	0
54	MG	BA	3281	1/1	0.80	0.15	84,84,84,84	0
54	MG	DA	3307	1/1	0.80	0.13	73,73,73,73	0
54	MG	DA	3178	1/1	0.80	0.14	83,83,83,83	0
54	MG	AA	1755	1/1	0.80	0.14	103,103,103,103	0
54	MG	DA	3022	1/1	0.80	0.18	60,60,60,60	0
54	MG	AA	1735	1/1	0.80	0.06	104,104,104,104	0
54	MG	BA	3037	1/1	0.80	0.11	93,93,93,93	0
54	MG	BA	3038	1/1	0.80	0.15	65,65,65,65	0
54	MG	DA	3319	1/1	0.80	0.06	83,83,83,83	0
54	MG	CA	1708	1/1	0.80	0.10	143,143,143,143	0
54	MG	BA	3302	1/1	0.80	0.08	121,121,121,121	0
54	MG	CA	1718	1/1	0.80	0.09	78,78,78,78	0
54	MG	DB	214	1/1	0.80	0.15	90,90,90,90	0
54	MG	AA	1702	1/1	0.80	0.35	94,94,94,94	0
54	MG	BA	3004	1/1	0.80	0.28	74,74,74,74	0
54	MG	BA	3059	1/1	0.80	0.14	60,60,60,60	0
54	MG	D2	101	1/1	0.80	0.22	66,66,66,66	0
54	MG	BA	3114	1/1	0.81	0.25	78,78,78,78	0
54	MG	CA	1713	1/1	0.81	0.07	80,80,80,80	0
54	MG	DA	3103	1/1	0.81	0.24	79,79,79,79	0
54	MG	DA	3286	1/1	0.81	0.06	98,98,98,98	0
54	MG	AA	1621	1/1	0.81	0.35	74,74,74,74	0
54	MG	AA	1644	1/1	0.81	0.19	53,53,53,53	0
54	MG	DA	3299	1/1	0.81	0.15	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	AA	1752	1/1	0.81	0.26	81,81,81,81	0
54	MG	DA	3305	1/1	0.81	0.10	110,110,110,110	0
54	MG	DA	3230	1/1	0.81	0.11	63,63,63,63	0
54	MG	CA	1687	1/1	0.81	0.17	64,64,64,64	0
54	MG	BA	3049	1/1	0.81	0.18	86,86,86,86	0
54	MG	BA	3119	1/1	0.81	0.15	64,64,64,64	0
54	MG	DA	3143	1/1	0.81	0.07	77,77,77,77	0
54	MG	CA	1662	1/1	0.81	0.23	86,86,86,86	0
54	MG	BA	3219	1/1	0.81	0.23	66,66,66,66	0
54	MG	DA	3066	1/1	0.81	0.36	85,85,85,85	0
54	MG	AA	1724	1/1	0.81	0.13	85,85,85,85	0
54	MG	DA	3264	1/1	0.81	0.16	61,61,61,61	0
54	MG	DA	3166	1/1	0.81	0.15	87,87,87,87	0
54	MG	DA	3074	1/1	0.81	0.16	64,64,64,64	0
54	MG	CA	1623	1/1	0.81	0.25	99,99,99,99	0
54	MG	BA	3226	1/1	0.81	0.11	81,81,81,81	0
54	MG	DA	3272	1/1	0.81	0.22	41,41,41,41	0
54	MG	BA	3229	1/1	0.81	0.21	62,62,62,62	0
54	MG	AA	1634	1/1	0.82	0.13	70,70,70,70	0
54	MG	DA	3267	1/1	0.82	0.13	76,76,76,76	0
54	MG	AA	1763	1/1	0.82	0.20	96,96,96,96	0
54	MG	BB	206	1/1	0.82	0.07	70,70,70,70	0
54	MG	CA	1706	1/1	0.82	0.30	101,101,101,101	0
54	MG	AA	1649	1/1	0.82	0.15	89,89,89,89	0
54	MG	AV	6301	1/1	0.82	0.07	72,72,72,72	0
54	MG	BB	210	1/1	0.82	0.18	100,100,100,100	0
54	MG	DA	3280	1/1	0.82	0.16	84,84,84,84	0
54	MG	DA	3170	1/1	0.82	0.10	80,80,80,80	0
54	MG	BA	3022	1/1	0.82	0.27	77,77,77,77	0
54	MG	AA	1693	1/1	0.82	0.12	74,74,74,74	0
54	MG	CA	1724	1/1	0.82	0.09	74,74,74,74	0
54	MG	BA	3026	1/1	0.82	0.11	82,82,82,82	0
54	MG	DA	3080	1/1	0.82	0.11	69,69,69,69	0
54	MG	BB	214	1/1	0.82	0.20	101,101,101,101	0
54	MG	DA	3187	1/1	0.82	0.22	90,90,90,90	0
54	MG	DA	3200	1/1	0.82	0.14	87,87,87,87	0
54	MG	DA	3209	1/1	0.82	0.29	80,80,80,80	0
54	MG	AA	1632	1/1	0.82	0.22	68,68,68,68	0
54	MG	BA	3067	1/1	0.82	0.11	86,86,86,86	0
54	MG	CP	101	1/1	0.82	0.09	96,96,96,96	0
54	MG	CA	1681	1/1	0.82	0.17	81,81,81,81	0
54	MG	BA	3170	1/1	0.82	0.08	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	DA	3105	1/1	0.82	0.18	75,75,75,75	0
54	MG	DA	3322	1/1	0.82	0.11	95,95,95,95	0
54	MG	CA	1621	1/1	0.82	0.21	67,67,67,67	0
54	MG	AA	1732	1/1	0.82	0.09	63,63,63,63	0
54	MG	DA	3246	1/1	0.82	0.27	67,67,67,67	0
54	MG	BA	3175	1/1	0.82	0.08	85,85,85,85	0
54	MG	DA	3119	1/1	0.82	0.15	88,88,88,88	0
54	MG	BA	3032	1/1	0.82	0.26	59,59,59,59	0
54	MG	BA	3075	1/1	0.82	0.12	67,67,67,67	0
54	MG	BA	3121	1/1	0.82	0.05	77,77,77,77	0
54	MG	DA	2924	1/1	0.83	0.24	41,41,41,41	0
54	MG	DA	3072	1/1	0.83	0.12	73,73,73,73	0
54	MG	CA	1647	1/1	0.83	0.24	77,77,77,77	0
54	MG	DA	2940	1/1	0.83	0.27	51,51,51,51	0
54	MG	BA	3112	1/1	0.83	0.07	68,68,68,68	0
54	MG	DA	3182	1/1	0.83	0.13	86,86,86,86	0
54	MG	BA	3258	1/1	0.83	0.11	104,104,104,104	0
54	MG	DA	2971	1/1	0.83	0.30	47,47,47,47	0
54	MG	CA	1652	1/1	0.83	0.15	85,85,85,85	0
54	MG	DA	3290	1/1	0.83	0.11	85,85,85,85	0
54	MG	CA	1717	1/1	0.83	0.22	84,84,84,84	0
54	MG	DA	3097	1/1	0.83	0.18	94,94,94,94	0
54	MG	DA	3298	1/1	0.83	0.18	79,79,79,79	0
54	MG	AA	1614	1/1	0.83	0.31	85,85,85,85	0
54	MG	DA	3104	1/1	0.83	0.07	99,99,99,99	0
54	MG	CA	1660	1/1	0.83	0.07	100,100,100,100	0
54	MG	AA	1733	1/1	0.83	0.10	91,91,91,91	0
54	MG	BA	3285	1/1	0.83	0.07	87,87,87,87	0
54	MG	DA	3113	1/1	0.83	0.09	71,71,71,71	0
54	MG	DA	3021	1/1	0.83	0.12	67,67,67,67	0
54	MG	DA	3236	1/1	0.83	0.23	63,63,63,63	0
54	MG	CA	1627	1/1	0.83	0.09	67,67,67,67	0
54	MG	DA	3242	1/1	0.83	0.27	96,96,96,96	0
54	MG	DA	3028	1/1	0.83	0.18	78,78,78,78	0
54	MG	DA	3029	1/1	0.83	0.08	70,70,70,70	0
54	MG	DA	3136	1/1	0.83	0.17	68,68,68,68	0
54	MG	AA	1757	1/1	0.83	0.08	89,89,89,89	0
54	MG	CA	1736	1/1	0.83	0.18	115,115,115,115	0
54	MG	CA	1739	1/1	0.83	0.07	99,99,99,99	0
54	MG	BA	3160	1/1	0.83	0.07	106,106,106,106	0
54	MG	AA	1629	1/1	0.83	0.34	72,72,72,72	0
54	MG	DA	3060	1/1	0.83	0.10	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	AA	1637	1/1	0.83	0.25	61,61,61,61	0
54	MG	BA	2996	1/1	0.84	0.17	54,54,54,54	0
54	MG	DA	3222	1/1	0.84	0.23	70,70,70,70	0
54	MG	DA	3134	1/1	0.84	0.11	71,71,71,71	0
54	MG	CA	1646	1/1	0.84	0.07	78,78,78,78	0
54	MG	AA	1631	1/1	0.84	0.17	70,70,70,70	0
54	MG	DA	3085	1/1	0.84	0.10	89,89,89,89	0
54	MG	AA	1645	1/1	0.84	0.24	79,79,79,79	0
54	MG	AA	1673	1/1	0.84	0.08	61,61,61,61	0
54	MG	DA	3154	1/1	0.84	0.35	94,94,94,94	0
54	MG	BA	3011	1/1	0.84	0.12	83,83,83,83	0
54	MG	BA	3165	1/1	0.84	0.14	71,71,71,71	0
54	MG	DA	3251	1/1	0.84	0.22	63,63,63,63	0
54	MG	CA	1711	1/1	0.84	0.17	87,87,87,87	0
54	MG	DA	3101	1/1	0.84	0.21	72,72,72,72	0
54	MG	DA	3258	1/1	0.84	0.23	72,72,72,72	0
54	MG	AA	1750	1/1	0.84	0.09	109,109,109,109	0
54	MG	AA	1758	1/1	0.84	0.06	73,73,73,73	0
54	MG	BA	3299	1/1	0.84	0.15	80,80,80,80	0
54	MG	DA	3320	1/1	0.84	0.17	58,58,58,58	0
54	MG	CA	1636	1/1	0.84	0.12	93,93,93,93	0
54	MG	BA	3207	1/1	0.84	0.25	94,94,94,94	0
54	MG	CA	1697	1/1	0.84	0.17	74,74,74,74	0
54	MG	DA	3115	1/1	0.84	0.12	65,65,65,65	0
54	MG	CA	1727	1/1	0.84	0.12	75,75,75,75	0
54	MG	DA	2987	1/1	0.84	0.22	70,70,70,70	0
54	MG	DA	3120	1/1	0.84	0.22	66,66,66,66	0
54	MG	DA	3122	1/1	0.84	0.12	87,87,87,87	0
54	MG	DA	2991	1/1	0.84	0.12	31,31,31,31	0
54	MG	BA	3124	1/1	0.85	0.09	89,89,89,89	0
54	MG	BB	216	1/1	0.85	0.14	79,79,79,79	0
54	MG	AA	1714	1/1	0.85	0.28	58,58,58,58	0
54	MG	DA	3256	1/1	0.85	0.14	82,82,82,82	0
54	MG	CA	1601	1/1	0.85	0.33	53,53,53,53	0
54	MG	CA	1606	1/1	0.85	0.20	68,68,68,68	0
54	MG	CA	1607	1/1	0.85	0.17	52,52,52,52	0
54	MG	BA	2994	1/1	0.85	0.21	56,56,56,56	0
54	MG	DA	3263	1/1	0.85	0.18	63,63,63,63	0
54	MG	DA	2986	1/1	0.85	0.12	55,55,55,55	0
54	MG	CA	1616	1/1	0.85	0.13	75,75,75,75	0
54	MG	AA	1651	1/1	0.85	0.17	97,97,97,97	0
54	MG	CA	1693	1/1	0.85	0.17	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	CA	1694	1/1	0.85	0.17	59,59,59,59	0
54	MG	DA	3013	1/1	0.85	0.13	44,44,44,44	0
54	MG	DA	3142	1/1	0.85	0.17	109,109,109,109	0
54	MG	CA	1620	1/1	0.85	0.14	79,79,79,79	0
54	MG	BA	3145	1/1	0.85	0.06	67,67,67,67	0
54	MG	BA	3096	1/1	0.85	0.16	65,65,65,65	0
54	MG	CA	1699	1/1	0.85	0.20	71,71,71,71	0
54	MG	AA	1677	1/1	0.85	0.11	64,64,64,64	0
54	MG	AA	1667	1/1	0.85	0.34	61,61,61,61	0
54	MG	AA	1741	1/1	0.85	0.12	74,74,74,74	0
54	MG	BA	3054	1/1	0.85	0.12	46,46,46,46	0
54	MG	AA	1610	1/1	0.85	0.18	78,78,78,78	0
54	MG	CA	1709	1/1	0.85	0.33	81,81,81,81	0
54	MG	BA	3291	1/1	0.85	0.10	68,68,68,68	0
54	MG	DA	3180	1/1	0.85	0.08	77,77,77,77	0
54	MG	CA	1645	1/1	0.85	0.16	72,72,72,72	0
54	MG	DA	3064	1/1	0.85	0.20	80,80,80,80	0
54	MG	BA	3294	1/1	0.85	0.12	64,64,64,64	0
54	MG	BA	3222	1/1	0.85	0.48	91,91,91,91	0
54	MG	BA	3162	1/1	0.85	0.15	94,94,94,94	0
54	MG	DA	3315	1/1	0.85	0.17	52,52,52,52	0
54	MG	BA	3017	1/1	0.85	0.20	69,69,69,69	0
54	MG	AA	1749	1/1	0.85	0.11	90,90,90,90	0
54	MG	AA	1680	1/1	0.85	0.13	90,90,90,90	0
54	MG	BA	3238	1/1	0.85	0.16	91,91,91,91	0
54	MG	AA	1681	1/1	0.85	0.15	99,99,99,99	0
54	MG	BA	3173	1/1	0.85	0.19	80,80,80,80	0
54	MG	DA	3089	1/1	0.85	0.10	76,76,76,76	0
54	MG	CA	1733	1/1	0.85	0.05	72,72,72,72	0
54	MG	BA	3174	1/1	0.85	0.11	84,84,84,84	0
54	MG	CA	1664	1/1	0.85	0.19	82,82,82,82	0
54	MG	CA	1665	1/1	0.85	0.16	89,89,89,89	0
54	MG	AA	1707	1/1	0.85	0.09	100,100,100,100	0
54	MG	AA	1712	1/1	0.85	0.25	75,75,75,75	0
54	MG	BA	3123	1/1	0.85	0.13	52,52,52,52	0
54	MG	BA	3034	1/1	0.86	0.38	102,102,102,102	0
54	MG	DA	3106	1/1	0.86	0.17	67,67,67,67	0
54	MG	DA	3274	1/1	0.86	0.12	62,62,62,62	0
54	MG	DA	3275	1/1	0.86	0.16	78,78,78,78	0
54	MG	CA	1622	1/1	0.86	0.16	79,79,79,79	0
54	MG	BB	209	1/1	0.86	0.14	83,83,83,83	0
54	MG	BA	3060	1/1	0.86	0.23	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	DA	3199	1/1	0.86	0.36	38,38,38,38	0
54	MG	CA	1667	1/1	0.86	0.07	67,67,67,67	0
54	MG	BA	3019	1/1	0.86	0.18	58,58,58,58	0
54	MG	DA	3287	1/1	0.86	0.11	69,69,69,69	0
54	MG	DA	2939	1/1	0.86	0.22	40,40,40,40	0
54	MG	BA	3066	1/1	0.86	0.19	56,56,56,56	0
54	MG	AA	1687	1/1	0.86	0.10	73,73,73,73	0
54	MG	DA	3297	1/1	0.86	0.15	49,49,49,49	0
54	MG	AA	1738	1/1	0.86	0.17	70,70,70,70	0
54	MG	BA	3072	1/1	0.86	0.11	67,67,67,67	0
54	MG	DA	3129	1/1	0.86	0.13	63,63,63,63	0
54	MG	DA	3302	1/1	0.86	0.18	77,77,77,77	0
54	MG	BB	217	1/1	0.86	0.08	78,78,78,78	0
54	MG	BA	3295	1/1	0.86	0.32	70,70,70,70	0
54	MG	DA	3078	1/1	0.86	0.08	79,79,79,79	0
54	MG	AA	1639	1/1	0.86	0.18	79,79,79,79	0
54	MG	DA	3243	1/1	0.86	0.12	72,72,72,72	0
54	MG	CA	1686	1/1	0.86	0.26	60,60,60,60	0
54	MG	AA	1713	1/1	0.86	0.16	93,93,93,93	0
54	MG	AA	1723	1/1	0.86	0.17	81,81,81,81	0
54	MG	DA	3153	1/1	0.86	0.06	85,85,85,85	0
54	MG	CA	1726	1/1	0.86	0.11	87,87,87,87	0
54	MG	DA	3012	1/1	0.86	0.11	45,45,45,45	0
54	MG	CA	1610	1/1	0.86	0.15	77,77,77,77	0
54	MG	DA	3092	1/1	0.86	0.12	98,98,98,98	0
54	MG	DB	203	1/1	0.86	0.20	82,82,82,82	0
54	MG	BA	3184	1/1	0.86	0.19	42,42,42,42	0
54	MG	DA	3095	1/1	0.86	0.14	67,67,67,67	0
54	MG	DB	212	1/1	0.86	0.10	70,70,70,70	0
54	MG	BA	3185	1/1	0.86	0.27	56,56,56,56	0
54	MG	DA	3176	1/1	0.86	0.18	83,83,83,83	0
54	MG	AA	1747	1/1	0.86	0.27	75,75,75,75	0
54	MG	BA	3082	1/1	0.86	0.10	61,61,61,61	0
54	MG	DA	3025	1/1	0.86	0.16	69,69,69,69	0
54	MG	DA	3273	1/1	0.87	0.15	85,85,85,85	0
54	MG	DA	2994	1/1	0.87	0.16	67,67,67,67	0
54	MG	BA	2905	1/1	0.87	0.19	12,12,12,12	0
54	MG	DA	3002	1/1	0.87	0.17	59,59,59,59	0
54	MG	CA	1626	1/1	0.87	0.16	65,65,65,65	0
54	MG	DA	3279	1/1	0.87	0.10	88,88,88,88	0
54	MG	CA	1715	1/1	0.87	0.17	74,74,74,74	0
54	MG	CA	1671	1/1	0.87	0.08	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	BA	2935	1/1	0.87	0.24	34,34,34,34	0
54	MG	DA	3193	1/1	0.87	0.19	51,51,51,51	0
54	MG	CA	1722	1/1	0.87	0.21	108,108,108,108	0
54	MG	CA	1673	1/1	0.87	0.08	73,73,73,73	0
54	MG	BA	2949	1/1	0.87	0.17	47,47,47,47	0
54	MG	CA	1630	1/1	0.87	0.18	70,70,70,70	0
54	MG	CA	1632	1/1	0.87	0.14	79,79,79,79	0
54	MG	AA	1748	1/1	0.87	0.10	96,96,96,96	0
54	MG	AA	1746	1/1	0.87	0.19	100,100,100,100	0
54	MG	BA	3090	1/1	0.87	0.15	69,69,69,69	0
54	MG	BA	3094	1/1	0.87	0.14	70,70,70,70	0
54	MG	BA	2992	1/1	0.87	0.21	70,70,70,70	0
54	MG	BA	3293	1/1	0.87	0.08	86,86,86,86	0
54	MG	DA	3130	1/1	0.87	0.11	82,82,82,82	0
54	MG	BA	3122	1/1	0.87	0.10	101,101,101,101	0
54	MG	BA	3098	1/1	0.87	0.16	78,78,78,78	0
54	MG	DA	3138	1/1	0.87	0.08	70,70,70,70	0
54	MG	DA	3065	1/1	0.87	0.14	56,56,56,56	0
54	MG	BA	3298	1/1	0.87	0.16	74,74,74,74	0
54	MG	BA	3042	1/1	0.87	0.09	90,90,90,90	0
54	MG	BA	3106	1/1	0.87	0.10	70,70,70,70	0
54	MG	CA	1612	1/1	0.87	0.24	58,58,58,58	0
54	MG	CA	1700	1/1	0.87	0.15	65,65,65,65	0
54	MG	DA	2941	1/1	0.87	0.19	37,37,37,37	0
54	MG	DA	3334	1/1	0.87	0.06	72,72,72,72	0
54	MG	DB	202	1/1	0.87	0.32	64,64,64,64	0
54	MG	BA	3030	1/1	0.87	0.16	57,57,57,57	0
54	MG	BA	3270	1/1	0.87	0.10	61,61,61,61	0
54	MG	BA	3014	1/1	0.87	0.15	47,47,47,47	0
54	MG	DA	3168	1/1	0.87	0.17	94,94,94,94	0
54	MG	CA	1705	1/1	0.87	0.08	54,54,54,54	0
54	MG	CA	1618	1/1	0.87	0.33	63,63,63,63	0
54	MG	BA	3308	1/1	0.87	0.09	94,94,94,94	0
54	MG	BA	3110	1/1	0.87	0.09	86,86,86,86	0
54	MG	BA	3274	1/1	0.87	0.15	78,78,78,78	0
54	MG	AA	1616	1/1	0.88	0.21	63,63,63,63	0
54	MG	BA	2990	1/1	0.88	0.11	54,54,54,54	0
54	MG	BA	3304	1/1	0.88	0.10	124,124,124,124	0
54	MG	AA	1624	1/1	0.88	0.26	67,67,67,67	0
54	MG	BA	3215	1/1	0.88	0.34	68,68,68,68	0
54	MG	BB	205	1/1	0.88	0.10	71,71,71,71	0
54	MG	DA	2993	1/1	0.88	0.16	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	AA	1688	1/1	0.88	0.07	68,68,68,68	0
54	MG	BA	2912	1/1	0.88	0.29	36,36,36,36	0
54	MG	DA	3098	1/1	0.88	0.20	71,71,71,71	0
54	MG	BA	3143	1/1	0.88	0.18	84,84,84,84	0
54	MG	CA	1674	1/1	0.88	0.13	74,74,74,74	0
54	MG	AA	1620	1/1	0.88	0.18	56,56,56,56	0
54	MG	CA	1676	1/1	0.88	0.14	82,82,82,82	0
54	MG	BA	3279	1/1	0.88	0.11	77,77,77,77	0
54	MG	DA	3292	1/1	0.88	0.23	33,33,33,33	0
54	MG	DA	3295	1/1	0.88	0.09	63,63,63,63	0
54	MG	BA	3178	1/1	0.88	0.12	72,72,72,72	0
54	MG	BA	2939	1/1	0.88	0.21	26,26,26,26	0
54	MG	AA	1731	1/1	0.88	0.13	76,76,76,76	0
54	MG	DA	3024	1/1	0.88	0.14	36,36,36,36	0
54	MG	BA	2960	1/1	0.88	0.19	40,40,40,40	0
54	MG	DA	3226	1/1	0.88	0.10	80,80,80,80	0
54	MG	DA	3118	1/1	0.88	0.27	62,62,62,62	0
54	MG	BA	3286	1/1	0.88	0.11	67,67,67,67	0
54	MG	DA	3310	1/1	0.88	0.08	52,52,52,52	0
54	MG	BA	2971	1/1	0.88	0.29	65,65,65,65	0
54	MG	DA	3030	1/1	0.88	0.23	71,71,71,71	0
54	MG	BA	3288	1/1	0.88	0.13	62,62,62,62	0
54	MG	DA	3037	1/1	0.88	0.14	77,77,77,77	0
54	MG	CA	1692	1/1	0.88	0.22	78,78,78,78	0
54	MG	AA	1692	1/1	0.88	0.20	84,84,84,84	0
54	MG	DA	3051	1/1	0.88	0.10	89,89,89,89	0
54	MG	BA	3097	1/1	0.88	0.15	53,53,53,53	0
54	MG	CA	1651	1/1	0.88	0.13	99,99,99,99	0
54	MG	DA	3254	1/1	0.88	0.11	79,79,79,79	0
54	MG	BA	3194	1/1	0.88	0.25	45,45,45,45	0
54	MG	DA	3326	1/1	0.88	0.05	85,85,85,85	0
54	MG	DA	3329	1/1	0.88	0.24	69,69,69,69	0
54	MG	DA	2929	1/1	0.88	0.22	39,39,39,39	0
54	MG	CA	1656	1/1	0.88	0.06	79,79,79,79	0
54	MG	CA	1608	1/1	0.88	0.20	61,61,61,61	0
54	MG	BA	3252	1/1	0.88	0.15	92,92,92,92	0
54	MG	DB	209	1/1	0.88	0.07	75,75,75,75	0
54	MG	DA	3262	1/1	0.88	0.16	82,82,82,82	0
54	MG	DA	3070	1/1	0.88	0.20	70,70,70,70	0
54	MG	BA	3069	1/1	0.88	0.12	109,109,109,109	0
54	MG	DA	2942	1/1	0.88	0.23	39,39,39,39	0
54	MG	DA	2966	1/1	0.88	0.23	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	BA	3199	1/1	0.88	0.24	68,68,68,68	0
54	MG	BA	3100	1/1	0.88	0.07	77,77,77,77	0
54	MG	DA	2932	1/1	0.89	0.21	38,38,38,38	0
54	MG	BA	2945	1/1	0.89	0.20	72,72,72,72	0
54	MG	BA	3108	1/1	0.89	0.20	99,99,99,99	0
54	MG	BA	3250	1/1	0.89	0.11	95,95,95,95	0
54	MG	DA	3282	1/1	0.89	0.08	96,96,96,96	0
54	MG	DA	3198	1/1	0.89	0.19	26,26,26,26	0
54	MG	BA	3289	1/1	0.89	0.16	65,65,65,65	0
54	MG	DA	3043	1/1	0.89	0.11	70,70,70,70	0
54	MG	DA	3289	1/1	0.89	0.07	92,92,92,92	0
54	MG	AA	1642	1/1	0.89	0.25	97,97,97,97	0
54	MG	DA	2953	1/1	0.89	0.21	58,58,58,58	0
54	MG	DA	2959	1/1	0.89	0.26	56,56,56,56	0
54	MG	DA	3221	1/1	0.89	0.09	68,68,68,68	0
54	MG	BA	3253	1/1	0.89	0.12	76,76,76,76	0
54	MG	DA	3125	1/1	0.89	0.18	81,81,81,81	0
54	MG	CA	1640	1/1	0.89	0.19	69,69,69,69	0
54	MG	DA	3063	1/1	0.89	0.15	79,79,79,79	0
54	MG	CA	1641	1/1	0.89	0.06	85,85,85,85	0
54	MG	CA	1644	1/1	0.89	0.22	77,77,77,77	0
54	MG	DA	3131	1/1	0.89	0.12	66,66,66,66	0
54	MG	CA	1680	1/1	0.89	0.23	58,58,58,58	0
54	MG	AA	1640	1/1	0.89	0.28	106,106,106,106	0
54	MG	BA	3084	1/1	0.89	0.19	51,51,51,51	0
54	MG	BA	2916	1/1	0.89	0.32	38,38,38,38	0
54	MG	BA	3093	1/1	0.89	0.23	83,83,83,83	0
54	MG	DA	3249	1/1	0.89	0.10	56,56,56,56	0
54	MG	BA	3050	1/1	0.89	0.05	41,41,41,41	0
54	MG	BA	3267	1/1	0.89	0.25	86,86,86,86	0
54	MG	BA	3071	1/1	0.89	0.16	72,72,72,72	0
54	MG	BA	3154	1/1	0.89	0.07	89,89,89,89	0
54	MG	DA	3004	1/1	0.89	0.21	67,67,67,67	0
54	MG	DA	3157	1/1	0.89	0.16	71,71,71,71	0
54	MG	DA	3161	1/1	0.89	0.07	74,74,74,74	0
54	MG	DA	3325	1/1	0.89	0.15	92,92,92,92	0
54	MG	DA	3006	1/1	0.89	0.09	74,74,74,74	0
54	MG	BA	3003	1/1	0.89	0.09	48,48,48,48	0
54	MG	AA	1666	1/1	0.89	0.11	100,100,100,100	0
54	MG	DA	3336	1/1	0.89	0.15	89,89,89,89	0
54	MG	BA	3024	1/1	0.89	0.20	67,67,67,67	0
54	MG	CA	1737	1/1	0.89	0.09	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	BA	3191	1/1	0.89	0.13	76,76,76,76	0
54	MG	DB	207	1/1	0.89	0.12	72,72,72,72	0
54	MG	DA	3173	1/1	0.89	0.09	97,97,97,97	0
54	MG	DA	3018	1/1	0.89	0.13	73,73,73,73	0
54	MG	BA	3230	1/1	0.89	0.29	44,44,44,44	0
54	MG	DA	3100	1/1	0.89	0.11	59,59,59,59	0
54	MG	BA	3232	1/1	0.89	0.24	24,24,24,24	0
54	MG	BA	3077	1/1	0.89	0.17	75,75,75,75	0
54	MG	DB	217	1/1	0.89	0.04	74,74,74,74	0
54	MG	BA	3193	1/1	0.89	0.15	53,53,53,53	0
54	MG	AA	1697	1/1	0.89	0.07	80,80,80,80	0
54	MG	AA	1664	1/1	0.90	0.07	103,103,103,103	0
54	MG	DA	3231	1/1	0.90	0.33	60,60,60,60	0
54	MG	AA	1606	1/1	0.90	0.25	53,53,53,53	0
54	MG	DA	3150	1/1	0.90	0.08	62,62,62,62	0
54	MG	BA	2914	1/1	0.90	0.23	31,31,31,31	0
54	MG	BA	3166	1/1	0.90	0.08	74,74,74,74	0
54	MG	BA	3148	1/1	0.90	0.11	68,68,68,68	0
54	MG	DA	3099	1/1	0.90	0.15	81,81,81,81	0
54	MG	BA	2963	1/1	0.90	0.18	54,54,54,54	0
54	MG	AA	1753	1/1	0.90	0.09	102,102,102,102	0
54	MG	CA	1625	1/1	0.90	0.10	94,94,94,94	0
54	MG	BA	3280	1/1	0.90	0.09	70,70,70,70	0
54	MG	DA	3054	1/1	0.90	0.12	75,75,75,75	0
54	MG	BA	3301	1/1	0.90	0.16	66,66,66,66	0
54	MG	DA	3057	1/1	0.90	0.12	59,59,59,59	0
54	MG	DA	2998	1/1	0.90	0.12	68,68,68,68	0
54	MG	DA	3314	1/1	0.90	0.25	102,102,102,102	0
54	MG	AA	1705	1/1	0.90	0.06	92,92,92,92	0
54	MG	DA	2904	1/1	0.90	0.28	4,4,4,4	0
54	MG	AA	1720	1/1	0.90	0.15	69,69,69,69	0
54	MG	DA	3179	1/1	0.90	0.05	68,68,68,68	0
54	MG	DA	3117	1/1	0.90	0.17	87,87,87,87	0
54	MG	BA	3259	1/1	0.90	0.12	75,75,75,75	0
54	MG	BA	3101	1/1	0.90	0.20	75,75,75,75	0
54	MG	DA	2934	1/1	0.90	0.21	25,25,25,25	0
54	MG	DA	3121	1/1	0.90	0.08	69,69,69,69	0
54	MG	CA	1716	1/1	0.90	0.13	77,77,77,77	0
54	MG	BA	3133	1/1	0.90	0.22	67,67,67,67	0
54	MG	DA	3076	1/1	0.90	0.12	63,63,63,63	0
54	MG	BB	202	1/1	0.90	0.13	75,75,75,75	0
54	MG	CA	1720	1/1	0.90	0.12	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	DA	3020	1/1	0.90	0.15	63,63,63,63	0
54	MG	DA	3205	1/1	0.90	0.17	48,48,48,48	0
54	MG	DA	3207	1/1	0.90	0.13	42,42,42,42	0
54	MG	CA	1638	1/1	0.90	0.07	65,65,65,65	0
54	MG	BB	203	1/1	0.90	0.11	83,83,83,83	0
54	MG	DA	3215	1/1	0.90	0.29	39,39,39,39	0
54	MG	BA	3008	1/1	0.90	0.14	57,57,57,57	0
54	MG	DA	2965	1/1	0.90	0.20	57,57,57,57	0
54	MG	DA	3285	1/1	0.90	0.19	113,113,113,113	0
54	MG	DA	3140	1/1	0.90	0.10	67,67,67,67	0
54	MG	DA	3090	1/1	0.90	0.07	71,71,71,71	0
54	MG	BA	3209	1/1	0.90	0.18	69,69,69,69	0
54	MG	BA	3220	1/1	0.91	0.14	56,56,56,56	0
54	MG	AA	1756	1/1	0.91	0.21	106,106,106,106	0
54	MG	BA	3035	1/1	0.91	0.07	44,44,44,44	0
54	MG	CA	1611	1/1	0.91	0.15	76,76,76,76	0
54	MG	AA	1744	1/1	0.91	0.07	82,82,82,82	0
54	MG	DA	3177	1/1	0.91	0.06	62,62,62,62	0
54	MG	BA	3081	1/1	0.91	0.11	65,65,65,65	0
54	MG	AA	1655	1/1	0.91	0.14	72,72,72,72	0
54	MG	DA	3010	1/1	0.91	0.17	51,51,51,51	0
54	MG	BA	2932	1/1	0.91	0.19	41,41,41,41	0
54	MG	AA	1675	1/1	0.91	0.06	77,77,77,77	0
54	MG	CA	1619	1/1	0.91	0.08	61,61,61,61	0
54	MG	BA	3086	1/1	0.91	0.16	102,102,102,102	0
54	MG	BA	3088	1/1	0.91	0.18	73,73,73,73	0
54	MG	BA	3126	1/1	0.91	0.05	54,54,54,54	0
54	MG	DA	3019	1/1	0.91	0.21	51,51,51,51	0
54	MG	CA	1729	1/1	0.91	0.11	98,98,98,98	0
54	MG	DA	3108	1/1	0.91	0.07	50,50,50,50	0
54	MG	BA	3244	1/1	0.91	0.34	47,47,47,47	0
54	MG	DA	3201	1/1	0.91	0.08	72,72,72,72	0
54	MG	AA	1638	1/1	0.91	0.13	63,63,63,63	0
54	MG	CA	1734	1/1	0.91	0.12	117,117,117,117	0
54	MG	CA	1679	1/1	0.91	0.05	93,93,93,93	0
54	MG	DA	3027	1/1	0.91	0.30	53,53,53,53	0
54	MG	DA	3301	1/1	0.91	0.10	80,80,80,80	0
54	MG	DA	3214	1/1	0.91	0.16	46,46,46,46	0
54	MG	BA	3132	1/1	0.91	0.23	79,79,79,79	0
54	MG	CA	1738	1/1	0.91	0.16	81,81,81,81	0
54	MG	BA	3251	1/1	0.91	0.12	64,64,64,64	0
54	MG	CA	1683	1/1	0.91	0.18	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	DA	3034	1/1	0.91	0.18	65,65,65,65	0
54	MG	BA	3188	1/1	0.91	0.24	45,45,45,45	0
54	MG	AA	1704	1/1	0.91	0.04	81,81,81,81	0
54	MG	BA	2947	1/1	0.91	0.02	14,14,14,14	0
54	MG	DA	3046	1/1	0.91	0.12	76,76,76,76	0
54	MG	BA	3257	1/1	0.91	0.30	64,64,64,64	0
54	MG	AA	1658	1/1	0.91	0.18	94,94,94,94	0
54	MG	BA	3138	1/1	0.91	0.07	100,100,100,100	0
54	MG	DA	3133	1/1	0.91	0.11	89,89,89,89	0
54	MG	BA	3260	1/1	0.91	0.13	62,62,62,62	0
54	MG	BA	2958	1/1	0.91	0.16	42,42,42,42	0
54	MG	AA	1654	1/1	0.91	0.25	76,76,76,76	0
54	MG	AA	1671	1/1	0.91	0.14	114,114,114,114	0
54	MG	BA	2966	1/1	0.91	0.13	75,75,75,75	0
54	MG	DA	3333	1/1	0.91	0.09	126,126,126,126	0
54	MG	AA	1709	1/1	0.91	0.12	83,83,83,83	0
54	MG	BA	2973	1/1	0.91	0.15	61,61,61,61	0
54	MG	BA	2974	1/1	0.91	0.09	45,45,45,45	0
54	MG	DA	3148	1/1	0.91	0.22	99,99,99,99	0
54	MG	BA	3273	1/1	0.91	0.07	83,83,83,83	0
54	MG	BA	2976	1/1	0.91	0.17	70,70,70,70	0
54	MG	AA	1727	1/1	0.91	0.12	100,100,100,100	0
54	MG	BA	3159	1/1	0.91	0.23	78,78,78,78	0
54	MG	CA	1655	1/1	0.91	0.09	80,80,80,80	0
54	MG	DA	3159	1/1	0.91	0.29	87,87,87,87	0
54	MG	BA	2983	1/1	0.91	0.27	62,62,62,62	0
54	MG	AA	1690	1/1	0.91	0.06	117,117,117,117	0
54	MG	BA	2988	1/1	0.91	0.15	60,60,60,60	0
54	MG	BA	3282	1/1	0.91	0.08	62,62,62,62	0
54	MG	CA	1712	1/1	0.91	0.13	78,78,78,78	0
54	MG	D4	101	1/1	0.91	0.18	55,55,55,55	0
54	MG	CA	1613	1/1	0.92	0.11	87,87,87,87	0
54	MG	DA	3164	1/1	0.92	0.13	88,88,88,88	0
54	MG	BA	2910	1/1	0.92	0.30	27,27,27,27	0
54	MG	DA	2995	1/1	0.92	0.18	48,48,48,48	0
54	MG	AA	1698	1/1	0.92	0.08	88,88,88,88	0
54	MG	DA	3088	1/1	0.92	0.13	70,70,70,70	0
54	MG	BA	2961	1/1	0.92	0.25	43,43,43,43	0
54	MG	DA	3174	1/1	0.92	0.09	42,42,42,42	0
54	MG	BA	3095	1/1	0.92	0.05	83,83,83,83	0
54	MG	DA	3003	1/1	0.92	0.11	41,41,41,41	0
54	MG	BA	3181	1/1	0.92	0.28	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	BA	2962	1/1	0.92	0.08	17,17,17,17	0
54	MG	DA	3009	1/1	0.92	0.09	49,49,49,49	0
54	MG	AA	1670	1/1	0.92	0.09	85,85,85,85	0
54	MG	BA	3028	1/1	0.92	0.22	62,62,62,62	0
54	MG	BA	2999	1/1	0.92	0.10	45,45,45,45	0
54	MG	DA	3183	1/1	0.92	0.07	83,83,83,83	0
54	MG	BA	3141	1/1	0.92	0.17	78,78,78,78	0
54	MG	BA	3068	1/1	0.92	0.08	59,59,59,59	0
54	MG	BA	3000	1/1	0.92	0.07	65,65,65,65	0
54	MG	BA	3104	1/1	0.92	0.14	63,63,63,63	0
54	MG	DA	3293	1/1	0.92	0.06	67,67,67,67	0
54	MG	AA	1635	1/1	0.92	0.10	68,68,68,68	0
54	MG	BA	3033	1/1	0.92	0.10	67,67,67,67	0
54	MG	BA	3306	1/1	0.92	0.08	74,74,74,74	0
54	MG	BA	2968	1/1	0.92	0.30	51,51,51,51	0
54	MG	BA	2929	1/1	0.92	0.20	37,37,37,37	0
54	MG	BA	3262	1/1	0.92	0.08	60,60,60,60	0
54	MG	BA	3200	1/1	0.92	0.16	64,64,64,64	0
54	MG	CA	1691	1/1	0.92	0.07	85,85,85,85	0
54	MG	DA	3303	1/1	0.92	0.18	66,66,66,66	0
54	MG	DA	2906	1/1	0.92	0.25	27,27,27,27	0
54	MG	BA	3203	1/1	0.92	0.14	41,41,41,41	0
54	MG	BA	3155	1/1	0.92	0.10	85,85,85,85	0
54	MG	DA	3217	1/1	0.92	0.10	56,56,56,56	0
54	MG	BA	3206	1/1	0.92	0.12	60,60,60,60	0
54	MG	BA	3268	1/1	0.92	0.18	58,58,58,58	0
54	MG	BA	3156	1/1	0.92	0.10	80,80,80,80	0
54	MG	DA	3223	1/1	0.92	0.37	45,45,45,45	0
54	MG	DA	3124	1/1	0.92	0.03	90,90,90,90	0
54	MG	BA	3007	1/1	0.92	0.16	55,55,55,55	0
54	MG	BA	3211	1/1	0.92	0.28	59,59,59,59	0
54	MG	CA	1649	1/1	0.92	0.14	80,80,80,80	0
54	MG	DA	3233	1/1	0.92	0.08	57,57,57,57	0
54	MG	DA	3049	1/1	0.92	0.10	56,56,56,56	0
54	MG	AA	1743	1/1	0.92	0.17	83,83,83,83	0
54	MG	DA	3324	1/1	0.92	0.23	78,78,78,78	0
54	MG	DA	2946	1/1	0.92	0.18	24,24,24,24	0
54	MG	DA	2952	1/1	0.92	0.19	50,50,50,50	0
54	MG	DA	3327	1/1	0.92	0.12	68,68,68,68	0
54	MG	AA	1708	1/1	0.92	0.08	101,101,101,101	0
54	MG	DA	3332	1/1	0.92	0.16	60,60,60,60	0
54	MG	AA	1689	1/1	0.92	0.06	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	DA	3059	1/1	0.92	0.06	67,67,67,67	0
54	MG	AA	1711	1/1	0.92	0.16	53,53,53,53	0
54	MG	DB	201	1/1	0.92	0.21	63,63,63,63	0
54	MG	BA	3043	1/1	0.92	0.13	70,70,70,70	0
54	MG	DA	2967	1/1	0.92	0.26	54,54,54,54	0
54	MG	BA	3045	1/1	0.92	0.08	80,80,80,80	0
54	MG	CA	1659	1/1	0.92	0.13	71,71,71,71	0
54	MG	BA	3046	1/1	0.92	0.27	87,87,87,87	0
54	MG	DB	210	1/1	0.92	0.08	74,74,74,74	0
54	MG	BA	3169	1/1	0.92	0.17	75,75,75,75	0
54	MG	DA	3151	1/1	0.92	0.18	82,82,82,82	0
54	MG	AA	1608	1/1	0.92	0.23	47,47,47,47	0
54	MG	DA	2985	1/1	0.92	0.20	48,48,48,48	0
54	MG	BA	3087	1/1	0.92	0.06	69,69,69,69	0
54	MG	DA	3077	1/1	0.92	0.24	67,67,67,67	0
54	MG	BA	3228	1/1	0.92	0.12	66,66,66,66	0
54	MG	AA	1602	1/1	0.92	0.30	49,49,49,49	0
54	MG	DA	3083	1/1	0.92	0.09	67,67,67,67	0
54	MG	DA	3240	1/1	0.93	0.20	60,60,60,60	0
54	MG	BA	3002	1/1	0.93	0.21	45,45,45,45	0
54	MG	CA	1657	1/1	0.93	0.11	78,78,78,78	0
54	MG	DA	3015	1/1	0.93	0.27	74,74,74,74	0
54	MG	DA	3016	1/1	0.93	0.07	74,74,74,74	0
54	MG	AA	1683	1/1	0.93	0.06	102,102,102,102	0
54	MG	BA	3134	1/1	0.93	0.14	64,64,64,64	0
54	MG	BA	2901	1/1	0.93	0.28	23,23,23,23	0
54	MG	BA	3005	1/1	0.93	0.16	69,69,69,69	0
54	MG	AA	1659	1/1	0.93	0.12	51,51,51,51	0
54	MG	AA	1668	1/1	0.93	0.10	90,90,90,90	0
54	MG	BA	3264	1/1	0.93	0.08	116,116,116,116	0
54	MG	AA	1662	1/1	0.93	0.08	53,53,53,53	0
54	MG	AA	1742	1/1	0.93	0.13	87,87,87,87	0
54	MG	DA	3132	1/1	0.93	0.10	70,70,70,70	0
54	MG	CA	1735	1/1	0.93	0.13	61,61,61,61	0
54	MG	B2	101	1/1	0.93	0.20	64,64,64,64	0
54	MG	BA	3202	1/1	0.93	0.31	63,63,63,63	0
54	MG	DA	3137	1/1	0.93	0.07	68,68,68,68	0
54	MG	CA	1603	1/1	0.93	0.29	48,48,48,48	0
54	MG	BA	3047	1/1	0.93	0.17	65,65,65,65	0
54	MG	DA	3035	1/1	0.93	0.21	77,77,77,77	0
54	MG	AA	1626	1/1	0.93	0.13	62,62,62,62	0
54	MG	DA	3038	1/1	0.93	0.23	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	DA	3041	1/1	0.93	0.07	51,51,51,51	0
54	MG	BA	3012	1/1	0.93	0.16	91,91,91,91	0
54	MG	DA	3149	1/1	0.93	0.17	74,74,74,74	0
54	MG	BA	3013	1/1	0.93	0.07	90,90,90,90	0
54	MG	BA	3208	1/1	0.93	0.10	48,48,48,48	0
54	MG	AA	1730	1/1	0.93	0.15	49,49,49,49	0
54	MG	DA	3048	1/1	0.93	0.09	66,66,66,66	0
54	MG	DA	2916	1/1	0.93	0.15	22,22,22,22	0
54	MG	DA	3050	1/1	0.93	0.09	105,105,105,105	0
54	MG	DA	2920	1/1	0.93	0.25	30,30,30,30	0
54	MG	CA	1677	1/1	0.93	0.15	85,85,85,85	0
54	MG	BA	3016	1/1	0.93	0.13	60,60,60,60	0
54	MG	BA	2931	1/1	0.93	0.16	32,32,32,32	0
54	MG	BA	3018	1/1	0.93	0.10	68,68,68,68	0
54	MG	DA	3058	1/1	0.93	0.06	54,54,54,54	0
54	MG	DA	2936	1/1	0.93	0.16	27,27,27,27	0
54	MG	BA	3062	1/1	0.93	0.12	76,76,76,76	0
54	MG	BA	3064	1/1	0.93	0.15	40,40,40,40	0
54	MG	BA	2977	1/1	0.93	0.13	52,52,52,52	0
54	MG	BA	3021	1/1	0.93	0.26	60,60,60,60	0
54	MG	BA	3111	1/1	0.93	0.24	46,46,46,46	0
54	MG	DA	2945	1/1	0.93	0.18	41,41,41,41	0
54	MG	BA	3221	1/1	0.93	0.11	48,48,48,48	0
54	MG	AA	1759	1/1	0.93	0.04	81,81,81,81	0
54	MG	DA	3073	1/1	0.93	0.12	80,80,80,80	0
54	MG	BA	3224	1/1	0.93	0.14	45,45,45,45	0
54	MG	BA	3113	1/1	0.93	0.09	71,71,71,71	0
54	MG	DA	2960	1/1	0.93	0.22	42,42,42,42	0
54	MG	DA	3308	1/1	0.93	0.07	91,91,91,91	0
54	MG	BA	3168	1/1	0.93	0.14	76,76,76,76	0
54	MG	AA	1719	1/1	0.93	0.19	78,78,78,78	0
54	MG	AA	1605	1/1	0.93	0.28	42,42,42,42	0
54	MG	CA	1631	1/1	0.93	0.08	68,68,68,68	0
54	MG	BA	2987	1/1	0.93	0.16	59,59,59,59	0
54	MG	DA	3189	1/1	0.93	0.10	37,37,37,37	0
54	MG	DA	3190	1/1	0.93	0.18	27,27,27,27	0
54	MG	BA	2941	1/1	0.93	0.38	50,50,50,50	0
54	MG	DA	3195	1/1	0.93	0.18	51,51,51,51	0
54	MG	CA	1635	1/1	0.93	0.06	67,67,67,67	0
54	MG	DA	2977	1/1	0.93	0.04	47,47,47,47	0
54	MG	BA	3297	1/1	0.93	0.13	67,67,67,67	0
54	MG	AA	1721	1/1	0.93	0.31	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	DA	3203	1/1	0.93	0.11	46,46,46,46	0
54	MG	CA	1702	1/1	0.93	0.24	68,68,68,68	0
54	MG	BA	3029	1/1	0.93	0.20	63,63,63,63	0
54	MG	DA	2988	1/1	0.93	0.20	41,41,41,41	0
54	MG	BA	3239	1/1	0.93	0.09	82,82,82,82	0
54	MG	AA	1672	1/1	0.93	0.18	101,101,101,101	0
54	MG	BA	3241	1/1	0.93	0.08	60,60,60,60	0
54	MG	BA	3242	1/1	0.93	0.15	44,44,44,44	0
54	MG	DA	3335	1/1	0.93	0.09	90,90,90,90	0
54	MG	BA	2993	1/1	0.93	0.28	58,58,58,58	0
54	MG	AA	1604	1/1	0.93	0.12	57,57,57,57	0
54	MG	DA	3102	1/1	0.93	0.20	68,68,68,68	0
54	MG	DA	3001	1/1	0.93	0.18	56,56,56,56	0
54	MG	DB	204	1/1	0.93	0.10	75,75,75,75	0
54	MG	DB	205	1/1	0.93	0.04	79,79,79,79	0
54	MG	BA	3246	1/1	0.93	0.12	73,73,73,73	0
54	MG	BA	2957	1/1	0.93	0.21	35,35,35,35	0
54	MG	DA	3227	1/1	0.93	0.16	34,34,34,34	0
54	MG	DA	3228	1/1	0.93	0.19	51,51,51,51	0
54	MG	DA	3229	1/1	0.93	0.17	64,64,64,64	0
54	MG	BA	3249	1/1	0.93	0.09	37,37,37,37	0
54	MG	AA	1736	1/1	0.93	0.08	79,79,79,79	0
54	MG	DA	3008	1/1	0.93	0.16	59,59,59,59	0
54	MG	BA	3186	1/1	0.93	0.24	52,52,52,52	0
54	MG	BA	3127	1/1	0.93	0.18	56,56,56,56	0
54	MG	CA	1654	1/1	0.93	0.05	111,111,111,111	0
54	MG	DA	3237	1/1	0.93	0.34	87,87,87,87	0
54	MG	AA	1751	1/1	0.93	0.09	72,72,72,72	0
54	MG	DA	3266	1/1	0.94	0.11	83,83,83,83	0
54	MG	AA	1710	1/1	0.94	0.15	65,65,65,65	0
54	MG	CA	1629	1/1	0.94	0.09	106,106,106,106	0
54	MG	DA	3172	1/1	0.94	0.16	81,81,81,81	0
54	MG	BA	3164	1/1	0.94	0.17	88,88,88,88	0
54	MG	BA	3051	1/1	0.94	0.08	66,66,66,66	0
54	MG	AA	1628	1/1	0.94	0.17	62,62,62,62	0
54	MG	BA	3055	1/1	0.94	0.05	60,60,60,60	0
54	MG	DA	3093	1/1	0.94	0.20	69,69,69,69	0
54	MG	BB	201	1/1	0.94	0.26	56,56,56,56	0
54	MG	DA	3277	1/1	0.94	0.16	52,52,52,52	0
54	MG	BA	3056	1/1	0.94	0.09	62,62,62,62	0
54	MG	BA	3214	1/1	0.94	0.22	53,53,53,53	0
54	MG	BB	204	1/1	0.94	0.08	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	AA	1695	1/1	0.94	0.14	83,83,83,83	0
54	MG	CA	1690	1/1	0.94	0.17	61,61,61,61	0
54	MG	BA	3216	1/1	0.94	0.17	65,65,65,65	0
54	MG	AA	1674	1/1	0.94	0.12	79,79,79,79	0
54	MG	CA	1642	1/1	0.94	0.06	71,71,71,71	0
54	MG	CA	1643	1/1	0.94	0.06	58,58,58,58	0
54	MG	DA	2933	1/1	0.94	0.26	30,30,30,30	0
54	MG	CA	1695	1/1	0.94	0.13	80,80,80,80	0
54	MG	DA	3026	1/1	0.94	0.09	48,48,48,48	0
54	MG	BA	3128	1/1	0.94	0.16	59,59,59,59	0
54	MG	DA	3196	1/1	0.94	0.24	39,39,39,39	0
54	MG	DA	3294	1/1	0.94	0.21	61,61,61,61	0
54	MG	DA	3197	1/1	0.94	0.17	28,28,28,28	0
54	MG	BA	2948	1/1	0.94	0.26	39,39,39,39	0
54	MG	DA	3111	1/1	0.94	0.19	67,67,67,67	0
54	MG	BA	2982	1/1	0.94	0.13	41,41,41,41	0
54	MG	DA	3114	1/1	0.94	0.18	83,83,83,83	0
54	MG	BA	2919	1/1	0.94	0.16	24,24,24,24	0
54	MG	DA	3204	1/1	0.94	0.13	54,54,54,54	0
54	MG	BA	2984	1/1	0.94	0.13	41,41,41,41	0
54	MG	BA	3099	1/1	0.94	0.16	78,78,78,78	0
54	MG	DA	3304	1/1	0.94	0.11	59,59,59,59	0
54	MG	DA	3208	1/1	0.94	0.23	49,49,49,49	0
54	MG	DA	3306	1/1	0.94	0.08	51,51,51,51	0
54	MG	BA	3182	1/1	0.94	0.21	20,20,20,20	0
54	MG	BA	3065	1/1	0.94	0.08	61,61,61,61	0
54	MG	DA	3309	1/1	0.94	0.21	30,30,30,30	0
54	MG	DA	3213	1/1	0.94	0.24	66,66,66,66	0
54	MG	DA	2949	1/1	0.94	0.18	41,41,41,41	0
54	MG	BA	3276	1/1	0.94	0.11	65,65,65,65	0
54	MG	BA	3227	1/1	0.94	0.12	48,48,48,48	0
54	MG	DA	2957	1/1	0.94	0.16	63,63,63,63	0
54	MG	BA	2955	1/1	0.94	0.10	50,50,50,50	0
54	MG	CA	1707	1/1	0.94	0.11	104,104,104,104	0
54	MG	BA	3139	1/1	0.94	0.17	78,78,78,78	0
54	MG	BA	2920	1/1	0.94	0.15	28,28,28,28	0
54	MG	DA	3225	1/1	0.94	0.08	80,80,80,80	0
54	MG	BA	2926	1/1	0.94	0.18	31,31,31,31	0
54	MG	BA	3234	1/1	0.94	0.10	61,61,61,61	0
54	MG	BA	2989	1/1	0.94	0.27	53,53,53,53	0
54	MG	BA	2927	1/1	0.94	0.20	37,37,37,37	0
54	MG	AV	6303	1/1	0.94	0.09	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	DA	2975	1/1	0.94	0.09	58,58,58,58	0
54	MG	BA	3041	1/1	0.94	0.05	67,67,67,67	0
54	MG	DA	2978	1/1	0.94	0.11	44,44,44,44	0
54	MG	DA	3331	1/1	0.94	0.09	52,52,52,52	0
54	MG	DA	2980	1/1	0.94	0.18	63,63,63,63	0
54	MG	DA	3062	1/1	0.94	0.14	65,65,65,65	0
54	MG	DA	2981	1/1	0.94	0.20	55,55,55,55	0
54	MG	AA	1660	1/1	0.94	0.18	59,59,59,59	0
54	MG	AA	1717	1/1	0.94	0.13	81,81,81,81	0
54	MG	BA	3076	1/1	0.94	0.14	68,68,68,68	0
54	MG	DA	3068	1/1	0.94	0.22	72,72,72,72	0
54	MG	BA	3292	1/1	0.94	0.13	72,72,72,72	0
54	MG	BA	3044	1/1	0.94	0.11	64,64,64,64	0
54	MG	BA	2933	1/1	0.94	0.21	32,32,32,32	0
54	MG	BA	3201	1/1	0.94	0.14	80,80,80,80	0
54	MG	BA	2934	1/1	0.94	0.22	28,28,28,28	0
54	MG	DB	208	1/1	0.94	0.05	96,96,96,96	0
54	MG	AA	1676	1/1	0.94	0.03	63,63,63,63	0
54	MG	DA	3255	1/1	0.94	0.13	101,101,101,101	0
54	MG	DA	3158	1/1	0.94	0.06	59,59,59,59	0
54	MG	DA	2996	1/1	0.94	0.12	43,43,43,43	0
54	MG	DA	3160	1/1	0.94	0.12	71,71,71,71	0
54	MG	BA	3048	1/1	0.94	0.13	67,67,67,67	0
54	MG	BA	3205	1/1	0.94	0.12	38,38,38,38	0
54	MG	BA	3001	1/1	0.94	0.16	59,59,59,59	0
54	MG	CA	1731	1/1	0.94	0.03	90,90,90,90	0
54	MG	CA	1732	1/1	0.94	0.15	73,73,73,73	0
54	MG	BA	3254	1/1	0.94	0.10	81,81,81,81	0
54	MG	BA	3092	1/1	0.95	0.05	63,63,63,63	0
54	MG	DA	2954	1/1	0.95	0.18	28,28,28,28	0
54	MG	BA	2964	1/1	0.95	0.15	30,30,30,30	0
54	MG	BA	2997	1/1	0.95	0.17	57,57,57,57	0
54	MG	BA	2902	1/1	0.95	0.22	16,16,16,16	0
54	MG	DA	3039	1/1	0.95	0.28	48,48,48,48	0
54	MG	DA	2962	1/1	0.95	0.14	37,37,37,37	0
54	MG	DA	2963	1/1	0.95	0.24	53,53,53,53	0
54	MG	CA	1605	1/1	0.95	0.12	56,56,56,56	0
54	MG	BA	2904	1/1	0.95	0.23	13,13,13,13	0
54	MG	BA	2969	1/1	0.95	0.08	37,37,37,37	0
54	MG	BA	3063	1/1	0.95	0.08	56,56,56,56	0
54	MG	CA	1609	1/1	0.95	0.14	93,93,93,93	0
54	MG	DA	3288	1/1	0.95	0.07	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	BA	3235	1/1	0.95	0.05	62,62,62,62	0
54	MG	BA	2970	1/1	0.95	0.24	45,45,45,45	0
54	MG	BA	3237	1/1	0.95	0.08	60,60,60,60	0
54	MG	DA	3206	1/1	0.95	0.19	37,37,37,37	0
54	MG	DA	3126	1/1	0.95	0.07	77,77,77,77	0
54	MG	DA	3053	1/1	0.95	0.23	61,61,61,61	0
54	MG	AA	1740	1/1	0.95	0.11	80,80,80,80	0
54	MG	BA	3142	1/1	0.95	0.09	89,89,89,89	0
54	MG	AA	1661	1/1	0.95	0.23	65,65,65,65	0
54	MG	BA	3290	1/1	0.95	0.14	42,42,42,42	0
54	MG	DA	2982	1/1	0.95	0.07	33,33,33,33	0
54	MG	DA	3216	1/1	0.95	0.17	46,46,46,46	0
54	MG	BA	2911	1/1	0.95	0.17	23,23,23,23	0
54	MG	DA	3061	1/1	0.95	0.17	75,75,75,75	0
54	MG	DA	3135	1/1	0.95	0.05	65,65,65,65	0
54	MG	BA	3146	1/1	0.95	0.18	83,83,83,83	0
54	MG	BA	2937	1/1	0.95	0.20	36,36,36,36	0
54	MG	BA	3105	1/1	0.95	0.10	60,60,60,60	0
54	MG	AA	1656	1/1	0.95	0.09	72,72,72,72	0
54	MG	BA	2913	1/1	0.95	0.18	16,16,16,16	0
54	MG	DA	3067	1/1	0.95	0.08	63,63,63,63	0
54	MG	CA	1624	1/1	0.95	0.03	66,66,66,66	0
54	MG	DA	3146	1/1	0.95	0.07	95,95,95,95	0
54	MG	BA	3153	1/1	0.95	0.08	67,67,67,67	0
54	MG	BA	2980	1/1	0.95	0.09	40,40,40,40	0
54	MG	DA	3232	1/1	0.95	0.14	39,39,39,39	0
54	MG	BA	2981	1/1	0.95	0.07	48,48,48,48	0
54	MG	AA	1716	1/1	0.95	0.08	120,120,120,120	0
54	MG	CA	1682	1/1	0.95	0.09	97,97,97,97	0
54	MG	BA	3074	1/1	0.95	0.04	61,61,61,61	0
54	MG	AA	1725	1/1	0.95	0.15	72,72,72,72	0
54	MG	AA	1601	1/1	0.95	0.24	31,31,31,31	0
54	MG	BA	3256	1/1	0.95	0.19	79,79,79,79	0
54	MG	AA	1611	1/1	0.95	0.08	49,49,49,49	0
54	MG	BA	2923	1/1	0.95	0.16	29,29,29,29	0
54	MG	BA	3210	1/1	0.95	0.09	48,48,48,48	0
54	MG	DA	3245	1/1	0.95	0.24	54,54,54,54	0
54	MG	DA	2914	1/1	0.95	0.26	27,27,27,27	0
54	MG	DA	3247	1/1	0.95	0.17	40,40,40,40	0
54	MG	DA	3248	1/1	0.95	0.20	75,75,75,75	0
54	MG	BA	2924	1/1	0.95	0.23	47,47,47,47	0
54	MG	DA	3250	1/1	0.95	0.34	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	BA	3261	1/1	0.95	0.15	53,53,53,53	0
54	MG	BA	2925	1/1	0.95	0.19	29,29,29,29	0
54	MG	DA	2928	1/1	0.95	0.25	43,43,43,43	0
54	MG	DA	3167	1/1	0.95	0.04	68,68,68,68	0
54	MG	AA	1703	1/1	0.95	0.07	83,83,83,83	0
54	MG	BA	2991	1/1	0.95	0.06	36,36,36,36	0
54	MG	BA	3120	1/1	0.95	0.07	57,57,57,57	0
54	MG	BA	3023	1/1	0.95	0.14	64,64,64,64	0
54	MG	BA	3085	1/1	0.95	0.08	68,68,68,68	0
54	MG	DA	3261	1/1	0.95	0.28	73,73,73,73	0
54	MG	BA	3171	1/1	0.95	0.06	68,68,68,68	0
54	MG	BA	3052	1/1	0.95	0.17	56,56,56,56	0
54	MG	AA	1627	1/1	0.95	0.14	85,85,85,85	0
54	MG	BA	2928	1/1	0.95	0.27	42,42,42,42	0
54	MG	AA	1607	1/1	0.95	0.20	54,54,54,54	0
54	MG	DB	213	1/1	0.95	0.22	63,63,63,63	0
54	MG	DA	2944	1/1	0.95	0.18	35,35,35,35	0
54	MG	BB	215	1/1	0.95	0.09	131,131,131,131	0
54	MG	BA	3091	1/1	0.95	0.06	56,56,56,56	0
54	MG	DA	3270	1/1	0.95	0.10	81,81,81,81	0
54	MG	BA	3177	1/1	0.95	0.18	93,93,93,93	0
54	MG	CA	1653	1/1	0.95	0.11	84,84,84,84	0
54	MG	DA	3107	1/1	0.95	0.19	67,67,67,67	0
55	ZN	CN	101	1/1	0.95	0.06	144,144,144,144	0
54	MG	BA	2908	1/1	0.96	0.25	18,18,18,18	0
54	MG	CA	1714	1/1	0.96	0.11	74,74,74,74	0
54	MG	DA	2921	1/1	0.96	0.20	17,17,17,17	0
54	MG	DA	3040	1/1	0.96	0.08	41,41,41,41	0
54	MG	AA	1630	1/1	0.96	0.13	70,70,70,70	0
54	MG	DA	2925	1/1	0.96	0.21	24,24,24,24	0
54	MG	DA	2927	1/1	0.96	0.13	22,22,22,22	0
54	MG	BA	3179	1/1	0.96	0.21	19,19,19,19	0
54	MG	BA	2995	1/1	0.96	0.15	47,47,47,47	0
54	MG	DA	2989	1/1	0.96	0.12	45,45,45,45	0
54	MG	BA	2918	1/1	0.96	0.21	17,17,17,17	0
54	MG	BA	3183	1/1	0.96	0.17	27,27,27,27	0
54	MG	CA	1721	1/1	0.96	0.10	101,101,101,101	0
54	MG	DA	2935	1/1	0.96	0.22	30,30,30,30	0
54	MG	DA	3241	1/1	0.96	0.31	54,54,54,54	0
54	MG	BA	2965	1/1	0.96	0.15	47,47,47,47	0
54	MG	DA	2997	1/1	0.96	0.05	35,35,35,35	0
54	MG	BA	3137	1/1	0.96	0.15	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	BA	2903	1/1	0.96	0.13	14,14,14,14	0
54	MG	BA	3015	1/1	0.96	0.12	58,58,58,58	0
54	MG	BA	3269	1/1	0.96	0.10	63,63,63,63	0
54	MG	BA	2952	1/1	0.96	0.16	38,38,38,38	0
54	MG	CA	1634	1/1	0.96	0.07	60,60,60,60	0
54	MG	BA	2954	1/1	0.96	0.11	52,52,52,52	0
54	MG	DA	3007	1/1	0.96	0.08	43,43,43,43	0
54	MG	AA	1617	1/1	0.96	0.13	77,77,77,77	0
54	MG	DA	2947	1/1	0.96	0.14	40,40,40,40	0
54	MG	DA	2948	1/1	0.96	0.20	52,52,52,52	0
54	MG	DA	3188	1/1	0.96	0.23	9,9,9,9	0
54	MG	BA	3245	1/1	0.96	0.18	54,54,54,54	0
54	MG	BA	3167	1/1	0.96	0.08	50,50,50,50	0
54	MG	DA	3192	1/1	0.96	0.15	30,30,30,30	0
54	MG	BA	2922	1/1	0.96	0.24	25,25,25,25	0
54	MG	DA	3194	1/1	0.96	0.16	10,10,10,10	0
54	MG	BA	3020	1/1	0.96	0.25	62,62,62,62	0
54	MG	DA	3071	1/1	0.96	0.07	64,64,64,64	0
54	MG	DA	3330	1/1	0.96	0.08	69,69,69,69	0
54	MG	DA	2956	1/1	0.96	0.08	45,45,45,45	0
54	MG	BA	3277	1/1	0.96	0.12	71,71,71,71	0
54	MG	BA	3307	1/1	0.96	0.11	68,68,68,68	0
54	MG	BA	3147	1/1	0.96	0.05	72,72,72,72	0
54	MG	BA	3195	1/1	0.96	0.09	53,53,53,53	0
54	MG	DA	3202	1/1	0.96	0.36	44,44,44,44	0
54	MG	BA	3197	1/1	0.96	0.22	57,57,57,57	0
54	MG	DA	3079	1/1	0.96	0.05	38,38,38,38	0
54	MG	DA	3139	1/1	0.96	0.07	60,60,60,60	0
54	MG	BA	3089	1/1	0.96	0.16	59,59,59,59	0
54	MG	BA	3125	1/1	0.96	0.14	87,87,87,87	0
54	MG	DA	3023	1/1	0.96	0.09	49,49,49,49	0
54	MG	AA	1615	1/1	0.96	0.15	42,42,42,42	0
54	MG	DA	3210	1/1	0.96	0.09	59,59,59,59	0
54	MG	DA	3144	1/1	0.96	0.06	72,72,72,72	0
54	MG	DA	2901	1/1	0.96	0.20	7,7,7,7	0
54	MG	DA	2969	1/1	0.96	0.18	42,42,42,42	0
54	MG	BA	2959	1/1	0.96	0.13	55,55,55,55	0
54	MG	BA	2942	1/1	0.96	0.12	22,22,22,22	0
54	MG	DA	2909	1/1	0.96	0.15	5,5,5,5	0
54	MG	DA	3218	1/1	0.96	0.13	48,48,48,48	0
54	MG	DA	2911	1/1	0.96	0.15	7,7,7,7	0
54	MG	DA	3031	1/1	0.96	0.09	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	DA	3032	1/1	0.96	0.09	49,49,49,49	0
54	MG	DA	2913	1/1	0.96	0.26	17,17,17,17	0
54	MG	BA	2943	1/1	0.96	0.20	42,42,42,42	0
54	MG	DA	2979	1/1	0.96	0.05	69,69,69,69	0
54	MG	DA	3081	1/1	0.97	0.06	71,71,71,71	0
54	MG	DA	3082	1/1	0.97	0.20	70,70,70,70	0
54	MG	DA	2990	1/1	0.97	0.06	35,35,35,35	0
54	MG	AA	1619	1/1	0.97	0.12	80,80,80,80	0
54	MG	CA	1669	1/1	0.97	0.08	66,66,66,66	0
54	MG	BA	2940	1/1	0.97	0.20	29,29,29,29	0
54	MG	BA	2956	1/1	0.97	0.14	35,35,35,35	0
54	MG	BA	2972	1/1	0.97	0.18	49,49,49,49	0
54	MG	DA	3252	1/1	0.97	0.05	44,44,44,44	0
54	MG	BA	2921	1/1	0.97	0.17	21,21,21,21	0
54	MG	AA	1663	1/1	0.97	0.13	70,70,70,70	0
54	MG	BA	3053	1/1	0.97	0.25	67,67,67,67	0
54	MG	DA	3044	1/1	0.97	0.05	59,59,59,59	0
54	MG	DA	3045	1/1	0.97	0.17	48,48,48,48	0
54	MG	DA	3145	1/1	0.97	0.18	70,70,70,70	0
54	MG	AA	1603	1/1	0.97	0.15	35,35,35,35	0
54	MG	BA	3196	1/1	0.97	0.23	51,51,51,51	0
54	MG	DA	3096	1/1	0.97	0.19	40,40,40,40	0
54	MG	BA	3223	1/1	0.97	0.08	54,54,54,54	0
54	MG	DA	2903	1/1	0.97	0.17	7,7,7,7	0
54	MG	DA	3005	1/1	0.97	0.05	33,33,33,33	0
54	MG	DA	3321	1/1	0.97	0.21	30,30,30,30	0
54	MG	BA	2907	1/1	0.97	0.15	7,7,7,7	0
54	MG	BA	2946	1/1	0.97	0.17	33,33,33,33	0
54	MG	BA	3078	1/1	0.97	0.12	83,83,83,83	0
54	MG	DA	3211	1/1	0.97	0.14	38,38,38,38	0
54	MG	BA	2979	1/1	0.97	0.09	40,40,40,40	0
54	MG	BA	2998	1/1	0.97	0.12	46,46,46,46	0
54	MG	DA	3328	1/1	0.97	0.11	45,45,45,45	0
54	MG	DA	3056	1/1	0.97	0.07	48,48,48,48	0
54	MG	BA	3102	1/1	0.97	0.15	69,69,69,69	0
54	MG	DA	2915	1/1	0.97	0.20	14,14,14,14	0
54	MG	BA	3151	1/1	0.97	0.29	56,56,56,56	0
54	MG	DA	2919	1/1	0.97	0.12	45,45,45,45	0
54	MG	AA	1633	1/1	0.97	0.10	73,73,73,73	0
54	MG	DA	3165	1/1	0.97	0.12	71,71,71,71	0
54	MG	CA	1719	1/1	0.97	0.06	78,78,78,78	0
54	MG	DA	2923	1/1	0.97	0.06	17,17,17,17	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	BA	3233	1/1	0.97	0.20	52,52,52,52	0
54	MG	DA	2973	1/1	0.97	0.27	50,50,50,50	0
54	MG	DA	2974	1/1	0.97	0.07	46,46,46,46	0
54	MG	DA	3283	1/1	0.97	0.29	53,53,53,53	0
54	MG	DA	3171	1/1	0.97	0.07	61,61,61,61	0
54	MG	BA	2909	1/1	0.97	0.17	24,24,24,24	0
54	MG	BA	2936	1/1	0.97	0.14	43,43,43,43	0
54	MG	BA	2950	1/1	0.97	0.09	32,32,32,32	0
54	MG	AA	1715	1/1	0.97	0.18	63,63,63,63	0
54	MG	DA	2930	1/1	0.97	0.19	36,36,36,36	0
54	MG	BA	3130	1/1	0.97	0.04	78,78,78,78	0
54	MG	DA	3123	1/1	0.97	0.05	59,59,59,59	0
54	MG	BA	3296	1/1	0.97	0.08	47,47,47,47	0
54	MG	BA	2985	1/1	0.97	0.26	54,54,54,54	0
54	MG	DA	3075	1/1	0.97	0.05	64,64,64,64	0
54	MG	BA	2967	1/1	0.97	0.09	24,24,24,24	0
54	MG	DE	301	1/1	0.97	0.08	44,44,44,44	0
54	MG	BA	2953	1/1	0.97	0.10	37,37,37,37	0
54	MG	CA	1602	1/1	0.97	0.10	64,64,64,64	0
54	MG	BA	3161	1/1	0.97	0.06	62,62,62,62	0
54	MG	CA	1604	1/1	0.97	0.12	59,59,59,59	0
54	MG	DA	2926	1/1	0.98	0.16	43,43,43,43	0
54	MG	CA	1615	1/1	0.98	0.05	51,51,51,51	0
54	MG	DA	2902	1/1	0.98	0.16	10,10,10,10	0
54	MG	BA	3144	1/1	0.98	0.07	75,75,75,75	0
54	MG	DA	2964	1/1	0.98	0.08	34,34,34,34	0
54	MG	BA	3131	1/1	0.98	0.07	67,67,67,67	0
54	MG	DA	2931	1/1	0.98	0.12	23,23,23,23	0
54	MG	DA	3000	1/1	0.98	0.08	35,35,35,35	0
54	MG	DA	2905	1/1	0.98	0.15	9,9,9,9	0
54	MG	BA	2975	1/1	0.98	0.04	37,37,37,37	0
54	MG	DA	3036	1/1	0.98	0.06	51,51,51,51	0
54	MG	DA	2907	1/1	0.98	0.18	7,7,7,7	0
54	MG	DA	2908	1/1	0.98	0.14	24,24,24,24	0
54	MG	BA	2906	1/1	0.98	0.08	5,5,5,5	0
54	MG	DA	2937	1/1	0.98	0.14	25,25,25,25	0
54	MG	DA	2910	1/1	0.98	0.09	6,6,6,6	0
54	MG	DA	3219	1/1	0.98	0.16	67,67,67,67	0
54	MG	BA	2917	1/1	0.98	0.11	8,8,8,8	0
54	MG	DA	2912	1/1	0.98	0.15	18,18,18,18	0
54	MG	DA	3112	1/1	0.98	0.04	60,60,60,60	0
54	MG	DA	2976	1/1	0.98	0.09	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	BA	3057	1/1	0.98	0.15	63,63,63,63	0
54	MG	BA	3010	1/1	0.98	0.06	37,37,37,37	0
54	MG	AA	1686	1/1	0.98	0.10	72,72,72,72	0
54	MG	BA	3231	1/1	0.98	0.09	22,22,22,22	0
54	MG	DA	2917	1/1	0.98	0.18	22,22,22,22	0
54	MG	DA	3191	1/1	0.98	0.18	24,24,24,24	0
54	MG	DA	2918	1/1	0.98	0.16	15,15,15,15	0
54	MG	DA	3155	1/1	0.98	0.06	124,124,124,124	0
54	MG	AA	1636	1/1	0.98	0.08	76,76,76,76	0
54	MG	BA	3247	1/1	0.98	0.13	52,52,52,52	0
54	MG	DA	2951	1/1	0.98	0.10	38,38,38,38	0
54	MG	BA	3040	1/1	0.98	0.06	58,58,58,58	0
54	MG	DA	2922	1/1	0.98	0.14	7,7,7,7	0
54	MG	BA	2930	1/1	0.98	0.16	34,34,34,34	0
54	MG	BA	2944	1/1	0.98	0.09	17,17,17,17	0
54	MG	DA	3239	1/1	0.98	0.12	42,42,42,42	0
54	MG	BA	2915	1/1	0.98	0.06	4,4,4,4	0
55	ZN	CD	301	1/1	0.98	0.18	131,131,131,131	0
54	MG	DA	2992	1/1	0.98	0.07	46,46,46,46	0
54	MG	DA	2943	1/1	0.99	0.16	32,32,32,32	0
54	MG	DA	2955	1/1	0.99	0.14	40,40,40,40	0
54	MG	BA	3180	1/1	0.99	0.16	26,26,26,26	0
54	MG	DA	2950	1/1	0.99	0.06	29,29,29,29	0
54	MG	BA	2938	1/1	0.99	0.06	10,10,10,10	0
54	MG	DA	2984	1/1	0.99	0.10	66,66,66,66	0
54	MG	DA	3156	1/1	0.99	0.06	78,78,78,78	0
54	MG	BA	2951	1/1	0.99	0.12	28,28,28,28	0
55	ZN	AN	101	1/1	0.99	0.06	120,120,120,120	0
54	MG	DA	2961	1/1	0.99	0.08	29,29,29,29	0
54	MG	BA	3140	1/1	0.99	0.08	76,76,76,76	0
55	ZN	AD	301	1/1	1.00	0.19	80,80,80,80	0
54	MG	DA	2958	1/1	1.00	0.04	2,2,2,2	0

6.5 Other polymers [i](#)

There are no such residues in this entry.