



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 22, 2024 – 06:22 PM EDT

PDB ID : 4V84  
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>.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

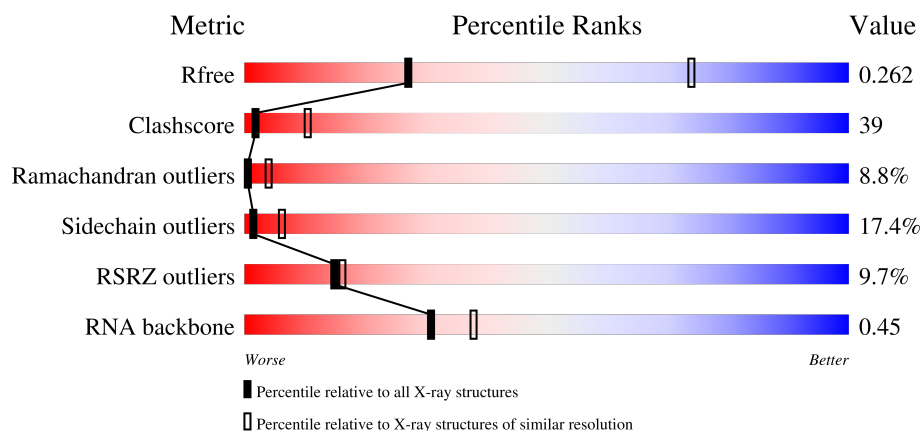
# 1 Overall quality at a glance

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))
$R_{free}$	164625	1140 (3.46-3.34)
Clashscore	180529	1172 (3.46-3.34)
Ramachandran outliers	177936	1172 (3.46-3.34)
Sidechain outliers	177891	1172 (3.46-3.34)
RSRZ outliers	164620	1140 (3.46-3.34)
RNA backbone	3690	1033 (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  $\geq 3$ , 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	<div> <div>5%</div> <div>20%</div> <div>63%</div> <div>16%</div> <div>.</div> </div>
1	CA	1506	<div> <div>5%</div> <div>19%</div> <div>64%</div> <div>18%</div> </div>
2	AB	234	<div> <div>13%</div> <div>33%</div> <div>53%</div> <div>13%</div> </div>
2	CB	234	<div> <div>13%</div> <div>32%</div> <div>56%</div> <div>12%</div> </div>

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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
54	MG	DA	3260	-	-	-	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 (three-letter code: 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

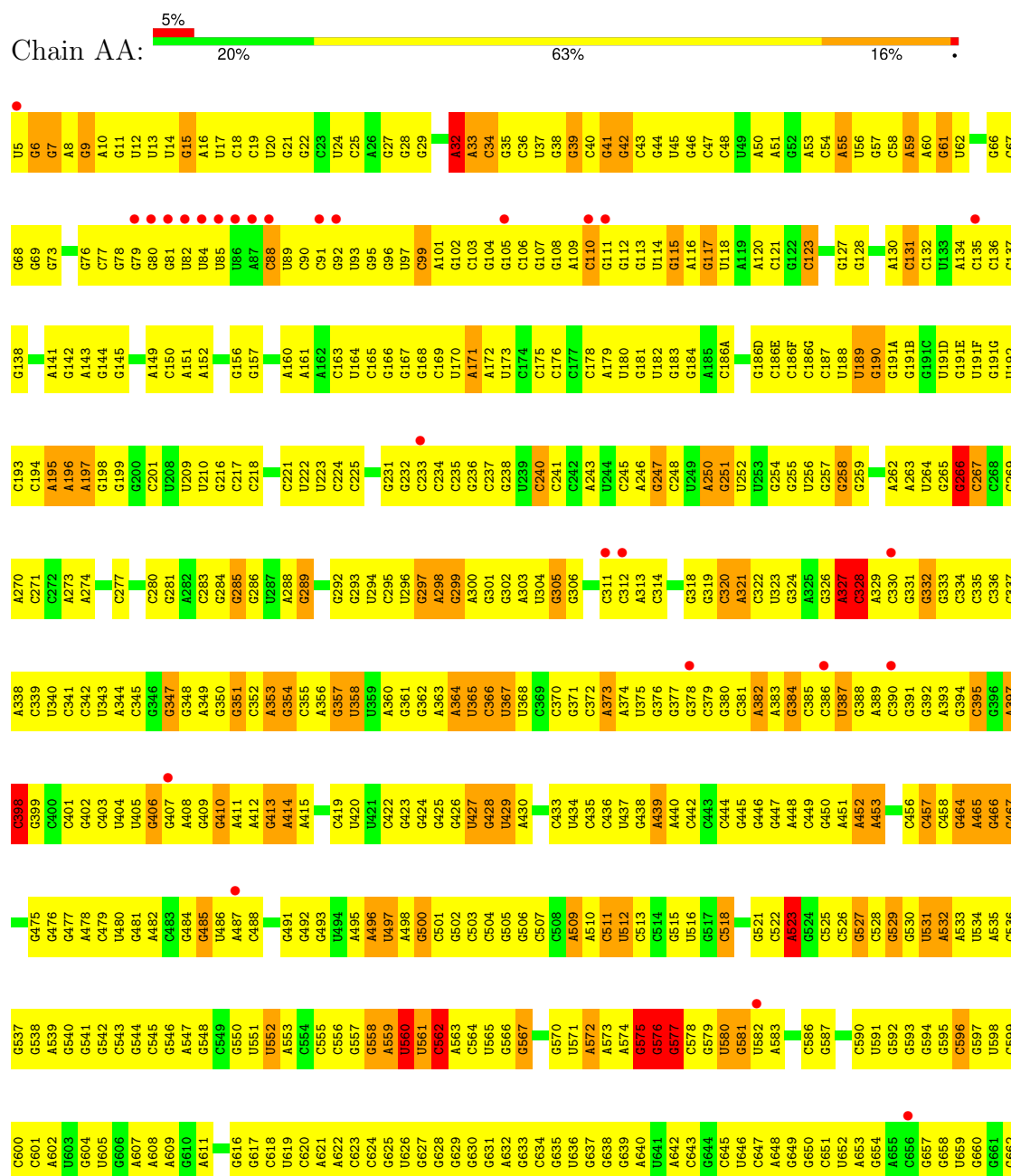
- Molecule 55 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

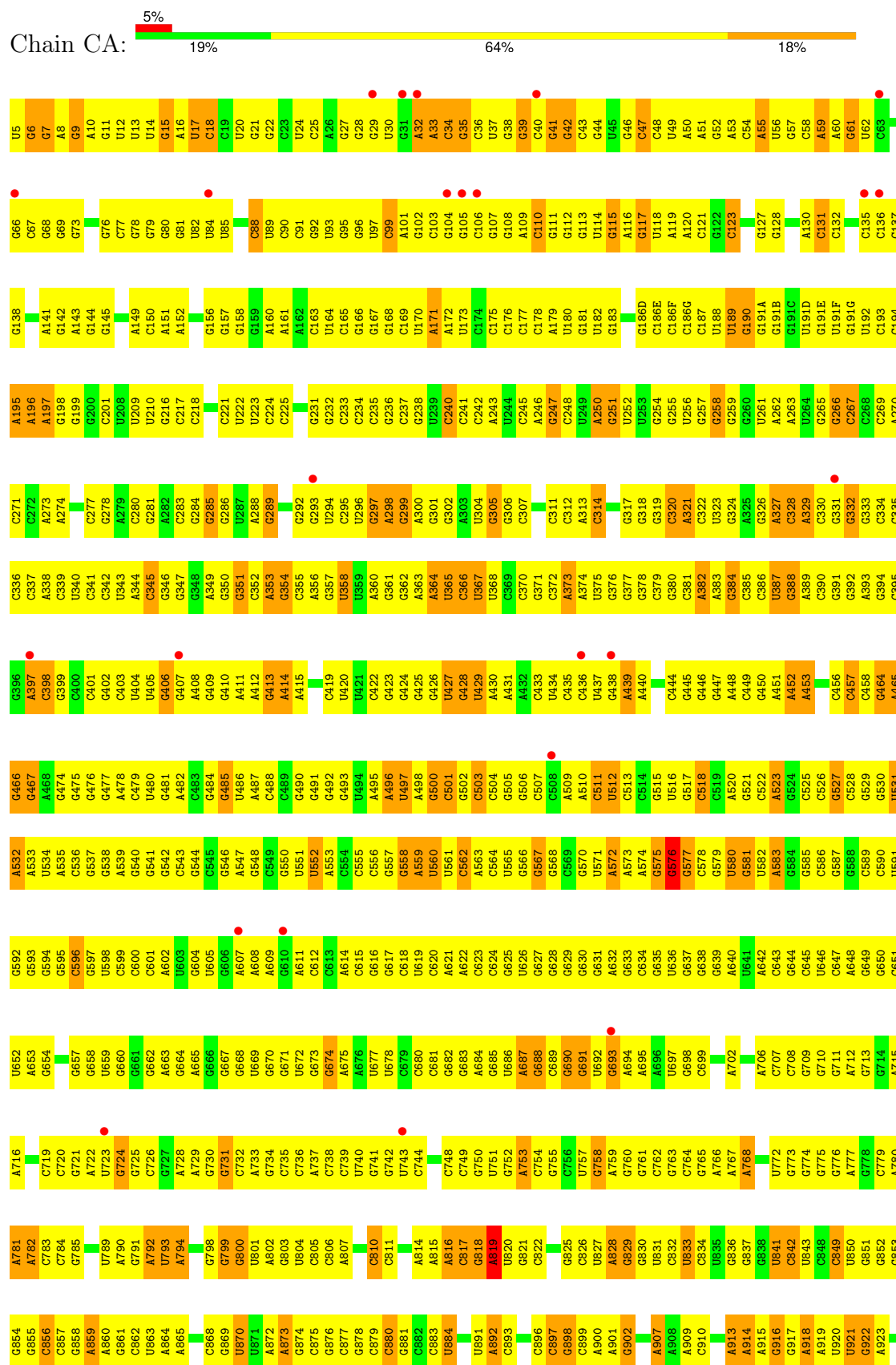
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

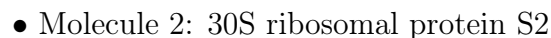
#### • Molecule 1: ribosomal RNA 16S

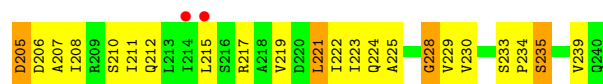


G1517	A1446	U1380	C1320	A1252	G1190	U1125	C1063	U992	C931	G861	A790	C726	A663
A1518	G1447	U1381	C1321	G1253	A1191	U1126	G1064	G993	C932	C862	G791	G727	G664
A1519	C1448	C1382	G1322	G1254	G1192	G1127	U1065	A994	G933	U863	A792	A728	A665
G1520	C1449	C1383	G1323	G1255	G1193	G1128	C1066	U997	C934	A864	U793	A729	G666
A1521	U1450	C1384	A1324	A1256	U1194	C1129	A1067	G998A	A935	A865	G794	G730	G667
U1522	G1451	C1385	C1325	U1257	C1195	A1130	U1068	U997	C936	G797	C797	C732	G668
G1523	C1452	C1386	C1326	G1258	U1196	U1131	C1069	G998A	A937	C868	G798	G733	U669
C1524	G1453	G1387	C1327	C1259	G1197	U1135	U1070	A1000	A938	C869	G799	A734	G670
G1525	G1454	C1388	C1328	C1260	G1198	U1136	U1071	G1001	G939	U870	G799	C735	G671
G1526	C1455	C1389	A1329	A1261	U1199	U1137	U1072	G1002	C940	G800	G799	C736	U672
C1527	C1459	U1390	U1330	C1262	C1200	C1137	U1073	G1003	G941	A873	U801	C737	G673
U1528	U1460	U1391	A1331	C1263	A1201	G1138	G1074	A1004	G942	C874	A802	A737	G674
G1529	G1461	C1392	A1332	G1264	G1202	G1139	C1075	A1005	U943	C875	G803	C738	A675
G1530	G1462	U1393	C1333	C1270	G1203	C1140	C1076	G1006	G944	C876	U804	C739	A676
U1531	G1464	C1394	A1334	G1271	A1204	C1141	G1077	U1009	G945	C877	C805	U677	U678
U1532	C1465	C1395	G1335	G1272	U1205	G1142	A1080	G1010	A946	C878	C806	G741	G679
C1533	C1466	A1396	G1336	G1273	G1206	G1143	U1081	G1011	G947	C879	A807	G742	U680
G1467	G1467	C1397	G1337	C1274	G1207	G1144	G1082	G1012	C948	C880	C810	U743	G681
A1468	A1398	A1398	G1338	C1275	C1208	C1145	U1083	A1014	A949	C881	C811	C744	G682
G1469	C1399	C1399	A1339	U1276	G1209	C1146	G1084	A1015	G951	C882	G812	C745	G683
G1470	C1400	C1400	A1340	A1279	C1210	C1147	U1085	A1016	U952	U884	A814	C746	G684
G1471	C1401	G1401	U1341	U1280	U1211	U1148	U1086	G1017	G953	G892	A815	G750	A687
U1472	C1402	C1402	C1342	U1281	U1212	C1149	U1087	G1018	G954	C893	A816	U751	G688
G1473	C1403	C1403	G1343	C1282	A1213	U1150	G1088	G1022	U955	C894	A817	G752	C689
G1479	G1407	G1407	U1344	C1283	G1214	A1151	G1089	G1023	U956	C895	G818	A753	G690
G1480	U1481	U1481	U1345	A1285	C1217	A1152	U1090	G1024	U957	C896	U820	C754	G691
U1482	G1410	G1410	A1346	C1286	G1218	G1153	U1091	U1025	A958	C897	G821	C755	U692
A1483	C1411	C1411	U1347	U1287	U1219	G1154	G1092	G1026	C959	C898	C822	U757	A694
C1484	C1412	C1412	A1348	A1288	G1220	G1155	U1093	C1027	U960	C899	C823	G758	G695
U1485	A1413	A1413	A1350	U1289	G1221	U1156	G1094	G1028	U961	C901	C824	A759	U697
U1486	U1414	U1414	C1351	G1290	G1222	C1157	C1095	G1031	C962	G902	C825	G760	G698
G1487	G1415	G1415	C1352	G1291	C1223	C1158	C1096	A1034	G963	G903	U827	G761	G699
G1488	U1488	U1488	G1353	U1292	G1224	U1159	C1098	C1037	A964	C904	A828	C762	G700
C1490	A1418	A1418	U1354	G1293	A1225	C1160	G1099	U1037	A965	C905	A829	G763	G701
G1491	G1419	G1419	A1357	C1294	C1226	C1161	C1100	C1038	G966	U906	C830	G764	A702
A1492	G1420	G1420	U1358	G1295	A1227	C1162	C1101	C1039	C967	G906	U831	C765	G703
A1493	G1421	G1421	C1359	C1296	C1228	G1164	A1102	U1040	A968	A907	C832	G766	A704
G1494	G1422	G1422	U1360	C1297	A1229	C1165	C1103	A1041	A969	C906	U833	G767	U705
G1495	C1423	C1423	A1361	C1298	G1230	G1166	G1104	G1042	C970	C910	C834	A767	A706
G1496	C1424	C1424	G1362	A1299	G1231	A1167	A1105	C1043	C972	C911	U835	A768	C707
G1497	U1425	U1425	C1363	G1300	G1232	A1169	G1106	A1044	C973	C912	C836	G769	G708
U1500	C1426	C1426	A1364	U1301	G1233	A1170	C1107	C1045	G974	A913	C837	C770	G709
C1501	U1427	U1427	U1365	U1302	C1234	G1171	G1108	A1046	A975	A914	C838	G771	G710
A1502	A1428	A1428	U1366	C1303	U1235	C1172	C1109	G1047	A976	A915	U841	U772	G711
A1503	C1429	C1429	G1367	G1304	A1236	A1176	A1110	U1048	G976	C916	C842	G773	G712
G1504	C1430	C1430	C1368	G1305	C1237	G1177	A1111	G1049	A977	C917	U843	G774	A713
G1505	C1431	C1431	A1369	A1306	A1238	G1178	C1112	G1051	A978	A918	C844	G775	G713
U1506	G1432	G1432	G1368	U1307	C1239	G1179	G1113	U1052	C979	A919	C845	G776	G714
A1433	A1433	A1433	U1369	U1308	U1240	A1179	C1114	U1053	C980	U920	U850	A777	A715
A1507	A1434	A1434	G1370	G1309	G1241	A1180	G1115	G1054	U981	U921	C851	G778	A716
G1508	U1435	U1435	C1371	C1310	C1242	G1181	C1116	C1055	U982	C922	G852	C779	G717
C1509	U1436	U1436	G1372	G1311	G1243	A1182	G1117	U1056	A983	C923	G853	A780	G718
G1510	C1437	C1437	C1373	C1244	C1244	G1183	C1118	G1057	C984	C924	G854	A781	C719
G1438	A1374	A1374	C1374	A1245	G1184	G1184	C1119	G1058	G985	G925	G855	A782	G720
U1512	A1375	A1375	U1375	C1246	G1185	G1185	G1120	G1059	G986	G926	C856	C783	G721
A1513	U1376	U1376	U1376	U1247	G1186	G1186	U1121	C1060	G987	G927	C857	C784	A722
C1514	C1377	C1377	A1377	G1317	G1187	G1187	U1122	G1061	G988	G928	G858	G785	U723
C1515	G1442	G1442	C1378	A1318	A1188	A1123	A1123	C1062	G989	G929	A859	G786	G724
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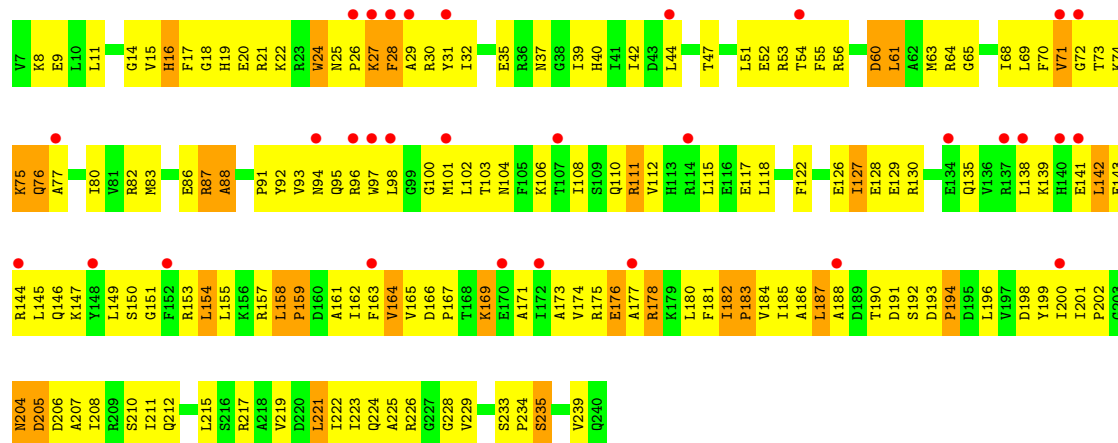
## ● Molecule 1: ribosomal RNA 16S



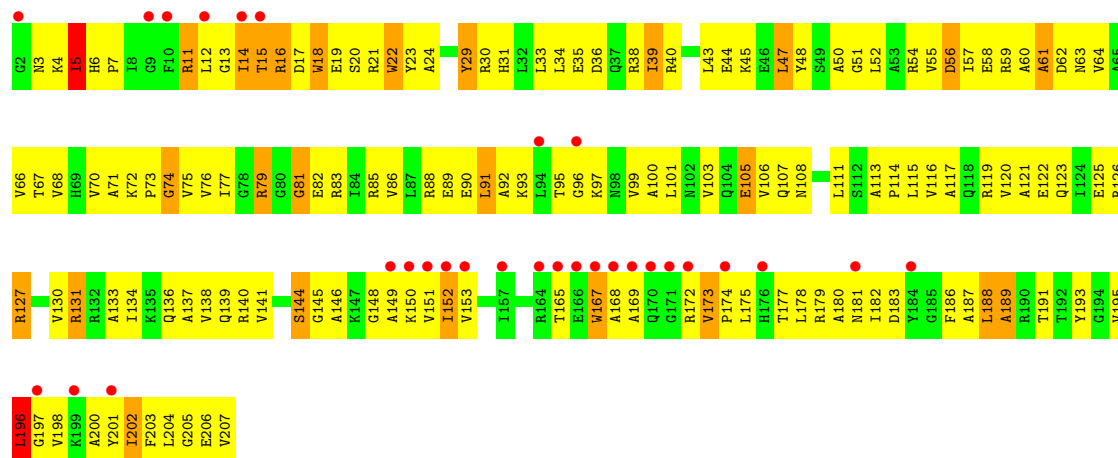




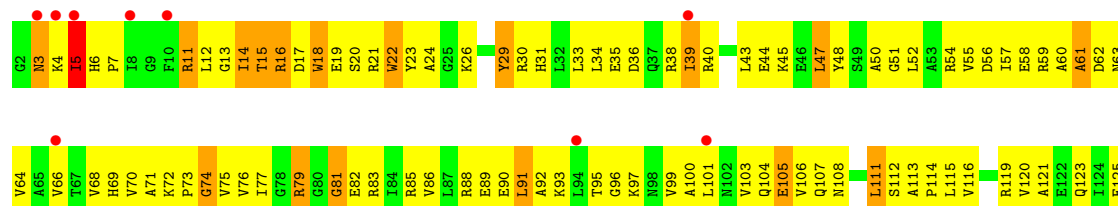
• Molecule 2: 30S ribosomal protein S2



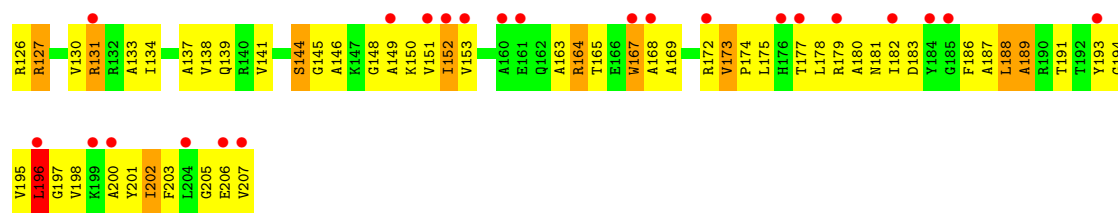
• Molecule 3: 30S ribosomal protein S3



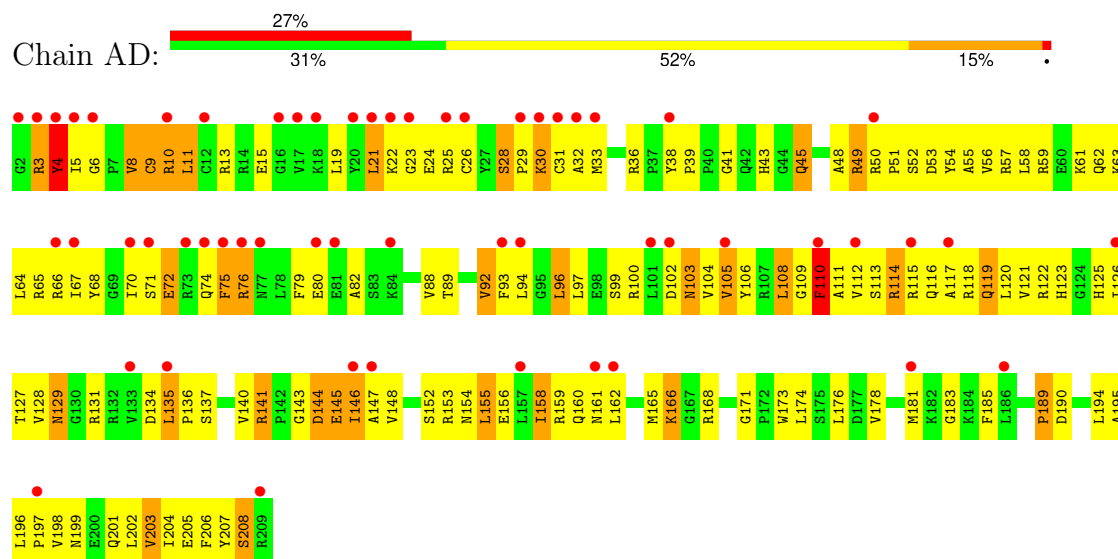
• Molecule 3: 30S ribosomal protein S3



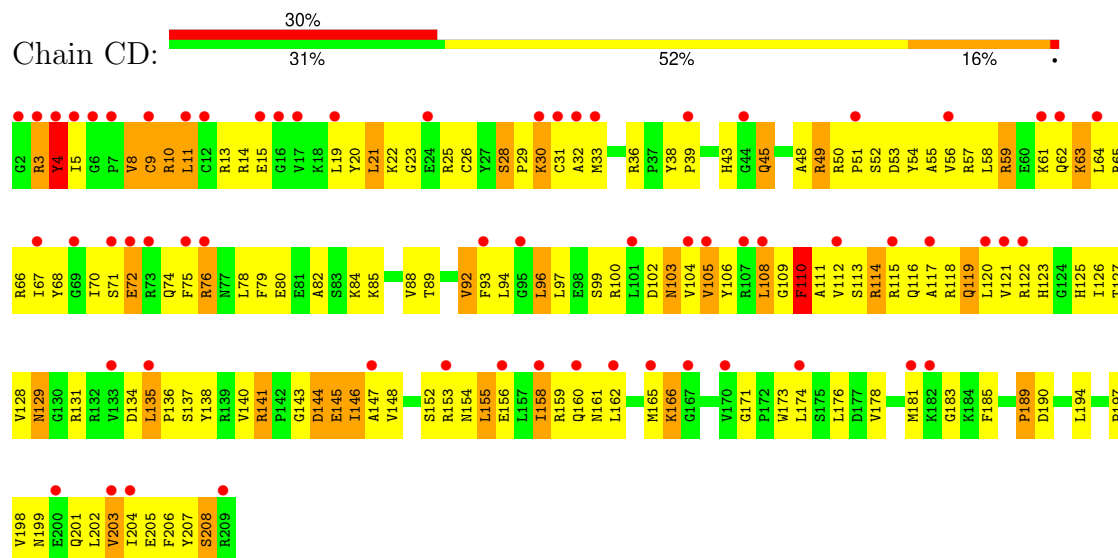




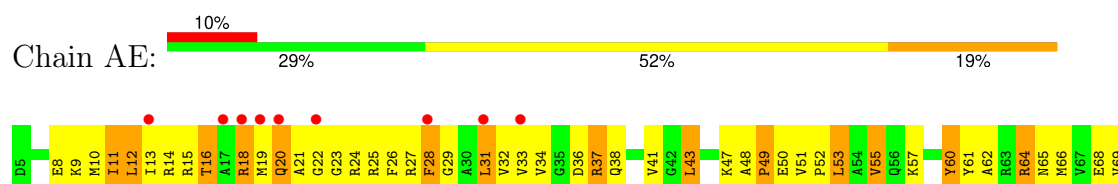
• Molecule 4: 30S ribosomal protein S4

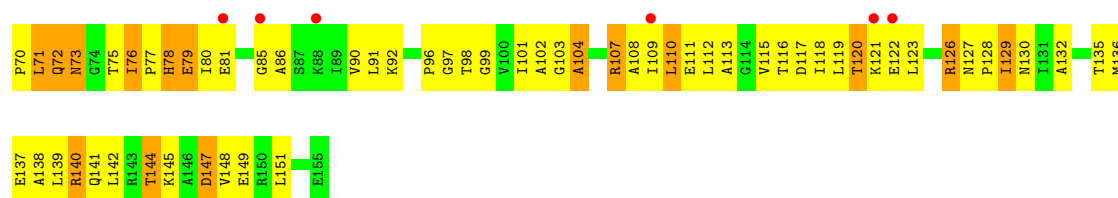


• Molecule 4: 30S ribosomal protein S4

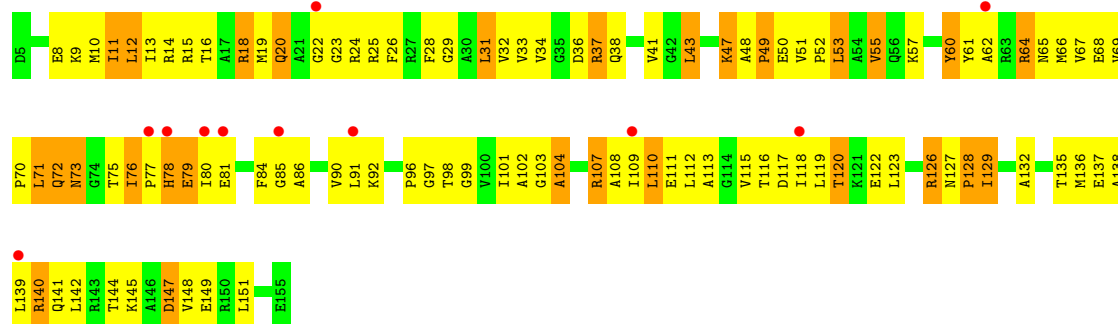


• Molecule 5: 30S ribosomal protein S5

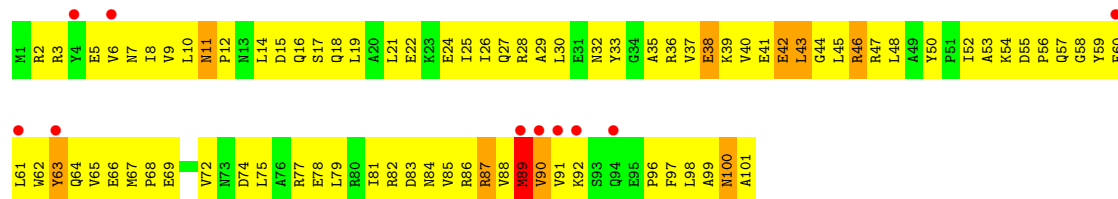




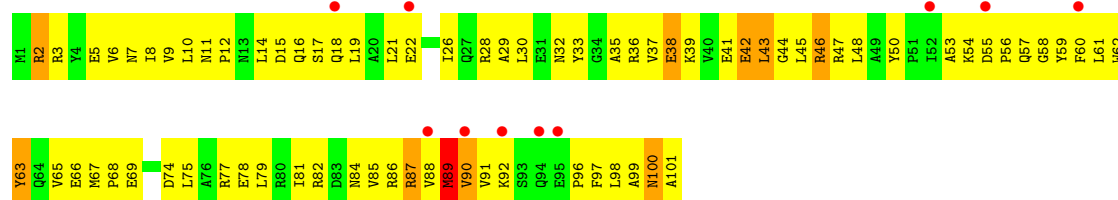
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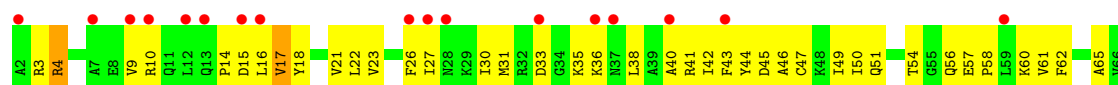
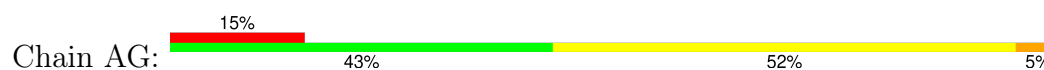
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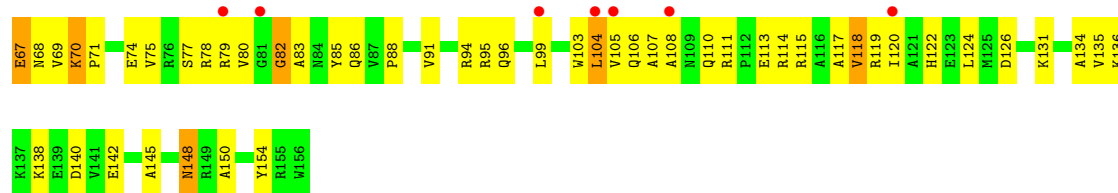


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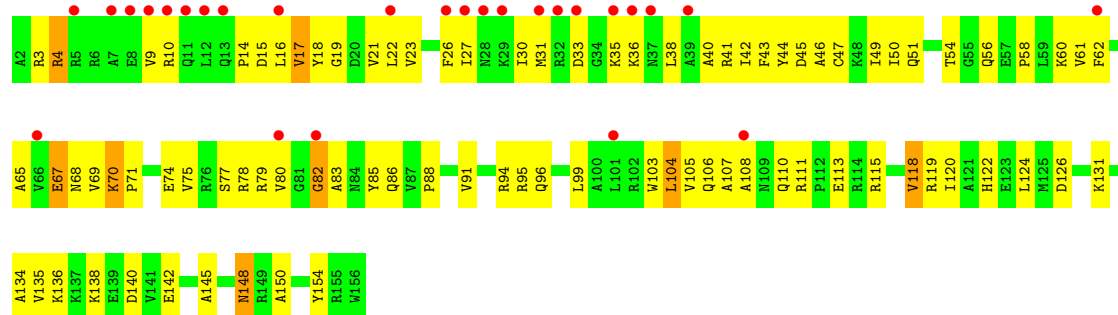


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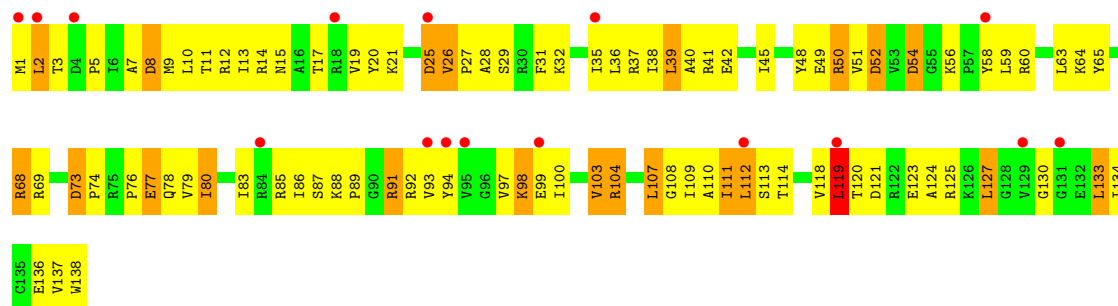




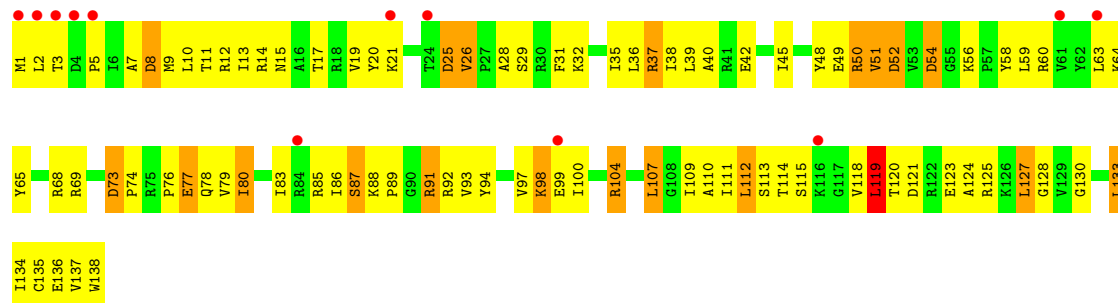
• Molecule 7: 30S ribosomal protein S7



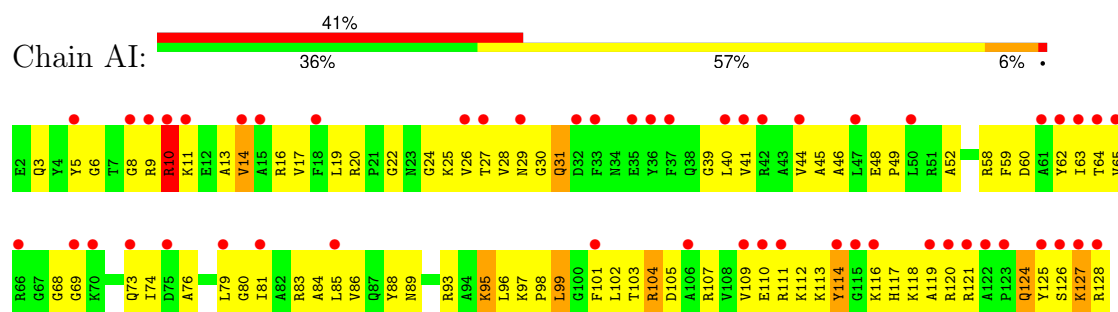
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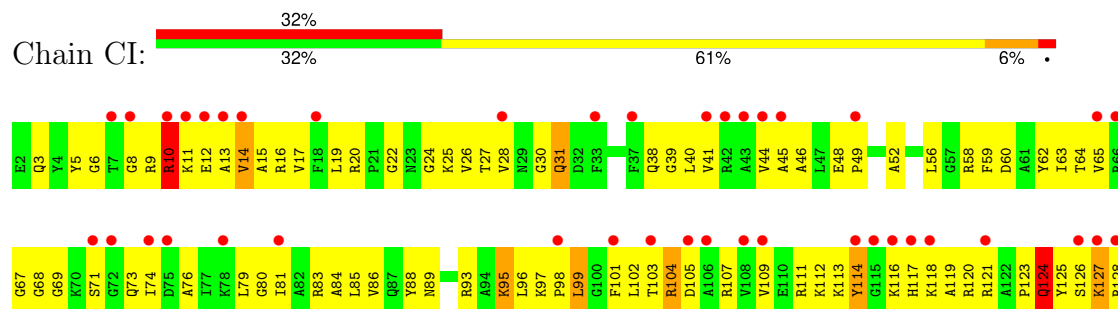
• Molecule 8: 30S ribosomal protein S8



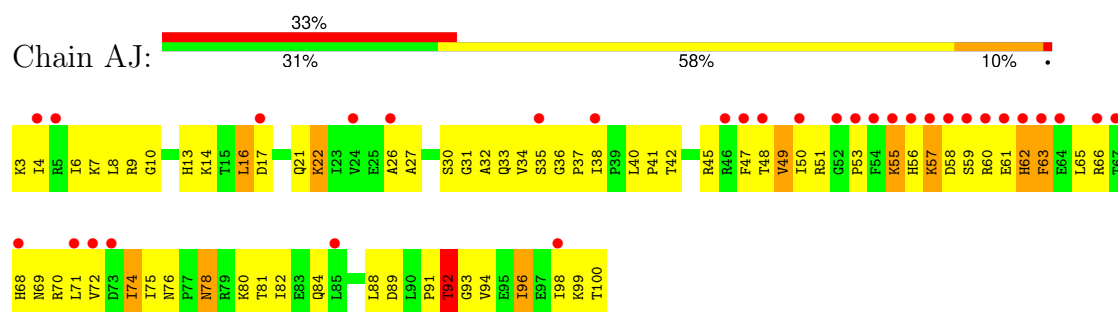
• Molecule 9: 30S ribosomal protein S9



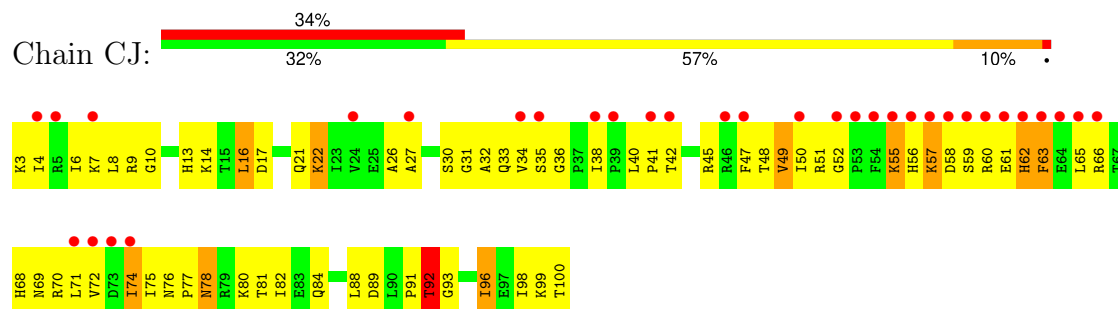
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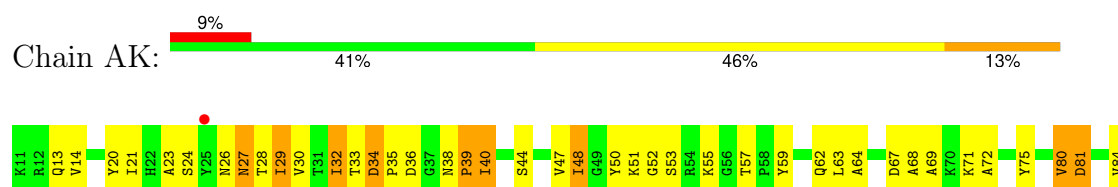
• Molecule 10: 30S ribosomal protein S10

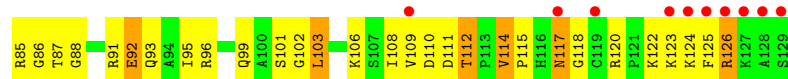


• Molecule 10: 30S ribosomal protein S10

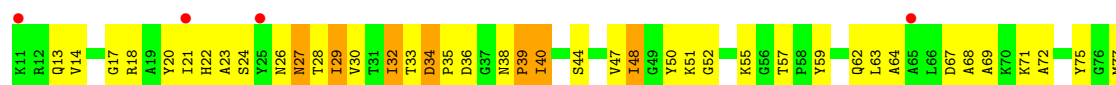


• Molecule 11: 30S ribosomal protein S11

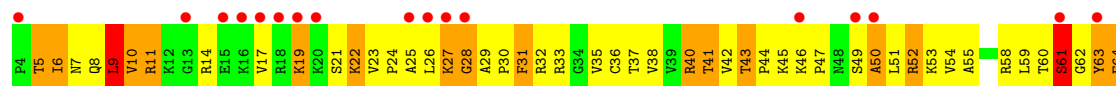




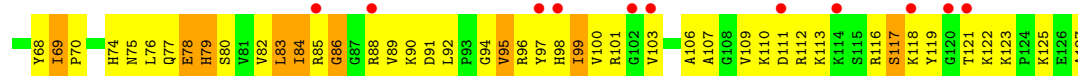
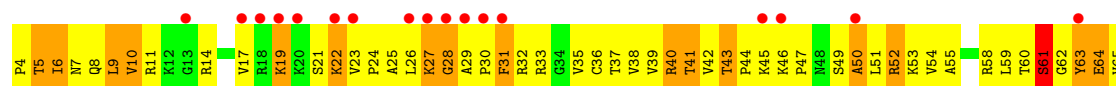
• Molecule 11: 30S ribosomal protein S11



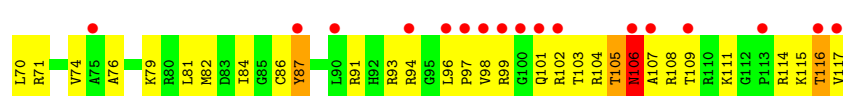
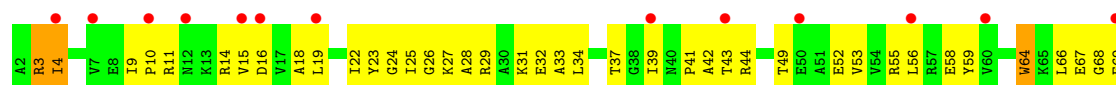
• Molecule 12: 30S ribosomal protein S12



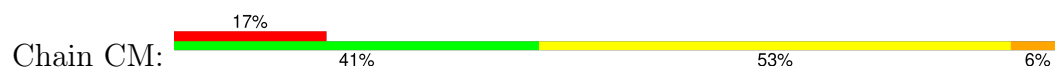
• Molecule 12: 30S ribosomal protein S12

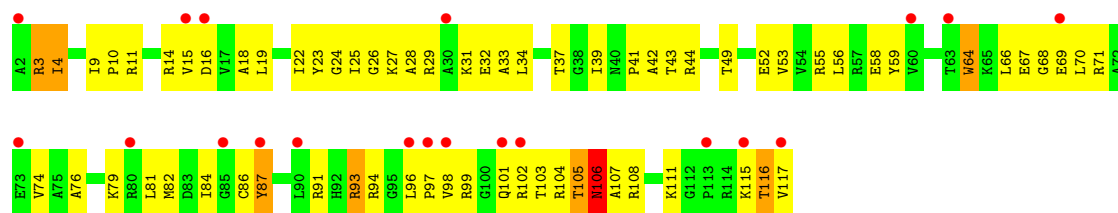


• Molecule 13: 30S ribosomal protein S13

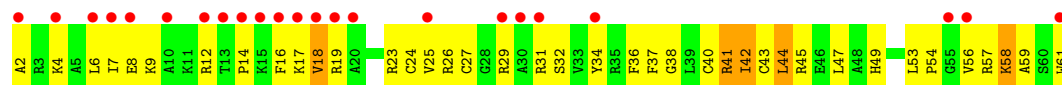


• Molecule 13: 30S ribosomal protein S13

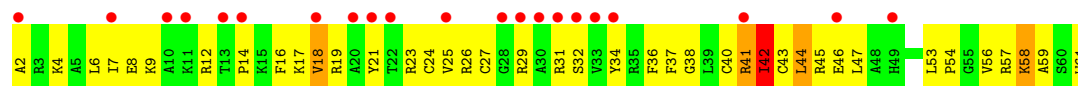




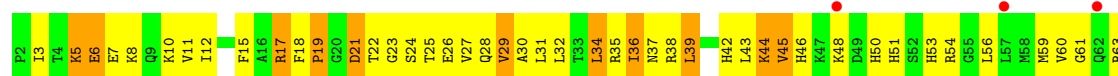
• Molecule 14: 30S ribosomal protein S14 type Z



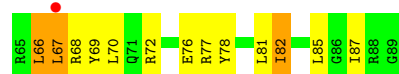
• Molecule 14: 30S ribosomal protein S14 type Z



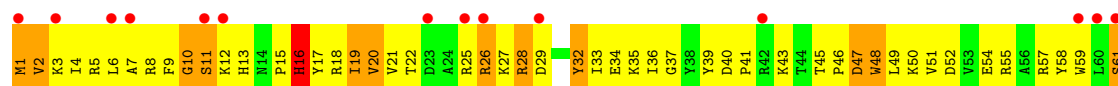
• Molecule 15: 30S ribosomal protein S15

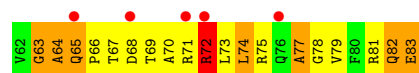


• Molecule 15: 30S ribosomal protein S15

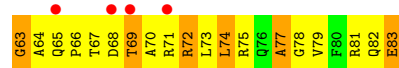
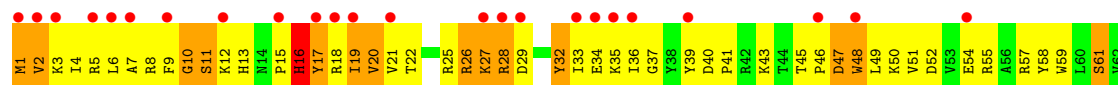


• Molecule 16: 30S ribosomal protein S16

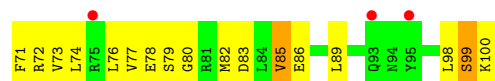
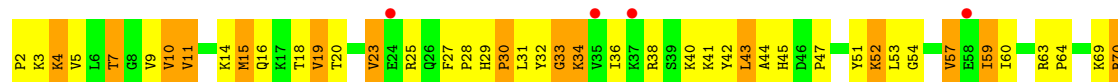
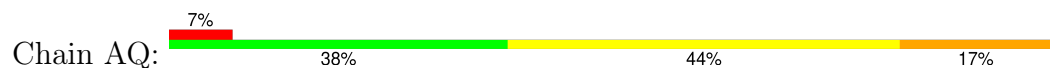




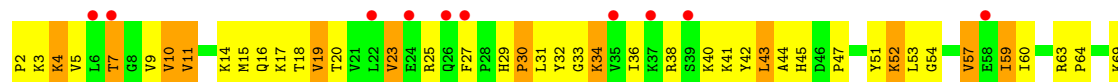
- Molecule 16: 30S ribosomal protein S16



- Molecule 17: 30S ribosomal protein S17



- Molecule 17: 30S ribosomal protein S17

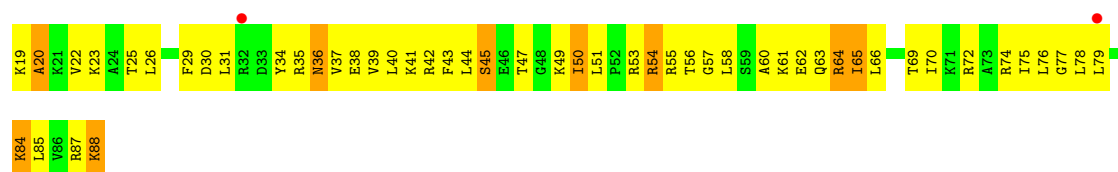


- Molecule 18: 30S ribosomal protein S18

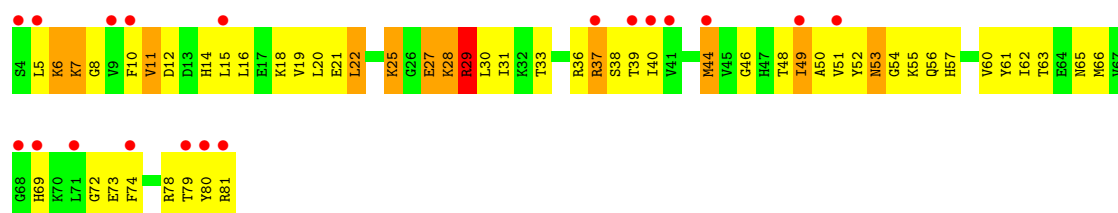


- Molecule 18: 30S ribosomal protein S18

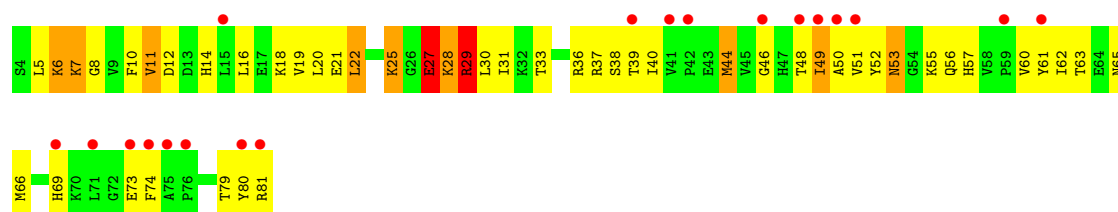




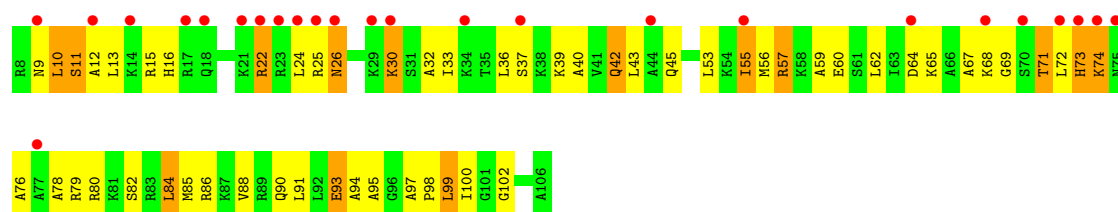
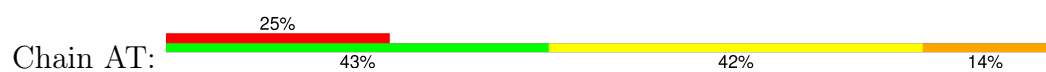
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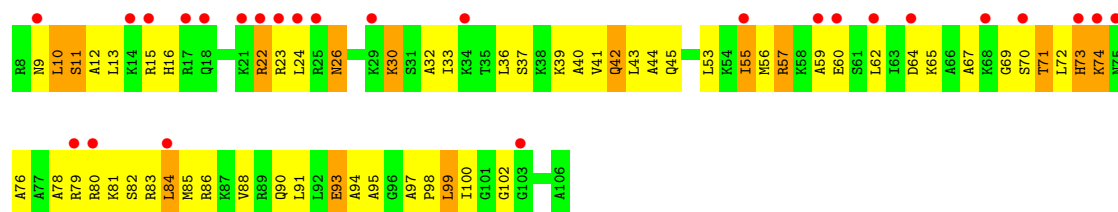
• Molecule 19: 30S ribosomal protein S19



• Molecule 20: 30S ribosomal protein S20

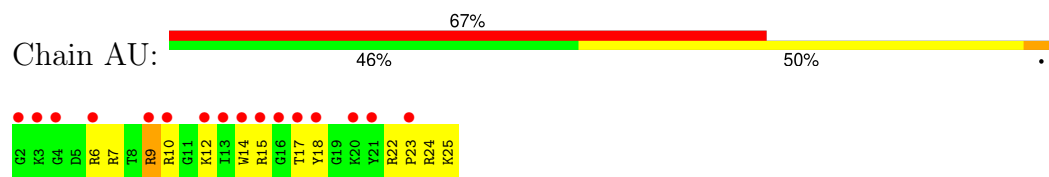


• Molecule 20: 30S ribosomal protein S20

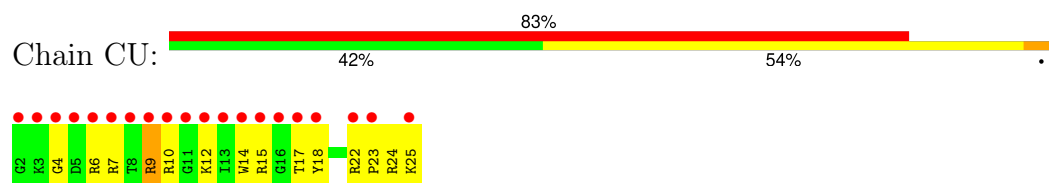




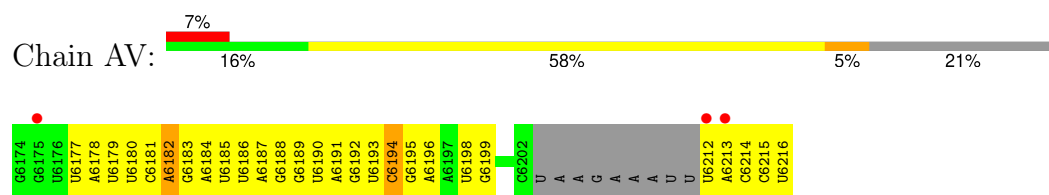
- Molecule 21: 30S ribosomal protein Thx



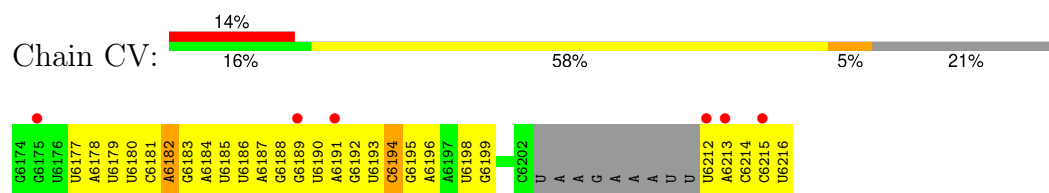
- Molecule 21: 30S ribosomal protein Thx



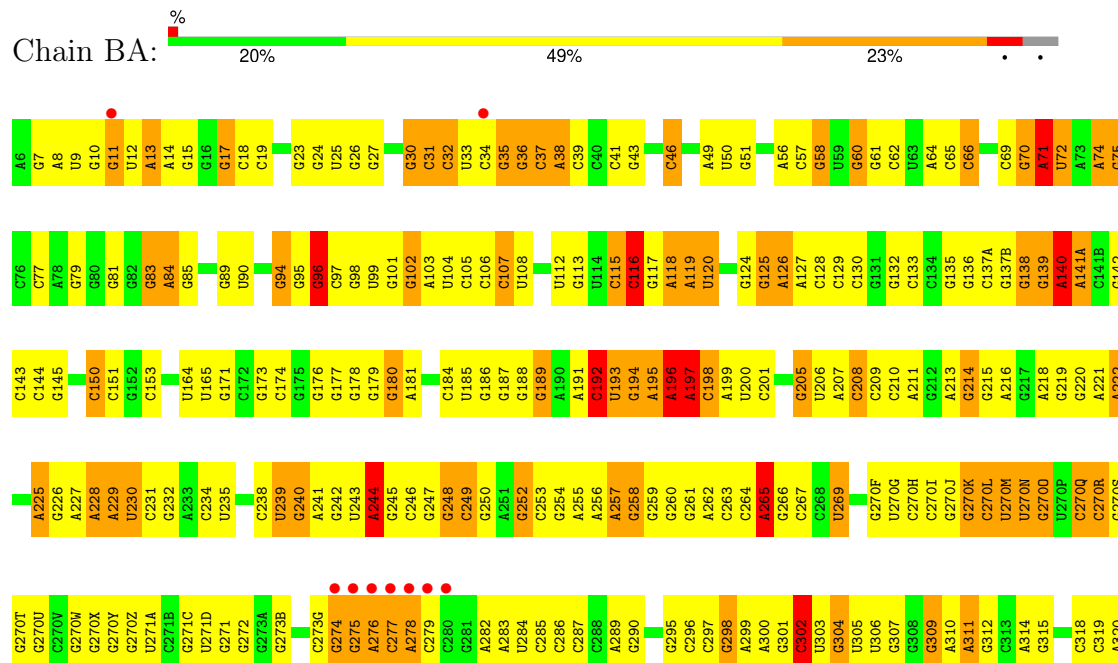
- Molecule 22: RNA (34-MER)



- Molecule 22: RNA (34-MER)

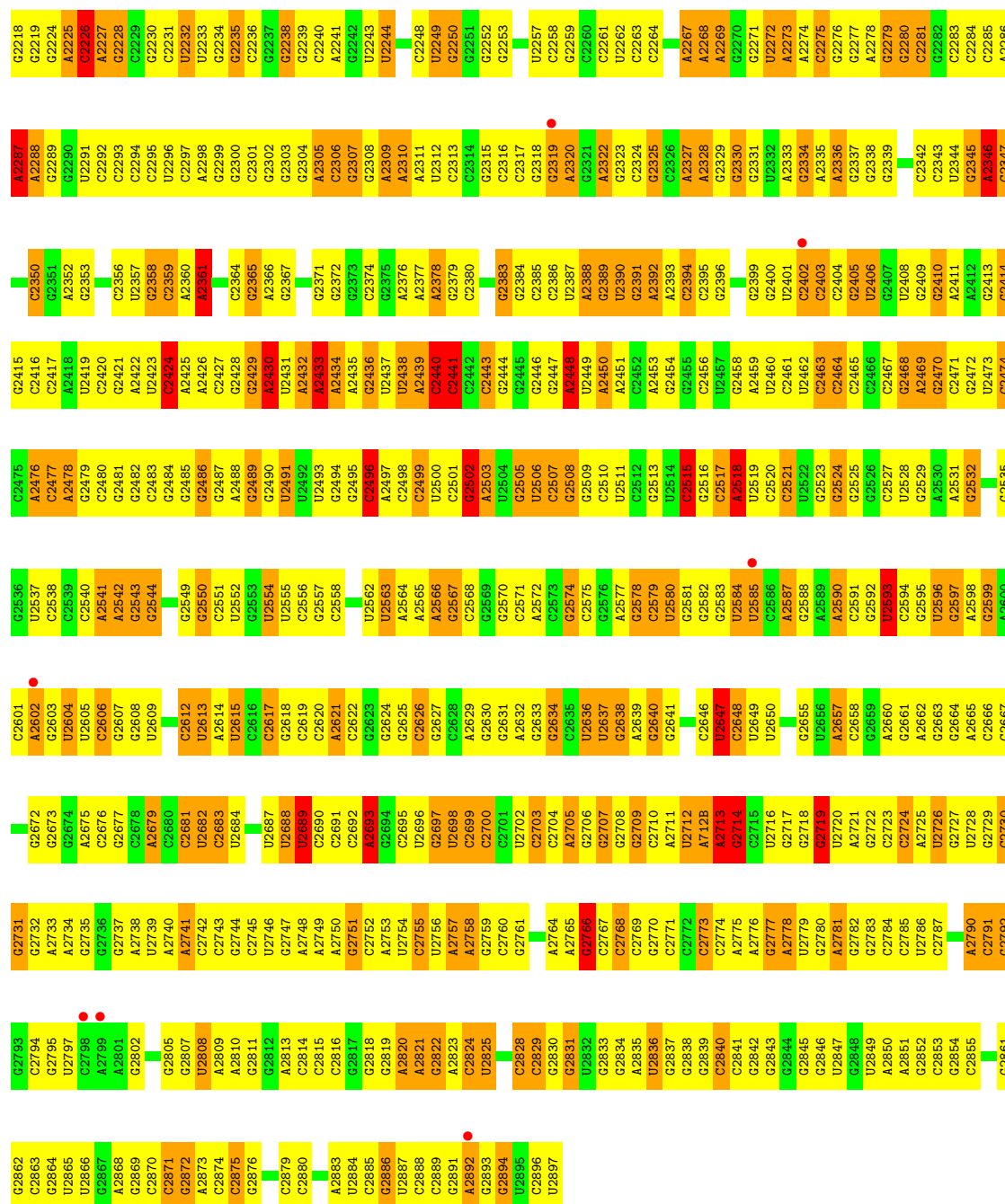


- Molecule 23: 23S ribosomal RNA

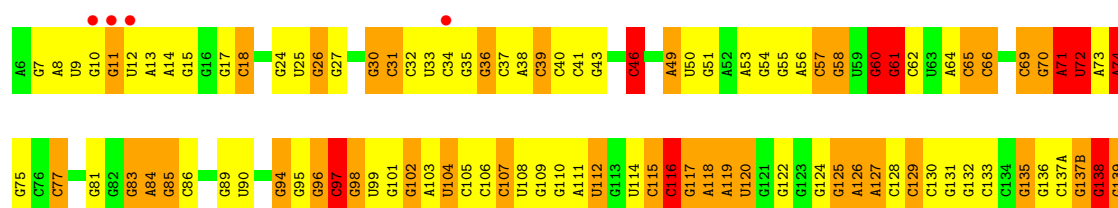
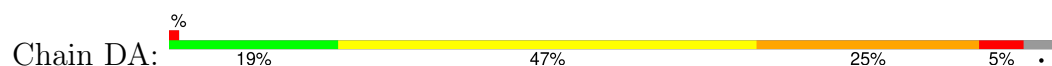


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G1243	A1181	C1118	A	C991	G928	C857	C795	G729	G600	A536	G469	C393	G323
G1244	A1182	G	G	C992	G929	U858	C796	G730	C601	C537	A470	A394	A324
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	C1185	G	U	C994	A933	A861	G799	G733	A603	C541	A472	G396	U328
	G1186	U	G	C995	G934	G862	A800	G734	G604	C542	G473	G397	U329
	G1187	U	G	A996	C935	A863	A801	A735	C605	C544	G474	G398	A330
	U1188	C	C	G997	C936	G864	A802	C736	U607	C545	G475	G399	A331
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	G1190	U	U	U999	G938	A866	A804	G738	A609A	C547	A479	G401	G333
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	G1192	G	G	A1001		U868	C806	U740	C610	A549	A481	C404	C335
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	A1194	A	A	G1003	G942	A870	G808	G745	G612	G551	A483	G406	C337
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	U1205	U	U	U1014	G954		A819	C758	U626	C564	A497	A428	G356
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	A1210	A	A	U1019	A959	A890	C825	U763	G632	U569	A502	C433	
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	G1214	U	U	G1023	U963	C898	A829	G769	G635	G573	A507	G444	G363D
	G1215	G	G	G1024	C964	A899	G830	G770	G636	C574	G508	C364	
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C	C2078	C2078	U2017	U1957	A1889	G1816	C1754	A1670	A1609	C1544	G1478	G1419	U1357
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# • Molecule 23: 23S ribosomal RNA



G1025	C965	A900	G832	G771	U703	U639	G579	A514	G450	C375	U306	C270H	A213	A140
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A1028	G968	C903	A835	U774	A706	G642	G582	C517	G453	C378	A310	G270K	G216	G142
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G1030	C970	U905	G837	G776	G708	A644	G584	U519	G455	U380	G312	U270M	G218	
G1031	C971	G906	C838	A777	U709	C645	G585	G520	C456	G381	C313	U270N	G219	G146
A1032	U907	U907	U839	G778		A646	A586	U524	A457	U384	A314	U270O	G220	U147
G973	C908	C908	C840	U779	G715	G647	C587	U525	G458		G315	G270P	A221	C148
U1033	A909	A909	G841	G780	A716	G648	U588	U526	U459	C385	G316	C270Q	A222	A149
G1034	C974A	A910	G842	A781	G717	G649	C589	A528	A460	C386	G317	C270R	A223	C150
U1035	G975	A911	G843	A782	A718	C650	A590	C527	C461	U387	C318	G270S	G224	G224
G1036	C976	C912	C844	A783	C719	G651		A528	C462	G388	C319	G270T	A225	C151
C1040	G977	U913	G845	A784		U652	G593	A529	G463	C389	A320	G270U	G226	G153
C1041	G978	C914	U846	G785	G723	C653	U594	G530	U464	A390	G321	C270V	A227	
A1045	G979	C915	U847	C786	U724	U654	C595	C531	G465		A322	G270W	A228	U161
A1046	G980	G916	G848	G725	A719	A655	G596	A532	A466	U395	A324	G270X	A229	U164
G1047	A983	A917	A849	U787	G726	U657	U597	G533	G467	G396		G270Y	U230	U165
A1048	C985	A918	C850	A789	A727	C658	G598	U534	G468	G397	U328	G270Z	C231	G171
C1049	G986	G919	U851	G790	G728	C659	G599	C535		G398	U329	U271A	G232	G172
A1050	G987	C923	G852	C791	G729	G660	G600	A536	A472	G399	G330	G271B	A233	C173
G987	G987	C924	G853	G792	C730	G661	C601	C537	G473	G400	A331	U271C	G234	G174
C1052	A988	C925	G854	A793	C731	C662	G602	C539	G474	A401	G332	U271D	U235	
G988	A989	C926	G855	G794	G732	G663	G603	C540	U475		A333	G271E		G175
A990	A990	G928	C856	C795	G733	G664	G604	C541	G476	C404	G334	G271F	G238	G176
G991	G991	G929	C857	C796	A734	C665	C605	G542		U405	C335	G271G	U239	G177
C992	C992	G930	U858	C797	A735	G666	U606	C543	A479	C336	G337	G271H	G240	G178
G993	G993	G931	G859	G798	C736	U667	U607	C544	A480	G407	A340	C273C	A241	G179
C994	C994	A932	U860	G799	G737		A608	G545	G481	G408	U339	G273G	G242	G180
C995	C995	A933	A861	G800	G738	C671	A609A	C546	A482	C409		G274	U243	A181
A996	A996	C935	G862	G801	G739	C672	G609B	A547	A483	C410		G275	G245	C184
G997	G997	C936	A863	A802	U740	C673	G610	A548	C484	G411		G276	G246	U185
G998	G998	U937	C865	G803	G741	C674	C611	G549	C485		C343	C277	G247	G186
U999	U999	G938	A866	A804	G742	A675	G612	C550	C487		G344	G278	G248	G187
C1000	C1000	G939	C867	G805	G743	A676	G615	U553	G488	C414	A345	C279	G249	G188
A1001	A1001	G940	U868	C806	G744	A677	A616	U554	G489	C415		C280	G250	G189
U1002	U1002	A941	G869	U807	A745	C678	G617	G556	G491	C417	G351	G281	A251	A190
G1003	G1003	G942	A870	G808	A746	C679	G618A	U557	A492		G352	A282	G252	A191
C1004	C1004	U943	U871	U810	G747	G680	C618B	G558	G493	U421	G353	A283	C253	C192
A1005	A1005	G944	A872	U811	G748	G681	G619	G559	G494	A422		U284	G254	U193
C1006	C1006	A945	G875	C812	A750	G682	G620	C560	G495	A423	G356	C285	A255	G194
G1007	G1007	G946	G876	U813	A751	C683	A621	G561	G496	G424		C286	A256	A195
A1008	A1008	G947	U877	C814	A752	G684	G622	U562	A497		U358	C287	A257	A196
C1009	C1009	G948	U878	C815	C753	A685	G623	G563	G498	A428	A359	C288	G258	A197
A1010	A1010	C949	G879	C816	C754	G686	G624	C564	U499	A429	G360	A289	G259	C198
C1011	C1011		G880	C817	C755	U688	U626	C565	G500	G430		G290	G260	A199
U1012	U1012	G952	G881	G818	C756		A627	U566	A501	U431	G363A		G261	U200
C1013	C1013	A953	G882	A819		C692	G628	A567	A502	A432	A363B	A294	G262	C201
U1014	U1014	G954			G760	C693	G629	U568	A503	C433	G363C	G295	C263	U202
G1015	G1015	C955	C886	U822	A761	C694	G630	U569	U504	U434	G363D	C296	C264	C203
U1016	U1016	G956	A887	G823	U762	G695	G631	G570	A505	U441		C297	G265	G205
C1017	C1017	A957	C888	A824	G763	G696	A631	A571	G506	C364		A298	U206	U206
U1018	U1018	C958	G889	G825	A764	G697	A632	A572	A507	C365A	A299	C298	G266	
U1019	U1019	A959	A890	G826	G765	C698	G633	G573	G508	A443	G366B	A300	U269	A207
A1020	A1020	A960		U827	C766	C699	G634	C574	C509	C444	G370	G301	C270A	C208
A1021	A1021	C861	A896	U828	U767	A699	C635	A575	C510		A371	C302	A270B	C209
G1022	G1022	G962	C897	A829	G768	G700	G636	U576	U511	A447	U373	U303	G270F	C210
U1023	U1023	U963	C898	G830	G769	G701	A637	G577	U512	U448		G304		A211
A1024	A1024	C964	A899	G831	G770		G638	A578	A513	A449	A374	U305	U270G	G212

G2003	G1799	G1728	A1655	A1529	G1466	U1406	G1346	A1286	G1216	G1151	G
G2004	C1800	A1729	C1656	G1530	C1467	C1407	G1347	A1287	C1217	C1152	U
A2005	G1801	G1733	C1657	C1531	C1468	C1408	G1348	U1288	G1218	C1153	G
A2006	A1802	G1734	C1658	U1535	A1470	C1411	A1349	C1289	G1219	G1154	C
C2007	A1803	C1734	U1659	U1536	G1471	C1412	C1350	C1290	A1220	A1155	G
C2008	A1804	C1735	C1660	A1536	A1472	C1413	C1351	C1291	C1221	A1156	U
G2009	U1805	G1743	G1661	C1537	A1472	G1414	U1352	U1292	C122A	A1157	A
G2010	C1806	C1742	C1662	G1538	G1475	U1415	A1353	C1293	C1222	C1158	A
U2011	G1811	G1743	C1663	U1539	C1476	U1416	G1355	U1294	G1223	U1159	U
A1884	A1812	G1746	A1664	U1540	C1476	C1417	G1356	G1295	C1224	A1160	A
A1952	C1886	G1747	A1665	U1541	A1477	C1418	U1357	G1296	G1225	C1161	G
A1953	G1813	G1748	G1666	G1542	G1478	G1419	U1358	G1297	A1226	G1162	C
A2014	G1814	A1749	G1667	A1543	G1479	A1419	G1358	C1298	G1227	U1163	U
U1955	A1815	G1750	A1668	C1544	G1480	U1420	A1359	G1299	G1227	G1164	C
U1956	A1816	C1754	A1669	A1545	U1481	G1421	A1360	U1300	C1230	U1165	A
C1957	G1817	G1755	C1670	A1546	G1483	G1422	G1361	A1301	G1231	C1166	C1104
C1958	U1818	A1756	U1671	C1548	G1484	G1423	C1362	A1302	G1232	U1167	U1105
A1890	A1819	G1757	C1672	C1549	G1485	G1424	C1363	G1303	C1233	G1168	G1106
A2020	A1820	U1757	U1673	C1548	A1486	G1425	G1364	C1304	U1234	G1169	G1107
C2021	A1821	G1758	G1674	C1549	G1487	G1426	A1365	C1305	G1235	G1170	U1108
U2022	G1822	C1759	C1675	U1550	G1488	G1427	A1366	C1306	G1236	G1171	C1109
C1963	U1823	A1759	A1677	G1551	U1489	G1428	G1368	A1307	G1237	G1172	G1110
U1998	G1824	A1760	C1678	G1552	A1490	G1429	A1367	A1308	U1240	A1174	A1111
G1964	C1825	G1761	U1679	A1553	G1491	C1430	G1369	G1309	U1241	U1175	G1112
A1900	A1825	A1762	U1680	A1554	G1492	U1431	C1370	G1310	A1241	U1176	U1113
C1967	G1826	G1763	G1681	G1555	C1493	C1432	G1371	G1311	A1242	A1177	G1114
G1968	C1827	G1764	G1682	C1556	A1494	U1433	U1372	U1312	G1243	C1178	G1115
A1969	U1828	U1766	C1683	C1557	A1495	A1434	G1373	U1313	G1248	C1179	G1116
C1970	A1829	C1767	C1684	C1558	A1496	G1435	G1374	C1314	U1248	G1180	G1117
A1970	G1830	U1768	C1685	U1559	U1497	G1436	C1375	C1315	U1249	C1181	G1118
C2031	G1831	U1769	C1686	G1560	C1498	C1437	G1376	G1316	G1252	U1182	U1119
A1972	C1832	G1770	G1687	C1561	C1499	U1438	G1377	A1317	A1253	G1183	C1121
G1973	U1833	C1771	U1688	C1562	G1500	A1439	A1378	C1318	A1254	G1184	G1122
C1974	G1834	C1772	A1689	U1566	C1501	G1440	G1379	G1319	U1255	C1185	C1123
U1975	A1835	A1773	C1691	A1567	C1502	G1441	G1380	C1320	G1256	G1186	C1124
C1976	C1837	G1774	U1691	G1568	U1503	G1442	G1381	A1321	C1257	G1187	G1125
A1915	G1838	U1775	U1692	C1569	C1504	G1443	G1382	A1322	U1258	U1188	A1126
U1916	G1839	G1776	U1693	A1570	C1505	G1444	C1383	U1323	G1259	A1127	A1127
C1917	U1840	U1777	C1694	C1571	C1506	A1445	A1384	G1324	C1261	G1190	A1128
A1918	U1841	U1778	G1697	A1572	A1508	C1446	G1385	G1325	A1262	A1129	A1129
C1919	G1842	U1779	A1698	C1573	A1509	C1447	G1386	U1326	U1263	G1192	U1130
G1984	C1843	A1780	G1699	U1576	A1510	G1448	C1387	G1327	G1264	G1193	G1131
A1985	G1844	G1781	U1700	U1577	A1511	A1498	G1388	G1328	A1265	A1194	A1132
C2045	U1845	C1782	C1708	C1578	C1512	G1449	G1389	U1329	G1266	U1133	U1133
G2046	G1846	A1783	G1703	U1578	C1513	C1450	U1390	C1330	U1267	C1135	C1135
U2047	A1847	U1784	G1704	C1581	U1514	C1451	A1392	A1331	A1268	G1136	G1136
G2048	C1848	A1785	G1705	C1582	C1515	C1452	A1393	G1332	A1269	G1137	G1137
C2049	U1850	G1786	U1706	C1583	U1516	A1453	A1394	C1333	C1270	G1138	G1138
C2050	C1851	U1787	G1707	A1584	G1517	U1454	U1395	G1334	G1271	A1204	A1204
A2051	G1852	C1788	C1708	C1585	C1518	G1455	A1396	U1335	A1272	U1205	U1205
G1928	A1853	A1789	U1709	A1586	G1519	G1456	U1397	A1336	U1273	C1206	C1206
C1929	U1854	C1790	C1710	A1587	U1520	A1457	U1398	G1337	A1274	U1141	U1141
G1930	G1855	A1791	C1711	C1588	G1521	G1458	C1398	G1338	A1275	C1207	C1207
U1931	C1856	G1792	C1712	C1589	G1522	G1459	C1399	G1339	A1276	G1208	A1148
A1932	G1857	U1793	U1716	U1590	U1523	A1460	G1401	U1340	A1210	A1143	A1143
C1933	G1858	U1794	G1717	G1591	G1524	G1461	G1402	U1341	C1211	C1145	C1145
C1934	A1859	C1795	G1718	C1592	G1525	C1462	C1403	A1342	U1282	G1212	G1212
G1935	U1860	U1796	G1725	G1593	G1526	C1463	C1404	G1343	A1284	A1213	A1213
A1936	C1862	C1797	G1726	G1594	G1527	G1464	C1404	G1344	G1283	G1214	G1214
G2001	U1862	U1798	G1727	G1595	A1528	G1465	U1405	C1345	G1285	G1149	C1150
A2002	G1863	U1798	U1727	G1595	A1528	G1465	U1405	C1345	G1285	G1149	C1150



Chain BB:

Category	Percentage
Red	8%
Green	16%
Yellow	66%
Orange	17%

U1 C2 C3 C4 C5 C6 C7 C8 C9 C10 C11 C12 C13 C14 C15 C16 C17 C18 C19 C20 C21 C22 C23 C24 C25 C26 C27 C28 C29 C30 C31 C32 C33 C34 C35 C36 C37 C38 C39 C40 C41 C42 C43 C44 C45 C46 C47 C48 C49 C50 C51 C52 C53 C54 C55 C56 C57 C58 C59 C60

Category	Percentage
Red	8%
Green	16%
Yellow	66%
Orange	17%

G61 G62 G63 G64 G65 G66 G67 G68 G69 G70 G71 G72 G73 G74 G75 G76 G77 G78 G79 G80 G81 G82 G83 G84 G85 G86 G87 G88 G89 G90 G91 G92 G93 G94 G95 G96 G97 G98 G99 G100 G101 G102 G103 G104 G105 G106 G107 G108 G109 G110 G111 G112 G113 G114 G115 G116 G117 G118

Category	Percentage
Red	8%
Green	16%
Yellow	66%
Orange	17%

Chain DB:

Category	Percentage
8%	8%
17%	17%
64%	64%
18%	18%

Chain BC:

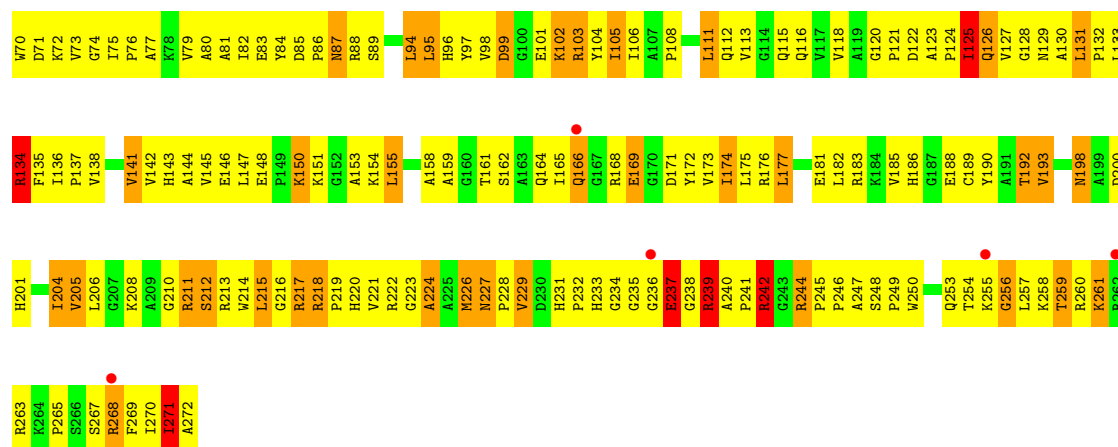
Category	Percentage
K258	7%
T259	23%
R260	56%
K261	19%
R262	7%
R263	23%
R264	56%
P265	19%
S266	7%
S267	23%
R268	56%
P269	19%
L270	7%
L271	23%
A272	56%
K68	7%
R69	23%
W70	56%
D71	19%
K72	7%
W73	23%
G74	56%
I75	19%
P76	7%
A77	23%
K78	56%
W79	19%
A80	7%
A81	23%
E82	56%
E83	19%
E84	7%
D85	23%
P86	56%
N87	19%
R88	7%
A93	23%
L94	56%
L95	19%
H96	7%
Y97	23%
V98	56%
D99	19%
G100	7%
E101	23%
K102	56%
K103	19%
L104	7%
Y105	23%
I106	56%
A107	19%
P108	7%
L111	23%
Q112	56%
V113	19%
G114	7%
Q115	23%
Q116	56%
V117	19%
V118	7%
A119	23%
G120	56%
P121	19%
D122	7%
A123	23%
P124	56%
I125	19%
Q126	7%
V127	23%
G128	56%
N129	19%
A130	7%
L131	23%
L132	56%
L133	19%
R134	7%
F135	23%
I136	56%
P137	19%
V138	7%
G139	23%
T140	56%
V141	19%
V142	7%
H143	23%
A144	56%
E145	19%
E146	7%
L147	23%
E148	56%
F149	19%
K150	7%
K151	23%
G152	56%
A153	19%
K154	7%
L155	23%
A156	56%
R157	19%
A158	7%
A159	23%
G160	56%
T161	19%
S162	7%
A163	23%
Q164	56%
T165	19%
Q166	7%
G167	23%
R168	56%
E169	19%
G170	7%
D171	23%
V172	56%
V173	19%
L174	7%
L175	23%
R176	56%
L177	19%
E181	7%
L182	23%
R183	56%
K184	19%
A185	7%
H186	23%
G187	56%
E188	19%
C189	7%
A190	23%
A191	56%
T192	19%
L193	7%
Q253	23%
T254	56%
K255	19%
G256	7%
L257	23%

Chain DC:

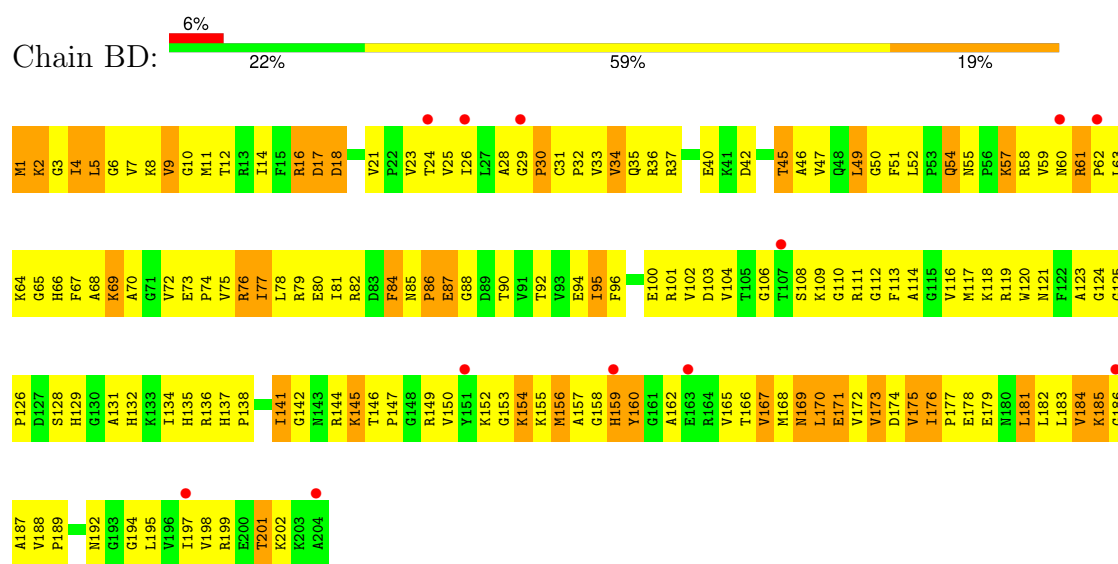
5% 24% 56% 18%

A2 V3 K4 P8 Y9 T10 S12 R13 R14 F15 M16 T17 F21 I24 T25 K26 T27 E28 P29 E30 K31 S32 L33 V34 K35 P36 L37 K38 K39 T40 G41 G42 R43 N44 N45 Q46 G47 R48 L49 T50 V51 R52 F53 R54 H58 K59 R60 L61 Y62 R63 I64 F67 K68 R69

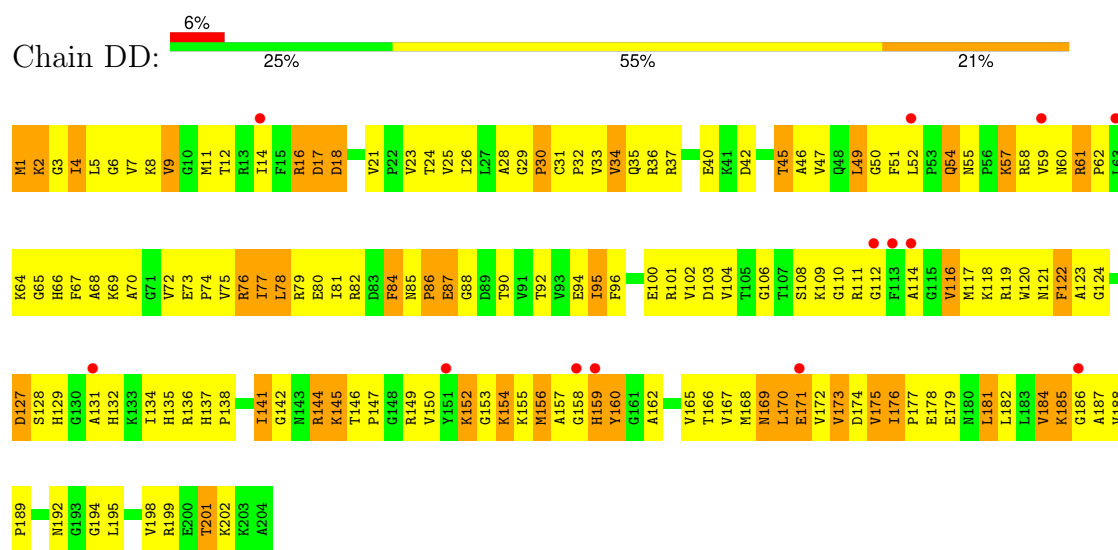




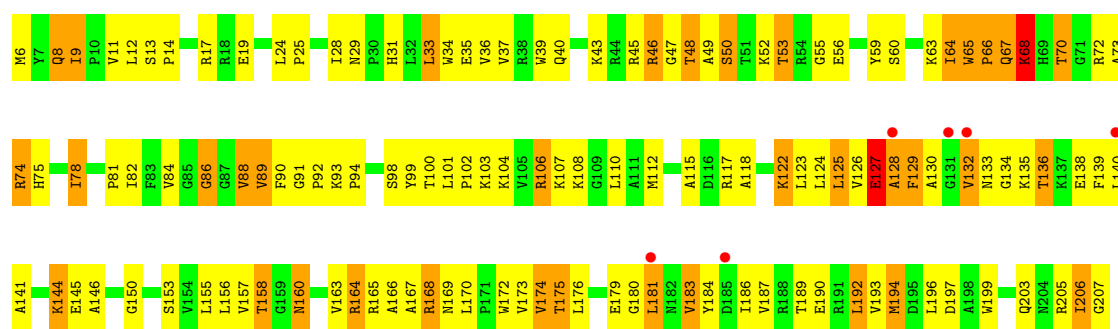
• Molecule 26: 50S ribosomal protein L3



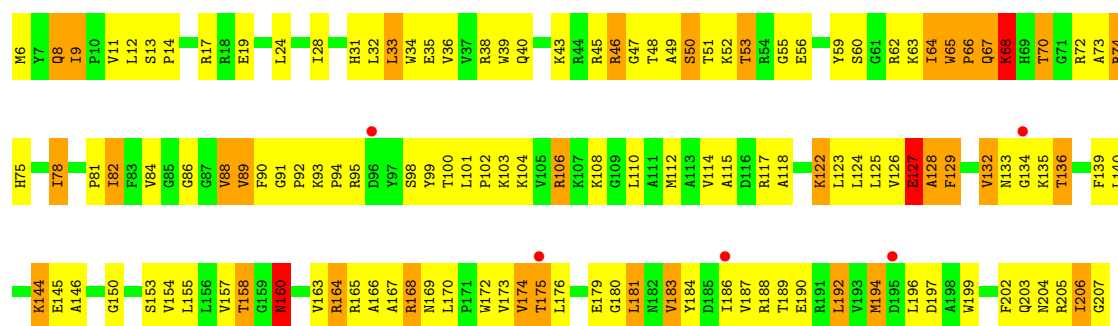
• Molecule 26: 50S ribosomal protein L3



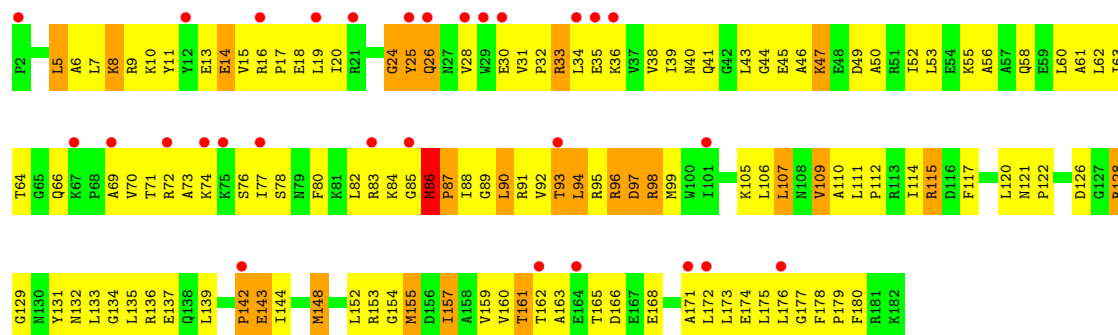
• Molecule 27: 50S ribosomal protein L4



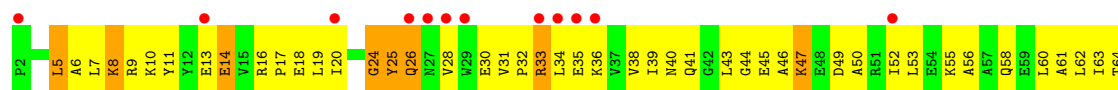
• Molecule 27: 50S ribosomal protein L4

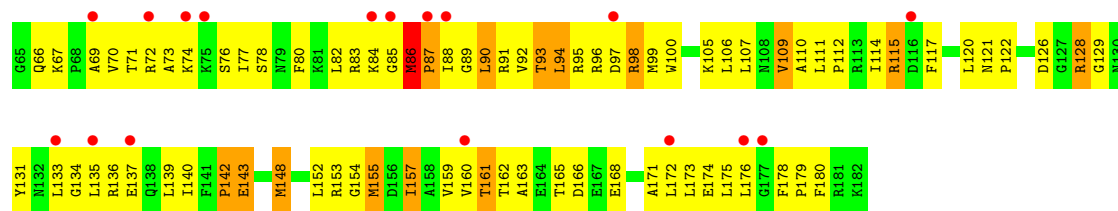


• Molecule 28: 50S ribosomal protein L5

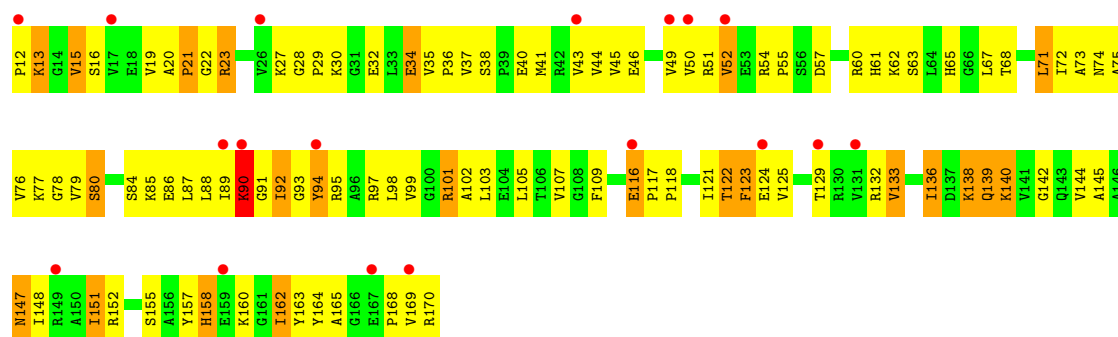


• Molecule 28: 50S ribosomal protein L5

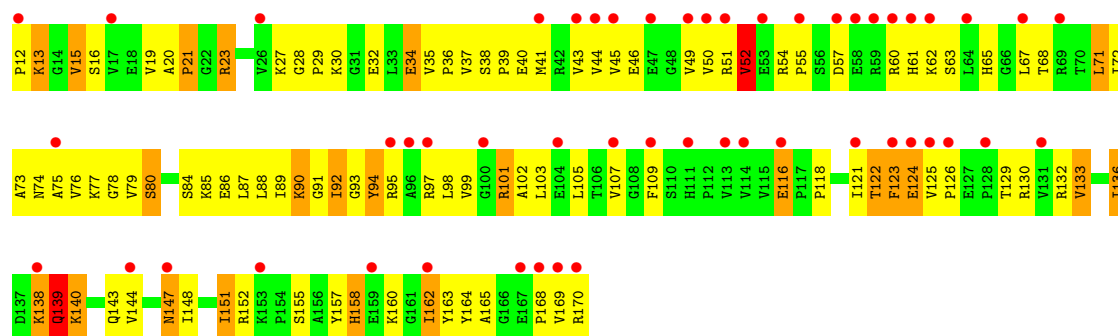




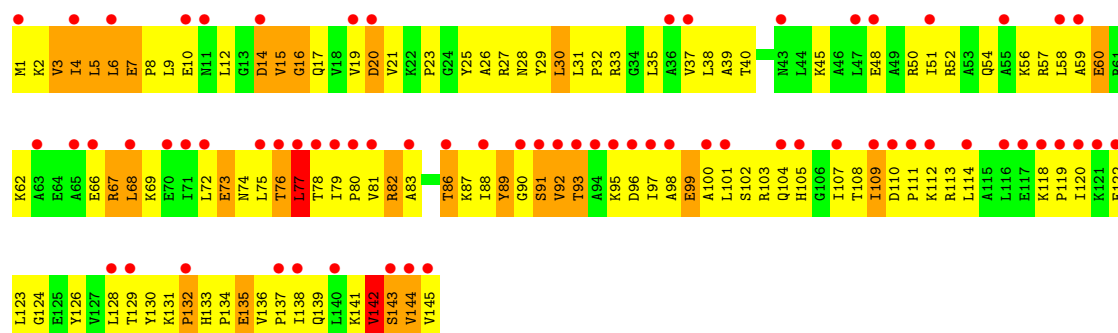
• Molecule 29: 50S ribosomal protein L6



• Molecule 29: 50S ribosomal protein L6



• Molecule 30: 50S ribosomal protein L9



Chain DH:

Category	Percentage
Red	45%
Green	24%
Yellow	54%
Orange	20%

Labels (from top to bottom):

- M1, K2, V3, I4, L5, L6, E7, L9, E10, M11, L12, G13, D14, V15, G16, Q17, V18, V19, D20, V21, K22, G24, Y25, A26, R27, N28, Y29, L30, P32, R33, L35, A36, V37, L38, A39, T40, K45, E48, A49, R50, I51, R52, K56, R57, L58, A59, E60, R61, K62, A63, E64, A65, E66
- R67, L68, K69, E70, I71, L72, E73, N74, L75, T76, R77, T78, I79, P80, V81, R82, A83, G84, E85, R86, K87, L88, Y89, G90, S91, Y92, T93, A94, K95, D96, I97, A98, E99, A100, L101, S102, R103, Q104, H105, G106, I107, T108, I109, D110, P111, K112, R113, L114, A115, L116, E117, K118, P119, T120, K121, E122, L123, G124, A125, Y126
- V127, L128, T129, V130, K131, P132, H133, E135, V136, P137, L138, Q139, L140, K141, V142, V143, V144, V145
- R67, L68, K69, E70, I71, L72, E73, N74, L75, T76, R77, T78, I79, P80, V81, R82, A83, G84, E85, R86, K87, L88, Y89, G90, S91, Y92, T93, A94, K95, D96, I97, A98, E99, A100, L101, S102, R103, Q104, H105, G106, I107, T108, I109, D110, P111, K112, R113, L114, A115, L116, E117, K118, P119, T120, K121, E122, L123, G124, A125, Y126

Chain BI:

Color	Percentage
Red	17%
Green	32%
Yellow	17%
Grey	51%

A horizontal bar chart titled "Chain BI:" showing four categories represented by different colors: Red (17%), Green (32%), Yellow (17%), and Grey (51%). The bars are stacked horizontally from left to right.

Chain DI:

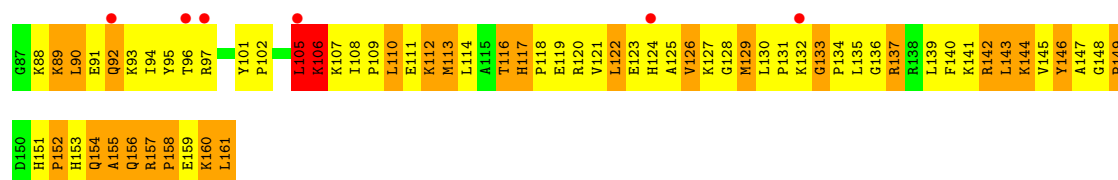
Amino Acid	Chain DI (%)
N3	9%
K4	32%
R5	32%
N6	32%
V7	32%
E8	32%
L9	32%
K14	32%
K15	32%
G22	32%
SER	32%
PHE	32%
PHI	32%
LEU	32%
VAL	32%
ASN	32%
TYR	32%
GLN	32%
GLY	32%
LEU	32%
PRO	32%
ALA	32%
LYS	32%
GLU	32%
THR	32%
HIS	32%
ALA	32%
LEU	32%
ARG	32%
GLN	32%
ALA	32%
LEU	32%
LEU	32%
LYS	32%
GLN	32%
ASN	32%
GLY	32%
ALA	32%
ARG	32%
LEU	32%
PHE	32%
VAL	32%
ALA	32%
LYS	32%
N55	32%
T57	32%
L58	32%
T59	32%
R60	32%
L61	32%
A62	32%
L63	32%
K64	32%
F65	32%
L66	32%

Chain BJ:

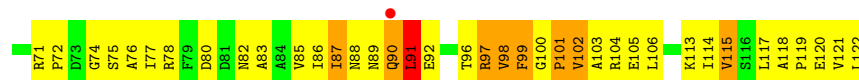
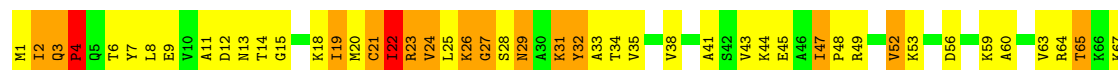
Category	Value
P149	4%
D150	18%
H151	55%
P152	25%
H153	0%
Q154	0%
Q156	0%
Q157	0%
P158	0%
E159	0%
K160	0%
L161	0%
T86	0%
G87	0%
K88	0%
K89	0%
L90	0%
E91	0%
Q92	0%
K93	0%
L94	0%
Y95	0%
T96	0%
R97	0%
Y101	0%
P102	0%
L103	0%
K106	0%
K107	0%
L108	0%
P109	0%
L110	0%
E111	0%
A112	0%
M113	0%
L114	0%
A115	0%
T116	0%
H117	0%
P118	0%
E119	0%
R120	0%
V121	0%
L122	0%
E123	0%
H124	0%
A125	0%
P126	0%
K127	0%
G128	0%
M129	0%
L130	0%
P131	0%
K132	0%
G133	0%
P134	0%
L135	0%
G136	0%
R137	0%
L138	0%
P139	0%
F140	0%
K141	0%
R142	0%
L143	0%
L144	0%
V145	0%
Y146	0%
A147	0%
C148	0%
K25	0%
T26	0%
Y27	0%
K30	0%
Q31	0%
V32	0%
E33	0%
P34	0%
R35	0%
W36	0%
V37	0%
L38	0%
L39	0%
D40	0%
A41	0%
E42	0%
G43	0%
K44	0%
T45	0%
L46	0%
G47	0%
R48	0%
L49	0%
A50	0%
T51	0%
K52	0%
E53	0%
A54	0%
T55	0%
L56	0%
L57	0%
R58	0%
G59	0%
K60	0%
H61	0%
P62	0%
D63	0%
D64	0%
W65	0%
T66	0%
P67	0%
N68	0%
V69	0%
A70	0%
M71	0%
G72	0%
D73	0%
F74	0%
V75	0%
V76	0%
V77	0%
N78	0%
N79	0%
A80	0%
D81	0%
K82	0%
L83	0%
R84	0%
V85	0%

Chain DJ:

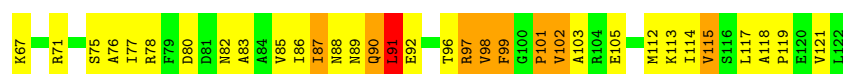
Category	Percentage
K25	6%
T26	19%
Y27	54%
K30	26%
Q31	
V32	
E33	
V36	
V37	
L38	
I39	
D40	
A41	
E42	
G43	
K44	
L45	
L46	
G47	
R48	
L49	
A50	
T51	
K52	
I53	
A54	
T55	
L56	
L57	
R58	
G59	
K60	
H61	
R62	
P63	
D64	
B65	
T66	
P67	
N68	
V69	
A70	
M71	
G72	
D73	
F74	
V75	
V76	
V77	
V78	
N79	
A80	
D81	
K82	
I83	
R84	
B85	
V86	



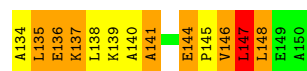
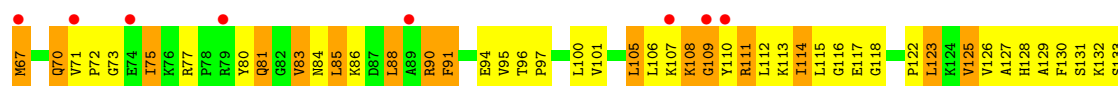
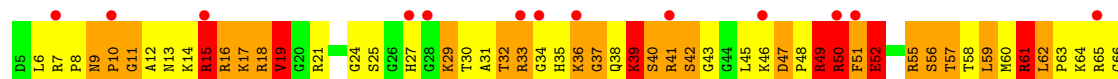
- Molecule 33: 50S ribosomal protein L14



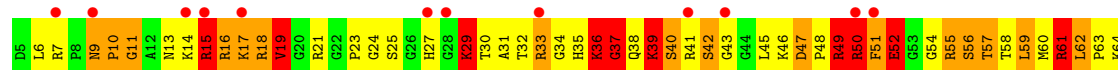
- Molecule 33: 50S ribosomal protein L14

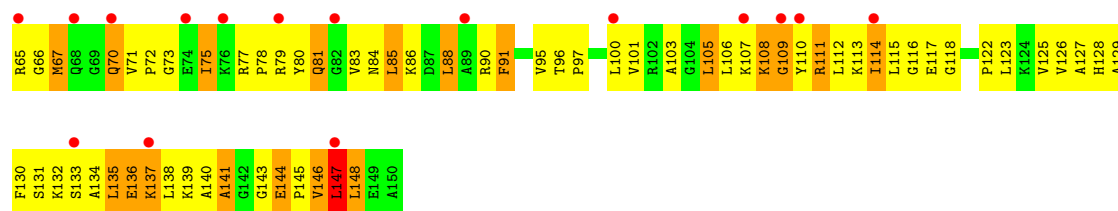


- Molecule 34: 50S ribosomal protein L15

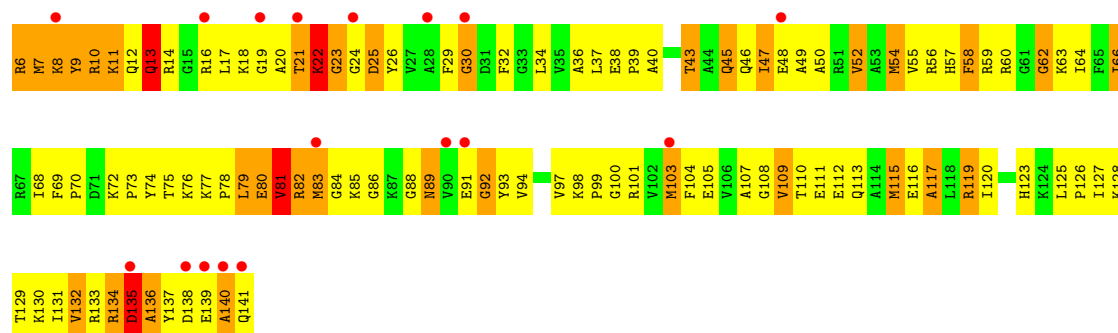


- Molecule 34: 50S ribosomal protein L15

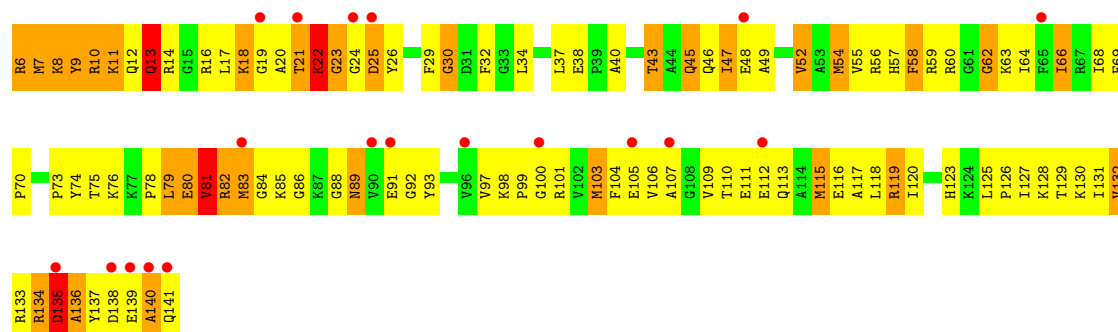




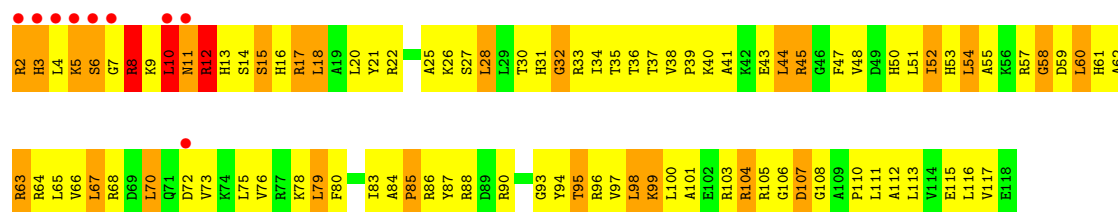
• Molecule 35: 50S ribosomal protein L16



• Molecule 35: 50S ribosomal protein L16

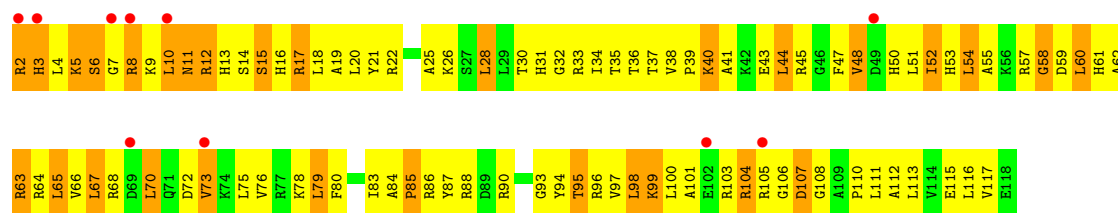


• Molecule 36: 50S ribosomal protein L17

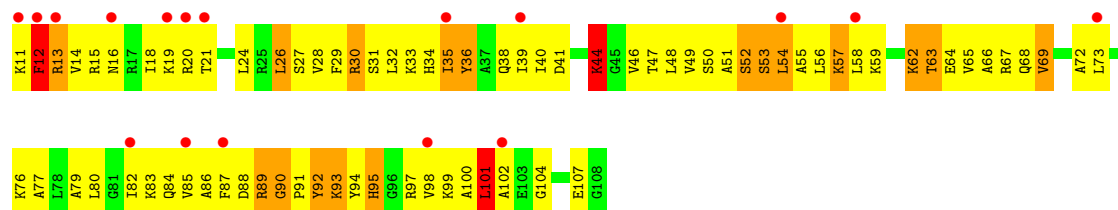


• Molecule 36: 50S ribosomal protein L17

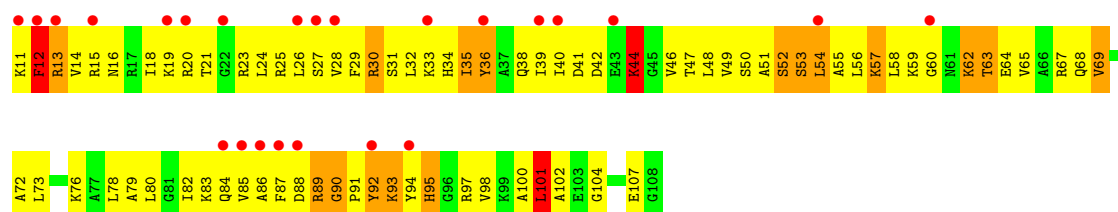




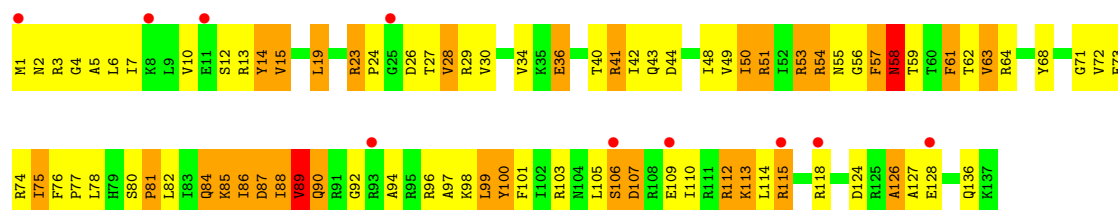
• Molecule 37: 50S ribosomal protein L18



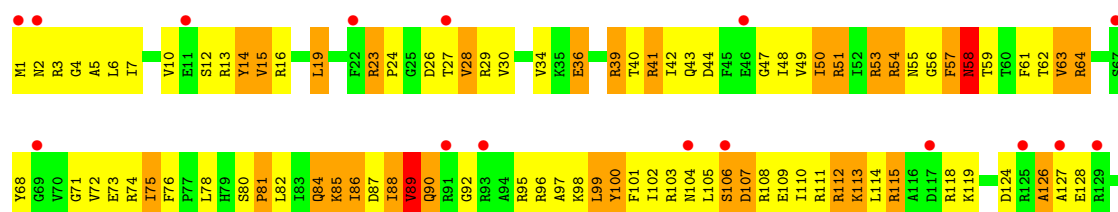
• Molecule 37: 50S ribosomal protein L18



• Molecule 38: 50S ribosomal protein L19



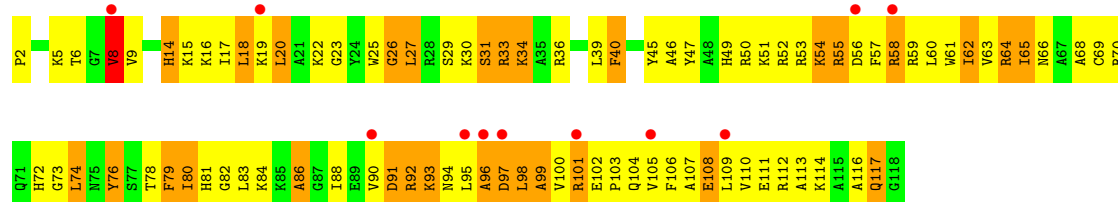
• Molecule 38: 50S ribosomal protein L19



Q136  
R137

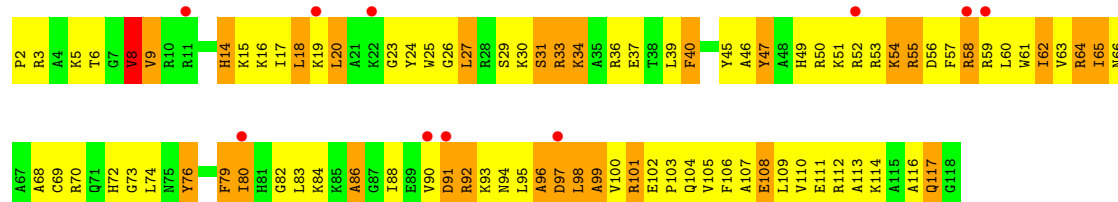
• Molecule 39: 50S ribosomal protein L20

Chain BQ: 9% 23% 50% 26%



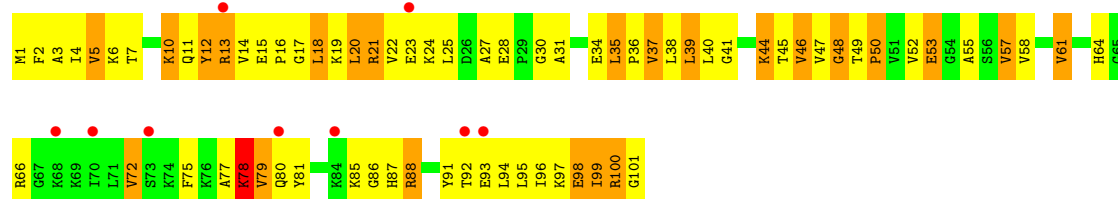
• Molecule 39: 50S ribosomal protein L20

Chain DQ: 9% 23% 51% 25%



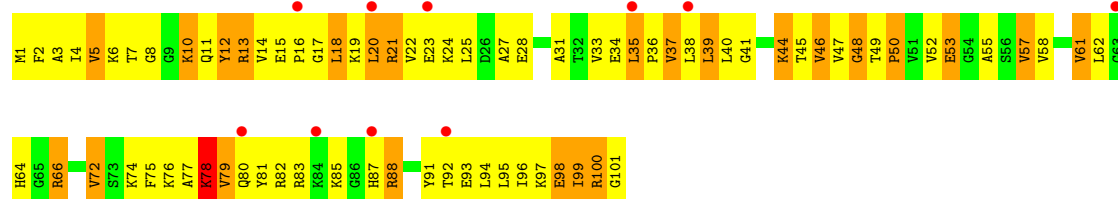
• Molecule 40: 50S ribosomal protein L21

Chain BR: 9% 29% 48% 23%



• Molecule 40: 50S ribosomal protein L21

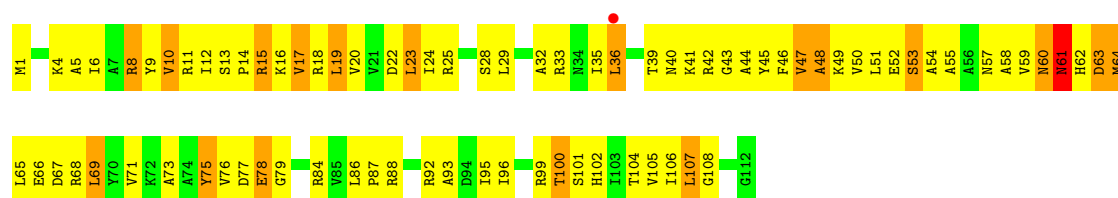
Chain DR: 10% 24% 51% 24%



• Molecule 41: 50S ribosomal protein L22

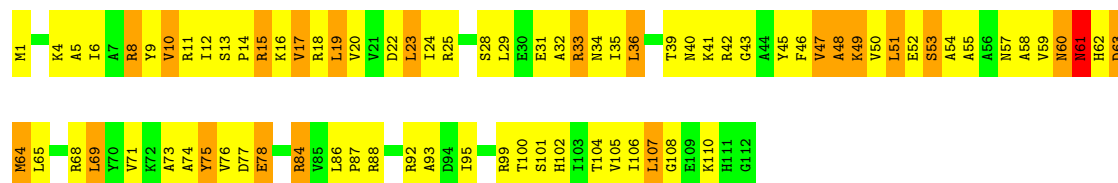
Chain BS: % 28% 55% 16%





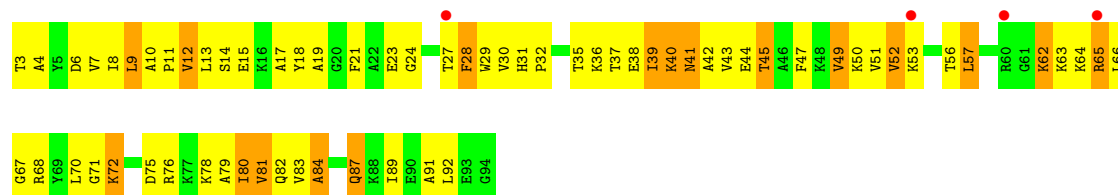
• Molecule 41: 50S ribosomal protein L22

Chain DS: 29% 52% 19%



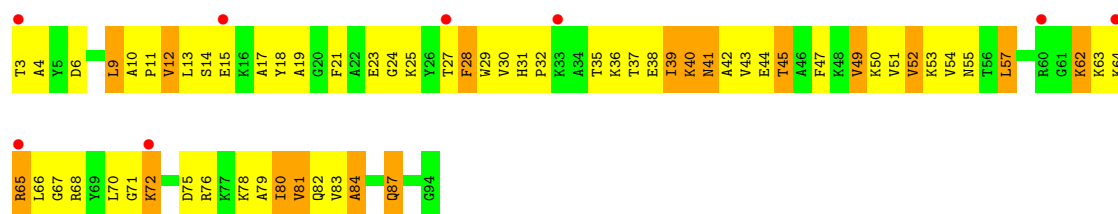
• Molecule 42: 50S ribosomal protein L23

Chain BT: 4% 28% 53% 18%



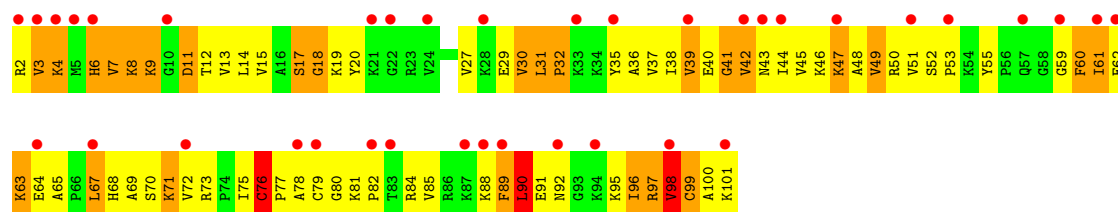
• Molecule 42: 50S ribosomal protein L23

Chain DT: 9% 32% 50% 18%

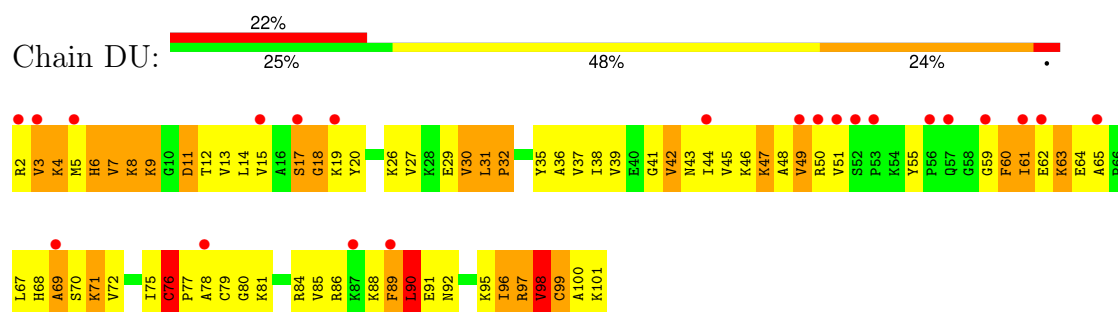


• Molecule 43: 50S ribosomal protein L24

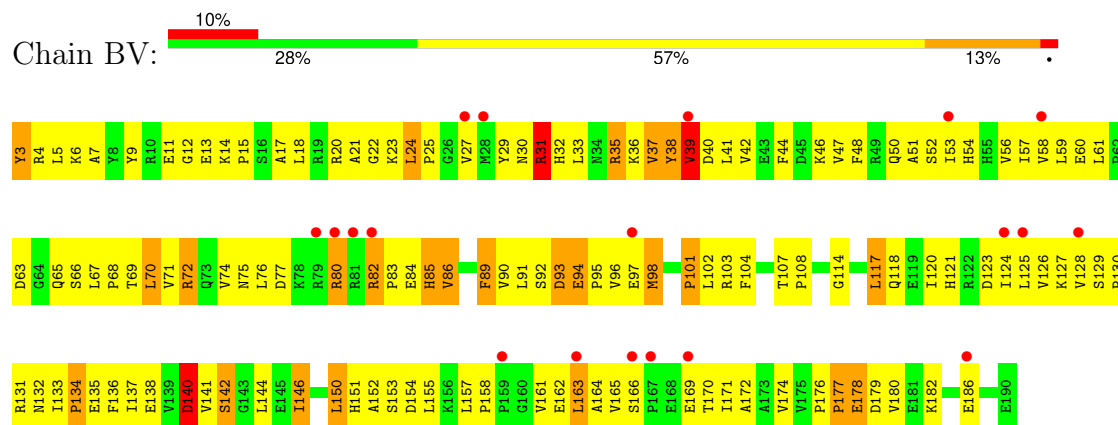
Chain BU: 37% 23% 48% 26%



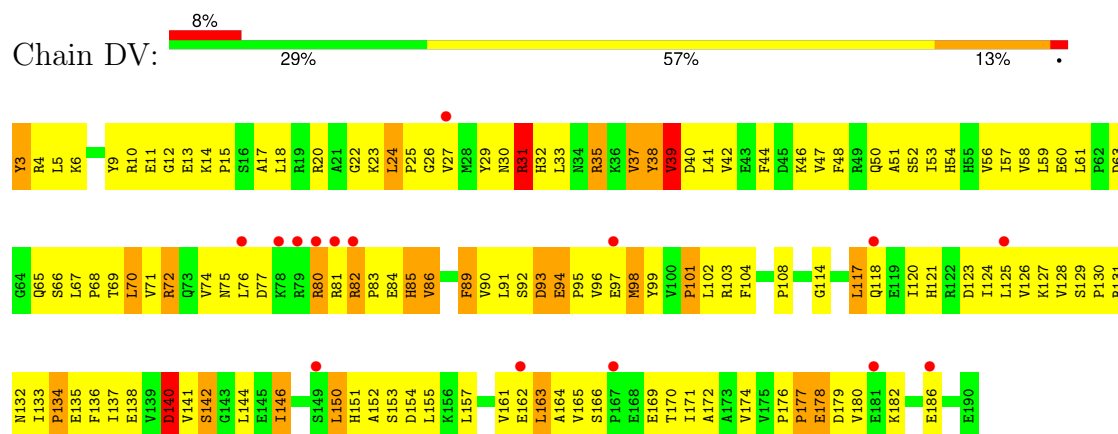
• Molecule 43: 50S ribosomal protein L24



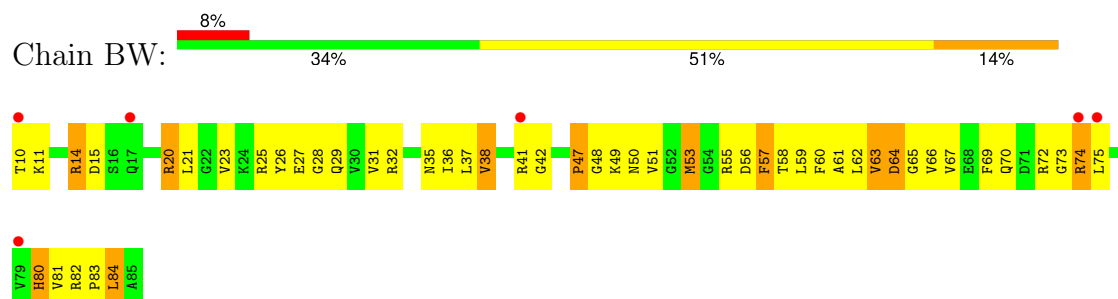
• Molecule 44: 50S ribosomal protein L25



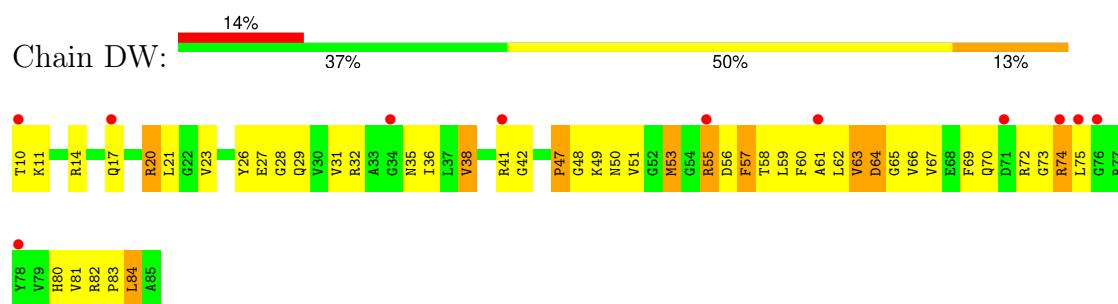
• Molecule 44: 50S ribosomal protein L25



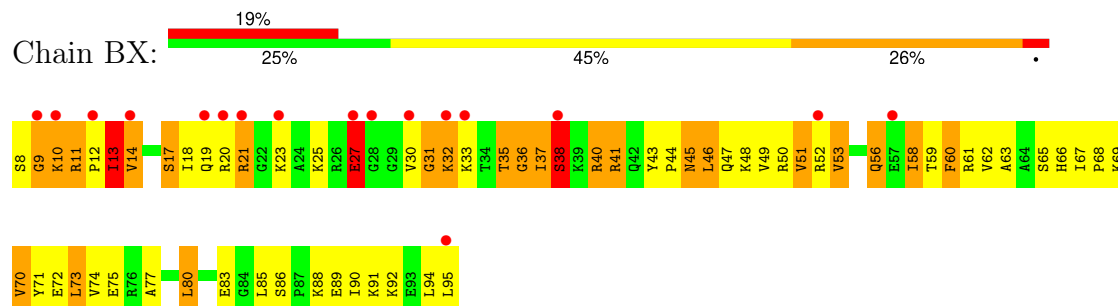
• Molecule 45: 50S ribosomal protein L27



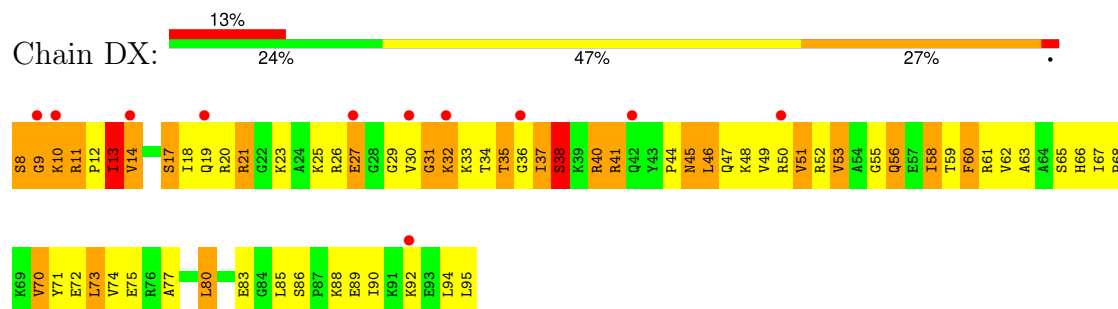
• Molecule 45: 50S ribosomal protein L27



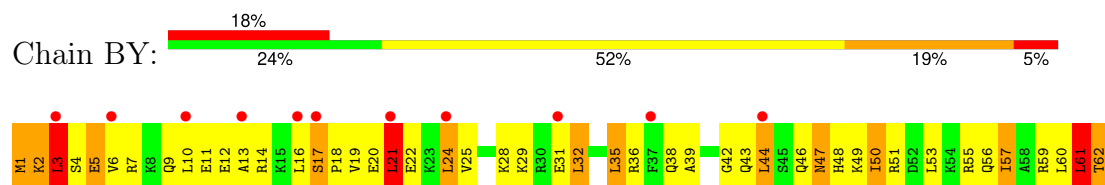
- Molecule 46: 50S ribosomal protein L28



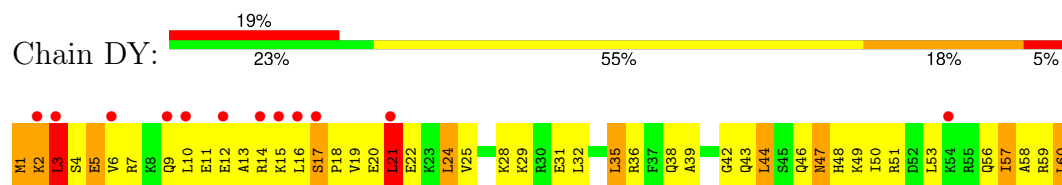
- Molecule 46: 50S ribosomal protein L28



- Molecule 47: 50S ribosomal protein L29

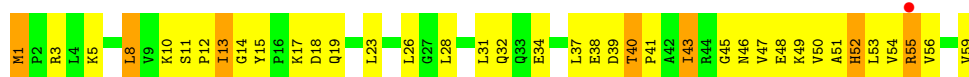


- Molecule 47: 50S ribosomal protein L29

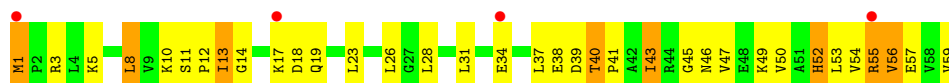


- Molecule 48: 50S ribosomal protein L30

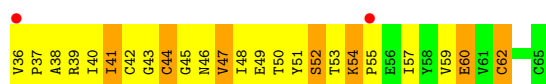




- Molecule 48: 50S ribosomal protein L30



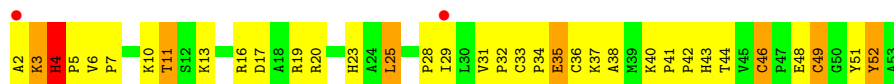
- Molecule 49: 50S ribosomal protein L31



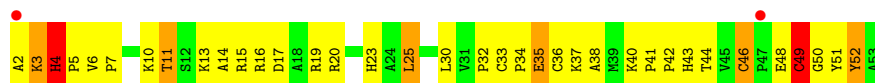
- Molecule 49: 50S ribosomal protein L31



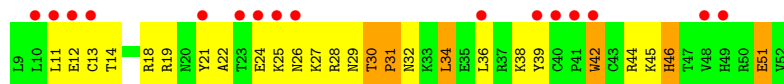
- Molecule 50: 50S ribosomal protein L32



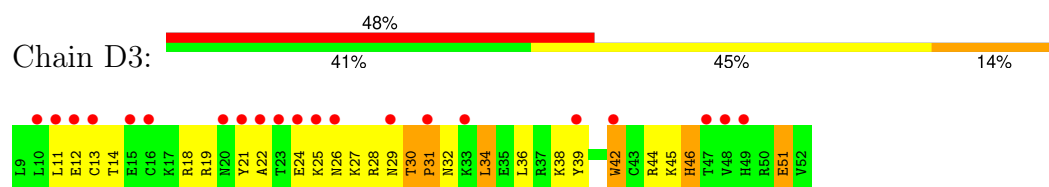
- Molecule 50: 50S ribosomal protein L32



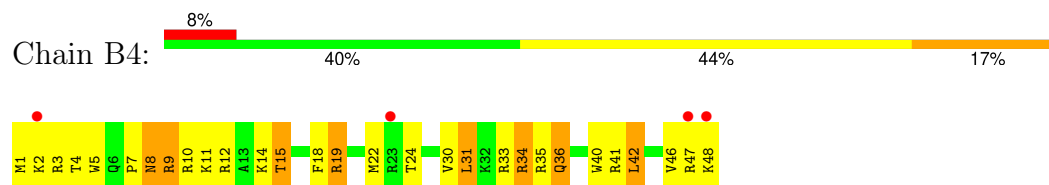
- Molecule 51: 50S ribosomal protein L33



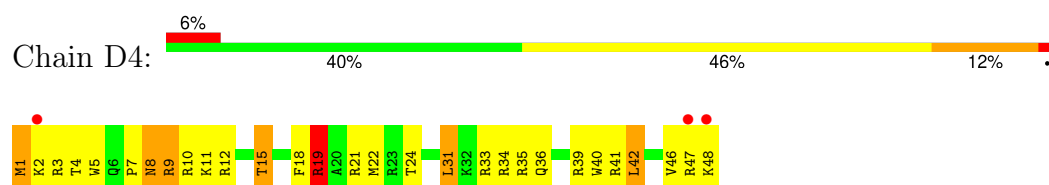
- Molecule 51: 50S ribosomal protein L33



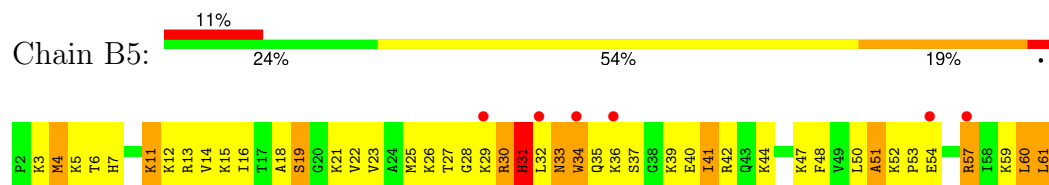
- Molecule 52: 50S ribosomal protein L34



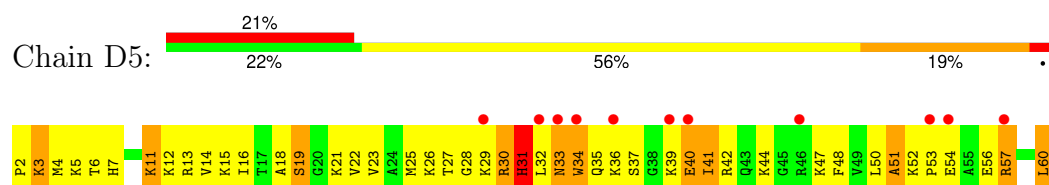
- Molecule 52: 50S ribosomal protein L34



- 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, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 <sup>2</sup> )	86.0	Xtriage
Anisotropy	0.391	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 95.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	AA	0.63	4/36238 (0.0%)	1.02	99/56561 (0.2%)
1	CA	0.57	0/36238	0.96	75/56561 (0.1%)
2	AB	0.31	0/1936	0.51	0/2609
2	CB	0.28	0/1936	0.50	0/2609
3	AC	0.31	0/1637	0.47	0/2205
3	CC	0.29	0/1637	0.47	0/2205
4	AD	0.41	0/1733	0.59	0/2318
4	CD	0.34	0/1733	0.56	0/2318
5	AE	0.41	0/1172	0.61	0/1576
5	CE	0.36	0/1172	0.57	0/1576
6	AF	0.33	0/856	0.57	0/1154
6	CF	0.37	0/856	0.59	0/1154
7	AG	0.27	0/1276	0.46	0/1709
7	CG	0.27	0/1276	0.46	0/1709
8	AH	0.39	0/1136	0.61	0/1527
8	CH	0.33	0/1136	0.58	0/1527
9	AI	0.29	0/1029	0.45	0/1378
9	CI	0.27	0/1029	0.45	0/1378
10	AJ	0.28	0/808	0.48	0/1085
10	CJ	0.27	0/808	0.46	0/1085
11	AK	0.39	0/900	0.59	0/1213
11	CK	0.41	0/900	0.61	0/1213
12	AL	0.47	0/987	0.70	1/1320 (0.1%)
12	CL	0.44	0/987	0.68	0/1320
13	AM	0.25	0/939	0.44	0/1258
13	CM	0.24	0/939	0.44	0/1258
14	AN	0.31	0/501	0.50	0/664
14	CN	0.31	0/501	0.52	0/664
15	AO	0.39	0/745	0.57	0/992
15	CO	0.37	0/745	0.56	0/992
16	AP	0.42	0/717	0.62	0/963
16	CP	0.34	0/717	0.59	0/963

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	AQ	0.43	0/837	0.60	0/1117
17	CQ	0.37	0/837	0.56	0/1117
18	AR	0.38	0/579	0.61	0/768
18	CR	0.37	0/579	0.60	0/768
19	AS	0.25	0/643	0.43	0/865
19	CS	0.25	0/643	0.42	0/865
20	AT	0.38	0/764	0.57	0/1006
20	CT	0.33	0/764	0.54	0/1006
21	AU	0.23	0/213	0.43	0/277
21	CU	0.24	0/213	0.42	0/277
22	AV	0.43	0/802	0.68	0/1245
22	CV	0.43	0/802	0.69	0/1245
23	BA	1.07	153/66570 (0.2%)	1.48	1344/103918 (1.3%)
23	DA	1.19	253/66575 (0.4%)	1.59	1756/103930 (1.7%)
24	BB	0.58	0/2853	1.00	9/4451 (0.2%)
24	DB	0.59	0/2853	1.04	3/4451 (0.1%)
25	BC	0.71	1/2155 (0.0%)	0.90	3/2905 (0.1%)
25	DC	0.74	1/2155 (0.0%)	0.91	5/2905 (0.2%)
26	BD	0.58	0/1597	0.77	0/2153
26	DD	0.62	1/1597 (0.1%)	0.81	0/2153
27	BE	0.63	0/1622	0.77	0/2194
27	DE	0.67	0/1622	0.78	0/2194
28	BF	0.28	0/1500	0.49	0/2017
28	DF	0.28	0/1500	0.49	0/2017
29	BG	0.32	0/1246	0.58	0/1682
29	DG	0.44	0/1246	0.64	0/1682
30	BH	0.33	0/1148	0.56	0/1552
30	DH	0.38	0/1148	0.56	0/1552
31	BI	0.25	0/252	0.44	0/333
31	DI	0.27	0/252	0.46	0/333
32	BJ	0.56	0/1124	0.75	0/1515
32	DJ	0.59	0/1124	0.76	0/1515
33	BK	0.57	0/942	0.76	0/1268
33	DK	0.61	0/942	0.77	0/1268
34	BL	0.74	1/1131 (0.1%)	1.01	1/1504 (0.1%)
34	DL	0.75	2/1131 (0.2%)	1.03	5/1504 (0.3%)
35	BM	0.61	0/1099	0.83	2/1468 (0.1%)
35	DM	0.60	0/1099	0.83	1/1468 (0.1%)
36	BN	0.59	0/974	0.85	0/1302
36	DN	0.59	0/974	0.83	1/1302 (0.1%)
37	BO	0.36	0/779	0.58	0/1036
37	DO	0.39	0/779	0.61	0/1036
38	BP	0.50	0/1158	0.68	0/1544



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
38	DP	0.51	0/1158	0.69	0/1544
39	BQ	0.63	0/970	0.81	0/1290
39	DQ	0.67	0/970	0.81	0/1290
40	BR	0.58	0/790	0.73	1/1057 (0.1%)
40	DR	0.61	0/790	0.74	1/1057 (0.1%)
41	BS	0.63	0/902	0.78	0/1209
41	DS	0.66	0/902	0.76	0/1209
42	BT	0.64	0/740	0.79	0/993
42	DT	0.74	0/740	0.84	0/993
43	BU	0.53	0/789	0.76	0/1051
43	DU	0.56	0/789	0.76	0/1051
44	BV	0.36	0/1524	0.57	0/2068
44	DV	0.38	0/1524	0.57	0/2068
45	BW	0.50	0/613	0.71	0/816
45	DW	0.52	0/613	0.72	0/816
46	BX	0.73	0/702	0.98	2/932 (0.2%)
46	DX	0.82	0/702	1.04	2/932 (0.2%)
47	BY	0.55	0/523	0.87	1/690 (0.1%)
47	DY	0.72	0/523	0.98	3/690 (0.4%)
48	BZ	0.52	0/473	0.68	0/634
48	DZ	0.50	0/473	0.65	0/634
49	B1	0.23	0/229	0.40	0/309
49	D1	0.22	0/229	0.41	0/309
50	B2	0.61	0/419	0.80	0/567
50	D2	0.58	0/419	0.79	0/567
51	B3	0.28	0/388	0.46	0/518
51	D3	0.27	0/388	0.46	0/518
52	B4	0.72	0/427	0.89	0/561
52	D4	0.84	0/427	1.05	1/561 (0.2%)
53	B5	0.68	0/516	0.88	0/679
53	D5	0.69	0/516	0.88	1/679 (0.1%)
All	All	0.85	416/305211 (0.1%)	1.21	3317/456064 (0.7%)

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 416 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	DA	774	A	N9-C4	-13.87	1.29	1.37
23	DA	1332	G	N9-C4	-11.99	1.28	1.38
23	DA	1602	U	C4-O4	11.31	1.32	1.23
23	BA	1332	G	N9-C4	-11.02	1.29	1.38
23	DA	2249	U	C4-O4	10.67	1.32	1.23

The worst 5 of 3317 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	DA	761	A	N1-C6-N6	30.82	137.09	118.60
23	BA	761	A	N1-C6-N6	25.08	133.65	118.60
23	DA	1332	G	N3-C4-N9	-24.42	111.35	126.00
23	DA	1332	G	N3-C4-C5	23.85	140.52	128.60
23	BA	1332	G	N3-C4-N9	-22.46	112.52	126.00

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	1680	0
1	CA	32372	0	16339	1784	0
2	AB	1901	0	1951	173	0
2	CB	1901	0	1951	180	0
3	AC	1613	0	1677	180	0
3	CC	1613	0	1677	186	0
4	AD	1703	0	1764	192	0
4	CD	1703	0	1764	182	1
5	AE	1156	0	1213	141	0
5	CE	1156	0	1213	141	0
6	AF	843	0	857	96	1
6	CF	843	0	857	93	0
7	AG	1257	0	1296	95	0
7	CG	1257	0	1296	92	0
8	AH	1116	0	1177	133	0
8	CH	1116	0	1177	140	0
9	AI	1011	0	1043	100	0
9	CI	1011	0	1043	112	0
10	AJ	795	0	840	93	0
10	CJ	795	0	840	92	0
11	AK	885	0	904	76	0
11	CK	885	0	904	72	0
12	AL	971	0	1057	126	0
12	CL	971	0	1057	139	0
13	AM	929	0	987	83	0
13	CM	929	0	987	83	0
14	AN	492	0	530	49	0
14	CN	492	0	532	61	0
15	AO	734	0	771	66	0
15	CO	734	0	771	60	0
16	AP	701	0	720	96	0
16	CP	701	0	720	90	0
17	AQ	824	0	893	66	0
17	CQ	824	0	893	77	0
18	AR	574	0	644	70	0
18	CR	574	0	644	70	0
19	AS	630	0	652	70	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	CS	630	0	652	60	0
20	AT	762	0	859	64	0
20	CT	762	0	859	70	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	2618	0
23	DA	59442	0	29965	2593	0
24	BB	2551	0	1295	147	0
24	DB	2551	0	1295	148	0
25	BC	2105	0	2182	353	0
25	DC	2105	0	2182	347	0
26	BD	1564	0	1629	224	0
26	DD	1564	0	1629	224	0
27	BE	1587	0	1632	147	0
27	DE	1587	0	1632	155	0
28	BF	1475	0	1537	155	0
28	DF	1475	0	1537	150	0
29	BG	1223	0	1282	114	0
29	DG	1223	0	1282	121	0
30	BH	1133	0	1220	131	0
30	DH	1133	0	1220	133	0
31	BI	254	0	275	8	0
31	DI	254	0	275	8	0
32	BJ	1097	0	1168	170	0
32	DJ	1097	0	1168	158	0
33	BK	932	0	994	97	0
33	DK	932	0	994	100	0
34	BL	1114	0	1187	270	0
34	DL	1114	0	1187	279	0
35	BM	1079	0	1127	170	0
35	DM	1079	0	1127	172	0
36	BN	960	0	1021	153	0
36	DN	960	0	1021	142	0
37	BO	771	0	832	95	0
37	DO	771	0	832	100	0
38	BP	1144	0	1211	129	0
38	DP	1144	0	1211	132	0
39	BQ	953	0	1013	150	0
39	DQ	953	0	1013	155	0
40	BR	779	0	852	131	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	DR	779	0	852	128	0
41	BS	891	0	951	106	0
41	DS	891	0	951	110	0
42	BT	726	0	778	88	0
42	DT	726	0	778	92	0
43	BU	776	0	870	138	0
43	DU	776	0	870	139	0
44	BV	1492	0	1513	174	0
44	DV	1492	0	1513	171	0
45	BW	605	0	628	71	0
45	DW	605	0	628	63	0
46	BX	695	0	764	112	0
46	DX	695	0	764	106	0
47	BY	521	0	575	81	0
47	DY	521	0	575	81	0
48	BZ	468	0	523	46	0
48	DZ	468	0	523	46	0
49	B1	226	0	225	23	0
49	D1	226	0	225	24	0
50	B2	405	0	420	61	0
50	D2	405	0	420	64	0
51	B3	381	0	391	25	0
51	D3	381	0	391	26	0
52	B4	419	0	467	50	0
52	D4	419	0	467	48	0
53	B5	508	0	576	111	0
53	D5	508	0	576	110	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	18333	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 39.

The worst 5 of 18333 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)
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
52:D4:8:ASN:HD22	52:D4:8:ASN:C	1.42	1.18

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%)	<b>0</b> <b>4</b>
2	CB	232/234 (99%)	173 (75%)	38 (16%)	21 (9%)	<b>0</b> <b>4</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	AC	204/206 (99%)	136 (67%)	43 (21%)	25 (12%)	0	2
3	CC	204/206 (99%)	134 (66%)	45 (22%)	25 (12%)	0	2
4	AD	206/208 (99%)	152 (74%)	38 (18%)	16 (8%)	1	5
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	18
7	CG	153/155 (99%)	121 (79%)	27 (18%)	5 (3%)	3	18
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%)	5	23
9	CI	125/127 (98%)	89 (71%)	32 (26%)	4 (3%)	3	18
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	14
11	CK	117/119 (98%)	82 (70%)	30 (26%)	5 (4%)	2	14
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	2
13	AM	114/116 (98%)	93 (82%)	17 (15%)	4 (4%)	3	17
13	CM	114/116 (98%)	93 (82%)	17 (15%)	4 (4%)	3	17
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	2
17	AQ	97/99 (98%)	74 (76%)	16 (16%)	7 (7%)	1	6
17	CQ	97/99 (98%)	75 (77%)	16 (16%)	6 (6%)	1	8
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	7
20	AT	97/99 (98%)	67 (69%)	23 (24%)	7 (7%)	1	6
20	CT	97/99 (98%)	67 (69%)	23 (24%)	7 (7%)	1	6
21	AU	22/24 (92%)	13 (59%)	8 (36%)	1 (4%)	2	13
21	CU	22/24 (92%)	13 (59%)	8 (36%)	1 (4%)	2	13
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	5
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	7
28	DF	179/181 (99%)	136 (76%)	31 (17%)	12 (7%)	1	7
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	1
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	4
32	DJ	135/137 (98%)	97 (72%)	24 (18%)	14 (10%)	0	3
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	7
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	2
39	DQ	114/116 (98%)	82 (72%)	20 (18%)	12 (10%)	0	3
40	BR	99/101 (98%)	70 (71%)	20 (20%)	9 (9%)	0	4
40	DR	99/101 (98%)	70 (71%)	20 (20%)	9 (9%)	0	4
41	BS	110/112 (98%)	88 (80%)	17 (16%)	5 (4%)	2	13
41	DS	110/112 (98%)	87 (79%)	17 (16%)	6 (6%)	1	10
42	BT	90/92 (98%)	69 (77%)	16 (18%)	5 (6%)	1	10
42	DT	90/92 (98%)	67 (74%)	18 (20%)	5 (6%)	1	10
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	4
44	DV	186/188 (99%)	135 (73%)	34 (18%)	17 (9%)	0	4
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%)	7	27
48	DZ	57/59 (97%)	50 (88%)	6 (10%)	1 (2%)	7	27
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	5
50	D2	50/52 (96%)	39 (78%)	7 (14%)	4 (8%)	1	5
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	4

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%)	4	16
2	CB	202/202 (100%)	179 (89%)	23 (11%)	4	17
3	AC	160/160 (100%)	146 (91%)	14 (9%)	8	28
3	CC	160/160 (100%)	145 (91%)	15 (9%)	7	25
4	AD	180/180 (100%)	150 (83%)	30 (17%)	2	7
4	CD	180/180 (100%)	150 (83%)	30 (17%)	2	7
5	AE	116/116 (100%)	92 (79%)	24 (21%)	1	2
5	CE	116/116 (100%)	94 (81%)	22 (19%)	1	4
6	AF	90/90 (100%)	82 (91%)	8 (9%)	8	27
6	CF	90/90 (100%)	83 (92%)	7 (8%)	10	33
7	AG	126/126 (100%)	121 (96%)	5 (4%)	27	52
7	CG	126/126 (100%)	121 (96%)	5 (4%)	27	52
8	AH	119/119 (100%)	102 (86%)	17 (14%)	2	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	CH	119/119 (100%)	104 (87%)	15 (13%)	3	14
9	AI	98/98 (100%)	88 (90%)	10 (10%)	6	22
9	CI	98/98 (100%)	88 (90%)	10 (10%)	6	22
10	AJ	88/88 (100%)	78 (89%)	10 (11%)	4	17
10	CJ	88/88 (100%)	78 (89%)	10 (11%)	4	17
11	AK	90/90 (100%)	75 (83%)	15 (17%)	2	7
11	CK	90/90 (100%)	76 (84%)	14 (16%)	2	8
12	AL	104/104 (100%)	83 (80%)	21 (20%)	1	3
12	CL	104/104 (100%)	83 (80%)	21 (20%)	1	3
13	AM	94/94 (100%)	87 (93%)	7 (7%)	11	35
13	CM	94/94 (100%)	87 (93%)	7 (7%)	11	35
14	AN	49/49 (100%)	45 (92%)	4 (8%)	9	31
14	CN	49/49 (100%)	45 (92%)	4 (8%)	9	31
15	AO	79/79 (100%)	69 (87%)	10 (13%)	3	14
15	CO	79/79 (100%)	69 (87%)	10 (13%)	3	14
16	AP	72/72 (100%)	57 (79%)	15 (21%)	1	2
16	CP	72/72 (100%)	56 (78%)	16 (22%)	1	2
17	AQ	94/94 (100%)	78 (83%)	16 (17%)	1	6
17	CQ	94/94 (100%)	79 (84%)	15 (16%)	2	8
18	AR	61/61 (100%)	58 (95%)	3 (5%)	21	48
18	CR	61/61 (100%)	58 (95%)	3 (5%)	21	48
19	AS	69/69 (100%)	60 (87%)	9 (13%)	3	13
19	CS	69/69 (100%)	60 (87%)	9 (13%)	3	13
20	AT	76/76 (100%)	65 (86%)	11 (14%)	2	10
20	CT	76/76 (100%)	65 (86%)	11 (14%)	2	10
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%)	164 (77%)	49 (23%)	0	2
25	DC	213/213 (100%)	162 (76%)	51 (24%)	0	1
26	BD	165/165 (100%)	129 (78%)	36 (22%)	1	2
26	DD	165/165 (100%)	129 (78%)	36 (22%)	1	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
27	BE	161/161 (100%)	124 (77%)	37 (23%)	0	2
27	DE	161/161 (100%)	124 (77%)	37 (23%)	0	2
28	BF	155/155 (100%)	132 (85%)	23 (15%)	2	9
28	DF	155/155 (100%)	134 (86%)	21 (14%)	3	12
29	BG	132/132 (100%)	108 (82%)	24 (18%)	1	5
29	DG	132/132 (100%)	107 (81%)	25 (19%)	1	4
30	BH	122/122 (100%)	103 (84%)	19 (16%)	2	8
30	DH	122/122 (100%)	103 (84%)	19 (16%)	2	8
31	BI	27/53 (51%)	25 (93%)	2 (7%)	11	35
31	DI	27/53 (51%)	25 (93%)	2 (7%)	11	35
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%)	78 (78%)	22 (22%)	1	2
33	DK	100/100 (100%)	78 (78%)	22 (22%)	1	2
34	BL	112/112 (100%)	75 (67%)	37 (33%)	0	0
34	DL	112/112 (100%)	76 (68%)	36 (32%)	0	0
35	BM	106/106 (100%)	82 (77%)	24 (23%)	1	2
35	DM	106/106 (100%)	81 (76%)	25 (24%)	0	1
36	BN	100/100 (100%)	75 (75%)	25 (25%)	0	1
36	DN	100/100 (100%)	76 (76%)	24 (24%)	0	1
37	BO	77/77 (100%)	63 (82%)	14 (18%)	1	5
37	DO	77/77 (100%)	63 (82%)	14 (18%)	1	5
38	BP	121/121 (100%)	96 (79%)	25 (21%)	1	2
38	DP	121/121 (100%)	94 (78%)	27 (22%)	1	2
39	BQ	92/92 (100%)	71 (77%)	21 (23%)	0	2
39	DQ	92/92 (100%)	71 (77%)	21 (23%)	0	2
40	BR	82/82 (100%)	63 (77%)	19 (23%)	0	2
40	DR	82/82 (100%)	61 (74%)	21 (26%)	0	1
41	BS	91/91 (100%)	65 (71%)	26 (29%)	0	1
41	DS	91/91 (100%)	65 (71%)	26 (29%)	0	1
42	BT	74/74 (100%)	60 (81%)	14 (19%)	1	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
42	DT	74/74 (100%)	60 (81%)	14 (19%)	1	4
43	BU	84/84 (100%)	66 (79%)	18 (21%)	1	2
43	DU	84/84 (100%)	67 (80%)	17 (20%)	1	3
44	BV	163/163 (100%)	142 (87%)	21 (13%)	3	13
44	DV	163/163 (100%)	141 (86%)	22 (14%)	3	12
45	BW	61/61 (100%)	52 (85%)	9 (15%)	2	9
45	DW	61/61 (100%)	53 (87%)	8 (13%)	3	13
46	BX	73/73 (100%)	50 (68%)	23 (32%)	0	1
46	DX	73/73 (100%)	50 (68%)	23 (32%)	0	1
47	BY	58/58 (100%)	46 (79%)	12 (21%)	1	2
47	DY	58/58 (100%)	46 (79%)	12 (21%)	1	2
48	BZ	51/51 (100%)	43 (84%)	8 (16%)	2	8
48	DZ	51/51 (100%)	43 (84%)	8 (16%)	2	8
49	B1	27/27 (100%)	26 (96%)	1 (4%)	29	54
49	D1	27/27 (100%)	26 (96%)	1 (4%)	29	54
50	B2	45/45 (100%)	40 (89%)	5 (11%)	5	18
50	D2	45/45 (100%)	39 (87%)	6 (13%)	3	12
51	B3	43/43 (100%)	38 (88%)	5 (12%)	4	17
51	D3	43/43 (100%)	38 (88%)	5 (12%)	4	17
52	B4	41/41 (100%)	29 (71%)	12 (29%)	0	1
52	D4	41/41 (100%)	28 (68%)	13 (32%)	0	1
53	B5	53/53 (100%)	42 (79%)	11 (21%)	1	2
53	D5	53/53 (100%)	43 (81%)	10 (19%)	1	4
All	All	9462/9514 (100%)	7811 (83%)	1651 (17%)	1	6

5 of 1651 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	CG	104	LEU
26	DD	141	ILE
47	DY	5	GLU
9	CI	124	GLN
7	CG	91	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 245 such sidechains are listed below:

Mol	Chain	Res	Type
48	BZ	19	GLN
42	DT	55	ASN
9	CI	124	GLN
42	DT	31	HIS
48	DZ	52	HIS

### 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%)	584 (21%)	27 (0%)
23	DA	2757/2879 (95%)	589 (21%)	29 (1%)
24	BB	118/119 (99%)	26 (22%)	0
24	DB	118/119 (99%)	27 (22%)	0
All	All	8822/9094 (97%)	1819 (20%)	84 (0%)

5 of 1819 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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	AA	1506/1506 (100%)	0.45	79 (5%) 34 30	51, 122, 245, 498	0
1	CA	1506/1506 (100%)	0.48	68 (4%) 39 34	51, 126, 251, 414	0
2	AB	234/234 (100%)	0.92	30 (12%) 9 11	113, 174, 244, 298	0
2	CB	234/234 (100%)	0.97	31 (13%) 8 11	111, 177, 259, 325	0
3	AC	206/206 (100%)	0.94	30 (14%) 7 9	106, 160, 225, 263	0
3	CC	206/206 (100%)	0.92	32 (15%) 6 8	105, 161, 226, 271	0
4	AD	208/208 (100%)	1.48	56 (26%) 2 4	90, 142, 199, 247	0
4	CD	208/208 (100%)	1.62	63 (30%) 1 3	94, 146, 220, 300	0
5	AE	151/151 (100%)	0.64	15 (9%) 14 16	73, 114, 172, 272	0
5	CE	151/151 (100%)	0.55	11 (7%) 22 22	72, 117, 188, 252	0
6	AF	101/101 (100%)	0.81	10 (9%) 14 16	83, 135, 192, 270	0
6	CF	101/101 (100%)	0.65	10 (9%) 14 16	79, 131, 184, 246	0
7	AG	155/155 (100%)	0.97	24 (15%) 6 8	118, 187, 237, 333	0
7	CG	155/155 (100%)	1.06	27 (17%) 5 7	119, 187, 237, 286	0
8	AH	138/138 (100%)	0.97	16 (11%) 11 14	77, 121, 166, 199	0
8	CH	138/138 (100%)	0.77	12 (8%) 17 18	81, 123, 167, 219	0
9	AI	127/127 (100%)	1.99	52 (40%) 1 1	119, 225, 289, 345	0
9	CI	127/127 (100%)	1.69	41 (32%) 1 2	121, 225, 286, 354	0
10	AJ	98/98 (100%)	1.53	32 (32%) 1 2	118, 198, 278, 356	0
10	CJ	98/98 (100%)	1.58	33 (33%) 1 2	122, 197, 264, 351	0
11	AK	119/119 (100%)	0.57	11 (9%) 16 17	71, 111, 171, 263	0
11	CK	119/119 (100%)	0.63	13 (10%) 12 14	74, 111, 178, 264	0
12	AL	124/124 (100%)	1.16	25 (20%) 3 6	67, 107, 165, 268	0
12	CL	124/124 (100%)	1.46	28 (22%) 3 5	70, 109, 178, 252	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	AM	116/116 (100%)	1.54	30 (25%) 2 4	134, 213, 299, 335	0
13	CM	116/116 (100%)	1.07	20 (17%) 5 7	135, 214, 309, 362	0
14	AN	60/60 (100%)	1.74	23 (38%) 1 1	114, 166, 217, 235	0
14	CN	60/60 (100%)	1.89	21 (35%) 1 2	116, 167, 227, 281	0
15	AO	88/88 (100%)	0.37	4 (4%) 39 34	66, 108, 159, 227	0
15	CO	88/88 (100%)	0.49	4 (4%) 39 34	67, 110, 166, 241	0
16	AP	83/83 (100%)	1.54	19 (22%) 2 5	84, 118, 174, 214	0
16	CP	83/83 (100%)	1.61	28 (33%) 1 2	87, 123, 177, 210	0
17	AQ	99/99 (100%)	0.71	7 (7%) 23 23	78, 112, 169, 216	0
17	CQ	99/99 (100%)	0.96	10 (10%) 14 16	79, 116, 166, 215	0
18	AR	70/70 (100%)	0.63	5 (7%) 23 23	84, 128, 183, 284	0
18	CR	70/70 (100%)	0.53	2 (2%) 54 46	82, 128, 192, 232	0
19	AS	78/78 (100%)	1.33	19 (24%) 2 4	152, 210, 275, 321	0
19	CS	78/78 (100%)	1.39	19 (24%) 2 4	151, 216, 291, 350	0
20	AT	99/99 (100%)	1.48	25 (25%) 2 4	86, 134, 203, 241	0
20	CT	99/99 (100%)	1.65	26 (26%) 2 4	92, 136, 212, 269	0
21	AU	24/24 (100%)	3.10	16 (66%) 0 0	160, 225, 264, 322	0
21	CU	24/24 (100%)	3.68	20 (83%) 0 0	163, 218, 265, 364	0
22	AV	34/43 (79%)	0.73	3 (8%) 17 18	89, 196, 324, 362	0
22	CV	34/43 (79%)	0.97	6 (17%) 4 7	92, 198, 333, 339	0
23	BA	2760/2879 (95%)	-0.32	28 (1%) 79 71	27, 65, 180, 398	0
23	DA	2760/2879 (95%)	-0.26	33 (1%) 76 68	25, 63, 178, 410	0
24	BB	119/119 (100%)	0.41	10 (8%) 18 19	76, 129, 182, 232	0
24	DB	119/119 (100%)	0.44	10 (8%) 18 19	78, 129, 184, 236	0
25	BC	271/271 (100%)	0.16	18 (6%) 26 25	25, 58, 109, 175	0
25	DC	271/271 (100%)	0.11	13 (4%) 36 32	18, 57, 109, 177	0
26	BD	204/204 (100%)	0.30	12 (5%) 29 28	36, 73, 146, 341	0
26	DD	204/204 (100%)	0.31	13 (6%) 27 26	33, 71, 145, 347	0
27	BE	202/202 (100%)	0.21	6 (2%) 52 45	31, 73, 155, 246	0
27	DE	202/202 (100%)	0.16	5 (2%) 58 50	25, 73, 155, 192	0
28	BF	181/181 (100%)	1.01	29 (16%) 6 8	102, 182, 254, 314	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
28	DF	181/181 (100%)	0.98	29 (16%) 6 8	104, 185, 268, 331	0
29	BG	159/159 (100%)	0.89	18 (11%) 11 14	85, 143, 221, 343	0
29	DG	159/159 (100%)	1.78	51 (32%) 1 2	79, 136, 186, 235	0
30	BH	145/145 (100%)	2.32	69 (47%) 0 1	67, 243, 391, 482	0
30	DH	145/145 (100%)	2.33	65 (44%) 1 1	64, 236, 379, 480	0
31	BI	32/65 (49%)	1.52	11 (34%) 1 2	171, 246, 347, 355	0
31	DI	32/65 (49%)	1.38	6 (18%) 4 6	168, 253, 310, 334	0
32	BJ	137/137 (100%)	0.33	5 (3%) 46 39	51, 81, 142, 201	0
32	DJ	137/137 (100%)	0.37	8 (5%) 30 28	52, 81, 146, 194	0
33	BK	122/122 (100%)	-0.00	1 (0%) 82 75	42, 70, 111, 150	0
33	DK	122/122 (100%)	-0.01	1 (0%) 82 75	41, 69, 111, 162	0
34	BL	146/146 (100%)	0.92	21 (14%) 7 9	34, 97, 166, 309	0
34	DL	146/146 (100%)	1.12	28 (19%) 4 6	32, 97, 163, 293	0
35	BM	136/136 (100%)	0.66	17 (12%) 9 12	49, 89, 199, 370	0
35	DM	136/136 (100%)	0.79	19 (13%) 7 10	48, 88, 205, 406	0
36	BN	117/117 (100%)	0.48	9 (7%) 21 21	45, 73, 137, 249	0
36	DN	117/117 (100%)	0.47	10 (8%) 18 19	43, 73, 134, 235	0
37	BO	98/98 (100%)	1.20	17 (17%) 5 7	82, 137, 197, 223	0
37	DO	98/98 (100%)	1.30	24 (24%) 2 4	80, 136, 190, 215	0
38	BP	137/137 (100%)	0.50	10 (7%) 22 22	58, 93, 185, 250	0
38	DP	137/137 (100%)	0.76	16 (11%) 10 14	55, 92, 190, 272	0
39	BQ	116/116 (100%)	0.36	11 (9%) 15 17	35, 75, 124, 239	0
39	DQ	116/116 (100%)	0.61	10 (8%) 18 19	26, 74, 126, 248	0
40	BR	101/101 (100%)	0.74	9 (8%) 17 18	41, 105, 164, 264	0
40	DR	101/101 (100%)	0.95	10 (9%) 14 16	41, 110, 156, 259	0
41	BS	112/112 (100%)	0.04	1 (0%) 81 73	44, 59, 137, 254	0
41	DS	112/112 (100%)	-0.10	0 100 100	43, 59, 134, 255	0
42	BT	92/92 (100%)	0.54	4 (4%) 40 35	45, 77, 129, 170	0
42	DT	92/92 (100%)	0.66	8 (8%) 17 18	36, 73, 127, 169	0
43	BU	100/100 (100%)	1.69	37 (37%) 1 1	62, 104, 257, 396	0
43	DU	100/100 (100%)	1.27	22 (22%) 3 5	61, 102, 251, 408	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
44	BV	188/188 (100%)	0.77	19 (10%) 14 16	83, 138, 195, 245	0
44	DV	188/188 (100%)	0.72	15 (7%) 20 20	83, 139, 194, 230	0
45	BW	76/76 (100%)	0.41	6 (7%) 20 20	58, 84, 138, 261	0
45	DW	76/76 (100%)	0.78	11 (14%) 7 9	59, 84, 135, 256	0
46	BX	88/88 (100%)	1.02	17 (19%) 4 6	37, 74, 153, 322	0
46	DX	88/88 (100%)	0.87	11 (12%) 9 12	39, 70, 153, 326	0
47	BY	62/62 (100%)	1.12	11 (17%) 4 7	57, 98, 209, 292	0
47	DY	62/62 (100%)	1.33	12 (19%) 4 6	51, 96, 212, 328	0
48	BZ	59/59 (100%)	0.42	1 (1%) 69 59	43, 81, 156, 299	0
48	DZ	59/59 (100%)	0.59	4 (6%) 25 24	45, 85, 157, 305	0
49	B1	30/30 (100%)	0.56	2 (6%) 25 25	184, 253, 295, 311	0
49	D1	30/30 (100%)	0.59	3 (10%) 14 16	183, 261, 306, 358	0
50	B2	52/52 (100%)	0.30	2 (3%) 44 38	26, 71, 187, 233	0
50	D2	52/52 (100%)	0.33	2 (3%) 44 38	21, 72, 197, 229	0
51	B3	44/44 (100%)	1.91	16 (36%) 1 1	139, 249, 299, 320	0
51	D3	44/44 (100%)	2.12	21 (47%) 0 1	141, 245, 312, 333	0
52	B4	48/48 (100%)	0.28	4 (8%) 19 20	33, 43, 93, 194	0
52	D4	48/48 (100%)	0.09	3 (6%) 27 26	21, 41, 91, 200	0
53	B5	63/63 (100%)	0.64	7 (11%) 12 14	45, 68, 131, 215	0
53	D5	63/63 (100%)	0.93	13 (20%) 3 5	45, 70, 132, 216	0
All	All	20230/20552 (98%)	0.50	1960 (9%) 15 16	18, 104, 241, 498	0

The worst 5 of 1960 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
12	CL	27	LYS	11.4
35	BM	140	ALA	10.9
13	AM	99	ARG	10.8
30	BH	72	LEU	10.6
1	AA	82	U	10.3

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	0.12	0.32	146,146,146,146	0
54	MG	DA	3313	1/1	0.24	0.20	107,107,107,107	0
54	MG	BA	3236	1/1	0.30	0.32	119,119,119,119	0
54	MG	DA	3184	1/1	0.30	0.14	117,117,117,117	0
54	MG	CA	1668	1/1	0.30	0.25	116,116,116,116	0
54	MG	BA	3278	1/1	0.33	0.32	115,115,115,115	0
54	MG	CA	1658	1/1	0.36	0.32	110,110,110,110	0
54	MG	BA	3305	1/1	0.44	0.11	103,103,103,103	0
54	MG	AV	6302	1/1	0.44	0.27	121,121,121,121	0
54	MG	CA	1701	1/1	0.45	0.27	112,112,112,112	0
54	MG	CA	1704	1/1	0.46	0.17	108,108,108,108	0
54	MG	BA	3217	1/1	0.46	0.22	111,111,111,111	0
54	MG	DA	3312	1/1	0.49	0.16	66,66,66,66	0
54	MG	AA	1682	1/1	0.49	0.17	85,85,85,85	0
54	MG	CA	1670	1/1	0.52	0.26	128,128,128,128	0
54	MG	CA	1696	1/1	0.52	0.21	133,133,133,133	0
54	MG	DA	3234	1/1	0.53	0.18	130,130,130,130	0
54	MG	DA	3276	1/1	0.53	0.20	128,128,128,128	0
54	MG	AA	1739	1/1	0.53	0.21	129,129,129,129	0
54	MG	CA	1637	1/1	0.53	0.19	112,112,112,112	0
54	MG	DA	3317	1/1	0.53	0.26	97,97,97,97	0
54	MG	CA	1698	1/1	0.55	0.12	117,117,117,117	0
54	MG	AA	1754	1/1	0.56	0.19	110,110,110,110	0
54	MG	DA	3116	1/1	0.56	0.15	115,115,115,115	0
54	MG	CA	1730	1/1	0.58	0.13	122,122,122,122	0
54	MG	DA	3265	1/1	0.58	0.18	120,120,120,120	0
54	MG	BA	3287	1/1	0.60	0.21	74,74,74,74	0
54	MG	BA	3079	1/1	0.60	0.24	86,86,86,86	0
54	MG	BA	3272	1/1	0.60	0.11	119,119,119,119	0
54	MG	BA	3061	1/1	0.60	0.15	91,91,91,91	0
54	MG	CA	1648	1/1	0.61	0.11	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	BA	3083	1/1	0.61	0.10	87,87,87,87	0
54	MG	AA	1728	1/1	0.61	0.27	105,105,105,105	0
54	MG	AA	1718	1/1	0.62	0.33	98,98,98,98	0
54	MG	BA	3275	1/1	0.62	0.26	87,87,87,87	0
54	MG	BA	3189	1/1	0.62	0.17	88,88,88,88	0
54	MG	DA	3269	1/1	0.63	0.35	91,91,91,91	0
54	MG	CA	1703	1/1	0.63	0.21	108,108,108,108	0
54	MG	CA	1650	1/1	0.63	0.11	108,108,108,108	0
54	MG	BA	3271	1/1	0.63	0.20	91,91,91,91	0
54	MG	CA	1688	1/1	0.63	0.24	99,99,99,99	0
54	MG	DA	3163	1/1	0.64	0.14	83,83,83,83	0
54	MG	BA	3157	1/1	0.64	0.15	68,68,68,68	0
54	MG	DA	3284	1/1	0.64	0.23	134,134,134,134	0
54	MG	DA	2983	1/1	0.66	0.17	70,70,70,70	0
54	MG	DA	3033	1/1	0.66	0.20	101,101,101,101	0
54	MG	DA	3186	1/1	0.66	0.14	90,90,90,90	0
54	MG	DA	3212	1/1	0.66	0.36	78,78,78,78	0
54	MG	AA	1684	1/1	0.66	0.26	95,95,95,95	0
54	MG	BA	3006	1/1	0.66	0.28	77,77,77,77	0
54	MG	CA	1617	1/1	0.67	0.24	90,90,90,90	0
54	MG	CA	1710	1/1	0.67	0.18	119,119,119,119	0
54	MG	CA	1725	1/1	0.67	0.17	105,105,105,105	0
54	MG	BA	3163	1/1	0.67	0.15	72,72,72,72	0
54	MG	DA	3316	1/1	0.67	0.09	97,97,97,97	0
54	MG	AA	1761	1/1	0.67	0.16	104,104,104,104	0
54	MG	DA	3011	1/1	0.68	0.17	99,99,99,99	0
54	MG	AA	1623	1/1	0.68	0.21	93,93,93,93	0
54	MG	AA	1706	1/1	0.68	0.07	103,103,103,103	0
54	MG	DA	2938	1/1	0.68	0.29	66,66,66,66	0
54	MG	CA	1718	1/1	0.68	0.10	78,78,78,78	0
54	MG	DA	3169	1/1	0.68	0.17	112,112,112,112	0
54	MG	DA	2972	1/1	0.69	0.22	47,47,47,47	0
54	MG	AA	1699	1/1	0.69	0.08	91,91,91,91	0
54	MG	AA	1669	1/1	0.69	0.21	110,110,110,110	0
54	MG	DA	3311	1/1	0.69	0.13	95,95,95,95	0
54	MG	AA	1696	1/1	0.69	0.19	132,132,132,132	0
54	MG	CA	1678	1/1	0.69	0.10	107,107,107,107	0
54	MG	BK	201	1/1	0.69	0.20	91,91,91,91	0
54	MG	DA	3152	1/1	0.69	0.16	77,77,77,77	0
54	MG	DG	201	1/1	0.69	0.24	101,101,101,101	0
54	MG	AA	1657	1/1	0.70	0.11	101,101,101,101	0
54	MG	DA	3087	1/1	0.70	0.21	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	AA	1691	1/1	0.70	0.11	78,78,78,78	0
54	MG	DB	215	1/1	0.70	0.22	103,103,103,103	0
54	MG	BA	3172	1/1	0.70	0.12	102,102,102,102	0
54	MG	AA	1643	1/1	0.71	0.15	70,70,70,70	0
54	MG	BA	3190	1/1	0.71	0.18	115,115,115,115	0
54	MG	AA	1734	1/1	0.71	0.16	103,103,103,103	0
54	MG	BB	211	1/1	0.71	0.23	112,112,112,112	0
54	MG	DA	3278	1/1	0.71	0.25	75,75,75,75	0
54	MG	BA	3039	1/1	0.71	0.11	94,94,94,94	0
54	MG	CA	1614	1/1	0.71	0.21	89,89,89,89	0
54	MG	CA	1740	1/1	0.71	0.15	117,117,117,117	0
54	MG	AA	1625	1/1	0.71	0.35	88,88,88,88	0
54	MG	DA	3181	1/1	0.71	0.08	106,106,106,106	0
54	MG	DA	2970	1/1	0.71	0.19	67,67,67,67	0
54	MG	BA	3073	1/1	0.71	0.11	89,89,89,89	0
54	MG	BA	3176	1/1	0.71	0.18	99,99,99,99	0
54	MG	DA	3014	1/1	0.72	0.22	69,69,69,69	0
54	MG	BA	3129	1/1	0.72	0.07	75,75,75,75	0
54	MG	DA	3047	1/1	0.72	0.16	66,66,66,66	0
54	MG	AA	1653	1/1	0.72	0.17	89,89,89,89	0
54	MG	BA	3070	1/1	0.72	0.12	75,75,75,75	0
54	MG	AA	1735	1/1	0.72	0.06	104,104,104,104	0
54	MG	AA	1679	1/1	0.72	0.09	78,78,78,78	0
54	MG	DA	3162	1/1	0.72	0.13	143,143,143,143	0
54	MG	BA	3058	1/1	0.72	0.12	114,114,114,114	0
54	MG	DA	3086	1/1	0.73	0.26	92,92,92,92	0
54	MG	AA	1701	1/1	0.73	0.21	83,83,83,83	0
54	MG	BA	3204	1/1	0.73	0.27	74,74,74,74	0
54	MG	BA	3031	1/1	0.73	0.47	87,87,87,87	0
54	MG	AA	1685	1/1	0.73	0.17	106,106,106,106	0
54	MG	BA	3240	1/1	0.73	0.18	114,114,114,114	0
54	MG	AA	1648	1/1	0.73	0.24	76,76,76,76	0
54	MG	AA	1722	1/1	0.73	0.23	83,83,83,83	0
54	MG	DA	3128	1/1	0.74	0.13	114,114,114,114	0
54	MG	DA	3268	1/1	0.74	0.26	81,81,81,81	0
54	MG	BA	3118	1/1	0.74	0.21	109,109,109,109	0
54	MG	CA	1728	1/1	0.74	0.12	82,82,82,82	0
54	MG	DA	3017	1/1	0.74	0.17	93,93,93,93	0
54	MG	BA	3027	1/1	0.74	0.24	62,62,62,62	0
54	MG	BA	3255	1/1	0.74	0.21	57,57,57,57	0
54	MG	AA	1650	1/1	0.74	0.25	103,103,103,103	0
54	MG	BA	3192	1/1	0.74	0.28	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	AA	1641	1/1	0.74	0.27	85,85,85,85	0
54	MG	BA	3117	1/1	0.74	0.26	77,77,77,77	0
54	MG	DA	3318	1/1	0.74	0.12	101,101,101,101	0
54	MG	DA	3235	1/1	0.74	0.32	90,90,90,90	0
54	MG	DA	3257	1/1	0.74	0.14	94,94,94,94	0
54	MG	D2	101	1/1	0.74	0.23	66,66,66,66	0
54	MG	CV	6301	1/1	0.75	0.08	98,98,98,98	0
54	MG	AA	1729	1/1	0.75	0.16	75,75,75,75	0
54	MG	DA	3259	1/1	0.75	0.10	108,108,108,108	0
54	MG	DB	206	1/1	0.75	0.16	99,99,99,99	0
54	MG	DA	2968	1/1	0.75	0.14	56,56,56,56	0
54	MG	AA	1700	1/1	0.75	0.08	98,98,98,98	0
54	MG	CA	1685	1/1	0.75	0.40	106,106,106,106	0
54	MG	DA	3147	1/1	0.76	0.18	78,78,78,78	0
54	MG	BA	3225	1/1	0.76	0.19	74,74,74,74	0
54	MG	DA	2999	1/1	0.76	0.30	76,76,76,76	0
54	MG	CA	1723	1/1	0.76	0.20	141,141,141,141	0
54	MG	DA	3166	1/1	0.76	0.16	87,87,87,87	0
54	MG	BA	3109	1/1	0.76	0.09	90,90,90,90	0
54	MG	DA	3291	1/1	0.76	0.19	78,78,78,78	0
54	MG	DA	3296	1/1	0.76	0.07	104,104,104,104	0
54	MG	AA	1760	1/1	0.76	0.16	84,84,84,84	0
54	MG	AA	1680	1/1	0.76	0.14	90,90,90,90	0
54	MG	BA	3265	1/1	0.76	0.17	80,80,80,80	0
54	MG	DA	3209	1/1	0.76	0.30	80,80,80,80	0
54	MG	AA	1745	1/1	0.76	0.08	97,97,97,97	0
54	MG	AA	1646	1/1	0.76	0.23	99,99,99,99	0
54	MG	BA	3158	1/1	0.76	0.12	105,105,105,105	0
54	MG	DA	3238	1/1	0.76	0.08	58,58,58,58	0
54	MG	BA	3213	1/1	0.76	0.20	101,101,101,101	0
54	MG	AV	6304	1/1	0.76	0.16	118,118,118,118	0
54	MG	AA	1609	1/1	0.77	0.27	70,70,70,70	0
54	MG	AA	1694	1/1	0.77	0.21	129,129,129,129	0
54	MG	CA	1633	1/1	0.77	0.26	102,102,102,102	0
54	MG	BA	3218	1/1	0.77	0.24	75,75,75,75	0
54	MG	DA	3094	1/1	0.77	0.10	76,76,76,76	0
54	MG	DA	3300	1/1	0.77	0.11	68,68,68,68	0
54	MG	CA	1639	1/1	0.77	0.20	66,66,66,66	0
54	MG	BA	3116	1/1	0.77	0.14	85,85,85,85	0
54	MG	BA	3075	1/1	0.77	0.13	67,67,67,67	0
54	MG	DA	3253	1/1	0.77	0.11	92,92,92,92	0
54	MG	BA	3283	1/1	0.77	0.09	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	BA	3198	1/1	0.77	0.33	81,81,81,81	0
54	MG	BA	3248	1/1	0.77	0.13	77,77,77,77	0
54	MG	DB	211	1/1	0.77	0.08	109,109,109,109	0
54	MG	BA	3036	1/1	0.77	0.12	92,92,92,92	0
54	MG	BA	3263	1/1	0.77	0.09	80,80,80,80	0
54	MG	DA	3272	1/1	0.77	0.25	41,41,41,41	0
54	MG	CA	1675	1/1	0.78	0.24	107,107,107,107	0
54	MG	BA	3107	1/1	0.78	0.16	87,87,87,87	0
54	MG	AA	1737	1/1	0.78	0.08	86,86,86,86	0
54	MG	DA	3042	1/1	0.78	0.32	79,79,79,79	0
54	MG	DA	3175	1/1	0.78	0.14	81,81,81,81	0
54	MG	DA	3281	1/1	0.78	0.17	73,73,73,73	0
54	MG	DA	3178	1/1	0.78	0.17	83,83,83,83	0
54	MG	CA	1628	1/1	0.78	0.13	100,100,100,100	0
54	MG	BA	3115	1/1	0.78	0.09	91,91,91,91	0
54	MG	AA	1634	1/1	0.78	0.14	70,70,70,70	0
54	MG	AA	1726	1/1	0.78	0.14	108,108,108,108	0
54	MG	AA	1752	1/1	0.78	0.28	81,81,81,81	0
54	MG	DA	3220	1/1	0.78	0.13	70,70,70,70	0
54	MG	DA	3109	1/1	0.78	0.12	54,54,54,54	0
54	MG	DA	3110	1/1	0.78	0.12	86,86,86,86	0
54	MG	AA	1665	1/1	0.78	0.19	82,82,82,82	0
54	MG	DA	3127	1/1	0.78	0.28	90,90,90,90	0
54	MG	BA	3080	1/1	0.78	0.11	73,73,73,73	0
54	MG	BB	213	1/1	0.78	0.33	84,84,84,84	0
54	MG	DA	3260	1/1	0.78	0.41	102,102,102,102	0
54	MG	BA	2986	1/1	0.78	0.10	67,67,67,67	0
54	MG	CA	1622	1/1	0.79	0.17	79,79,79,79	0
54	MG	AA	1612	1/1	0.79	0.16	64,64,64,64	0
54	MG	AA	1613	1/1	0.79	0.14	47,47,47,47	0
54	MG	AA	1621	1/1	0.79	0.35	74,74,74,74	0
54	MG	DA	3271	1/1	0.79	0.07	97,97,97,97	0
54	MG	AA	1622	1/1	0.79	0.33	88,88,88,88	0
54	MG	BA	3300	1/1	0.79	0.15	83,83,83,83	0
54	MG	BA	3212	1/1	0.79	0.09	69,69,69,69	0
54	MG	BB	207	1/1	0.79	0.10	105,105,105,105	0
54	MG	DA	3052	1/1	0.79	0.21	107,107,107,107	0
54	MG	DA	3182	1/1	0.79	0.12	86,86,86,86	0
54	MG	DA	3295	1/1	0.79	0.12	63,63,63,63	0
54	MG	DA	3055	1/1	0.79	0.13	93,93,93,93	0
54	MG	DA	3185	1/1	0.79	0.14	108,108,108,108	0
54	MG	CA	1661	1/1	0.79	0.25	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	DA	3085	1/1	0.79	0.10	89,89,89,89	0
54	MG	CA	1666	1/1	0.79	0.15	116,116,116,116	0
54	MG	BB	208	1/1	0.79	0.14	109,109,109,109	0
54	MG	DA	3224	1/1	0.79	0.26	72,72,72,72	0
54	MG	AA	1678	1/1	0.79	0.11	115,115,115,115	0
54	MG	CA	1672	1/1	0.79	0.10	62,62,62,62	0
54	MG	BA	3187	1/1	0.79	0.28	40,40,40,40	0
54	MG	DB	214	1/1	0.79	0.15	90,90,90,90	0
54	MG	BA	3266	1/1	0.79	0.28	98,98,98,98	0
54	MG	DB	216	1/1	0.79	0.15	88,88,88,88	0
54	MG	BA	3135	1/1	0.79	0.09	77,77,77,77	0
54	MG	BA	3219	1/1	0.79	0.24	66,66,66,66	0
54	MG	DA	3256	1/1	0.80	0.14	82,82,82,82	0
54	MG	BA	3302	1/1	0.80	0.08	121,121,121,121	0
54	MG	DA	3115	1/1	0.80	0.12	65,65,65,65	0
54	MG	BA	3243	1/1	0.80	0.14	82,82,82,82	0
54	MG	CP	101	1/1	0.80	0.10	96,96,96,96	0
54	MG	BA	3004	1/1	0.80	0.28	74,74,74,74	0
54	MG	DA	3141	1/1	0.80	0.06	95,95,95,95	0
54	MG	BA	3149	1/1	0.80	0.31	82,82,82,82	0
54	MG	BA	3152	1/1	0.80	0.09	75,75,75,75	0
54	MG	BA	3049	1/1	0.80	0.18	86,86,86,86	0
54	MG	AA	1714	1/1	0.80	0.29	58,58,58,58	0
54	MG	DA	3280	1/1	0.80	0.17	84,84,84,84	0
54	MG	CA	1684	1/1	0.80	0.07	117,117,117,117	0
54	MG	BA	3059	1/1	0.80	0.14	60,60,60,60	0
54	MG	CA	1616	1/1	0.80	0.14	75,75,75,75	0
54	MG	CA	1689	1/1	0.80	0.20	83,83,83,83	0
54	MG	BA	3009	1/1	0.80	0.12	87,87,87,87	0
54	MG	DA	3029	1/1	0.80	0.09	70,70,70,70	0
54	MG	DA	3305	1/1	0.80	0.11	110,110,110,110	0
54	MG	BA	3026	1/1	0.80	0.11	82,82,82,82	0
54	MG	CA	1623	1/1	0.80	0.25	99,99,99,99	0
54	MG	AA	1757	1/1	0.80	0.09	89,89,89,89	0
54	MG	DA	3200	1/1	0.80	0.14	87,87,87,87	0
54	MG	BA	3281	1/1	0.80	0.14	84,84,84,84	0
54	MG	CA	1708	1/1	0.80	0.10	143,143,143,143	0
54	MG	BA	3226	1/1	0.80	0.12	81,81,81,81	0
54	MG	CA	1711	1/1	0.80	0.18	87,87,87,87	0
54	MG	DA	3230	1/1	0.80	0.11	63,63,63,63	0
54	MG	BA	3284	1/1	0.80	0.17	85,85,85,85	0
54	MG	AA	1652	1/1	0.80	0.18	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	BA	3299	1/1	0.80	0.15	80,80,80,80	0
54	MG	AA	1693	1/1	0.80	0.12	74,74,74,74	0
54	MG	CA	1736	1/1	0.81	0.19	115,115,115,115	0
54	MG	BA	2978	1/1	0.81	0.29	59,59,59,59	0
54	MG	DA	3064	1/1	0.81	0.20	80,80,80,80	0
54	MG	DA	3069	1/1	0.81	0.11	81,81,81,81	0
54	MG	AA	1702	1/1	0.81	0.36	94,94,94,94	0
54	MG	BA	3119	1/1	0.81	0.15	64,64,64,64	0
54	MG	AA	1647	1/1	0.81	0.12	85,85,85,85	0
54	MG	BA	3229	1/1	0.81	0.21	62,62,62,62	0
54	MG	DA	3286	1/1	0.81	0.06	98,98,98,98	0
54	MG	DA	3187	1/1	0.81	0.22	90,90,90,90	0
54	MG	DA	3091	1/1	0.81	0.08	125,125,125,125	0
54	MG	BB	214	1/1	0.81	0.20	101,101,101,101	0
54	MG	DA	3299	1/1	0.81	0.15	68,68,68,68	0
54	MG	DA	3105	1/1	0.81	0.20	75,75,75,75	0
54	MG	AA	1618	1/1	0.81	0.19	91,91,91,91	0
54	MG	DA	3307	1/1	0.81	0.14	73,73,73,73	0
54	MG	BA	3136	1/1	0.81	0.10	87,87,87,87	0
54	MG	DA	2986	1/1	0.81	0.14	55,55,55,55	0
54	MG	AD	302	1/1	0.81	0.11	87,87,87,87	0
54	MG	BA	3022	1/1	0.81	0.27	77,77,77,77	0
54	MG	CA	1713	1/1	0.81	0.07	80,80,80,80	0
54	MG	DA	3242	1/1	0.81	0.26	96,96,96,96	0
54	MG	AA	1755	1/1	0.81	0.15	103,103,103,103	0
54	MG	DA	3143	1/1	0.81	0.07	77,77,77,77	0
54	MG	DA	3028	1/1	0.81	0.18	78,78,78,78	0
54	MG	AA	1629	1/1	0.81	0.35	72,72,72,72	0
54	MG	BA	3072	1/1	0.81	0.12	67,67,67,67	0
54	MG	BA	3303	1/1	0.81	0.17	98,98,98,98	0
54	MG	CA	1687	1/1	0.81	0.17	64,64,64,64	0
54	MG	CA	1739	1/1	0.82	0.07	99,99,99,99	0
54	MG	DA	3170	1/1	0.82	0.10	80,80,80,80	0
54	MG	BA	3025	1/1	0.82	0.14	65,65,65,65	0
54	MG	DA	3274	1/1	0.82	0.14	62,62,62,62	0
54	MG	DA	3072	1/1	0.82	0.13	73,73,73,73	0
54	MG	DA	3074	1/1	0.82	0.17	64,64,64,64	0
54	MG	DA	3080	1/1	0.82	0.11	69,69,69,69	0
54	MG	AA	1673	1/1	0.82	0.09	61,61,61,61	0
54	MG	CA	1694	1/1	0.82	0.17	59,59,59,59	0
54	MG	CA	1646	1/1	0.82	0.08	78,78,78,78	0
54	MG	DA	3290	1/1	0.82	0.10	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	BB	212	1/1	0.82	0.06	89,89,89,89	0
54	MG	AA	1724	1/1	0.82	0.13	85,85,85,85	0
54	MG	BA	3165	1/1	0.82	0.15	71,71,71,71	0
54	MG	DA	3103	1/1	0.82	0.24	79,79,79,79	0
54	MG	BA	3170	1/1	0.82	0.09	64,64,64,64	0
54	MG	CA	1706	1/1	0.82	0.30	101,101,101,101	0
54	MG	AA	1732	1/1	0.82	0.09	63,63,63,63	0
54	MG	BA	3175	1/1	0.82	0.09	85,85,85,85	0
54	MG	BA	3067	1/1	0.82	0.11	86,86,86,86	0
54	MG	CA	1621	1/1	0.82	0.21	67,67,67,67	0
54	MG	DA	3022	1/1	0.82	0.18	60,60,60,60	0
54	MG	CA	1674	1/1	0.82	0.14	74,74,74,74	0
54	MG	AA	1733	1/1	0.82	0.11	91,91,91,91	0
54	MG	DA	3319	1/1	0.82	0.06	83,83,83,83	0
54	MG	DA	3322	1/1	0.82	0.11	95,95,95,95	0
54	MG	CA	1724	1/1	0.82	0.09	74,74,74,74	0
54	MG	BA	3038	1/1	0.82	0.15	65,65,65,65	0
54	MG	CA	1627	1/1	0.82	0.09	67,67,67,67	0
54	MG	DA	3264	1/1	0.82	0.16	61,61,61,61	0
54	MG	BB	206	1/1	0.82	0.07	70,70,70,70	0
54	MG	DA	3267	1/1	0.82	0.13	76,76,76,76	0
54	MG	AA	1644	1/1	0.82	0.19	53,53,53,53	0
54	MG	BA	3285	1/1	0.83	0.08	87,87,87,87	0
54	MG	AA	1651	1/1	0.83	0.17	97,97,97,97	0
54	MG	DA	3097	1/1	0.83	0.18	94,94,94,94	0
54	MG	DA	3279	1/1	0.83	0.11	88,88,88,88	0
54	MG	DA	3101	1/1	0.83	0.21	72,72,72,72	0
54	MG	BA	3112	1/1	0.83	0.07	68,68,68,68	0
54	MG	CA	1722	1/1	0.83	0.22	108,108,108,108	0
54	MG	DA	3021	1/1	0.83	0.12	67,67,67,67	0
54	MG	BA	3114	1/1	0.83	0.26	78,78,78,78	0
54	MG	DA	3113	1/1	0.83	0.09	71,71,71,71	0
54	MG	AA	1763	1/1	0.83	0.20	96,96,96,96	0
54	MG	BA	3258	1/1	0.83	0.12	104,104,104,104	0
54	MG	DA	3119	1/1	0.83	0.14	88,88,88,88	0
54	MG	DA	3120	1/1	0.83	0.23	66,66,66,66	0
54	MG	BA	3160	1/1	0.83	0.08	106,106,106,106	0
54	MG	AA	1614	1/1	0.83	0.31	85,85,85,85	0
54	MG	DA	3244	1/1	0.83	0.15	87,87,87,87	0
54	MG	DA	3246	1/1	0.83	0.26	67,67,67,67	0
54	MG	BA	3060	1/1	0.83	0.23	74,74,74,74	0
54	MG	DA	3254	1/1	0.83	0.11	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	BA	3037	1/1	0.83	0.11	93,93,93,93	0
54	MG	BB	210	1/1	0.83	0.18	100,100,100,100	0
54	MG	CA	1647	1/1	0.83	0.24	77,77,77,77	0
54	MG	BA	2996	1/1	0.83	0.17	54,54,54,54	0
54	MG	DA	3323	1/1	0.83	0.08	69,69,69,69	0
54	MG	DA	3334	1/1	0.83	0.07	72,72,72,72	0
54	MG	DA	2924	1/1	0.83	0.24	41,41,41,41	0
54	MG	BA	3222	1/1	0.83	0.50	91,91,91,91	0
54	MG	BA	3121	1/1	0.83	0.05	77,77,77,77	0
54	MG	BA	3093	1/1	0.83	0.26	83,83,83,83	0
54	MG	CA	1663	1/1	0.83	0.19	86,86,86,86	0
54	MG	BA	3103	1/1	0.83	0.13	88,88,88,88	0
54	MG	AA	1632	1/1	0.83	0.21	68,68,68,68	0
54	MG	CA	1717	1/1	0.84	0.26	84,84,84,84	0
54	MG	CA	1636	1/1	0.84	0.12	93,93,93,93	0
54	MG	AA	1645	1/1	0.84	0.24	79,79,79,79	0
54	MG	AA	1681	1/1	0.84	0.15	99,99,99,99	0
54	MG	DA	3298	1/1	0.84	0.18	79,79,79,79	0
54	MG	DA	2971	1/1	0.84	0.30	47,47,47,47	0
54	MG	DA	3104	1/1	0.84	0.07	99,99,99,99	0
54	MG	BA	3150	1/1	0.84	0.06	79,79,79,79	0
54	MG	DA	3258	1/1	0.84	0.23	72,72,72,72	0
54	MG	DA	3180	1/1	0.84	0.08	77,77,77,77	0
54	MG	BA	3294	1/1	0.84	0.12	64,64,64,64	0
54	MG	DA	3060	1/1	0.84	0.10	87,87,87,87	0
54	MG	AA	1758	1/1	0.84	0.06	73,73,73,73	0
54	MG	DA	3066	1/1	0.84	0.35	85,85,85,85	0
54	MG	DA	2994	1/1	0.84	0.17	67,67,67,67	0
54	MG	CA	1676	1/1	0.84	0.15	82,82,82,82	0
54	MG	DA	3320	1/1	0.84	0.18	58,58,58,58	0
54	MG	BA	3253	1/1	0.84	0.13	76,76,76,76	0
54	MG	DA	3012	1/1	0.84	0.11	45,45,45,45	0
54	MG	AV	6301	1/1	0.84	0.07	72,72,72,72	0
54	MG	DA	3134	1/1	0.84	0.11	71,71,71,71	0
54	MG	DA	3222	1/1	0.84	0.23	70,70,70,70	0
54	MG	AA	1723	1/1	0.84	0.17	81,81,81,81	0
54	MG	CA	1662	1/1	0.84	0.23	86,86,86,86	0
54	MG	AA	1649	1/1	0.84	0.15	89,89,89,89	0
54	MG	DA	3090	1/1	0.84	0.10	71,71,71,71	0
54	MG	DA	3154	1/1	0.84	0.34	94,94,94,94	0
54	MG	AA	1667	1/1	0.85	0.35	61,61,61,61	0
54	MG	BA	2994	1/1	0.85	0.21	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	BA	3267	1/1	0.85	0.28	86,86,86,86	0
54	MG	BA	3162	1/1	0.85	0.15	94,94,94,94	0
54	MG	AA	1677	1/1	0.85	0.11	64,64,64,64	0
54	MG	BA	3101	1/1	0.85	0.21	75,75,75,75	0
54	MG	CA	1665	1/1	0.85	0.17	89,89,89,89	0
54	MG	BB	216	1/1	0.85	0.14	79,79,79,79	0
54	MG	BA	3166	1/1	0.85	0.09	74,74,74,74	0
54	MG	CA	1610	1/1	0.85	0.15	77,77,77,77	0
54	MG	BA	3122	1/1	0.85	0.12	101,101,101,101	0
54	MG	BA	3123	1/1	0.85	0.13	52,52,52,52	0
54	MG	BA	3173	1/1	0.85	0.19	80,80,80,80	0
54	MG	DA	3297	1/1	0.85	0.15	49,49,49,49	0
54	MG	CA	1620	1/1	0.85	0.14	79,79,79,79	0
54	MG	DA	3051	1/1	0.85	0.11	89,89,89,89	0
54	MG	CA	1733	1/1	0.85	0.06	72,72,72,72	0
54	MG	DA	3302	1/1	0.85	0.18	77,77,77,77	0
54	MG	DA	3236	1/1	0.85	0.23	63,63,63,63	0
54	MG	DA	3129	1/1	0.85	0.14	63,63,63,63	0
54	MG	BA	3174	1/1	0.85	0.11	84,84,84,84	0
54	MG	DA	3136	1/1	0.85	0.17	68,68,68,68	0
54	MG	BA	3032	1/1	0.85	0.27	59,59,59,59	0
54	MG	DA	3251	1/1	0.85	0.23	63,63,63,63	0
54	MG	DA	3142	1/1	0.85	0.17	109,109,109,109	0
54	MG	BA	3291	1/1	0.85	0.09	68,68,68,68	0
54	MG	CA	1686	1/1	0.85	0.29	60,60,60,60	0
54	MG	BA	3238	1/1	0.85	0.17	91,91,91,91	0
54	MG	BA	3034	1/1	0.85	0.37	102,102,102,102	0
54	MG	AA	1631	1/1	0.85	0.17	70,70,70,70	0
54	MG	DA	2940	1/1	0.85	0.28	51,51,51,51	0
54	MG	DB	203	1/1	0.85	0.20	82,82,82,82	0
54	MG	DA	3263	1/1	0.85	0.17	63,63,63,63	0
54	MG	AA	1712	1/1	0.85	0.26	75,75,75,75	0
54	MG	DB	212	1/1	0.85	0.10	70,70,70,70	0
54	MG	DA	3168	1/1	0.85	0.18	94,94,94,94	0
54	MG	AA	1713	1/1	0.85	0.16	93,93,93,93	0
54	MG	AA	1749	1/1	0.85	0.11	90,90,90,90	0
54	MG	AA	1750	1/1	0.85	0.10	109,109,109,109	0
54	MG	BA	3199	1/1	0.85	0.25	68,68,68,68	0
54	MG	CA	1726	1/1	0.86	0.11	87,87,87,87	0
54	MG	BA	3017	1/1	0.86	0.21	69,69,69,69	0
54	MG	DA	3153	1/1	0.86	0.06	85,85,85,85	0
54	MG	BA	3207	1/1	0.86	0.24	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	DA	3063	1/1	0.86	0.16	79,79,79,79	0
54	MG	BA	2905	1/1	0.86	0.19	12,12,12,12	0
54	MG	CA	1681	1/1	0.86	0.19	81,81,81,81	0
54	MG	DA	3275	1/1	0.86	0.16	78,78,78,78	0
54	MG	CA	1630	1/1	0.86	0.18	70,70,70,70	0
54	MG	BB	209	1/1	0.86	0.14	83,83,83,83	0
54	MG	BA	3124	1/1	0.86	0.09	89,89,89,89	0
54	MG	DA	3078	1/1	0.86	0.08	79,79,79,79	0
54	MG	AA	1637	1/1	0.86	0.26	61,61,61,61	0
54	MG	BA	3178	1/1	0.86	0.14	72,72,72,72	0
54	MG	BA	3184	1/1	0.86	0.19	42,42,42,42	0
54	MG	DA	2939	1/1	0.86	0.22	40,40,40,40	0
54	MG	BA	3293	1/1	0.86	0.09	86,86,86,86	0
54	MG	DA	2965	1/1	0.86	0.22	57,57,57,57	0
54	MG	AA	1741	1/1	0.86	0.12	74,74,74,74	0
54	MG	DA	3092	1/1	0.86	0.12	98,98,98,98	0
54	MG	CA	1697	1/1	0.86	0.18	74,74,74,74	0
54	MG	DA	3095	1/1	0.86	0.14	67,67,67,67	0
54	MG	BB	217	1/1	0.86	0.08	78,78,78,78	0
54	MG	DA	3098	1/1	0.86	0.20	71,71,71,71	0
54	MG	CA	1699	1/1	0.86	0.22	71,71,71,71	0
54	MG	CA	1652	1/1	0.86	0.14	85,85,85,85	0
54	MG	DA	3226	1/1	0.86	0.10	80,80,80,80	0
54	MG	BA	3295	1/1	0.86	0.32	70,70,70,70	0
54	MG	CA	1660	1/1	0.86	0.07	100,100,100,100	0
54	MG	DA	3315	1/1	0.86	0.17	52,52,52,52	0
54	MG	CA	1705	1/1	0.86	0.08	54,54,54,54	0
54	MG	DA	3002	1/1	0.86	0.17	59,59,59,59	0
54	MG	CA	1601	1/1	0.86	0.32	53,53,53,53	0
54	MG	CA	1606	1/1	0.86	0.21	68,68,68,68	0
54	MG	DA	3243	1/1	0.86	0.12	72,72,72,72	0
54	MG	CA	1709	1/1	0.86	0.34	81,81,81,81	0
54	MG	BA	3298	1/1	0.86	0.16	74,74,74,74	0
54	MG	DA	3327	1/1	0.86	0.13	68,68,68,68	0
54	MG	CA	1664	1/1	0.86	0.19	82,82,82,82	0
54	MG	DA	3122	1/1	0.86	0.12	87,87,87,87	0
54	MG	AA	1624	1/1	0.86	0.27	67,67,67,67	0
54	MG	DA	3025	1/1	0.86	0.16	69,69,69,69	0
54	MG	BA	3145	1/1	0.86	0.07	67,67,67,67	0
54	MG	BA	3148	1/1	0.86	0.13	68,68,68,68	0
54	MG	BA	3011	1/1	0.86	0.12	83,83,83,83	0
54	MG	BA	3082	1/1	0.86	0.10	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	CA	1673	1/1	0.86	0.08	73,73,73,73	0
54	MG	BA	3308	1/1	0.86	0.09	94,94,94,94	0
54	MG	BA	3066	1/1	0.87	0.19	56,56,56,56	0
54	MG	DA	3273	1/1	0.87	0.17	85,85,85,85	0
54	MG	BA	3030	1/1	0.87	0.16	57,57,57,57	0
54	MG	DA	3176	1/1	0.87	0.17	83,83,83,83	0
54	MG	DA	3089	1/1	0.87	0.11	76,76,76,76	0
54	MG	BA	3274	1/1	0.87	0.16	78,78,78,78	0
54	MG	BA	2988	1/1	0.87	0.16	60,60,60,60	0
54	MG	AA	1639	1/1	0.87	0.18	79,79,79,79	0
54	MG	AA	1692	1/1	0.87	0.19	84,84,84,84	0
54	MG	DA	2987	1/1	0.87	0.22	70,70,70,70	0
54	MG	AA	1655	1/1	0.87	0.16	72,72,72,72	0
54	MG	DA	3287	1/1	0.87	0.14	69,69,69,69	0
54	MG	AA	1738	1/1	0.87	0.17	70,70,70,70	0
54	MG	DA	3199	1/1	0.87	0.36	38,38,38,38	0
54	MG	AA	1610	1/1	0.87	0.18	78,78,78,78	0
54	MG	AA	1687	1/1	0.87	0.10	73,73,73,73	0
54	MG	CA	1607	1/1	0.87	0.17	52,52,52,52	0
54	MG	DA	3013	1/1	0.87	0.13	44,44,44,44	0
54	MG	DA	3106	1/1	0.87	0.17	67,67,67,67	0
54	MG	BA	3288	1/1	0.87	0.12	62,62,62,62	0
54	MG	CA	1611	1/1	0.87	0.15	76,76,76,76	0
54	MG	CA	1612	1/1	0.87	0.24	58,58,58,58	0
54	MG	BA	3042	1/1	0.87	0.09	90,90,90,90	0
54	MG	BA	3084	1/1	0.87	0.20	51,51,51,51	0
54	MG	BA	3090	1/1	0.87	0.15	69,69,69,69	0
54	MG	AA	1707	1/1	0.87	0.10	100,100,100,100	0
54	MG	BA	3143	1/1	0.87	0.17	84,84,84,84	0
54	MG	BA	3250	1/1	0.87	0.12	95,95,95,95	0
54	MG	CA	1680	1/1	0.87	0.26	58,58,58,58	0
54	MG	BA	3252	1/1	0.87	0.15	92,92,92,92	0
54	MG	DA	3130	1/1	0.87	0.10	82,82,82,82	0
54	MG	BA	3097	1/1	0.87	0.15	53,53,53,53	0
54	MG	BA	3054	1/1	0.87	0.13	46,46,46,46	0
54	MG	BA	2935	1/1	0.87	0.24	34,34,34,34	0
54	MG	BA	2949	1/1	0.87	0.17	47,47,47,47	0
54	MG	AA	1747	1/1	0.87	0.26	75,75,75,75	0
54	MG	DB	202	1/1	0.87	0.32	64,64,64,64	0
54	MG	BA	3110	1/1	0.87	0.09	86,86,86,86	0
54	MG	DA	2934	1/1	0.87	0.24	25,25,25,25	0
54	MG	DB	209	1/1	0.87	0.07	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	DA	3070	1/1	0.87	0.21	70,70,70,70	0
54	MG	CA	1693	1/1	0.87	0.17	65,65,65,65	0
54	MG	AA	1748	1/1	0.87	0.10	96,96,96,96	0
54	MG	CA	1645	1/1	0.87	0.16	72,72,72,72	0
54	MG	DA	2941	1/1	0.87	0.19	37,37,37,37	0
54	MG	BA	3270	1/1	0.87	0.10	61,61,61,61	0
54	MG	DA	2966	1/1	0.87	0.23	70,70,70,70	0
54	MG	BA	3185	1/1	0.88	0.28	56,56,56,56	0
54	MG	DA	3065	1/1	0.88	0.14	56,56,56,56	0
54	MG	DA	3215	1/1	0.88	0.31	39,39,39,39	0
54	MG	BA	3301	1/1	0.88	0.17	66,66,66,66	0
54	MG	BA	3077	1/1	0.88	0.17	75,75,75,75	0
54	MG	DA	3289	1/1	0.88	0.07	92,92,92,92	0
54	MG	CA	1715	1/1	0.88	0.18	74,74,74,74	0
54	MG	BA	3279	1/1	0.88	0.11	77,77,77,77	0
54	MG	BA	3304	1/1	0.88	0.09	124,124,124,124	0
54	MG	DA	3233	1/1	0.88	0.09	57,57,57,57	0
54	MG	BA	2939	1/1	0.88	0.21	26,26,26,26	0
54	MG	DA	3138	1/1	0.88	0.08	70,70,70,70	0
54	MG	BA	2912	1/1	0.88	0.33	36,36,36,36	0
54	MG	CA	1651	1/1	0.88	0.13	99,99,99,99	0
54	MG	BB	205	1/1	0.88	0.10	71,71,71,71	0
54	MG	BA	3050	1/1	0.88	0.05	41,41,41,41	0
54	MG	DA	3150	1/1	0.88	0.08	62,62,62,62	0
54	MG	DA	3310	1/1	0.88	0.08	52,52,52,52	0
54	MG	CA	1727	1/1	0.88	0.13	75,75,75,75	0
54	MG	BA	3259	1/1	0.88	0.14	75,75,75,75	0
54	MG	BA	2992	1/1	0.88	0.22	70,70,70,70	0
54	MG	BA	3071	1/1	0.88	0.16	72,72,72,72	0
54	MG	BA	3289	1/1	0.88	0.18	65,65,65,65	0
54	MG	DA	3018	1/1	0.88	0.13	73,73,73,73	0
54	MG	BA	2971	1/1	0.88	0.28	65,65,65,65	0
54	MG	CA	1626	1/1	0.88	0.17	65,65,65,65	0
54	MG	AA	1666	1/1	0.88	0.11	100,100,100,100	0
54	MG	DA	3262	1/1	0.88	0.16	82,82,82,82	0
54	MG	CA	1700	1/1	0.88	0.15	65,65,65,65	0
54	MG	DA	2904	1/1	0.88	0.29	4,4,4,4	0
54	MG	DA	3329	1/1	0.88	0.25	69,69,69,69	0
54	MG	CA	1667	1/1	0.88	0.08	67,67,67,67	0
54	MG	DA	3037	1/1	0.88	0.14	77,77,77,77	0
54	MG	DA	2929	1/1	0.88	0.22	39,39,39,39	0
54	MG	BA	3019	1/1	0.88	0.18	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	BA	3098	1/1	0.88	0.16	78,78,78,78	0
54	MG	CA	1671	1/1	0.88	0.09	74,74,74,74	0
54	MG	CA	1632	1/1	0.88	0.14	79,79,79,79	0
54	MG	BA	3244	1/1	0.88	0.33	47,47,47,47	0
54	MG	DA	3193	1/1	0.88	0.20	51,51,51,51	0
54	MG	DA	3118	1/1	0.88	0.27	62,62,62,62	0
54	MG	DB	217	1/1	0.88	0.04	74,74,74,74	0
54	MG	BA	3215	1/1	0.88	0.35	68,68,68,68	0
54	MG	DA	3207	1/1	0.88	0.14	42,42,42,42	0
54	MG	DA	3131	1/1	0.89	0.12	66,66,66,66	0
54	MG	DA	3133	1/1	0.89	0.12	89,89,89,89	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	3231	1/1	0.89	0.34	60,60,60,60	0
54	MG	DA	3006	1/1	0.89	0.08	74,74,74,74	0
54	MG	BA	3155	1/1	0.89	0.13	85,85,85,85	0
54	MG	AA	1606	1/1	0.89	0.27	53,53,53,53	0
54	MG	BA	3100	1/1	0.89	0.07	77,77,77,77	0
54	MG	AA	1746	1/1	0.89	0.20	100,100,100,100	0
54	MG	CA	1640	1/1	0.89	0.19	69,69,69,69	0
54	MG	CA	1641	1/1	0.89	0.06	85,85,85,85	0
54	MG	AA	1675	1/1	0.89	0.07	77,77,77,77	0
54	MG	DA	2932	1/1	0.89	0.20	38,38,38,38	0
54	MG	DA	3249	1/1	0.89	0.11	56,56,56,56	0
54	MG	CA	1608	1/1	0.89	0.19	61,61,61,61	0
54	MG	BA	3193	1/1	0.89	0.15	53,53,53,53	0
54	MG	BA	3194	1/1	0.89	0.27	45,45,45,45	0
54	MG	DA	3100	1/1	0.89	0.11	59,59,59,59	0
54	MG	DA	3030	1/1	0.89	0.24	71,71,71,71	0
54	MG	BA	3106	1/1	0.89	0.10	70,70,70,70	0
54	MG	CA	1716	1/1	0.89	0.14	77,77,77,77	0
54	MG	DA	2942	1/1	0.89	0.23	39,39,39,39	0
54	MG	DA	3043	1/1	0.89	0.11	70,70,70,70	0
54	MG	DA	2959	1/1	0.89	0.26	56,56,56,56	0
54	MG	AA	1642	1/1	0.89	0.26	97,97,97,97	0
54	MG	BA	3014	1/1	0.89	0.16	47,47,47,47	0
54	MG	BA	2990	1/1	0.89	0.12	54,54,54,54	0
54	MG	AA	1640	1/1	0.89	0.28	106,106,106,106	0
54	MG	BA	3286	1/1	0.89	0.11	67,67,67,67	0
54	MG	AA	1664	1/1	0.89	0.09	103,103,103,103	0
54	MG	BA	3257	1/1	0.89	0.30	64,64,64,64	0
54	MG	DB	207	1/1	0.89	0.12	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	DA	3198	1/1	0.89	0.19	26,26,26,26	0
54	MG	DA	3121	1/1	0.89	0.08	69,69,69,69	0
54	MG	BA	3024	1/1	0.89	0.21	67,67,67,67	0
54	MG	DA	3125	1/1	0.89	0.18	81,81,81,81	0
54	MG	BA	2960	1/1	0.89	0.20	40,40,40,40	0
54	MG	DA	2993	1/1	0.89	0.16	69,69,69,69	0
54	MG	BA	3096	1/1	0.89	0.17	65,65,65,65	0
54	MG	BA	3003	1/1	0.89	0.09	48,48,48,48	0
54	MG	DA	3221	1/1	0.89	0.10	68,68,68,68	0
54	MG	DA	3099	1/1	0.90	0.15	81,81,81,81	0
54	MG	BA	2968	1/1	0.90	0.33	51,51,51,51	0
54	MG	AA	1705	1/1	0.90	0.06	92,92,92,92	0
54	MG	DA	3183	1/1	0.90	0.07	83,83,83,83	0
54	MG	BA	3012	1/1	0.90	0.16	91,91,91,91	0
54	MG	DA	3020	1/1	0.90	0.15	63,63,63,63	0
54	MG	CA	1683	1/1	0.90	0.18	91,91,91,91	0
54	MG	BA	3209	1/1	0.90	0.18	69,69,69,69	0
54	MG	DA	3282	1/1	0.90	0.08	96,96,96,96	0
54	MG	BA	3211	1/1	0.90	0.28	59,59,59,59	0
54	MG	DA	3027	1/1	0.90	0.32	53,53,53,53	0
54	MG	CA	1638	1/1	0.90	0.07	65,65,65,65	0
54	MG	BA	2977	1/1	0.90	0.15	52,52,52,52	0
54	MG	BA	3081	1/1	0.90	0.11	65,65,65,65	0
54	MG	BA	3045	1/1	0.90	0.09	80,80,80,80	0
54	MG	CA	1692	1/1	0.90	0.22	78,78,78,78	0
54	MG	CA	1644	1/1	0.90	0.22	77,77,77,77	0
54	MG	AA	1756	1/1	0.90	0.21	106,106,106,106	0
54	MG	BA	2983	1/1	0.90	0.28	62,62,62,62	0
54	MG	BA	2914	1/1	0.90	0.23	31,31,31,31	0
54	MG	DA	3223	1/1	0.90	0.37	45,45,45,45	0
54	MG	BA	2916	1/1	0.90	0.35	38,38,38,38	0
54	MG	BA	3280	1/1	0.90	0.09	70,70,70,70	0
54	MG	DA	3057	1/1	0.90	0.12	59,59,59,59	0
54	MG	BA	3094	1/1	0.90	0.14	70,70,70,70	0
54	MG	BA	2932	1/1	0.90	0.18	41,41,41,41	0
54	MG	DA	3132	1/1	0.90	0.11	70,70,70,70	0
54	MG	DA	2949	1/1	0.90	0.20	41,41,41,41	0
54	MG	DA	3314	1/1	0.90	0.25	102,102,102,102	0
54	MG	DA	2953	1/1	0.90	0.22	58,58,58,58	0
54	MG	CA	1656	1/1	0.90	0.07	79,79,79,79	0
54	MG	AA	1616	1/1	0.90	0.21	63,63,63,63	0
54	MG	DA	3140	1/1	0.90	0.11	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	BA	3230	1/1	0.90	0.32	44,44,44,44	0
54	MG	BA	3232	1/1	0.90	0.24	24,24,24,24	0
54	MG	AA	1697	1/1	0.90	0.08	80,80,80,80	0
54	MG	BA	3138	1/1	0.90	0.07	100,100,100,100	0
54	MG	DA	3325	1/1	0.90	0.15	92,92,92,92	0
54	MG	DA	3326	1/1	0.90	0.05	85,85,85,85	0
54	MG	BA	3028	1/1	0.90	0.23	62,62,62,62	0
54	MG	BA	3241	1/1	0.90	0.09	60,60,60,60	0
54	MG	DA	3333	1/1	0.90	0.09	126,126,126,126	0
54	MG	BA	2945	1/1	0.90	0.20	72,72,72,72	0
54	MG	DA	3336	1/1	0.90	0.15	89,89,89,89	0
54	MG	BA	3188	1/1	0.90	0.24	45,45,45,45	0
54	MG	DA	3157	1/1	0.90	0.17	71,71,71,71	0
54	MG	DA	3161	1/1	0.90	0.07	74,74,74,74	0
54	MG	BA	3069	1/1	0.90	0.12	109,109,109,109	0
54	MG	AA	1753	1/1	0.90	0.10	102,102,102,102	0
54	MG	BA	3251	1/1	0.90	0.14	64,64,64,64	0
54	MG	CA	1720	1/1	0.90	0.12	63,63,63,63	0
54	MG	BA	3191	1/1	0.90	0.14	76,76,76,76	0
54	MG	AA	1744	1/1	0.90	0.09	82,82,82,82	0
54	MG	DA	3173	1/1	0.90	0.09	97,97,97,97	0
54	MG	BA	3108	1/1	0.90	0.21	99,99,99,99	0
54	MG	BA	2963	1/1	0.90	0.18	54,54,54,54	0
54	MG	BA	3008	1/1	0.90	0.15	57,57,57,57	0
54	MG	DA	3088	1/1	0.91	0.13	70,70,70,70	0
54	MG	BA	3088	1/1	0.91	0.18	73,73,73,73	0
54	MG	DA	2998	1/1	0.91	0.13	68,68,68,68	0
54	MG	CA	1679	1/1	0.91	0.05	93,93,93,93	0
54	MG	BA	2974	1/1	0.91	0.09	45,45,45,45	0
54	MG	BA	3159	1/1	0.91	0.26	78,78,78,78	0
54	MG	BA	3282	1/1	0.91	0.09	62,62,62,62	0
54	MG	DA	3177	1/1	0.91	0.06	62,62,62,62	0
54	MG	BA	3242	1/1	0.91	0.15	44,44,44,44	0
54	MG	DA	3179	1/1	0.91	0.05	68,68,68,68	0
54	MG	BA	3007	1/1	0.91	0.16	55,55,55,55	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	BA	3200	1/1	0.91	0.16	64,64,64,64	0
54	MG	DA	3285	1/1	0.91	0.19	113,113,113,113	0
54	MG	CA	1737	1/1	0.91	0.10	70,70,70,70	0
54	MG	DA	3019	1/1	0.91	0.21	51,51,51,51	0
54	MG	CA	1738	1/1	0.91	0.16	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	BA	3033	1/1	0.91	0.11	67,67,67,67	0
54	MG	DA	3190	1/1	0.91	0.20	27,27,27,27	0
54	MG	BA	3068	1/1	0.91	0.08	59,59,59,59	0
54	MG	DA	3196	1/1	0.91	0.25	39,39,39,39	0
54	MG	DA	3024	1/1	0.91	0.15	36,36,36,36	0
54	MG	B2	101	1/1	0.91	0.20	64,64,64,64	0
54	MG	AA	1727	1/1	0.91	0.12	100,100,100,100	0
54	MG	DA	3201	1/1	0.91	0.08	72,72,72,72	0
54	MG	DA	3301	1/1	0.91	0.10	80,80,80,80	0
54	MG	DA	3205	1/1	0.91	0.17	48,48,48,48	0
54	MG	CA	1649	1/1	0.91	0.14	80,80,80,80	0
54	MG	DA	3117	1/1	0.91	0.17	87,87,87,87	0
54	MG	CA	1605	1/1	0.91	0.13	56,56,56,56	0
54	MG	AA	1704	1/1	0.91	0.05	81,81,81,81	0
54	MG	BA	3132	1/1	0.91	0.23	79,79,79,79	0
54	MG	BA	3133	1/1	0.91	0.22	67,67,67,67	0
54	MG	BA	2984	1/1	0.91	0.13	41,41,41,41	0
54	MG	AA	1620	1/1	0.91	0.20	56,56,56,56	0
54	MG	BA	3260	1/1	0.91	0.13	62,62,62,62	0
54	MG	AA	1742	1/1	0.91	0.15	87,87,87,87	0
54	MG	AA	1731	1/1	0.91	0.12	76,76,76,76	0
54	MG	DA	3053	1/1	0.91	0.22	61,61,61,61	0
54	MG	DA	3054	1/1	0.91	0.12	75,75,75,75	0
54	MG	BA	3220	1/1	0.91	0.14	56,56,56,56	0
54	MG	CA	1707	1/1	0.91	0.11	104,104,104,104	0
54	MG	DA	3324	1/1	0.91	0.24	78,78,78,78	0
54	MG	DA	2956	1/1	0.91	0.09	45,45,45,45	0
54	MG	CA	1618	1/1	0.91	0.34	63,63,63,63	0
54	MG	BA	3043	1/1	0.91	0.13	70,70,70,70	0
54	MG	BA	2958	1/1	0.91	0.17	42,42,42,42	0
54	MG	DA	2967	1/1	0.91	0.27	54,54,54,54	0
54	MG	AA	1720	1/1	0.91	0.14	69,69,69,69	0
54	MG	AA	1658	1/1	0.91	0.19	94,94,94,94	0
54	MG	DB	201	1/1	0.91	0.22	63,63,63,63	0
54	MG	CA	1625	1/1	0.91	0.09	94,94,94,94	0
54	MG	DA	3148	1/1	0.91	0.21	99,99,99,99	0
54	MG	BB	202	1/1	0.91	0.14	75,75,75,75	0
54	MG	DA	3151	1/1	0.91	0.17	82,82,82,82	0
54	MG	DA	3077	1/1	0.91	0.26	67,67,67,67	0
54	MG	BB	203	1/1	0.91	0.11	83,83,83,83	0
54	MG	AA	1654	1/1	0.91	0.25	76,76,76,76	0
54	MG	AA	1671	1/1	0.91	0.13	114,114,114,114	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	DA	3159	1/1	0.91	0.31	87,87,87,87	0
54	MG	DA	2988	1/1	0.91	0.20	41,41,41,41	0
54	MG	DA	2991	1/1	0.91	0.13	31,31,31,31	0
54	MG	BA	3005	1/1	0.91	0.16	69,69,69,69	0
54	MG	DA	3164	1/1	0.91	0.13	88,88,88,88	0
54	MG	D4	101	1/1	0.91	0.19	55,55,55,55	0
54	MG	BA	3126	1/1	0.92	0.05	54,54,54,54	0
54	MG	AA	1736	1/1	0.92	0.09	79,79,79,79	0
54	MG	DA	3108	1/1	0.92	0.07	50,50,50,50	0
54	MG	BA	3095	1/1	0.92	0.05	83,83,83,83	0
54	MG	BA	3181	1/1	0.92	0.29	22,22,22,22	0
54	MG	BA	3064	1/1	0.92	0.15	40,40,40,40	0
54	MG	BA	3134	1/1	0.92	0.16	64,64,64,64	0
54	MG	CA	1655	1/1	0.92	0.09	80,80,80,80	0
54	MG	CA	1702	1/1	0.92	0.25	68,68,68,68	0
54	MG	BA	3186	1/1	0.92	0.24	52,52,52,52	0
54	MG	DA	2945	1/1	0.92	0.17	41,41,41,41	0
54	MG	BA	2929	1/1	0.92	0.20	37,37,37,37	0
54	MG	DA	3292	1/1	0.92	0.25	33,33,33,33	0
54	MG	DA	3293	1/1	0.92	0.06	67,67,67,67	0
54	MG	DA	3048	1/1	0.92	0.09	66,66,66,66	0
54	MG	DA	3049	1/1	0.92	0.10	56,56,56,56	0
54	MG	DA	3124	1/1	0.92	0.03	90,90,90,90	0
54	MG	DA	2952	1/1	0.92	0.19	50,50,50,50	0
54	MG	AA	1674	1/1	0.92	0.12	79,79,79,79	0
54	MG	DA	3214	1/1	0.92	0.16	46,46,46,46	0
54	MG	AA	1668	1/1	0.92	0.10	90,90,90,90	0
54	MG	BA	3141	1/1	0.92	0.17	78,78,78,78	0
54	MG	DA	3303	1/1	0.92	0.18	66,66,66,66	0
54	MG	BA	3246	1/1	0.92	0.13	73,73,73,73	0
54	MG	BA	2937	1/1	0.92	0.20	36,36,36,36	0
54	MG	DA	3308	1/1	0.92	0.07	91,91,91,91	0
54	MG	BA	3035	1/1	0.92	0.08	44,44,44,44	0
54	MG	BA	3104	1/1	0.92	0.15	63,63,63,63	0
54	MG	BA	3105	1/1	0.92	0.12	60,60,60,60	0
54	MG	CA	1619	1/1	0.92	0.08	61,61,61,61	0
54	MG	DA	3137	1/1	0.92	0.08	68,68,68,68	0
54	MG	AA	1672	1/1	0.92	0.18	101,101,101,101	0
54	MG	AA	1688	1/1	0.92	0.07	68,68,68,68	0
54	MG	AA	1689	1/1	0.92	0.06	68,68,68,68	0
54	MG	BA	2957	1/1	0.92	0.22	35,35,35,35	0
54	MG	DA	3073	1/1	0.92	0.12	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	DA	3146	1/1	0.92	0.08	95,95,95,95	0
54	MG	BA	3016	1/1	0.92	0.14	60,60,60,60	0
54	MG	DA	3076	1/1	0.92	0.12	63,63,63,63	0
54	MG	BA	2910	1/1	0.92	0.30	27,27,27,27	0
54	MG	BA	3306	1/1	0.92	0.08	74,74,74,74	0
54	MG	DA	3079	1/1	0.92	0.07	38,38,38,38	0
54	MG	CA	1677	1/1	0.92	0.15	85,85,85,85	0
54	MG	DA	2995	1/1	0.92	0.18	48,48,48,48	0
54	MG	DA	3332	1/1	0.92	0.15	60,60,60,60	0
54	MG	BA	3262	1/1	0.92	0.10	60,60,60,60	0
54	MG	BA	2991	1/1	0.92	0.06	36,36,36,36	0
54	MG	AA	1743	1/1	0.92	0.17	83,83,83,83	0
54	MG	DA	3003	1/1	0.92	0.11	41,41,41,41	0
54	MG	BA	2961	1/1	0.92	0.25	43,43,43,43	0
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	BA	3056	1/1	0.92	0.10	62,62,62,62	0
54	MG	BA	3086	1/1	0.92	0.17	102,102,102,102	0
54	MG	DB	210	1/1	0.92	0.08	74,74,74,74	0
54	MG	BA	2999	1/1	0.92	0.10	45,45,45,45	0
54	MG	BA	3273	1/1	0.92	0.07	83,83,83,83	0
54	MG	BA	3000	1/1	0.92	0.08	65,65,65,65	0
54	MG	BA	3221	1/1	0.92	0.11	48,48,48,48	0
54	MG	CA	1691	1/1	0.92	0.07	85,85,85,85	0
54	MG	BA	3091	1/1	0.92	0.09	56,56,56,56	0
54	MG	DA	3102	1/1	0.92	0.20	68,68,68,68	0
54	MG	AA	1670	1/1	0.92	0.09	85,85,85,85	0
54	MG	DA	2906	1/1	0.92	0.25	27,27,27,27	0
54	MG	BA	3156	1/1	0.93	0.10	80,80,80,80	0
54	MG	BA	3203	1/1	0.93	0.16	41,41,41,41	0
54	MG	DA	3149	1/1	0.93	0.18	74,74,74,74	0
54	MG	DA	3059	1/1	0.93	0.07	67,67,67,67	0
54	MG	DA	2946	1/1	0.93	0.19	24,24,24,24	0
54	MG	AA	1608	1/1	0.93	0.23	47,47,47,47	0
54	MG	BA	3206	1/1	0.93	0.12	60,60,60,60	0
54	MG	BA	3047	1/1	0.93	0.17	65,65,65,65	0
54	MG	BA	3208	1/1	0.93	0.10	48,48,48,48	0
54	MG	DA	3158	1/1	0.93	0.07	59,59,59,59	0
54	MG	BA	3264	1/1	0.93	0.08	116,116,116,116	0
54	MG	DA	2960	1/1	0.93	0.22	42,42,42,42	0
54	MG	BA	3018	1/1	0.93	0.10	68,68,68,68	0
54	MG	BA	3210	1/1	0.93	0.10	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	AA	1708	1/1	0.93	0.08	101,101,101,101	0
54	MG	BA	3268	1/1	0.93	0.18	58,58,58,58	0
54	MG	CA	1654	1/1	0.93	0.05	111,111,111,111	0
54	MG	BA	3021	1/1	0.93	0.27	60,60,60,60	0
54	MG	BA	3120	1/1	0.93	0.10	57,57,57,57	0
54	MG	DA	3171	1/1	0.93	0.08	61,61,61,61	0
54	MG	DA	2977	1/1	0.93	0.04	47,47,47,47	0
54	MG	CA	1657	1/1	0.93	0.11	78,78,78,78	0
54	MG	DA	2985	1/1	0.93	0.20	48,48,48,48	0
54	MG	BA	3214	1/1	0.93	0.22	53,53,53,53	0
54	MG	CA	1659	1/1	0.93	0.13	71,71,71,71	0
54	MG	BA	2993	1/1	0.93	0.28	58,58,58,58	0
54	MG	BA	3023	1/1	0.93	0.16	64,64,64,64	0
54	MG	BA	3168	1/1	0.93	0.14	76,76,76,76	0
54	MG	CA	1603	1/1	0.93	0.29	48,48,48,48	0
54	MG	BA	3169	1/1	0.93	0.18	75,75,75,75	0
54	MG	AA	1711	1/1	0.93	0.16	53,53,53,53	0
54	MG	AA	1698	1/1	0.93	0.08	88,88,88,88	0
54	MG	DA	3001	1/1	0.93	0.18	56,56,56,56	0
54	MG	AA	1659	1/1	0.93	0.12	51,51,51,51	0
54	MG	BA	3127	1/1	0.93	0.18	56,56,56,56	0
54	MG	BA	3062	1/1	0.93	0.12	76,76,76,76	0
54	MG	DA	3195	1/1	0.93	0.18	51,51,51,51	0
54	MG	BA	3228	1/1	0.93	0.12	66,66,66,66	0
54	MG	DA	3008	1/1	0.93	0.17	59,59,59,59	0
54	MG	CA	1613	1/1	0.93	0.11	87,87,87,87	0
54	MG	DA	3010	1/1	0.93	0.19	51,51,51,51	0
54	MG	CA	1729	1/1	0.93	0.11	98,98,98,98	0
54	MG	DA	3203	1/1	0.93	0.12	46,46,46,46	0
54	MG	BA	2966	1/1	0.93	0.13	75,75,75,75	0
54	MG	CA	1731	1/1	0.93	0.04	90,90,90,90	0
54	MG	BA	3002	1/1	0.93	0.20	45,45,45,45	0
54	MG	DA	3016	1/1	0.93	0.08	74,74,74,74	0
54	MG	DA	3111	1/1	0.93	0.19	67,67,67,67	0
54	MG	AA	1690	1/1	0.93	0.07	117,117,117,117	0
54	MG	CA	1735	1/1	0.93	0.13	61,61,61,61	0
54	MG	BA	3182	1/1	0.93	0.22	20,20,20,20	0
54	MG	AA	1759	1/1	0.93	0.04	81,81,81,81	0
54	MG	BA	3239	1/1	0.93	0.10	82,82,82,82	0
54	MG	BA	3292	1/1	0.93	0.13	72,72,72,72	0
54	MG	BA	2973	1/1	0.93	0.16	61,61,61,61	0
54	MG	DA	3227	1/1	0.93	0.16	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	AA	1717	1/1	0.93	0.13	81,81,81,81	0
54	MG	BA	3139	1/1	0.93	0.18	78,78,78,78	0
54	MG	AA	1662	1/1	0.93	0.08	53,53,53,53	0
54	MG	AA	1683	1/1	0.93	0.07	102,102,102,102	0
54	MG	DA	2914	1/1	0.93	0.26	27,27,27,27	0
54	MG	DA	2916	1/1	0.93	0.15	22,22,22,22	0
54	MG	DA	3237	1/1	0.93	0.34	87,87,87,87	0
54	MG	DA	3035	1/1	0.93	0.21	77,77,77,77	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	DA	2920	1/1	0.93	0.25	30,30,30,30	0
54	MG	DA	3038	1/1	0.93	0.24	71,71,71,71	0
54	MG	DA	3041	1/1	0.93	0.07	51,51,51,51	0
54	MG	AA	1605	1/1	0.93	0.31	42,42,42,42	0
54	MG	BA	2941	1/1	0.93	0.38	50,50,50,50	0
54	MG	DA	3046	1/1	0.93	0.13	76,76,76,76	0
54	MG	BA	3249	1/1	0.93	0.09	37,37,37,37	0
54	MG	AA	1602	1/1	0.93	0.30	49,49,49,49	0
54	MG	DA	2936	1/1	0.93	0.16	27,27,27,27	0
54	MG	BA	3013	1/1	0.93	0.07	90,90,90,90	0
54	MG	AA	1751	1/1	0.93	0.08	72,72,72,72	0
54	MG	BA	3113	1/1	0.93	0.10	71,71,71,71	0
54	MG	AA	1635	1/1	0.93	0.11	68,68,68,68	0
54	MG	AA	1617	1/1	0.94	0.14	77,77,77,77	0
54	MG	BA	3164	1/1	0.94	0.17	88,88,88,88	0
54	MG	BA	2989	1/1	0.94	0.27	53,53,53,53	0
54	MG	DA	3034	1/1	0.94	0.20	65,65,65,65	0
54	MG	DA	3250	1/1	0.94	0.34	74,74,74,74	0
54	MG	BA	3111	1/1	0.94	0.25	46,46,46,46	0
54	MG	BA	3224	1/1	0.94	0.15	45,45,45,45	0
54	MG	BA	3065	1/1	0.94	0.09	61,61,61,61	0
54	MG	DA	3255	1/1	0.94	0.13	101,101,101,101	0
54	MG	AA	1604	1/1	0.94	0.11	57,57,57,57	0
54	MG	DA	2933	1/1	0.94	0.26	30,30,30,30	0
54	MG	BA	3227	1/1	0.94	0.12	48,48,48,48	0
54	MG	BA	2943	1/1	0.94	0.21	42,42,42,42	0
54	MG	AV	6303	1/1	0.94	0.09	67,67,67,67	0
54	MG	BA	3290	1/1	0.94	0.15	42,42,42,42	0
54	MG	BA	2948	1/1	0.94	0.26	39,39,39,39	0
54	MG	DA	3050	1/1	0.94	0.09	105,105,105,105	0
54	MG	AA	1626	1/1	0.94	0.13	62,62,62,62	0
54	MG	DA	3266	1/1	0.94	0.11	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	BA	2955	1/1	0.94	0.10	50,50,50,50	0
54	MG	BA	2997	1/1	0.94	0.18	57,57,57,57	0
54	MG	CA	1629	1/1	0.94	0.09	106,106,106,106	0
54	MG	BA	2901	1/1	0.94	0.29	23,23,23,23	0
54	MG	CA	1695	1/1	0.94	0.13	80,80,80,80	0
54	MG	DA	3058	1/1	0.94	0.06	54,54,54,54	0
54	MG	CA	1631	1/1	0.94	0.08	68,68,68,68	0
54	MG	DA	2954	1/1	0.94	0.19	28,28,28,28	0
54	MG	DA	3061	1/1	0.94	0.18	75,75,75,75	0
54	MG	DA	3277	1/1	0.94	0.17	52,52,52,52	0
54	MG	BA	3297	1/1	0.94	0.13	67,67,67,67	0
54	MG	DA	2957	1/1	0.94	0.16	63,63,63,63	0
54	MG	BA	3074	1/1	0.94	0.05	61,61,61,61	0
54	MG	CA	1635	1/1	0.94	0.06	67,67,67,67	0
54	MG	DA	3068	1/1	0.94	0.21	72,72,72,72	0
54	MG	AA	1660	1/1	0.94	0.19	59,59,59,59	0
54	MG	BA	3001	1/1	0.94	0.17	59,59,59,59	0
54	MG	AA	1721	1/1	0.94	0.31	66,66,66,66	0
54	MG	AA	1709	1/1	0.94	0.12	83,83,83,83	0
54	MG	DA	3288	1/1	0.94	0.07	78,78,78,78	0
54	MG	AA	1710	1/1	0.94	0.15	65,65,65,65	0
54	MG	DA	3172	1/1	0.94	0.17	81,81,81,81	0
54	MG	BA	3128	1/1	0.94	0.17	59,59,59,59	0
54	MG	DA	3174	1/1	0.94	0.10	42,42,42,42	0
54	MG	CA	1642	1/1	0.94	0.06	71,71,71,71	0
54	MG	DA	2975	1/1	0.94	0.09	58,58,58,58	0
54	MG	CA	1643	1/1	0.94	0.06	58,58,58,58	0
54	MG	DA	2979	1/1	0.94	0.06	69,69,69,69	0
54	MG	DA	3083	1/1	0.94	0.10	67,67,67,67	0
54	MG	DA	2980	1/1	0.94	0.18	63,63,63,63	0
54	MG	DA	2981	1/1	0.94	0.20	55,55,55,55	0
54	MG	AA	1661	1/1	0.94	0.24	65,65,65,65	0
54	MG	BA	2964	1/1	0.94	0.16	30,30,30,30	0
54	MG	BA	3041	1/1	0.94	0.05	67,67,67,67	0
54	MG	DA	3304	1/1	0.94	0.11	59,59,59,59	0
54	MG	BB	201	1/1	0.94	0.26	56,56,56,56	0
54	MG	CA	1712	1/1	0.94	0.12	78,78,78,78	0
54	MG	BA	2919	1/1	0.94	0.16	24,24,24,24	0
54	MG	DA	3309	1/1	0.94	0.21	30,30,30,30	0
54	MG	DA	3189	1/1	0.94	0.11	37,37,37,37	0
54	MG	CA	1714	1/1	0.94	0.13	74,74,74,74	0
54	MG	DA	3093	1/1	0.94	0.19	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	BA	3087	1/1	0.94	0.06	69,69,69,69	0
54	MG	BB	204	1/1	0.94	0.09	87,87,87,87	0
54	MG	DA	3197	1/1	0.94	0.17	28,28,28,28	0
54	MG	BA	2924	1/1	0.94	0.23	47,47,47,47	0
54	MG	BA	3044	1/1	0.94	0.14	64,64,64,64	0
54	MG	CA	1653	1/1	0.94	0.11	84,84,84,84	0
54	MG	BA	2926	1/1	0.94	0.19	31,31,31,31	0
54	MG	BA	3046	1/1	0.94	0.30	87,87,87,87	0
54	MG	DA	3204	1/1	0.94	0.14	54,54,54,54	0
54	MG	BA	3202	1/1	0.94	0.32	63,63,63,63	0
54	MG	BA	3261	1/1	0.94	0.17	53,53,53,53	0
54	MG	BA	2927	1/1	0.94	0.20	37,37,37,37	0
54	MG	BA	3048	1/1	0.94	0.13	67,67,67,67	0
54	MG	DA	3213	1/1	0.94	0.24	66,66,66,66	0
54	MG	AA	1725	1/1	0.94	0.15	72,72,72,72	0
54	MG	DA	3331	1/1	0.94	0.09	52,52,52,52	0
54	MG	BA	2976	1/1	0.94	0.18	70,70,70,70	0
54	MG	DA	3217	1/1	0.94	0.11	56,56,56,56	0
54	MG	BA	3051	1/1	0.94	0.09	66,66,66,66	0
54	MG	DA	3335	1/1	0.94	0.09	90,90,90,90	0
54	MG	BA	3099	1/1	0.94	0.17	78,78,78,78	0
54	MG	CA	1732	1/1	0.94	0.15	73,73,73,73	0
54	MG	DA	3015	1/1	0.94	0.27	74,74,74,74	0
54	MG	DA	3114	1/1	0.94	0.19	83,83,83,83	0
54	MG	BA	3052	1/1	0.94	0.18	56,56,56,56	0
54	MG	BA	2931	1/1	0.94	0.17	32,32,32,32	0
54	MG	DA	3228	1/1	0.94	0.19	51,51,51,51	0
54	MG	DA	3229	1/1	0.94	0.17	64,64,64,64	0
54	MG	DB	208	1/1	0.94	0.05	96,96,96,96	0
54	MG	BA	3055	1/1	0.94	0.05	60,60,60,60	0
54	MG	AA	1695	1/1	0.94	0.14	83,83,83,83	0
54	MG	DA	3232	1/1	0.94	0.14	39,39,39,39	0
54	MG	BA	2981	1/1	0.94	0.08	48,48,48,48	0
54	MG	BA	2933	1/1	0.94	0.21	32,32,32,32	0
54	MG	BA	3216	1/1	0.94	0.17	65,65,65,65	0
54	MG	BA	3276	1/1	0.94	0.11	65,65,65,65	0
54	MG	CA	1609	1/1	0.94	0.14	93,93,93,93	0
54	MG	AA	1628	1/1	0.94	0.18	62,62,62,62	0
54	MG	DA	3240	1/1	0.94	0.22	60,60,60,60	0
54	MG	AA	1740	1/1	0.94	0.11	80,80,80,80	0
54	MG	DA	3032	1/1	0.95	0.09	49,49,49,49	0
54	MG	AA	1703	1/1	0.95	0.07	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	DA	3107	1/1	0.95	0.20	67,67,67,67	0
54	MG	AA	1656	1/1	0.95	0.09	72,72,72,72	0
54	MG	BA	3201	1/1	0.95	0.14	80,80,80,80	0
54	MG	DA	2962	1/1	0.95	0.14	37,37,37,37	0
54	MG	DA	2963	1/1	0.95	0.25	53,53,53,53	0
54	MG	DA	3040	1/1	0.95	0.09	41,41,41,41	0
54	MG	BA	2942	1/1	0.95	0.12	22,22,22,22	0
54	MG	BA	3076	1/1	0.95	0.14	68,68,68,68	0
54	MG	BA	2980	1/1	0.95	0.09	40,40,40,40	0
54	MG	CA	1624	1/1	0.95	0.04	66,66,66,66	0
54	MG	DA	2969	1/1	0.95	0.16	42,42,42,42	0
54	MG	BA	3205	1/1	0.95	0.12	38,38,38,38	0
54	MG	BA	3254	1/1	0.95	0.11	81,81,81,81	0
54	MG	BA	2918	1/1	0.95	0.23	17,17,17,17	0
54	MG	BA	2982	1/1	0.95	0.13	41,41,41,41	0
54	MG	AA	1730	1/1	0.95	0.16	49,49,49,49	0
54	MG	DA	2978	1/1	0.95	0.12	44,44,44,44	0
54	MG	DA	3126	1/1	0.95	0.07	77,77,77,77	0
54	MG	BA	2920	1/1	0.95	0.15	28,28,28,28	0
54	MG	DA	3294	1/1	0.95	0.21	61,61,61,61	0
54	MG	BA	2922	1/1	0.95	0.26	25,25,25,25	0
54	MG	DA	3210	1/1	0.95	0.09	59,59,59,59	0
54	MG	BA	2987	1/1	0.95	0.17	59,59,59,59	0
54	MG	DA	2982	1/1	0.95	0.08	33,33,33,33	0
54	MG	BA	3085	1/1	0.95	0.09	68,68,68,68	0
54	MG	BA	2952	1/1	0.95	0.16	38,38,38,38	0
54	MG	DA	3216	1/1	0.95	0.17	46,46,46,46	0
54	MG	BA	3020	1/1	0.95	0.28	62,62,62,62	0
54	MG	DA	3062	1/1	0.95	0.15	65,65,65,65	0
54	MG	DA	3135	1/1	0.95	0.05	65,65,65,65	0
54	MG	BA	2953	1/1	0.95	0.12	37,37,37,37	0
54	MG	DA	3306	1/1	0.95	0.07	51,51,51,51	0
54	MG	BA	2923	1/1	0.95	0.17	29,29,29,29	0
54	MG	BA	3171	1/1	0.95	0.07	68,68,68,68	0
54	MG	DA	3225	1/1	0.95	0.09	80,80,80,80	0
54	MG	DA	3139	1/1	0.95	0.08	60,60,60,60	0
54	MG	BA	3125	1/1	0.95	0.17	87,87,87,87	0
54	MG	CA	1690	1/1	0.95	0.18	61,61,61,61	0
54	MG	BA	3269	1/1	0.95	0.09	63,63,63,63	0
54	MG	DA	2997	1/1	0.95	0.06	35,35,35,35	0
54	MG	DA	3144	1/1	0.95	0.07	72,72,72,72	0
54	MG	AA	1611	1/1	0.95	0.08	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	BA	3092	1/1	0.95	0.05	63,63,63,63	0
54	MG	BA	2925	1/1	0.95	0.19	29,29,29,29	0
54	MG	AA	1607	1/1	0.95	0.20	54,54,54,54	0
54	MG	DA	2915	1/1	0.95	0.21	14,14,14,14	0
54	MG	AA	1627	1/1	0.95	0.15	85,85,85,85	0
54	MG	BB	215	1/1	0.95	0.10	131,131,131,131	0
54	MG	BA	2995	1/1	0.95	0.16	47,47,47,47	0
54	MG	DA	2928	1/1	0.95	0.25	43,43,43,43	0
54	MG	BA	2902	1/1	0.95	0.22	16,16,16,16	0
54	MG	BA	3029	1/1	0.95	0.21	63,63,63,63	0
54	MG	DA	3245	1/1	0.95	0.24	54,54,54,54	0
54	MG	DA	3330	1/1	0.95	0.08	69,69,69,69	0
54	MG	BA	2903	1/1	0.95	0.13	14,14,14,14	0
54	MG	DA	3247	1/1	0.95	0.17	40,40,40,40	0
54	MG	DA	3248	1/1	0.95	0.21	75,75,75,75	0
54	MG	DA	3160	1/1	0.95	0.12	71,71,71,71	0
54	MG	BA	2904	1/1	0.95	0.23	13,13,13,13	0
54	MG	DA	2935	1/1	0.95	0.22	30,30,30,30	0
54	MG	AA	1716	1/1	0.95	0.07	120,120,120,120	0
54	MG	BA	2934	1/1	0.95	0.22	28,28,28,28	0
54	MG	BA	3234	1/1	0.95	0.09	61,61,61,61	0
54	MG	DA	3167	1/1	0.95	0.04	68,68,68,68	0
54	MG	BA	3235	1/1	0.95	0.05	62,62,62,62	0
54	MG	BA	3142	1/1	0.95	0.09	89,89,89,89	0
54	MG	BA	3237	1/1	0.95	0.08	60,60,60,60	0
54	MG	DA	2944	1/1	0.95	0.20	35,35,35,35	0
54	MG	DA	3261	1/1	0.95	0.28	73,73,73,73	0
54	MG	DA	3096	1/1	0.95	0.18	40,40,40,40	0
54	MG	BA	2969	1/1	0.95	0.08	37,37,37,37	0
54	MG	BA	2970	1/1	0.95	0.23	45,45,45,45	0
54	MG	BA	3146	1/1	0.95	0.19	83,83,83,83	0
54	MG	DA	3026	1/1	0.95	0.09	48,48,48,48	0
54	MG	AA	1676	1/1	0.95	0.03	63,63,63,63	0
54	MG	BA	2936	1/1	0.95	0.15	43,43,43,43	0
54	MG	BA	3197	1/1	0.95	0.22	57,57,57,57	0
54	MG	DA	3270	1/1	0.95	0.10	81,81,81,81	0
54	MG	AA	1601	1/1	0.95	0.24	31,31,31,31	0
55	ZN	CN	101	1/1	0.95	0.06	144,144,144,144	0
54	MG	BA	3053	1/1	0.96	0.28	67,67,67,67	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	3183	1/1	0.96	0.17	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	AA	1633	1/1	0.96	0.10	73,73,73,73	0
54	MG	DA	3039	1/1	0.96	0.29	48,48,48,48	0
54	MG	BA	2911	1/1	0.96	0.17	23,23,23,23	0
54	MG	CA	1721	1/1	0.96	0.10	101,101,101,101	0
54	MG	AA	1719	1/1	0.96	0.22	78,78,78,78	0
54	MG	DA	2990	1/1	0.96	0.06	35,35,35,35	0
54	MG	DA	3044	1/1	0.96	0.05	59,59,59,59	0
54	MG	BA	3057	1/1	0.96	0.17	63,63,63,63	0
54	MG	BA	2928	1/1	0.96	0.27	42,42,42,42	0
54	MG	BA	2965	1/1	0.96	0.15	47,47,47,47	0
54	MG	BA	2938	1/1	0.96	0.08	10,10,10,10	0
54	MG	DA	2996	1/1	0.96	0.15	43,43,43,43	0
54	MG	CA	1634	1/1	0.96	0.06	60,60,60,60	0
54	MG	BA	3245	1/1	0.96	0.19	54,54,54,54	0
54	MG	BA	2954	1/1	0.96	0.12	52,52,52,52	0
54	MG	DA	3000	1/1	0.96	0.10	35,35,35,35	0
54	MG	DA	3241	1/1	0.96	0.31	54,54,54,54	0
54	MG	DA	3112	1/1	0.96	0.06	60,60,60,60	0
54	MG	BA	3167	1/1	0.96	0.08	50,50,50,50	0
54	MG	BA	2921	1/1	0.96	0.18	21,21,21,21	0
54	MG	BA	3063	1/1	0.96	0.08	56,56,56,56	0
54	MG	DA	2947	1/1	0.96	0.15	40,40,40,40	0
54	MG	DA	2948	1/1	0.96	0.20	52,52,52,52	0
54	MG	DA	3007	1/1	0.96	0.08	43,43,43,43	0
54	MG	CA	1669	1/1	0.96	0.09	66,66,66,66	0
54	MG	BA	3307	1/1	0.96	0.11	68,68,68,68	0
54	MG	BA	3195	1/1	0.96	0.10	53,53,53,53	0
54	MG	BA	3015	1/1	0.96	0.12	58,58,58,58	0
54	MG	BA	2985	1/1	0.96	0.26	54,54,54,54	0
54	MG	DA	3067	1/1	0.96	0.08	63,63,63,63	0
54	MG	BA	2907	1/1	0.96	0.15	7,7,7,7	0
54	MG	BA	2909	1/1	0.96	0.18	24,24,24,24	0
54	MG	DA	3188	1/1	0.96	0.23	9,9,9,9	0
54	MG	BA	3256	1/1	0.96	0.18	79,79,79,79	0
54	MG	DA	3071	1/1	0.96	0.08	64,64,64,64	0
54	MG	DA	3192	1/1	0.96	0.15	30,30,30,30	0
54	MG	BA	2972	1/1	0.96	0.18	49,49,49,49	0
54	MG	DA	3194	1/1	0.96	0.15	10,10,10,10	0
54	MG	BA	3153	1/1	0.96	0.08	67,67,67,67	0
54	MG	DA	2901	1/1	0.96	0.22	7,7,7,7	0
54	MG	BA	2959	1/1	0.96	0.13	55,55,55,55	0
54	MG	BA	3177	1/1	0.96	0.18	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	DA	2909	1/1	0.96	0.15	5,5,5,5	0
54	MG	DA	2911	1/1	0.96	0.15	7,7,7,7	0
54	MG	DA	3023	1/1	0.96	0.09	49,49,49,49	0
54	MG	DA	3202	1/1	0.96	0.36	44,44,44,44	0
54	MG	DA	3081	1/1	0.96	0.07	71,71,71,71	0
54	MG	DA	3082	1/1	0.96	0.20	70,70,70,70	0
54	MG	DA	2913	1/1	0.96	0.26	17,17,17,17	0
54	MG	DA	3206	1/1	0.96	0.20	37,37,37,37	0
54	MG	BA	3089	1/1	0.96	0.17	59,59,59,59	0
54	MG	DA	3208	1/1	0.96	0.24	49,49,49,49	0
54	MG	CA	1682	1/1	0.96	0.10	97,97,97,97	0
54	MG	DA	2974	1/1	0.96	0.07	46,46,46,46	0
54	MG	DB	213	1/1	0.96	0.23	63,63,63,63	0
54	MG	DA	3211	1/1	0.96	0.14	38,38,38,38	0
54	MG	BA	3179	1/1	0.96	0.22	19,19,19,19	0
54	MG	DA	3145	1/1	0.96	0.17	70,70,70,70	0
54	MG	BA	2917	1/1	0.96	0.12	8,8,8,8	0
54	MG	DA	2922	1/1	0.96	0.16	7,7,7,7	0
54	MG	DA	3031	1/1	0.96	0.09	62,62,62,62	0
54	MG	DA	2923	1/1	0.96	0.07	17,17,17,17	0
54	MG	DA	3218	1/1	0.96	0.13	48,48,48,48	0
54	MG	AA	1615	1/1	0.97	0.15	42,42,42,42	0
54	MG	BA	2998	1/1	0.97	0.13	46,46,46,46	0
54	MG	DA	3252	1/1	0.97	0.05	44,44,44,44	0
54	MG	BA	2906	1/1	0.97	0.08	5,5,5,5	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	BA	3161	1/1	0.97	0.07	62,62,62,62	0
54	MG	DA	2905	1/1	0.97	0.17	9,9,9,9	0
54	MG	BA	2950	1/1	0.97	0.09	32,32,32,32	0
54	MG	DA	3056	1/1	0.97	0.08	48,48,48,48	0
54	MG	BA	3277	1/1	0.97	0.11	71,71,71,71	0
54	MG	AA	1663	1/1	0.97	0.14	70,70,70,70	0
54	MG	CA	1615	1/1	0.97	0.06	51,51,51,51	0
54	MG	BA	3137	1/1	0.97	0.15	54,54,54,54	0
54	MG	BA	2967	1/1	0.97	0.10	24,24,24,24	0
54	MG	BA	2908	1/1	0.97	0.25	18,18,18,18	0
54	MG	DA	2917	1/1	0.97	0.18	22,22,22,22	0
54	MG	DA	2918	1/1	0.97	0.18	15,15,15,15	0
54	MG	DA	3321	1/1	0.97	0.22	30,30,30,30	0
54	MG	DA	2919	1/1	0.97	0.13	45,45,45,45	0
54	MG	DA	3165	1/1	0.97	0.12	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	BA	3078	1/1	0.97	0.12	83,83,83,83	0
54	MG	DA	2921	1/1	0.97	0.20	17,17,17,17	0
54	MG	DA	3219	1/1	0.97	0.17	67,67,67,67	0
54	MG	DA	2973	1/1	0.97	0.30	50,50,50,50	0
54	MG	CA	1719	1/1	0.97	0.06	78,78,78,78	0
54	MG	AA	1715	1/1	0.97	0.19	63,63,63,63	0
54	MG	BA	3223	1/1	0.97	0.08	54,54,54,54	0
54	MG	BA	3196	1/1	0.97	0.23	51,51,51,51	0
54	MG	AA	1630	1/1	0.97	0.14	70,70,70,70	0
54	MG	BA	3144	1/1	0.97	0.08	75,75,75,75	0
54	MG	DA	3123	1/1	0.97	0.05	59,59,59,59	0
54	MG	DA	3075	1/1	0.97	0.05	64,64,64,64	0
54	MG	BA	2956	1/1	0.97	0.14	35,35,35,35	0
54	MG	DA	3283	1/1	0.97	0.29	53,53,53,53	0
54	MG	DA	2930	1/1	0.97	0.20	36,36,36,36	0
54	MG	BA	2940	1/1	0.97	0.20	29,29,29,29	0
54	MG	BA	3147	1/1	0.97	0.05	72,72,72,72	0
54	MG	BA	3102	1/1	0.97	0.16	69,69,69,69	0
54	MG	BA	2930	1/1	0.97	0.16	34,34,34,34	0
54	MG	BA	3233	1/1	0.97	0.20	52,52,52,52	0
54	MG	DA	2989	1/1	0.97	0.12	45,45,45,45	0
54	MG	AA	1603	1/1	0.97	0.14	35,35,35,35	0
54	MG	BA	3151	1/1	0.97	0.29	56,56,56,56	0
54	MG	DA	2992	1/1	0.97	0.07	46,46,46,46	0
54	MG	BA	2975	1/1	0.97	0.04	37,37,37,37	0
54	MG	AA	1619	1/1	0.97	0.12	80,80,80,80	0
54	MG	CA	1602	1/1	0.97	0.10	64,64,64,64	0
54	MG	BA	2913	1/1	0.97	0.19	16,16,16,16	0
54	MG	CA	1604	1/1	0.97	0.13	59,59,59,59	0
54	MG	DE	301	1/1	0.97	0.09	44,44,44,44	0
54	MG	BA	2946	1/1	0.97	0.18	33,33,33,33	0
54	MG	DA	3045	1/1	0.97	0.17	48,48,48,48	0
54	MG	BA	2979	1/1	0.97	0.09	40,40,40,40	0
54	MG	BA	3130	1/1	0.97	0.04	78,78,78,78	0
54	MG	AA	1636	1/1	0.98	0.09	76,76,76,76	0
54	MG	BA	3296	1/1	0.98	0.08	47,47,47,47	0
54	MG	BA	3180	1/1	0.98	0.17	26,26,26,26	0
54	MG	BA	3247	1/1	0.98	0.13	52,52,52,52	0
54	MG	DA	2907	1/1	0.98	0.19	7,7,7,7	0
54	MG	DA	2908	1/1	0.98	0.14	24,24,24,24	0
54	MG	BA	3040	1/1	0.98	0.06	58,58,58,58	0
54	MG	DA	3239	1/1	0.98	0.12	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	DA	3191	1/1	0.98	0.18	24,24,24,24	0
54	MG	DA	2910	1/1	0.98	0.09	6,6,6,6	0
54	MG	BA	3131	1/1	0.98	0.07	67,67,67,67	0
54	MG	DA	3036	1/1	0.98	0.06	51,51,51,51	0
54	MG	DA	2912	1/1	0.98	0.15	18,18,18,18	0
54	MG	BA	3231	1/1	0.98	0.09	22,22,22,22	0
54	MG	DA	2951	1/1	0.98	0.10	38,38,38,38	0
54	MG	DA	2931	1/1	0.98	0.12	23,23,23,23	0
54	MG	DA	2976	1/1	0.98	0.09	37,37,37,37	0
54	MG	BA	3010	1/1	0.98	0.06	37,37,37,37	0
54	MG	BA	2944	1/1	0.98	0.09	17,17,17,17	0
54	MG	DA	2955	1/1	0.98	0.14	40,40,40,40	0
54	MG	DA	3155	1/1	0.98	0.06	124,124,124,124	0
54	MG	DA	3328	1/1	0.98	0.11	45,45,45,45	0
54	MG	AA	1686	1/1	0.98	0.10	72,72,72,72	0
54	MG	BA	2915	1/1	0.98	0.06	4,4,4,4	0
54	MG	DA	2902	1/1	0.98	0.17	10,10,10,10	0
55	ZN	CD	301	1/1	0.98	0.18	131,131,131,131	0
54	MG	DA	2937	1/1	0.98	0.14	25,25,25,25	0
54	MG	BA	2947	1/1	0.99	0.03	14,14,14,14	0
54	MG	DA	2964	1/1	0.99	0.08	34,34,34,34	0
54	MG	DA	2950	1/1	0.99	0.06	29,29,29,29	0
54	MG	DA	2984	1/1	0.99	0.09	66,66,66,66	0
54	MG	BA	2951	1/1	0.99	0.13	28,28,28,28	0
54	MG	DA	3156	1/1	0.99	0.06	78,78,78,78	0
54	MG	DA	2958	1/1	0.99	0.04	2,2,2,2	0
54	MG	BA	3140	1/1	0.99	0.08	76,76,76,76	0
54	MG	DA	2926	1/1	0.99	0.16	43,43,43,43	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	DA	2943	1/1	0.99	0.16	32,32,32,32	0
55	ZN	AD	301	1/1	1.00	0.19	80,80,80,80	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.