



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 13, 2024 – 06:35 PM EST

PDB ID : 4V87
Title : Crystal structure analysis of ribosomal decoding.
Authors : Demeshkina, N.; Jenner, L.; Yusupov, M.; Yusupova, G.
Deposited on : 2011-09-20
Resolution : 3.10 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4.02b-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

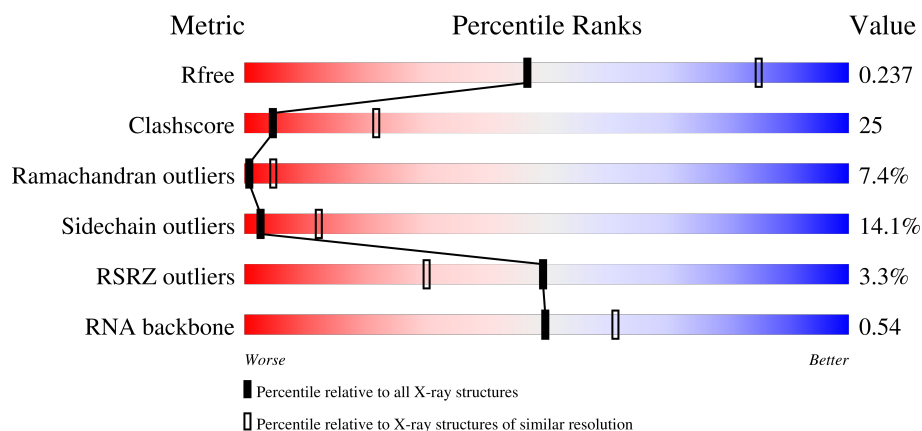
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	1351 (3.10-3.10)
Clashscore	180529	1454 (3.10-3.10)
Ramachandran outliers	177936	1391 (3.10-3.10)
Sidechain outliers	177891	1391 (3.10-3.10)
RSRZ outliers	164620	1351 (3.10-3.10)
RNA backbone	3690	1021 (3.36-2.84)

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

Mol	Chain	Length	Quality of chain
1	AA	2912	<div> <div></div> <div>41%</div> <div>45%</div> <div>14%</div> </div>
1	DA	2912	<div> <div>2%</div> <div>41%</div> <div>43%</div> <div>16%</div> </div>
2	AB	122	<div> <div></div> <div>37%</div> <div>45%</div> <div>16%</div> <div></div> </div>
2	DB	122	<div> <div></div> <div>33%</div> <div>48%</div> <div>19%</div> <div></div> </div>

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Mol	Chain	Length	Quality of chain
3	AD	272	
3	DD	272	
4	AE	205	
4	DE	205	
5	AF	208	
5	DF	208	
6	AG	181	
6	DG	181	
7	AH	170	
7	DH	170	
8	AK	146	
8	DK	146	
9	AM	138	
9	DM	138	
10	AN	122	
10	DN	122	
11	AO	150	
11	DO	150	
12	AP	141	
12	DP	141	
13	A0	118	
13	D0	118	
14	AQ	111	
14	DQ	111	
15	AR	137	


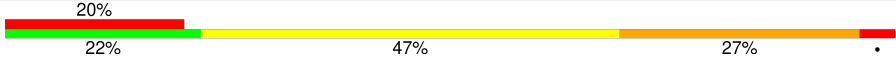

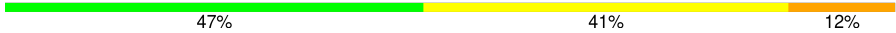
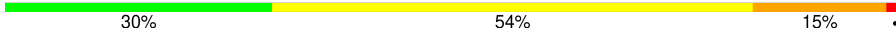




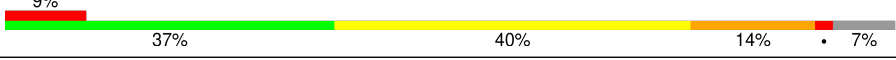
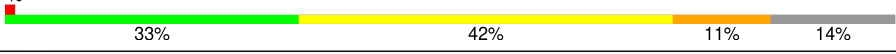
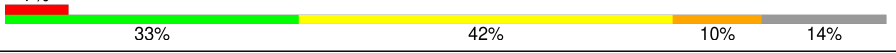


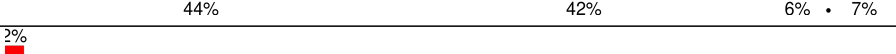
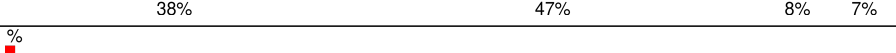
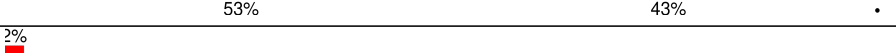
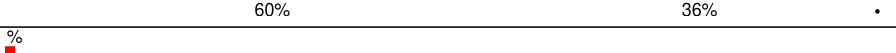

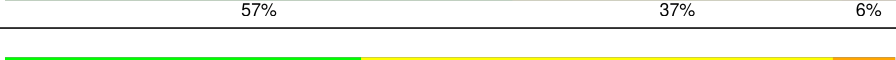
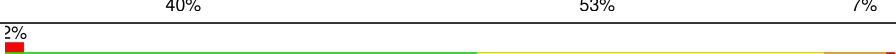
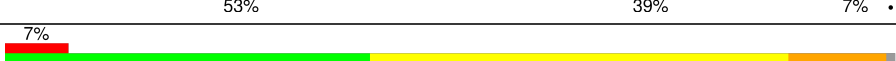
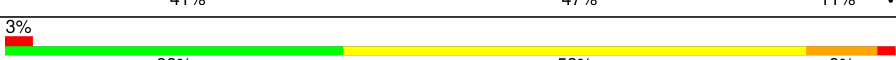
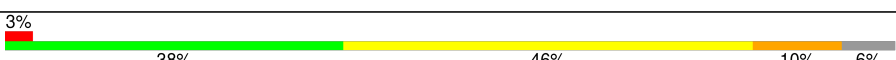

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Mol	Chain	Length	Quality of chain
15	DR	137	
16	A1	117	
16	D1	117	
17	A2	101	
17	D2	101	
18	AS	113	
18	DS	113	
19	AT	92	
19	DT	92	
20	AU	102	
20	DU	102	
21	AV	179	
21	DV	179	
22	A3	77	
22	D3	77	
23	AZ	97	
23	DZ	97	
24	AW	69	
24	DW	69	
25	AX	59	
25	DX	59	
26	A4	66	
26	D4	66	
27	A5	59	
27	D5	59	

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Mol	Chain	Length	Quality of chain
28	A6	45	
28	D6	45	
29	A7	49	
29	D7	49	
30	A8	61	
30	D8	61	
31	BA	1506	
31	CA	1506	
32	BE	256	
32	CE	256	
33	BF	239	
33	CF	239	
34	BG	208	
34	CG	208	
35	BH	162	
35	CH	162	
36	BI	101	
36	CI	101	
37	BJ	156	
37	CJ	156	
38	BK	138	
38	CK	138	
39	BL	128	
39	CL	128	
40	BM	105	

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Mol	Chain	Length	Quality of chain
40	CM	105	
41	BN	129	
41	CN	129	
42	BO	132	
42	CO	132	
43	BP	126	
43	CP	126	
44	BQ	61	
44	CQ	61	
45	BR	89	
45	CR	89	
46	BS	88	
46	CS	88	
47	BT	105	
47	CT	105	
48	BU	88	
48	CU	88	
49	BV	93	
49	CV	93	
50	BW	106	
50	CW	106	
51	BX	27	
51	CX	27	
52	BB	87	
52	CB	87	

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Mol	Chain	Length	Quality of chain
53	BC	77	
53	BD	77	
53	CC	77	
53	CD	77	
54	B1	10	
54	C1	10	

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
55	MG	AA	3058	-	-	-	X
55	MG	AA	3077	-	-	-	X
55	MG	AA	3108	-	-	-	X
55	MG	AA	3132	-	-	-	X
55	MG	AA	3236	-	-	-	X
55	MG	AA	3317	-	-	-	X
55	MG	AA	3353	-	-	-	X
55	MG	AA	3431	-	-	-	X
55	MG	AA	3460	-	-	-	X
55	MG	AA	3518	-	-	-	X
55	MG	AA	3521	-	-	-	X
55	MG	AA	3558	-	-	-	X
55	MG	AE	304	-	-	-	X
55	MG	BA	1628	-	-	-	X
55	MG	BA	1636	-	-	-	X
55	MG	BA	1674	-	-	-	X
55	MG	BA	1678	-	-	-	X
55	MG	BA	1709	-	-	-	X
55	MG	BA	1712	-	-	-	X
55	MG	BA	1778	-	-	-	X
55	MG	BA	1784	-	-	-	X
55	MG	BA	1831	-	-	-	X
55	MG	BA	1838	-	-	-	X
55	MG	CA	1634	-	-	-	X
55	MG	CA	1747	-	-	-	X
55	MG	CA	1759	-	-	-	X
55	MG	CA	1777	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	CC	107	-	-	-	X
55	MG	DA	3004	-	-	-	X
55	MG	DA	3060	-	-	-	X
55	MG	DA	3272	-	-	-	X
55	MG	DA	3301	-	-	-	X
55	MG	DA	3324	-	-	-	X
55	MG	DA	3332	-	-	-	X
55	MG	DA	3357	-	-	-	X
55	MG	DA	3372	-	-	-	X
55	MG	DA	3397	-	-	-	X
55	MG	DA	3404	-	-	-	X
55	MG	DA	3438	-	-	-	X
55	MG	DA	3447	-	-	-	X
55	MG	DA	3453	-	-	-	X

2 Entry composition

There are 56 unique types of molecules in this entry. The entry contains 299628 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 RNA (2909-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	2912	Total	C	N	O	P	0	0	0
			62707	27911	11722	20163	2911			
1	DA	2907	Total	C	N	O	P	0	0	0
			62607	27866	11712	20123	2906			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AA	161	U	-	insertion	GB AP008226.1
AA	654A	A	G	conflict	GB AP008226.1
AA	654E	C	G	conflict	GB AP008226.1
AA	654P	G	C	conflict	GB AP008226.1
AA	654T	A	C	conflict	GB AP008226.1
AA	1058	U	G	conflict	GB AP008226.1
AA	1080	A	C	conflict	GB AP008226.1
DA	166	U	-	expression tag	GB AP008226.1
DA	654A	A	G	conflict	GB AP008226.1
DA	654E	C	G	conflict	GB AP008226.1
DA	654P	G	C	conflict	GB AP008226.1
DA	654T	A	C	conflict	GB AP008226.1
DA	1058	U	G	conflict	GB AP008226.1
DA	1080	A	C	conflict	GB AP008226.1

- Molecule 2 is a RNA chain called 5S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AB	122	Total	C	N	O	P	0	0	0
			2617	1166	486	844	121			
2	DB	122	Total	C	N	O	P	0	0	0
			2617	1166	486	844	121			

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AD	272	Total	C	N	O	S	0	0	0
			2116	1335	420	358	3			
3	DD	272	Total	C	N	O	S	0	0	0
			2115	1335	420	357	3			

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AE	205	Total	C	N	O	S	0	0	0
			1569	991	300	272	6			
4	DE	205	Total	C	N	O	S	0	0	0
			1568	991	300	271	6			

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AF	203	Total	C	N	O	S	0	0	1
			1586	1011	298	275	2			
5	DF	208	Total	C	N	O	S	0	0	0
			1627	1037	304	283	3			

- Molecule 6 is a protein called 50S ribosomal protein L5.

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

- Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AH	170	Total	C	N	O	S	0	0	0
			1308	829	245	233	1			
7	DH	170	Total	C	N	O	S	0	0	0
			1307	829	245	232	1			

- Molecule 8 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AK	146	Total	C	N	O	S	0	0	0
			1137	726	201	209	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	DK	146	Total	C	N	O	S	0	0	0
			1136	726	201	208	1			

- Molecule 9 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	AM	138	Total	C	N	O	S	0	0	0
			1105	712	206	183	4			
9	DM	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			

- Molecule 10 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AN	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			
10	DN	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

- Molecule 11 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	AO	150	Total	C	N	O	S	0	0	0
			1145	712	232	198	3			
11	DO	150	Total	C	N	O	S	0	0	0
			1145	712	232	198	3			

- Molecule 12 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AP	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			
12	DP	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			

- Molecule 13 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	A0	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			
13	D0	117	Total	C	N	O	S	0	0	0
			960	599	202	159				

- Molecule 14 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	AQ	111	Total	C	N	O	0	0	0
			882	556	176	150			
14	DQ	111	Total	C	N	O	0	0	0
			882	556	176	150			

- Molecule 15 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AR	137	Total	C	N	O	S	0	0	0
			1142	710	234	197	1			
15	DR	137	Total	C	N	O	S	0	0	0
			1141	710	234	196	1			

- Molecule 16 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	A1	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			
16	D1	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			

- Molecule 17 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	A2	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			
17	D2	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			

- Molecule 18 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	AS	113	Total	C	N	O	S	0	0	0
			900	566	177	155	2			
18	DS	113	Total	C	N	O	S	0	0	0
			900	566	177	155	2			

- Molecule 19 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
19	AT	92	Total	C	N	O	0	0	0
			726	471	131	124			
19	DT	92	Total	C	N	O	0	0	0
			725	471	131	123			

- Molecule 20 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AU	102	Total	C	N	O	S	0	0	0
			786	505	150	126	5			
20	DU	102	Total	C	N	O	S	0	0	0
			785	505	150	125	5			

- Molecule 21 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	AV	175	Total	C	N	O	S	0	0	0
			1397	892	251	251	3			
21	DV	179	Total	C	N	O	S	0	0	0
			1428	911	255	259	3			

- Molecule 22 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	A3	76	Total	C	N	O	S	0	0	0
			607	376	128	102	1			
22	D3	77	Total	C	N	O	S	0	0	0
			613	379	129	104	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AZ	97	Total	C	N	O	S	0	0	0
			763	481	150	131	1			
23	DZ	97	Total	C	N	O	S	0	0	0
			763	481	150	131	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	AW	66	Total	C	N	O	S	0	0	0
			558	346	113	98	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	DW	69	Total	C	N	O	S	0	0	0
			581	358	118	104	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	AX	59	Total	C	N	O		0	0	0
			469	298	90	81				
25	DX	59	Total	C	N	O		0	0	0
			469	298	90	81				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	A4	66	Total	C	N	O	S	0	0	0
			533	335	96	97	5			
26	D4	63	Total	C	N	O	S	0	0	0
			515	326	93	91	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	A5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			
27	D5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	A6	45	Total	C	N	O	S	0	0	0
			390	241	79	66	4			
28	D6	45	Total	C	N	O	S	0	0	0
			389	241	79	65	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	A7	49	Total	C	N	O	S	0	0	0
			430	263	108	57	2			
29	D7	49	Total	C	N	O	S	0	0	0
			430	263	108	57	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	A8	61	Total	C	N	O	S	0	0	0
			488	312	99	75	2			
30	D8	61	Total	C	N	O	S	0	0	0
			488	312	99	75	2			

- Molecule 31 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	BA	1506	Total	C	N	O	P	0	0	0
			32369	14408	5997	10459	1505			
31	CA	1506	Total	C	N	O	P	0	0	0
			32372	14408	5997	10461	1506			

- Molecule 32 is a protein called 30S RIBOSOMAL PROTEIN S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	BE	237	Total	C	N	O	S	0	0	0
			1924	1228	344	347	5			
32	CE	237	Total	C	N	O	S	0	0	0
			1924	1228	344	347	5			

- Molecule 33 is a protein called 30S RIBOSOMAL PROTEIN S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	BF	205	Total	C	N	O	S	0	0	0
			1605	1011	313	280	1			
33	CF	206	Total	C	N	O	S	0	0	0
			1612	1016	314	281	1			

- Molecule 34 is a protein called 30S RIBOSOMAL PROTEIN S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	BG	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			
34	CG	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			

- Molecule 35 is a protein called 30S RIBOSOMAL PROTEIN S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BH	151	Total	C	N	O	S	0	0	0
			1155	729	218	204	4			
35	CH	151	Total	C	N	O	S	0	0	0
			1155	729	218	204	4			

- Molecule 36 is a protein called 30S RIBOSOMAL PROTEIN S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	BI	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			
36	CI	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			

- Molecule 37 is a protein called 30S RIBOSOMAL PROTEIN S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	BJ	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			
37	CJ	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			

- Molecule 38 is a protein called 30S RIBOSOMAL PROTEIN S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	BK	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			
38	CK	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			

- Molecule 39 is a protein called 30S RIBOSOMAL PROTEIN S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BL	127	Total	C	N	O		0	0	0
			1010	639	197	174				
39	CL	127	Total	C	N	O		0	0	0
			1010	639	197	174				

- Molecule 40 is a protein called 30S RIBOSOMAL PROTEIN S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	BM	99	Total	C	N	O	S	0	0	0
			801	504	157	139	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	CM	99	Total	C	N	O	S	0	0	0
			801	504	157	139	1			

- Molecule 41 is a protein called 30S RIBOSOMAL PROTEIN S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BN	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			
41	CN	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			

- Molecule 42 is a protein called 30S RIBOSOMAL PROTEIN S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BO	125	Total	C	N	O	S	0	0	0
			975	614	196	164	1			
42	CO	125	Total	C	N	O	S	0	0	0
			975	614	196	164	1			

- Molecule 43 is a protein called 30S RIBOSOMAL PROTEIN S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BP	116	Total	C	N	O	S	0	0	0
			928	574	191	161	2			
43	CP	117	Total	C	N	O	S	0	0	0
			933	577	192	162	2			

- Molecule 44 is a protein called 30S RIBOSOMAL PROTEIN S14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	BQ	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			
44	CQ	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			

- Molecule 45 is a protein called 30S RIBOSOMAL PROTEIN S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	BR	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			
45	CR	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			

- Molecule 46 is a protein called 30S RIBOSOMAL PROTEIN S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	BS	84	Total	C	N	O	S	0	0	0
			705	446	140	118	1			
46	CS	84	Total	C	N	O	S	0	0	0
			705	446	140	118	1			

- Molecule 47 is a protein called 30S RIBOSOMAL PROTEIN S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	BT	100	Total	C	N	O	S	0	0	0
			834	534	155	143	2			
47	CT	100	Total	C	N	O	S	0	0	0
			834	534	155	143	2			

- Molecule 48 is a protein called 30S RIBOSOMAL PROTEIN S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
48	BU	72	Total	C	N	O	0	0	0
			591	376	117	98			
48	CU	72	Total	C	N	O	0	0	0
			591	376	117	98			

- Molecule 49 is a protein called 30S RIBOSOMAL PROTEIN S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	BV	83	Total	C	N	O	S	0	0	0
			665	424	124	115	2			
49	CV	78	Total	C	N	O	S	0	0	0
			624	398	115	109	2			

- Molecule 50 is a protein called 30S RIBOSOMAL PROTEIN S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	BW	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			
50	CW	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			

- Molecule 51 is a protein called 30S RIBOSOMAL PROTEIN THX.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
51	BX	25	Total	C	N	O	0	0	0
			217	134	52	31			
51	CX	25	Total	C	N	O	0	0	0
			217	134	52	31			

- Molecule 52 is a RNA chain called TRNA-LEU.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	BB	87	Total	C	N	O	P	0	0	0
			1861	829	333	612	87			
52	CB	87	Total	C	N	O	P	0	0	0
			1861	829	333	612	87			

- Molecule 53 is a RNA chain called TRNA-FMET.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	BC	77	Total	C	N	O	P	0	0	0
			1643	732	298	536	77			
53	BD	77	Total	C	N	O	P	0	0	0
			1643	732	298	536	77			
53	CC	77	Total	C	N	O	P	0	0	0
			1643	732	298	536	77			
53	CD	77	Total	C	N	O	P	0	0	0
			1643	732	298	536	77			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BC	18	C	U	conflict	GB AP012306.1
BD	18	C	U	conflict	GB AP012306.1
CC	18	C	U	conflict	GB AP012306.1
CD	18	C	U	conflict	GB AP012306.1

- Molecule 54 is a RNA chain called MRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	B1	10	Total	C	N	O	P	0	0	0
			205	92	28	75	10			
54	C1	10	Total	C	N	O	P	0	0	0
			205	92	28	75	10			

- Molecule 55 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
55	AA	630	Total 630 Mg 630	0	0
55	AB	17	Total 17 Mg 17	0	0
55	AD	2	Total 2 Mg 2	0	0
55	AE	4	Total 4 Mg 4	0	0
55	AF	3	Total 3 Mg 3	0	0
55	AO	3	Total 3 Mg 3	0	0
55	A0	1	Total 1 Mg 1	0	0
55	A1	1	Total 1 Mg 1	0	0
55	A2	1	Total 1 Mg 1	0	0
55	AU	1	Total 1 Mg 1	0	0
55	A3	1	Total 1 Mg 1	0	0
55	A5	2	Total 2 Mg 2	0	0
55	A6	1	Total 1 Mg 1	0	0
55	A7	1	Total 1 Mg 1	0	0
55	BA	244	Total 244 Mg 244	0	0
55	BG	1	Total 1 Mg 1	0	0
55	BN	2	Total 2 Mg 2	0	0
55	BQ	2	Total 2 Mg 2	0	0
55	BB	8	Total 8 Mg 8	0	0
55	BC	9	Total 9 Mg 9	0	0
55	BD	1	Total 1 Mg 1	0	0
55	B1	2	Total 2 Mg 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	CA	209	Total 209	Mg 209	0	0
55	CG	3	Total 3	Mg 3	0	0
55	CH	1	Total 1	Mg 1	0	0
55	CS	1	Total 1	Mg 1	0	0
55	CB	5	Total 5	Mg 5	0	0
55	CC	8	Total 8	Mg 8	0	0
55	DA	528	Total 528	Mg 528	0	0
55	DB	14	Total 14	Mg 14	0	0
55	DE	3	Total 3	Mg 3	0	0
55	DP	1	Total 1	Mg 1	0	0
55	D0	1	Total 1	Mg 1	0	0
55	D1	2	Total 2	Mg 2	0	0
55	DU	1	Total 1	Mg 1	0	0
55	D3	1	Total 1	Mg 1	0	0
55	D5	1	Total 1	Mg 1	0	0

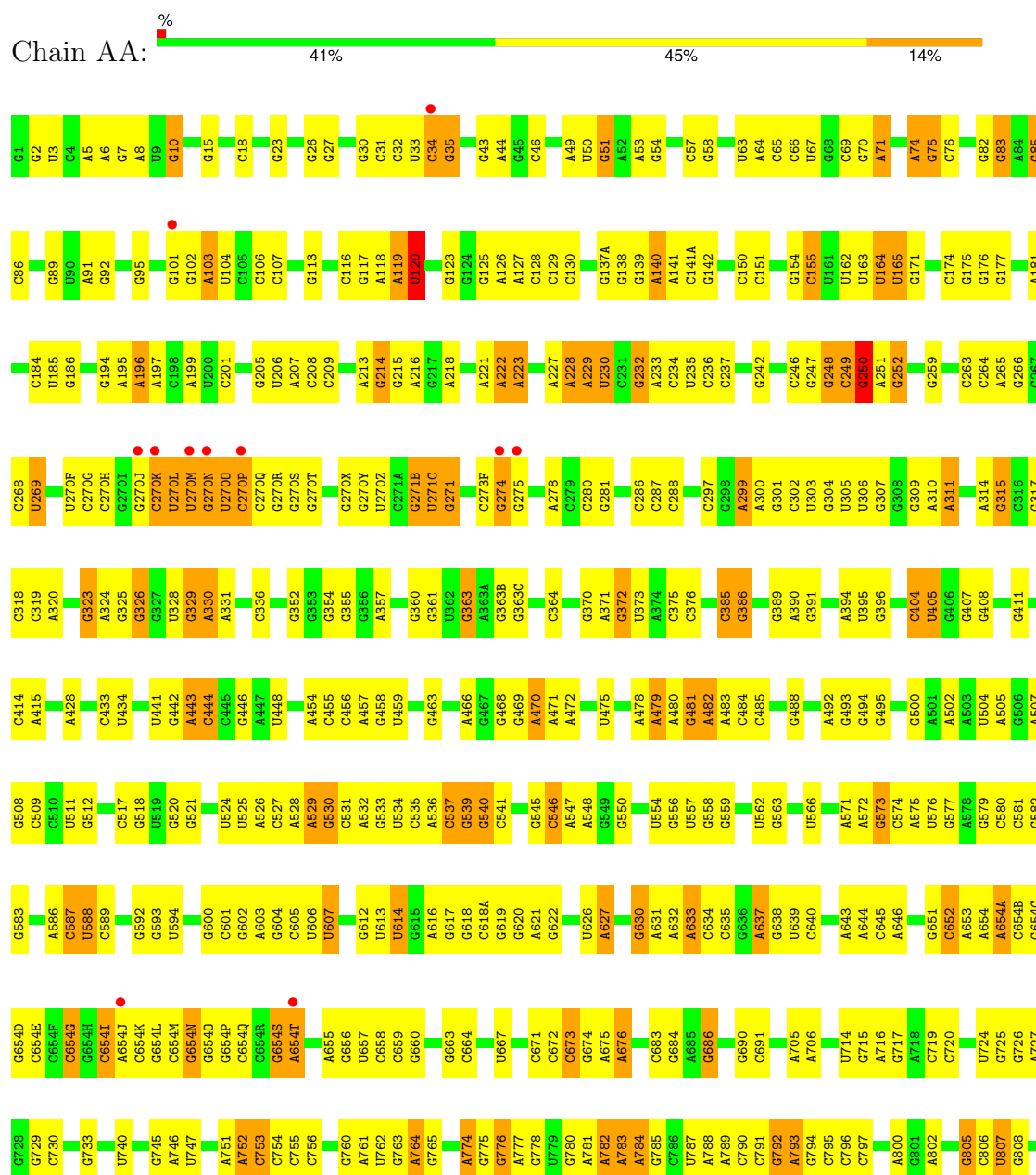
- Molecule 56 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	BG	1	Total 1	Zn 1	0	0
56	BQ	1	Total 1	Zn 1	0	0
56	CG	1	Total 1	Zn 1	0	0
56	CQ	1	Total 1	Zn 1	0	0

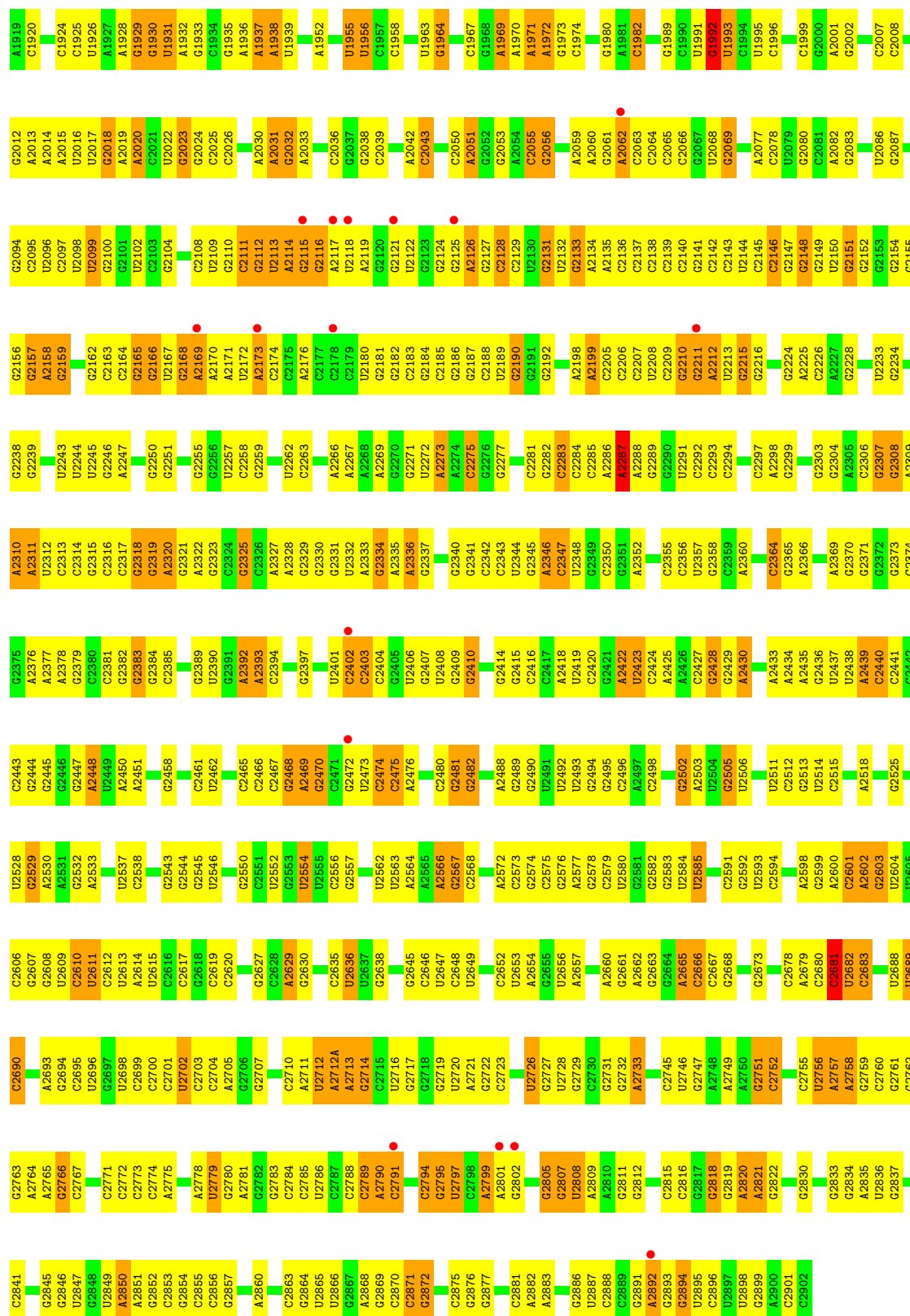
3 Residue-property plots [i](#)

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: RNA (2909-MER)



A1819	C1734	G1642	G1542	A1471	G1324	U1240	U1165	A1096	G1036	C967	C886	U811
U1820	C1735	G1643	A1543	C1474	G1325	A1241	U1166	U1097	G1037	G968	A887	C812
A1821	C1741	G1648	C1544	G1475	U1326	A1241	U1167	A1098	C1038	U969	C888	U813
A1825	G1743	G1649	A1545	C1476	G1327	G1244	G1168	U1099	G1039	C970	C889	C814
G1826	G1749	G1650	C1547	A1477	G1328	A1247	G1169	U1101	G1042	C971	C890	C815
C1827	C1548	G1651	C1548	G1478	U1329	A1247	G1170	U1102	G1043	G972	C892	C816
G1828	C1549	A1652	C1549	G1479	C1330	A1247	G1171	C1103	C1044	A973	C893	C817
A1829	C1550	G1653	C1550	G1480	A1331	G1250	G1172	A1104	G1045	G974	C894	C818
U1833	A1554	A1654	C1554	G1481	C1332	G1251	U1175	U1105	A1046	C974A	U895	A819
U1834	G1555	G1482	C1555	G1483	C1333	G1252	U1176	U1106	G1047	G975	A896	A821
G1835	G1556	G1483	C1556	G1484	G1337	A1253	G1177	G1110	A1048	G977	C897	A821
U1843	C1557	A1486	C1557	G1487	G1338	G1256	U1178	A1111	G1049	G978	C898	A824
A1847	A1558	G1487	A1558	G1488	G1339	G1256	C1179	A1112	C1050	G979	C899	A824
G1851	G1560	G1489	G1560	A1494	U1340	U1263	C1180	U1113	G1051	A900	C900	C825
U1851	G1568	A1495	G1568	A1496	C1344	A1264	C1181	U1113	G1052	A901	C902	U826
G1858	C1571	U1497	C1571	G1498	C1345	A1265	A1182	G1116	C1053	C982	C903	U827
A1859	A1570	C1502	C1570	G1499	G1348	U1267	C1185	G1117	A1054	A983	U905	U828
G1860	A1571	G1503	A1571	G1504	A1349	A1268	G1186	C1118	G1055	C986	U906	U829
G1861	C1577	C1505	C1577	C1506	U1352	A1269	G1187	C1119	G1056	C987	U907	U833
G1862	G1674	G1507	G1674	C1508	U1353	C1270	U1188	G1122	U1058	A988	U907	C834
G1863	G1678	A1510	A1578	A1509	A1354	A1271	U1189	G1123	U1059	C989	C908	C838
U1864	G1681	G1511	C1578	C1510	G1355	A1272	G1190	G1124	U1060	A990	C909	C839
G1869	C1686	C1512	C1579	A1511	G1356	U1273	G1191	G1125	U1061	C991	A910	U839
A1872	G1687	G1513	A1580	A1512	U1357	A1274	G1195	A1127	G1062	C992	A911	C840
C1878	G1688	C1514	C1581	G1513	G1358	G1276	U1201	U1130	U1063	C994	C915	C844
U1884	U1778	G1515	C1582	G1514	U1359	A1277	U1202	U1131	U1064	C995	G916	G846
G1885	U1779	G1516	C1583	G1515	G1360	A1278	G1203	G1131	U1065	A996	A917	C846
C1886	C1770	C1517	C1584	G1516	G1361	A1278	G1204	C1135	U1066	A1000	G919	G848
C1887	G1771	G1518	C1585	G1517	U1362	A1278	G1205	G1136	U1067	A1001	G929	G849
A1891	A1773	G1519	C1586	G1518	A1364	U1278	G1206	G1137	U1068	C1002	C860	C850
U1894	U1778	G1520	C1587	G1519	A1365	U1278	U1207	G1138	A1070	C1003	G932	U851
C1895	C1779	G1521	C1588	G1520	G1368	C1291	C1208	G1139	G1071	C1005	A933	C856
G1899	G1702	G1522	C1589	G1521	G1369	U1292	G1209	G1140	C1072	C1006	C857	C857
U1900	G1705	G1523	C1590	G1522	U1372	C1293	U1210	U1141	A1073	C1007	G938	U858
A1901	U1706	G1524	C1591	G1523	A1373	U1288	U1211	U1142	G1074	G1011	A941	U860
C1902	C1710	G1525	C1592	G1524	G1374	C1289	G1212	A1143	C1075	U1012	G942	U868
G1903	C1717	G1526	C1593	G1525	C1375	C1290	G1215	G1144	A1076	C1013	U943	A863
U1906	G1718	G1527	C1594	G1526	G1376	C1291	G1216	G1145	U1077	U1014	G944	G864
G1907	G1725	G1528	C1595	G1527	G1377	U1300	G1217	C1146	C1079	G1015	A945	C865
C1908	G1726	G1529	C1596	G1528	A1378	A1301	C1218	C1147	A1080	G1016	G946	A866
A1913	U1727	G1530	C1597	G1529	A1379	G1309	U1219	G1148	U1081	G1017	C950	C867
C1914	G1728	G1531	C1598	G1530	A1380	G1310	G1220	G1149	U1082	C1018	G951	U868
U1915	U1730	C1532	C1599	G1531	G1381	U1312	C1221	G1150	U1083	U1019	C952	A870
A1916	G1731	G1533	C1600	G1532	C1382	U1313	C1222	G1151	A1084	A1020	G953	U871
U1917	G1732	G1534	C1601	G1533	A1384	C1314	A1227	G1152	A1085	A1021	G954	A872
A1918	G1733	G1535	C1602	G1534	G1385	G1315	G1228	G1153	A1086	U1023	C955	G873
		G1536	C1603	G1535	C1386	U1316	G1229	A1154	G1087	G1024	G956	G879
		G1537	C1604	G1536	C1387	A1317	G1230	G1155	A1088	G1025	A957	G880
		G1538	C1605	G1537	G1388	G1319	G1231	G1156	U1090	U1026	U958	G881
		G1539	C1606	G1538	G1389	G1320	G1235	G1157	U1091	A1027	A959	G882
		G1540	C1607	G1539	U1396	A1322	G1236	G1160	C1092	A1028	A960	G883
		G1541	C1608	G1540	C1403	U1323	A1237	G1162	U1094	A1029	C961	C885

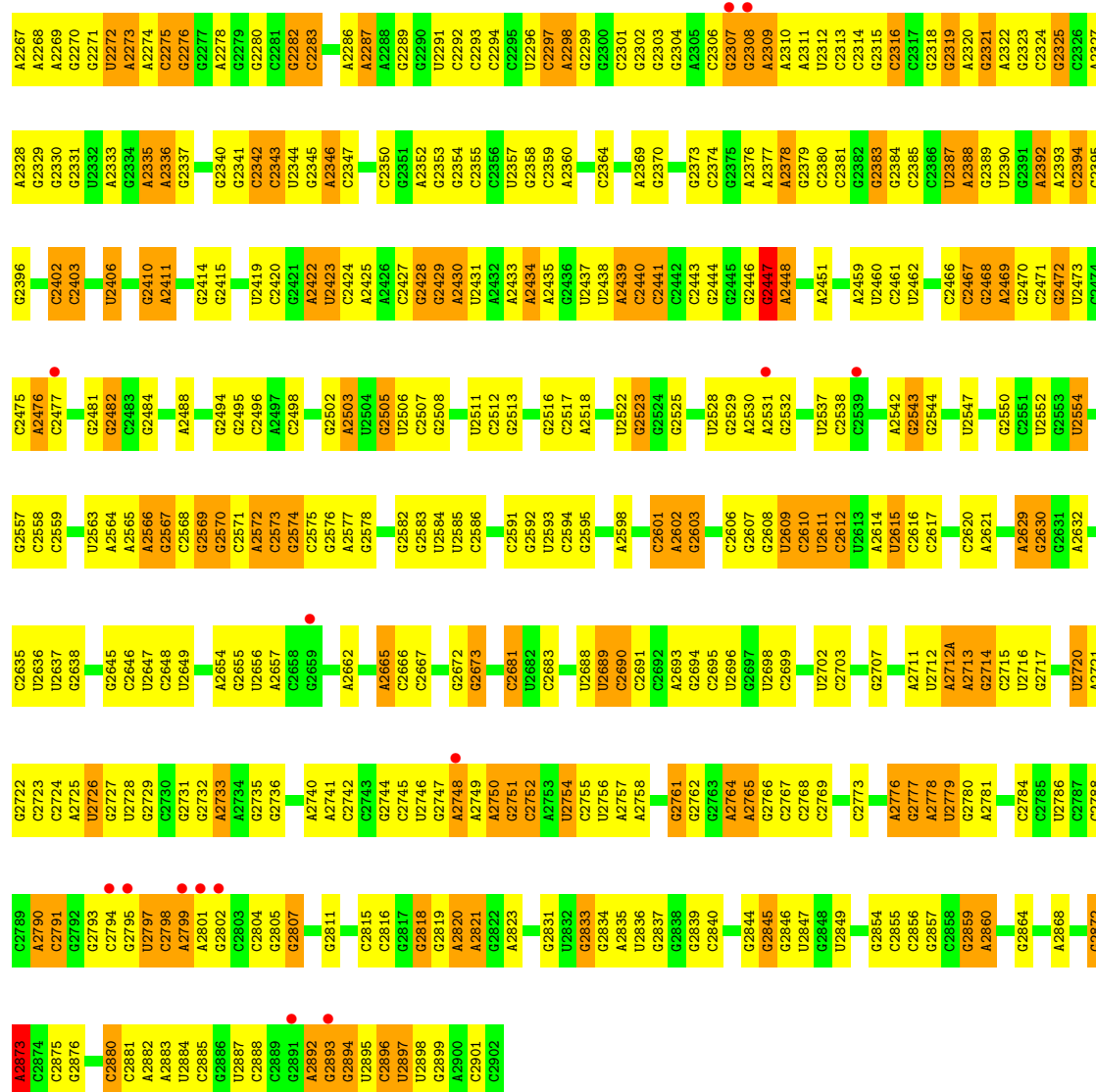


- Molecule 1: RNA (2909-MER)

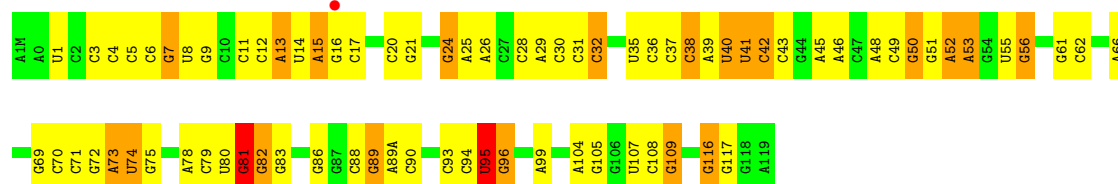


G1024	A959	A890	U828	U757	A670	G624	G556	A479	U383	C296	C249	U	U	G70	G1
G1025	A960	G922	A629	C758	C671	G625	U557	A480	U384	C297	G250	U	U	A71	G2
U1026	G961	C893	C830	G759	C672	U626	G558	A481	C385	C298	A251	U	U	U72	U3
A1027	G962	C894	C831	A761	C673	A627	G559	A482	G386	C299	G252	U	U	A73	C4
U1033	U963	U895	U832	A764	A675	G629	U562	C486	G389	A300	A255	C172	C172	A74	A5
G1034	C965	A896	C834	G765	A676	G630	G563	C487	G390	G307	A256	G173	G173	C76	A6
U1035	G966	C898	A835	G769	C679	A632	C564	C488	C392	G308	A257	C174	C174	C77	A7
G1036	C970	A899	C837	G769	C680	A633	C565	C489	C393	G309	G258	G175	G175	C78	A8
U1039	C971	A900	C838	G774	C681	A634	U566	C491	C394	G310	G259	G176	G176	C79	U9
C1040	G972	C902	U839	A775	G684	C635	G570	A492	U395	A311	G260	G177	G177	C84	G10
C1041	G973	C903	C840	G776	A685	A636	A571	C493	U405	G315	A265	C184	C184	A84	G11
G1042	G974	C904	A841	G777	G686	A637	A572	C494	G406	C316	G266	U185	U185	G85	U12
C1043	C974A	U905	G842	G778	C690	G638	A573	G495	G407	G317	U269	C186	C186	G89	G17
G1044	G975	C906	C843	U779	C691	U639	G574	G496	C409	A320	U269	A195	A195	U90	A21
A1045	G976	U907	C844	G780	C692	C640	A575	G497	C410	A321	A270	A196	A196	A91	C22
U1046	G977	C908	G845	A781	G696	G641	U576	C498	G411	A322	A270A	A197	A197	G92	G23
G1047	G978	A909	C846	A782	C697	G642	U577	A501	A412	G323	U270F	C198	C198	C93	G24
A1048	C979	A910	U847	A783	C698	A643	A578	A502	A413	G324	C270G	A199	A199	G94	U25
C1049	C980	A911	G848	A784	C699	G644	G579	A503	C420	A324	C270H	U200	U200	G95	G26
A1050	G981	C912	A849	G785	G700	A645	C580	U504	U421	U328	G270I	A204	A204	G96	G27
G1051	C913	U913	C850	G786	G701	G646	C581	A505	A428	A330	G270J	G205	G205	U99	U29
C1052	C914	C915	U851	U787	G702	G647	G582	A506	U429	A331	C270K	G206	G206	G101	U30
G1053	G916	G916	G854	A788	A705	G648	G583	A507	C433	A332	U270L	A207	A207	G102	C31
A1054	C917	G917	G855	A789	A706	G649	U586	G508	U434	G333	U270M	C208	C208	A103	G32
G1055	G918	A918	C856	G792	A707	G651	G598	G509	C435	G334	G270N	A207	A207	G110	U33
U1057	C919	G919	C857	G793	G707	C652	G599	C510	U448	G341	U270O	A218	A218	G111	C34
C1058	C920	G920	U858	A794	C708	A653	U588	U511	G451	G342	C270P	A219	A219	G112	G35
U1059	G921	G921	G859	G795	U709	A654	C589	G512	C444	G343	C270Q	G215	G215	G113	G36
G1060	C922	U922	U860	C796	G710	A654A	G592	A513	C445	G344	G270R	G216	G216	G114	C37
U1061	G923	G923	A861	C797	A717	G654B	G593	C517	U449	G345	U270S	A216	A216	G115	A38
G1062	C924	G924	G862	G798	G718	G654C	G594	U519	G450	G346	G270T	G217	G217	A118	C39
C1063	G925	G925	A863	A799	A719	G654D	G595	U520	G451	G347	G270U	A218	A218	C40	C40
U1064	G926	G926	G864	G799	G723	G654E	G596	G520	G452	G348	G270V	A222	A222	U120	C41
C1065	C927	G927	C865	A800	G724	G654F	G597	U521	C453	G349	G270W	A223	A223	G125	G43
U1066	U999	G932	A866	G801	G725	G654G	G602	U524	C454	G350	G270X	A224	A224	A126	A44
A1067	A1000	A933	C867	A802	G726	C654H	A603	U525	C455	G351	G270Y	A225	A225	A127	G45
G1068	A1001	G934	U868	G803	A727	A654J	G604	U526	C456	G352	U270Z	A226	A226	C128	C46
A1069	G1002	C935	C869	G805	G728	C654K	C605	A527	C457	G353	C273C	A227	A227	C129	A49
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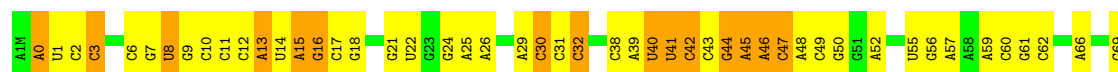
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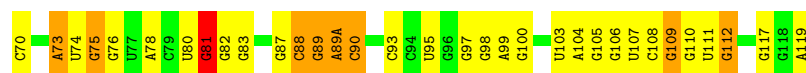


• Molecule 2: 5S RIBOSOMAL RNA

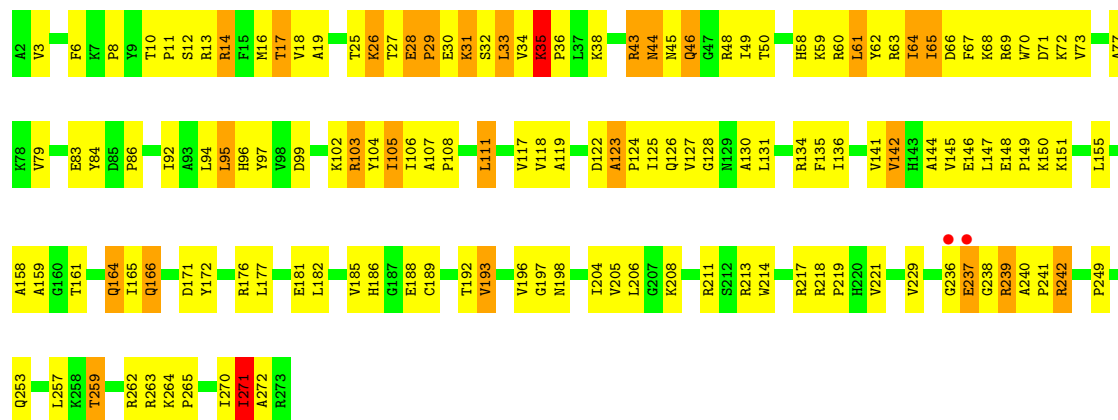


• Molecule 2: 5S RIBOSOMAL RNA

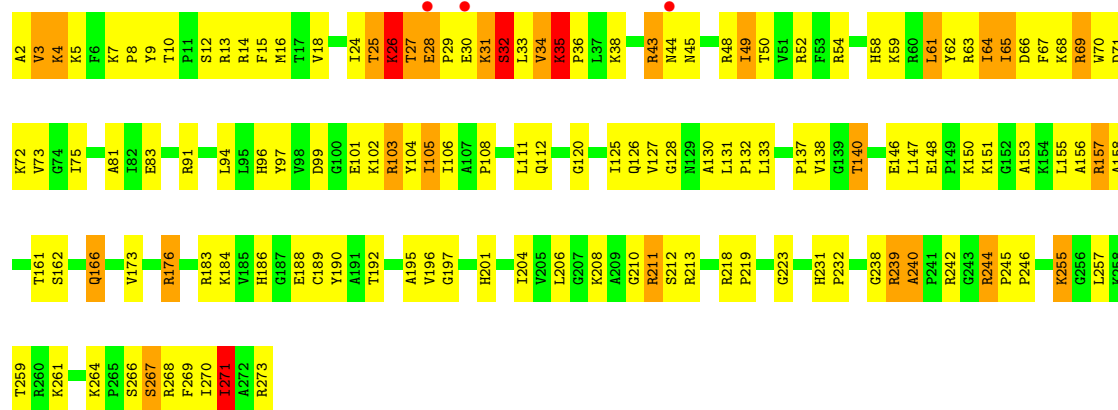




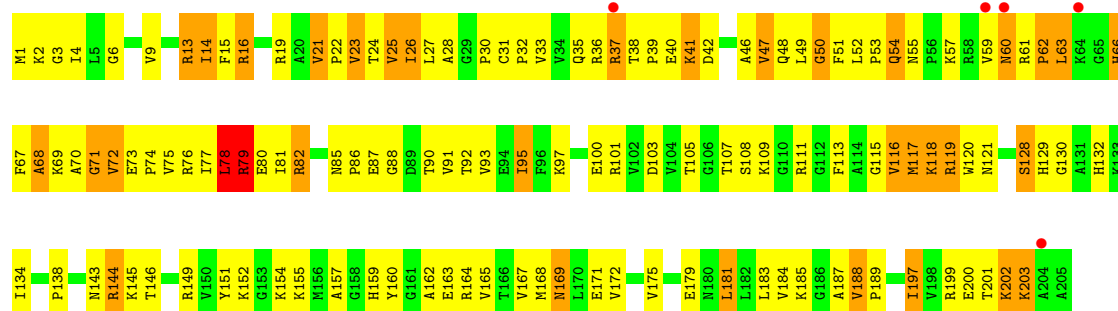
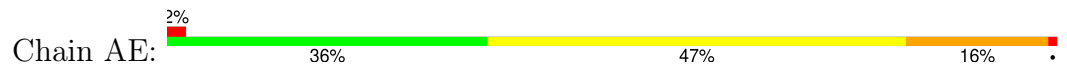
• Molecule 3: 50S ribosomal protein L2



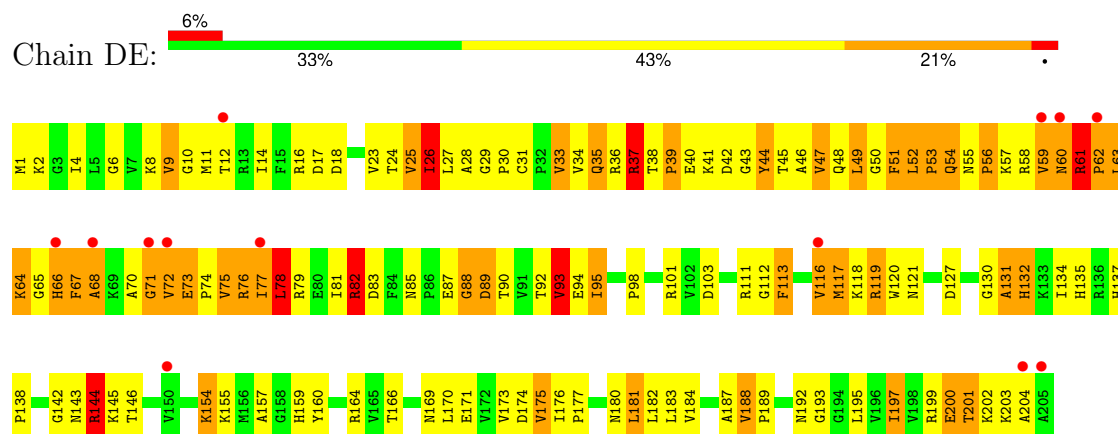
• Molecule 3: 50S ribosomal protein L2



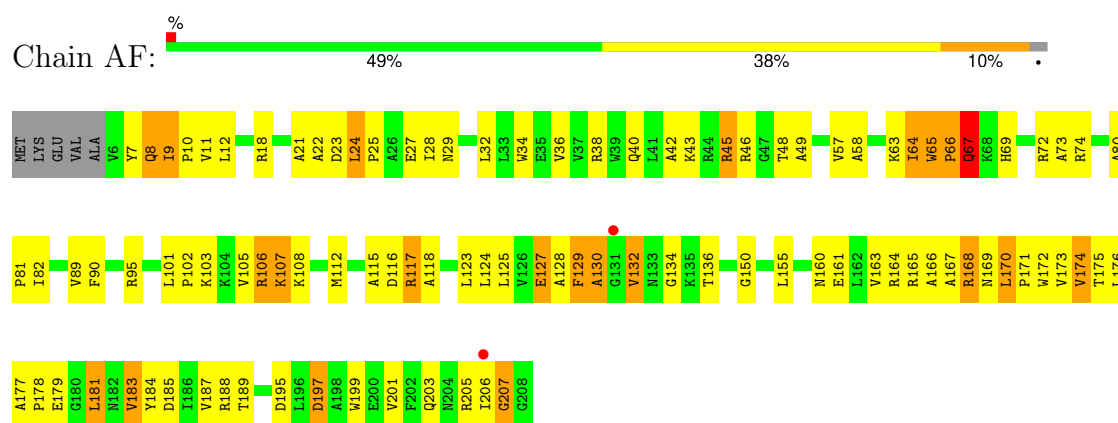
• Molecule 4: 50S ribosomal protein L3



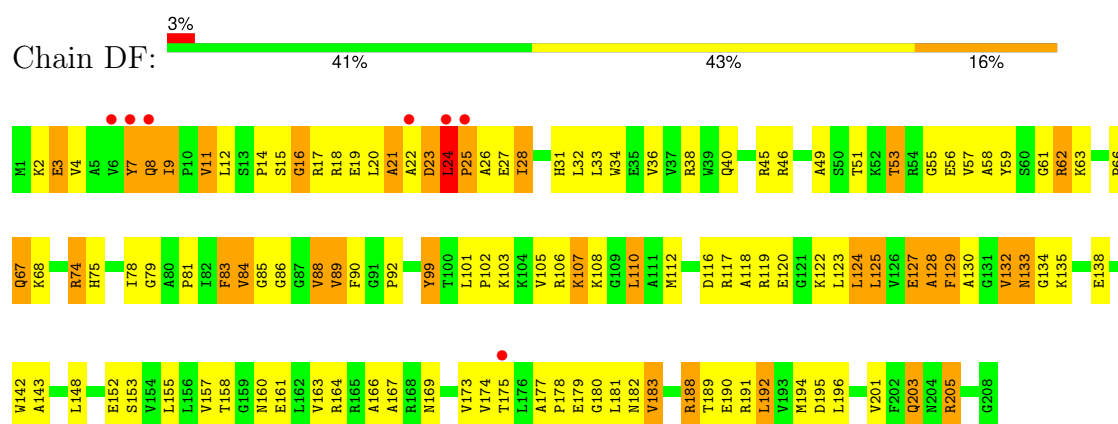
- Molecule 4: 50S ribosomal protein L3



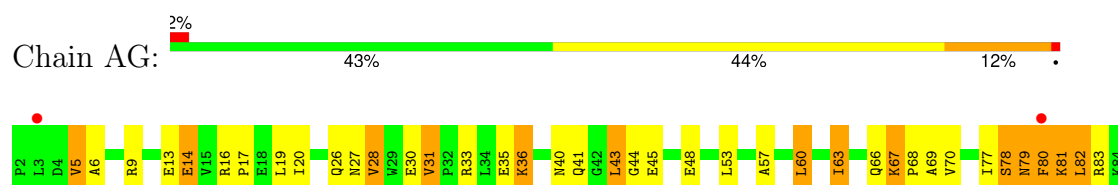
- Molecule 5: 50S ribosomal protein L4

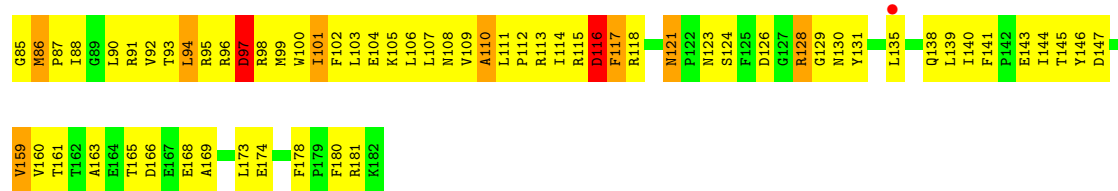


- Molecule 5: 50S ribosomal protein L4

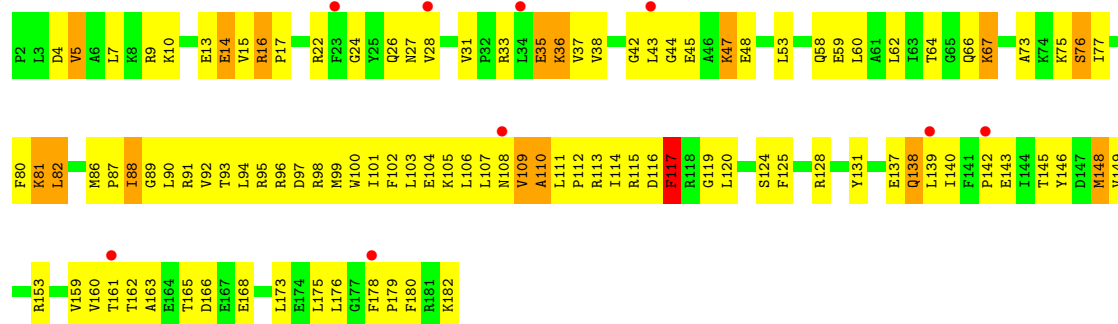
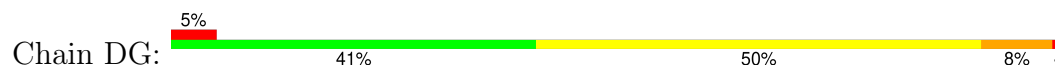


- Molecule 6: 50S ribosomal protein L5

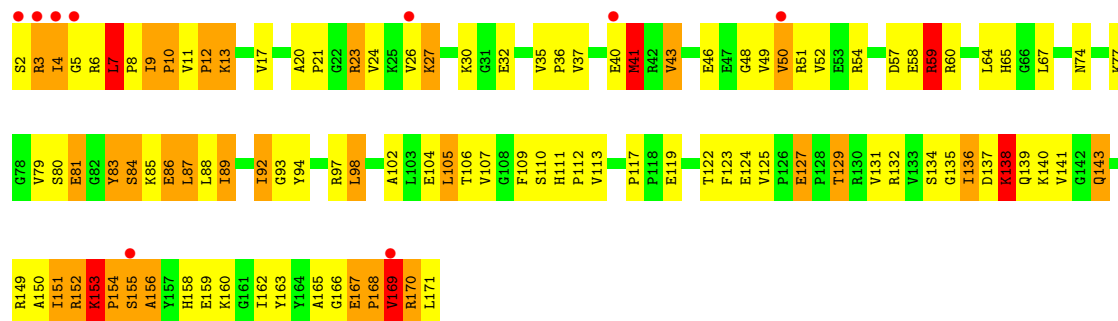




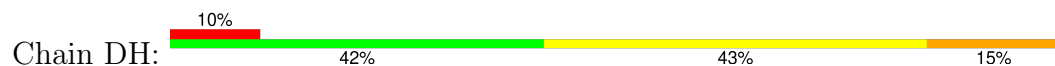
• Molecule 6: 50S ribosomal protein L5



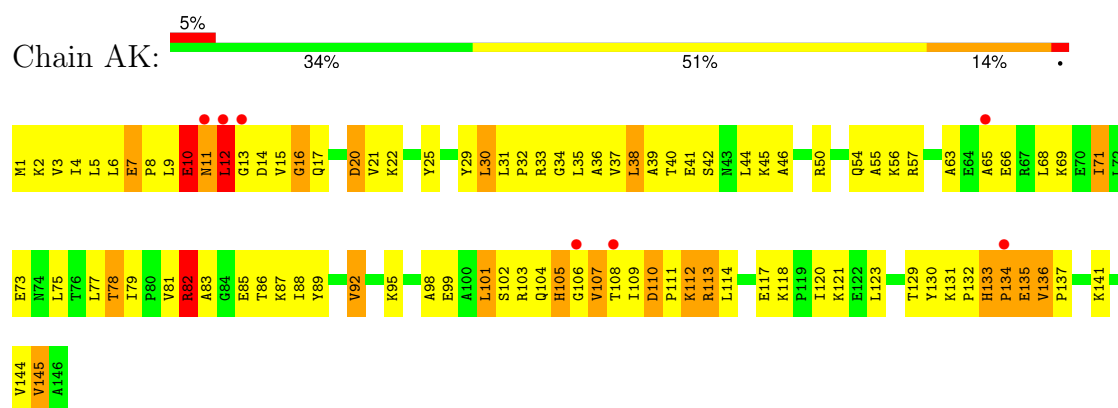
• Molecule 7: 50S ribosomal protein L6



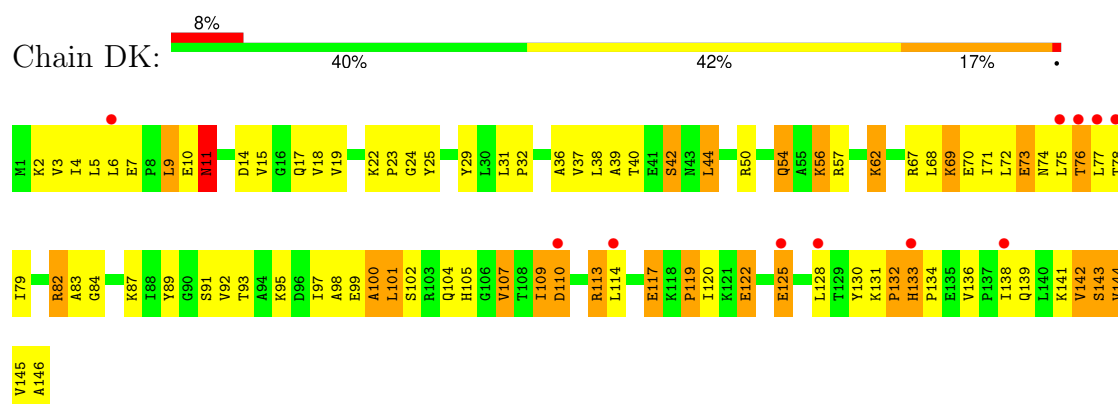
• Molecule 7: 50S ribosomal protein L6



• Molecule 8: 50S ribosomal protein L9



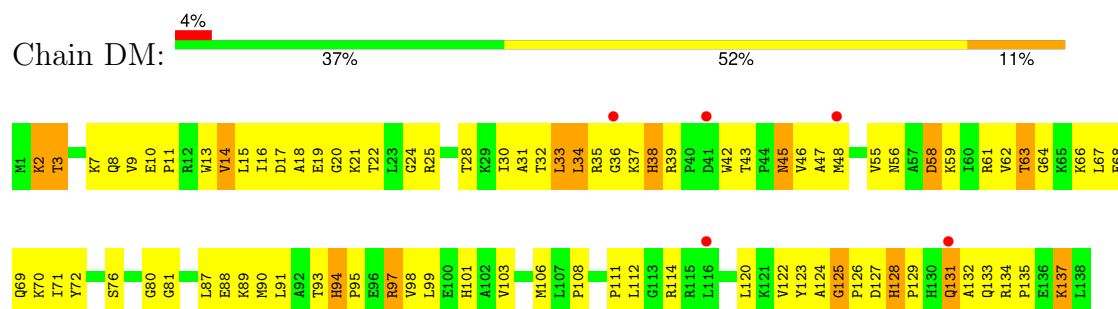
- Molecule 8: 50S ribosomal protein L9



- Molecule 9: 50S ribosomal protein L13

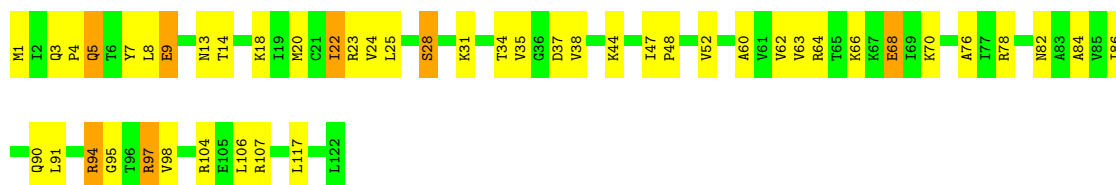


- Molecule 9: 50S ribosomal protein L13

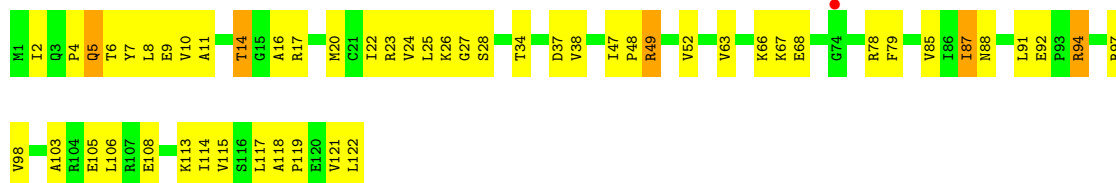


- Molecule 10: 50S ribosomal protein L14

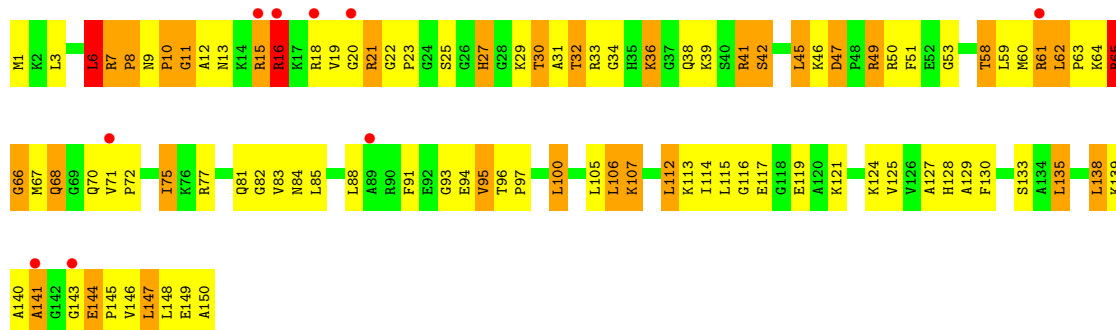




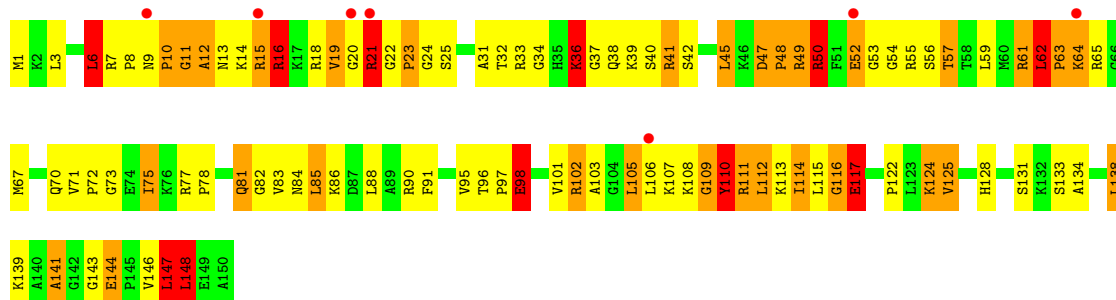
- Molecule 10: 50S ribosomal protein L14



- Molecule 11: 50S ribosomal protein L15

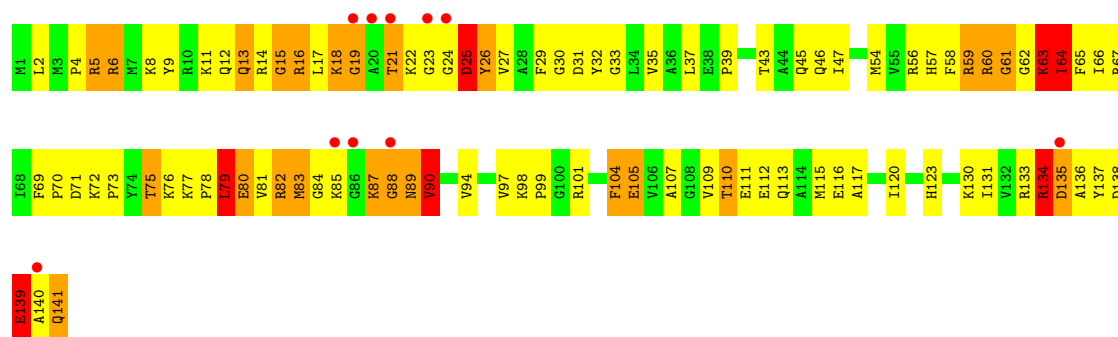


- Molecule 11: 50S ribosomal protein L15

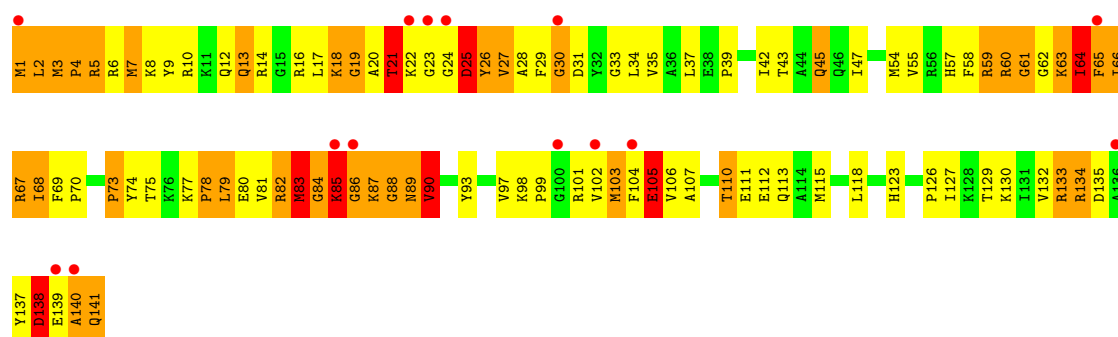


- Molecule 12: 50S ribosomal protein L16

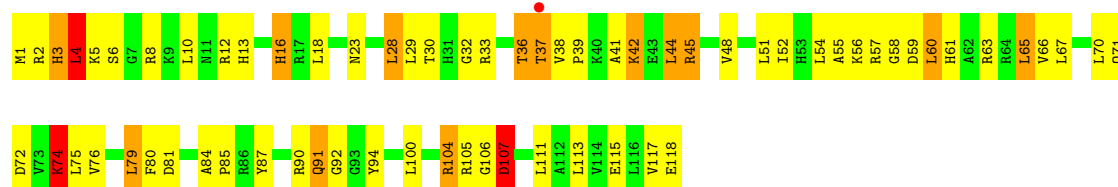
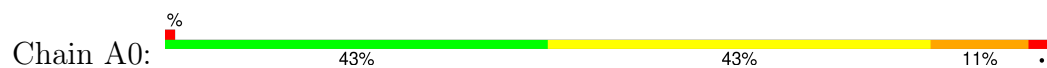




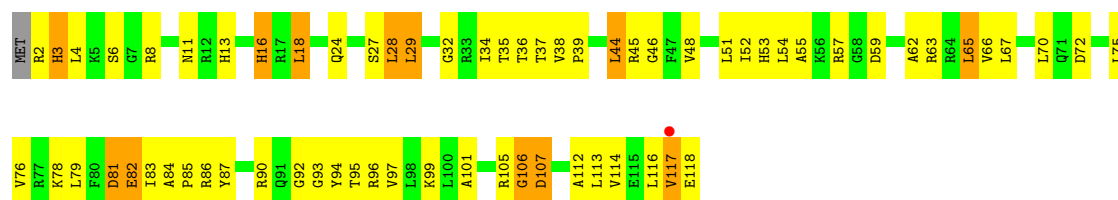
• Molecule 12: 50S ribosomal protein L16



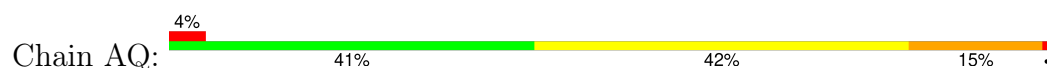
• Molecule 13: 50S ribosomal protein L17

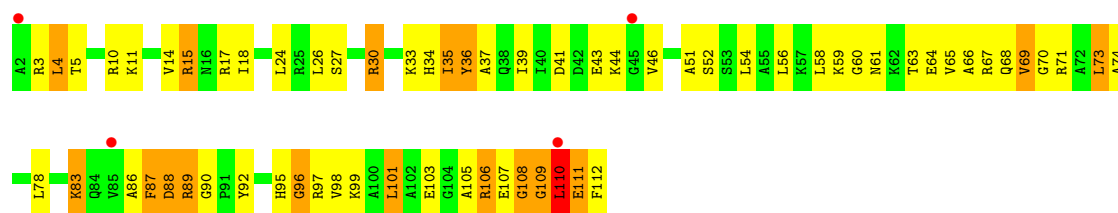


• Molecule 13: 50S ribosomal protein L17

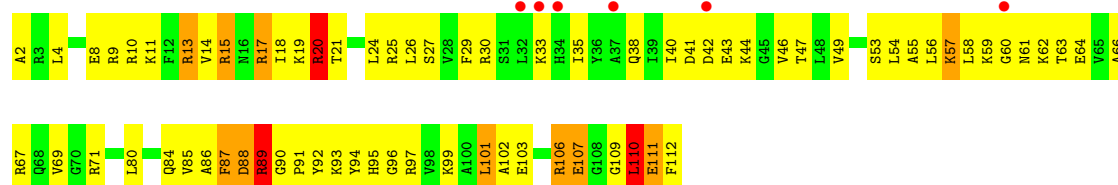


• Molecule 14: 50S ribosomal protein L18

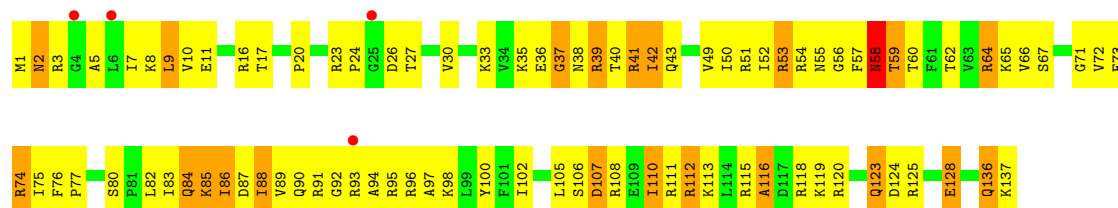




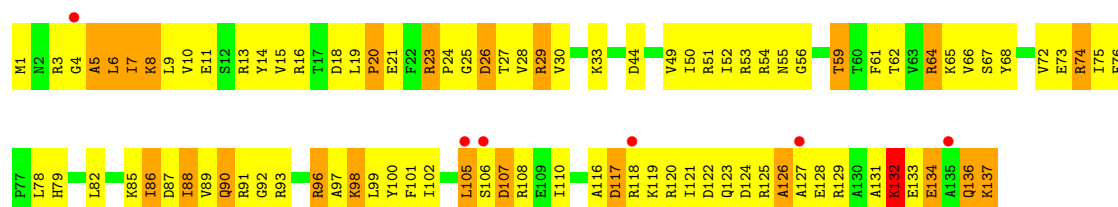
• Molecule 14: 50S ribosomal protein L18



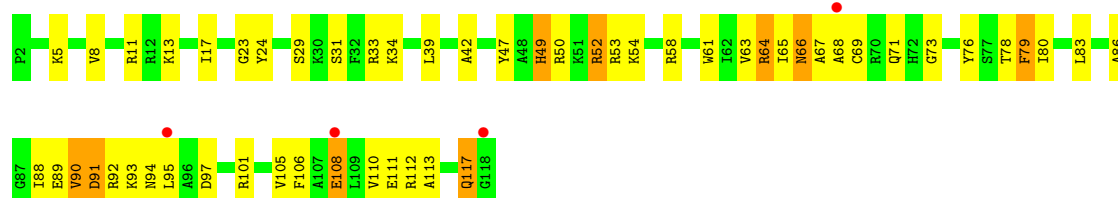
• Molecule 15: 50S ribosomal protein L19



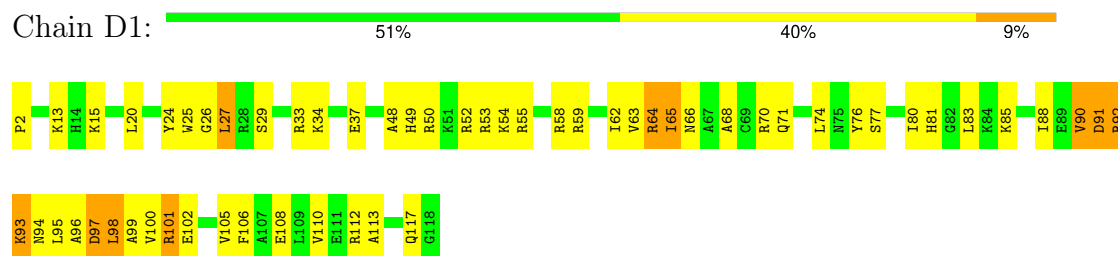
• Molecule 15: 50S ribosomal protein L19



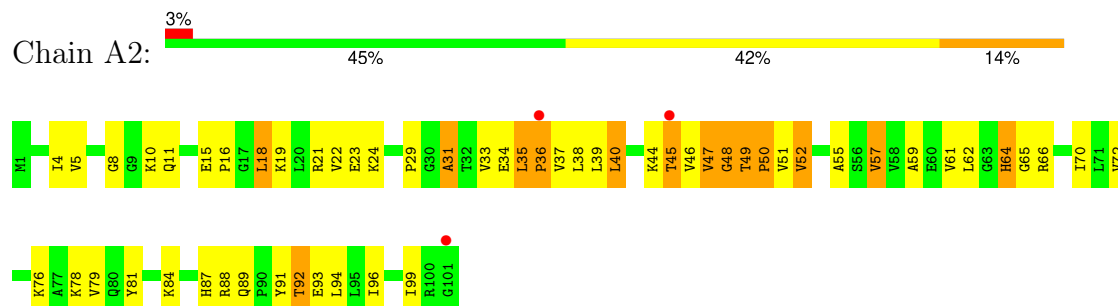
• Molecule 16: 50S ribosomal protein L20



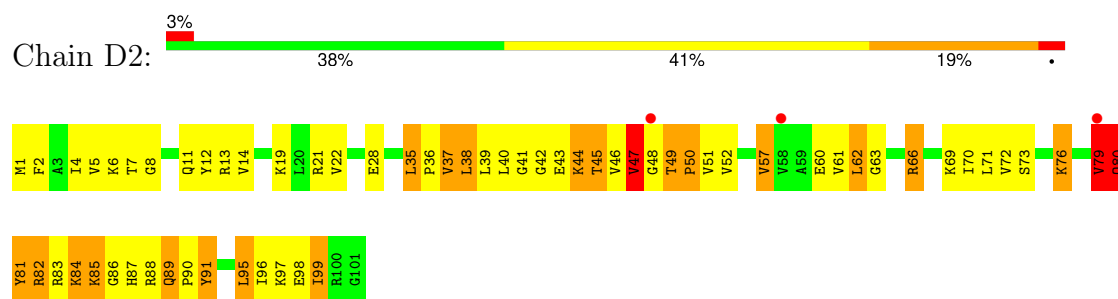
- Molecule 16: 50S ribosomal protein L20



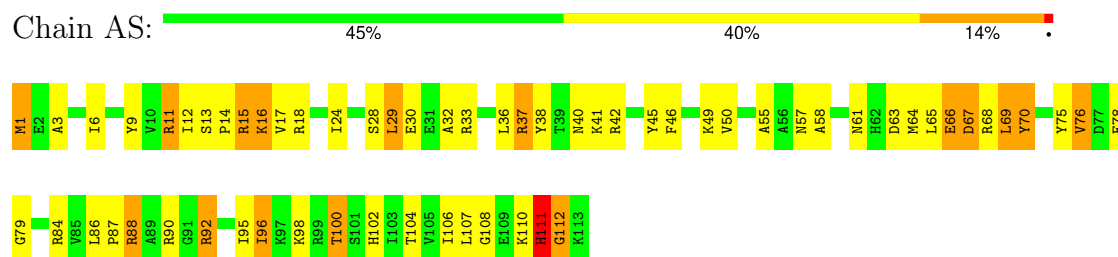
- Molecule 17: 50S ribosomal protein L21



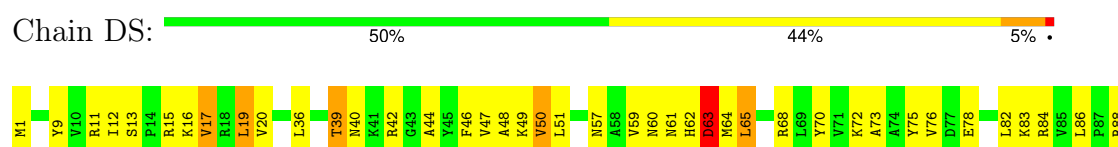
- Molecule 17: 50S ribosomal protein L21

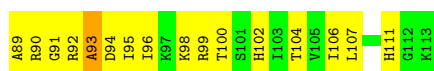


- Molecule 18: 50S ribosomal protein L22

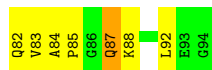
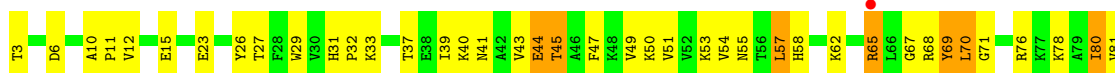


- Molecule 18: 50S ribosomal protein L22

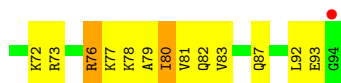




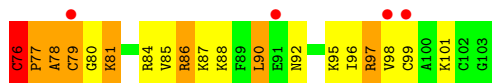
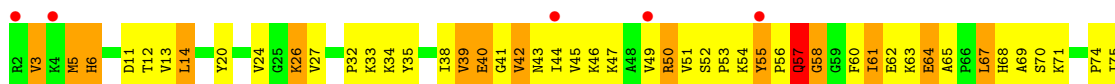
- Molecule 19: 50S ribosomal protein L23



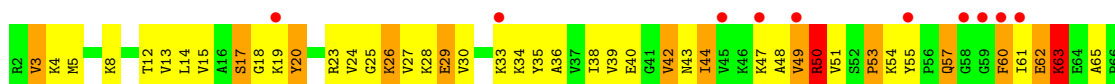
- Molecule 19: 50S ribosomal protein L23



- Molecule 20: 50S ribosomal protein L24

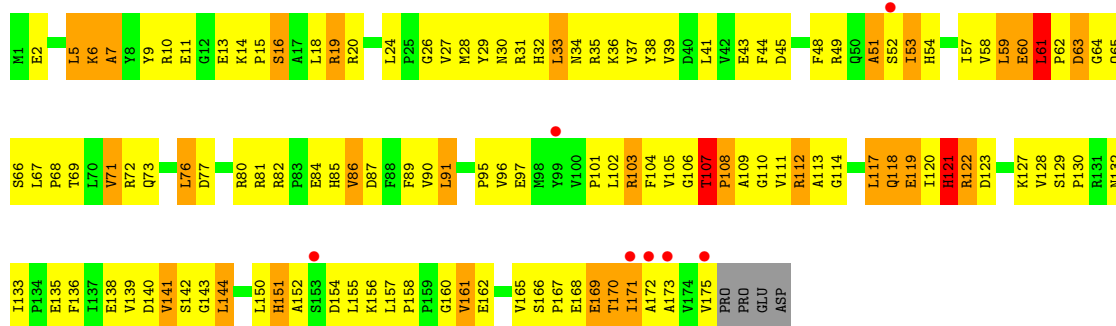


- Molecule 20: 50S ribosomal protein L24

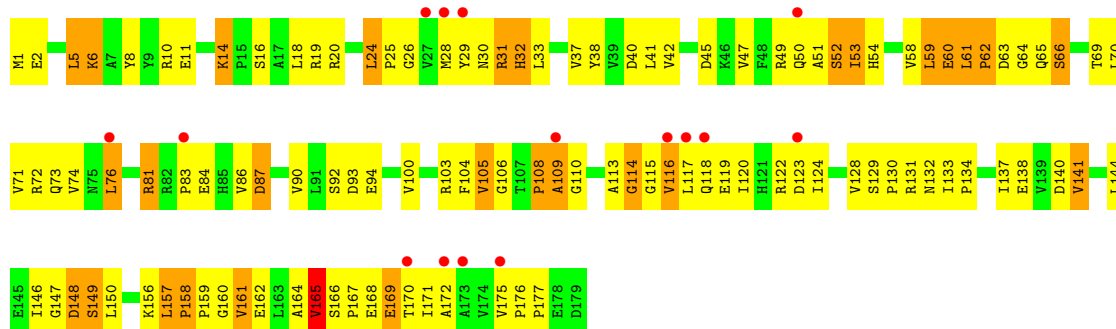


- Molecule 21: 50S ribosomal protein L25

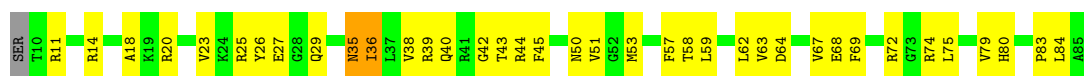




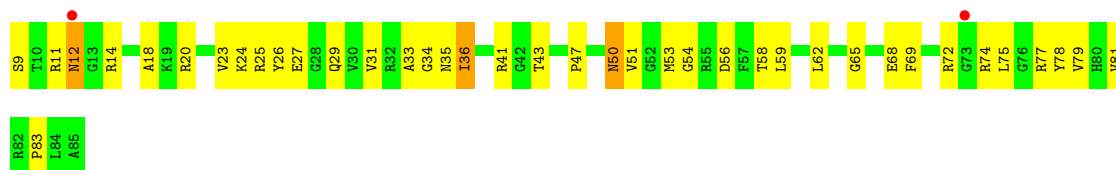
• Molecule 21: 50S ribosomal protein L25



• Molecule 22: 50S ribosomal protein L27

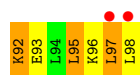


• Molecule 22: 50S ribosomal protein L27



• Molecule 23: 50S ribosomal protein L28

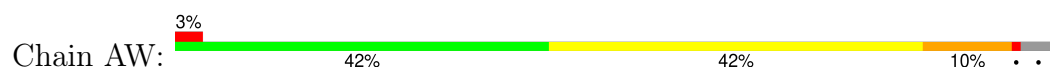




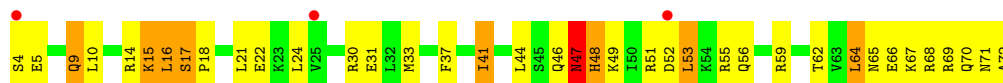
- Molecule 23: 50S ribosomal protein L28



- Molecule 24: 50S ribosomal protein L29



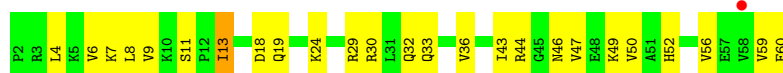
- Molecule 24: 50S ribosomal protein L29



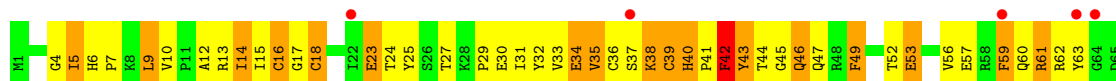
- Molecule 25: 50S ribosomal protein L30



- Molecule 25: 50S ribosomal protein L30

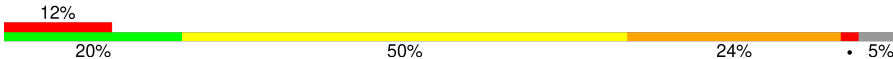


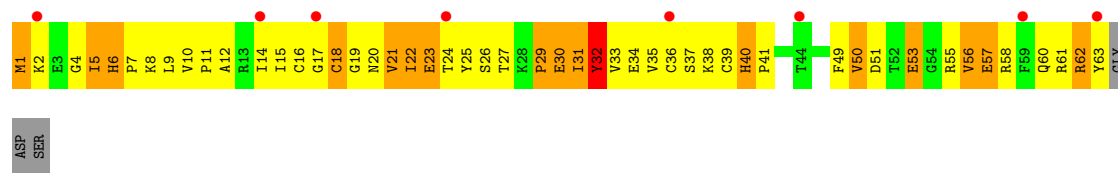
- Molecule 26: 50S ribosomal protein L31



S66

- Molecule 26: 50S ribosomal protein L31

Chain D4: 




- Molecule 27: 50S ribosomal protein L32

Chain A5: 




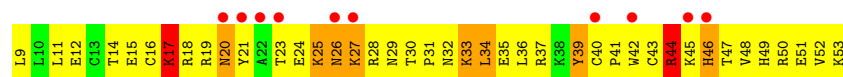
- Molecule 27: 50S ribosomal protein L32

Chain D5: 



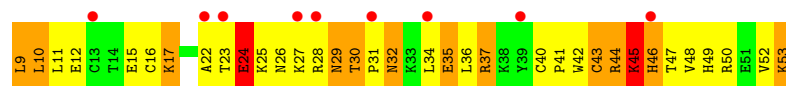
- Molecule 28: 50S ribosomal protein L33

Chain A6: 



- Molecule 28: 50S ribosomal protein L33

Chain D6: 



- Molecule 29: 50S ribosomal protein L34

Chain A7: 



- Molecule 29: 50S ribosomal protein L34

Chain D7: 



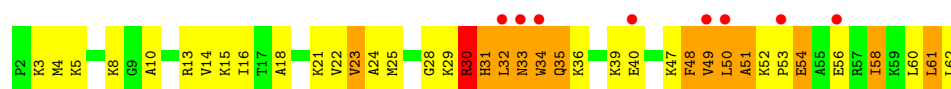
- Molecule 30: 50S ribosomal protein L35

Chain A8: 

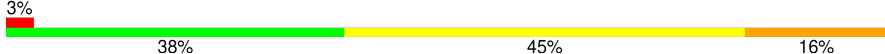


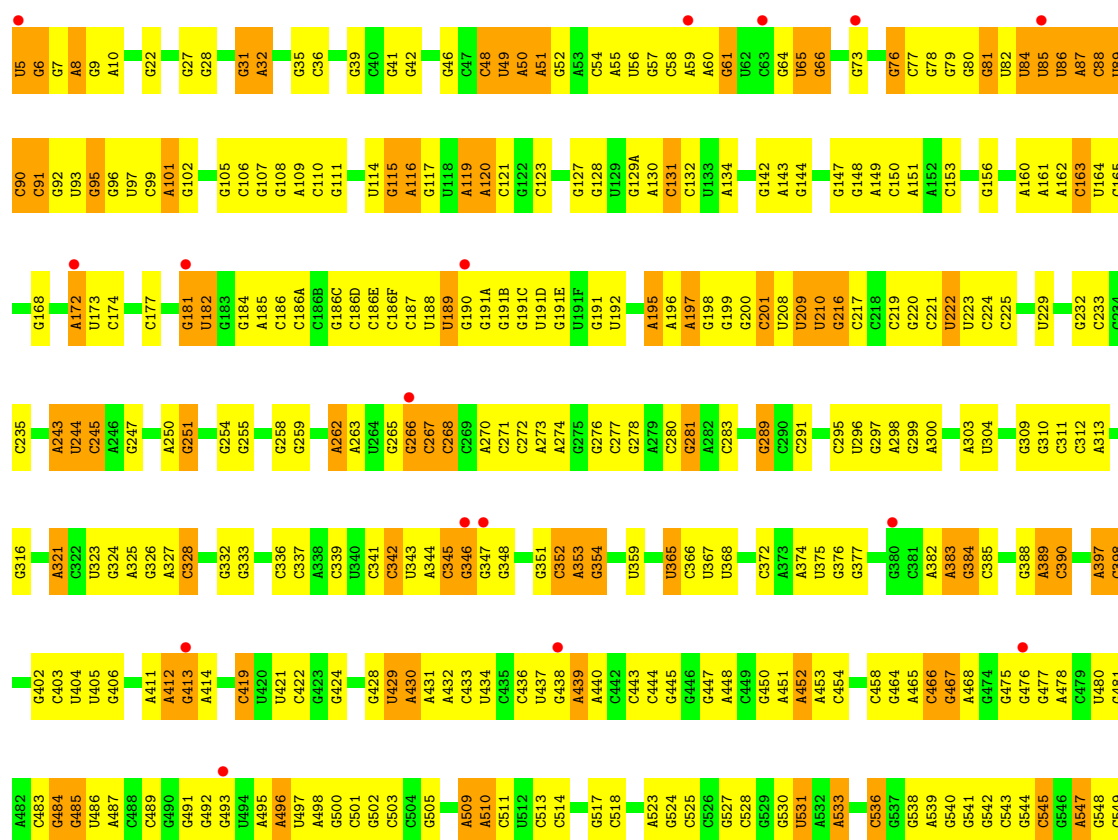
- Molecule 30: 50S ribosomal protein L35

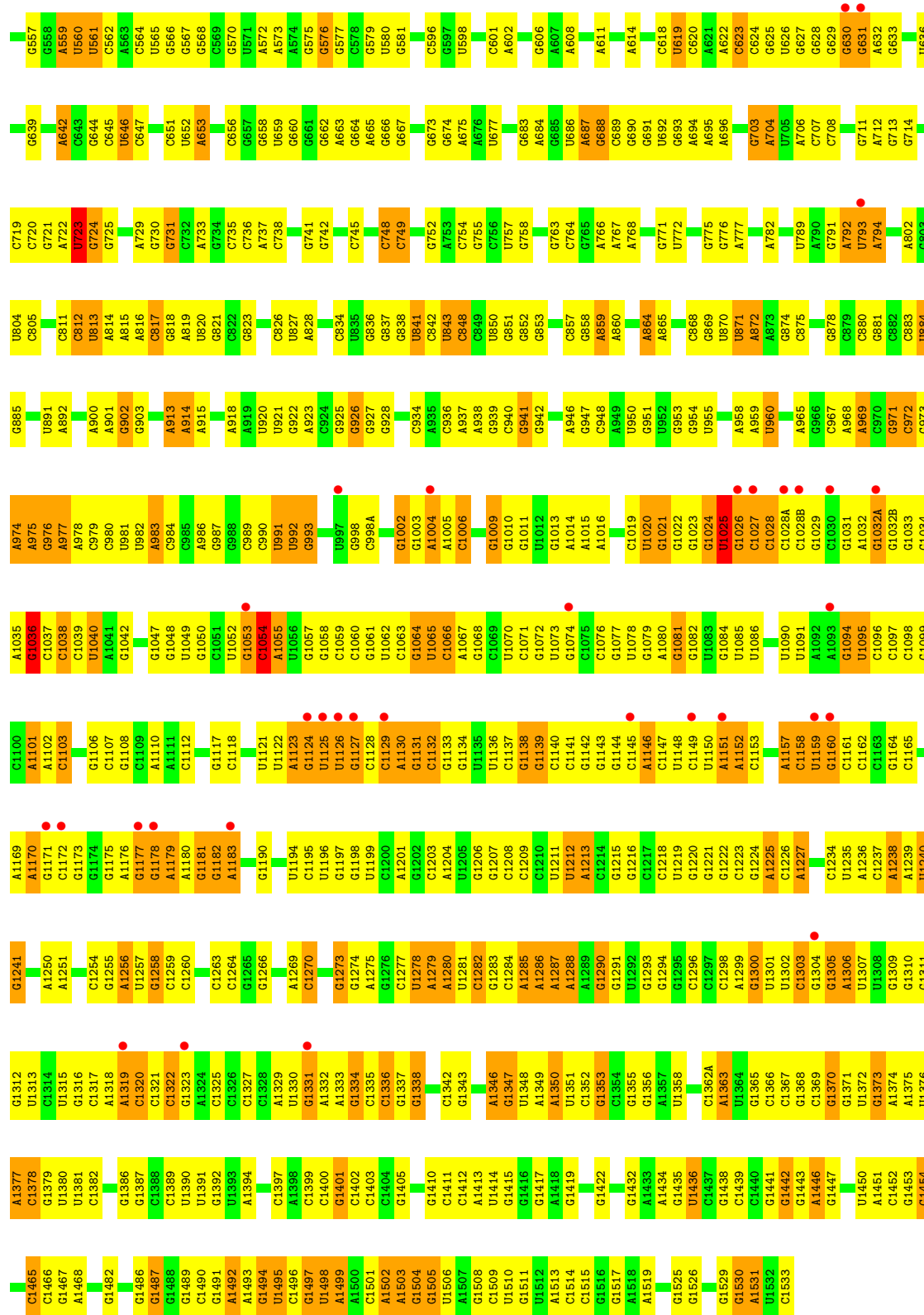
Chain D8: 



- Molecule 31: 16S ribosomal RNA

Chain BA: 

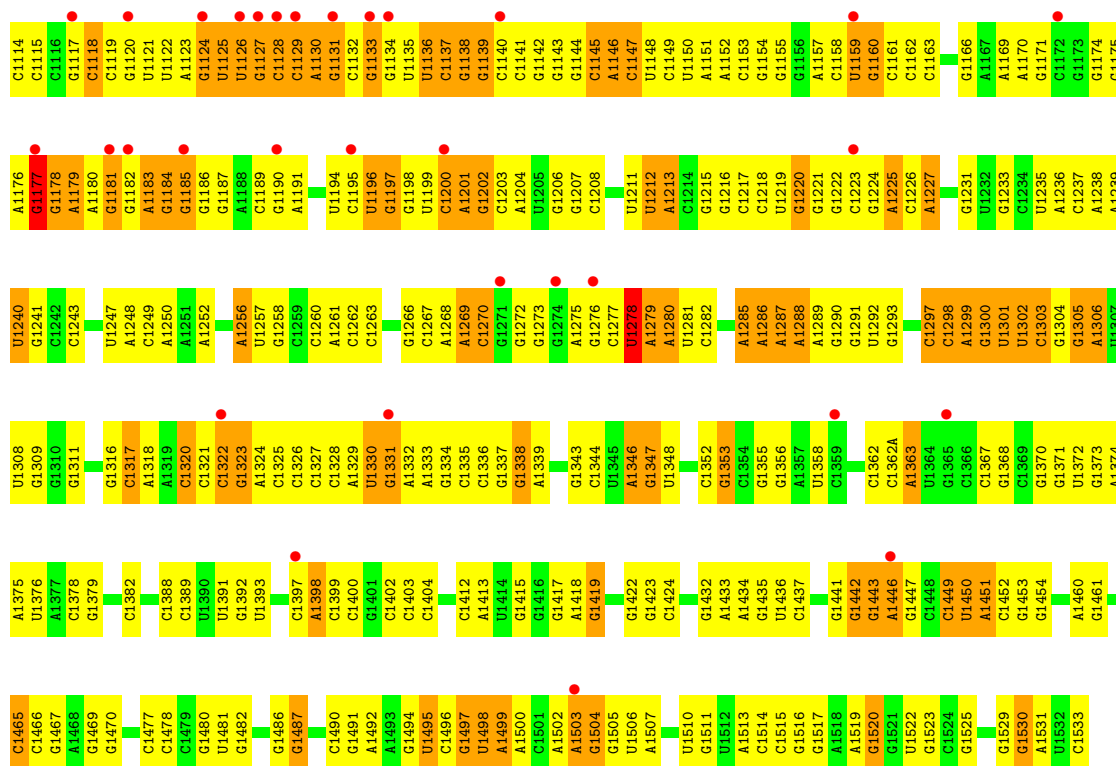




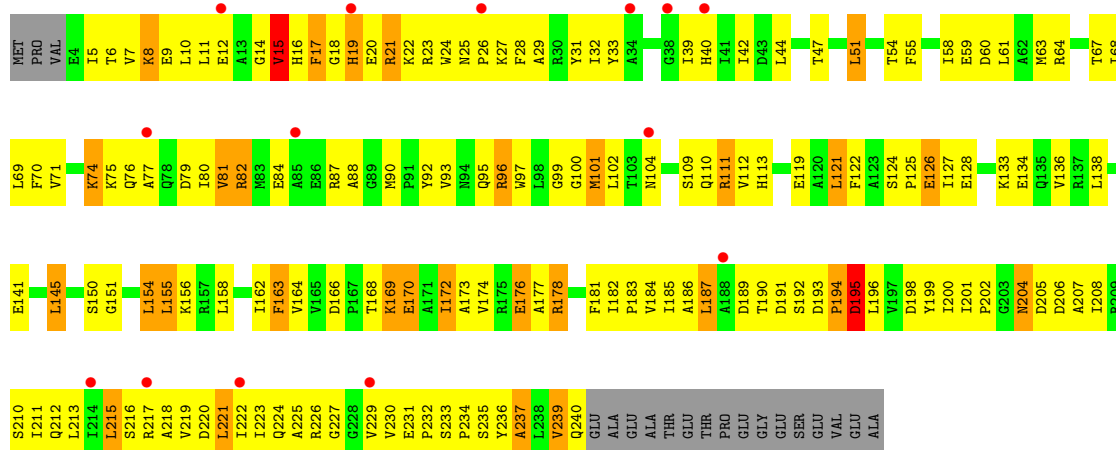
• Molecule 31: 16S ribosomal RNA



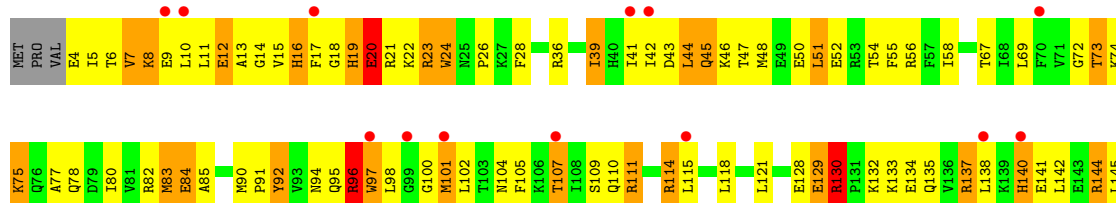


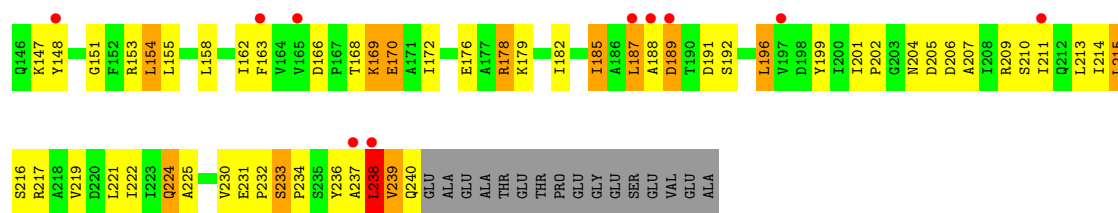


• Molecule 32: 30S RIBOSOMAL PROTEIN S2

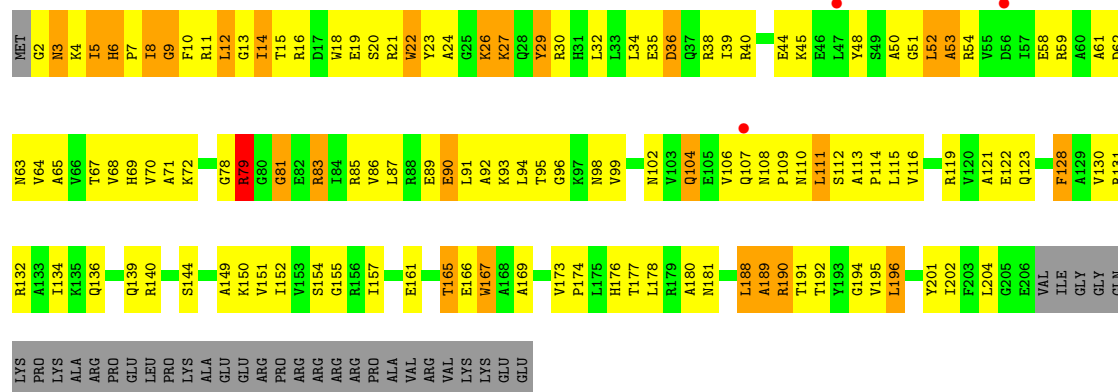


• Molecule 32: 30S RIBOSOMAL PROTEIN S2

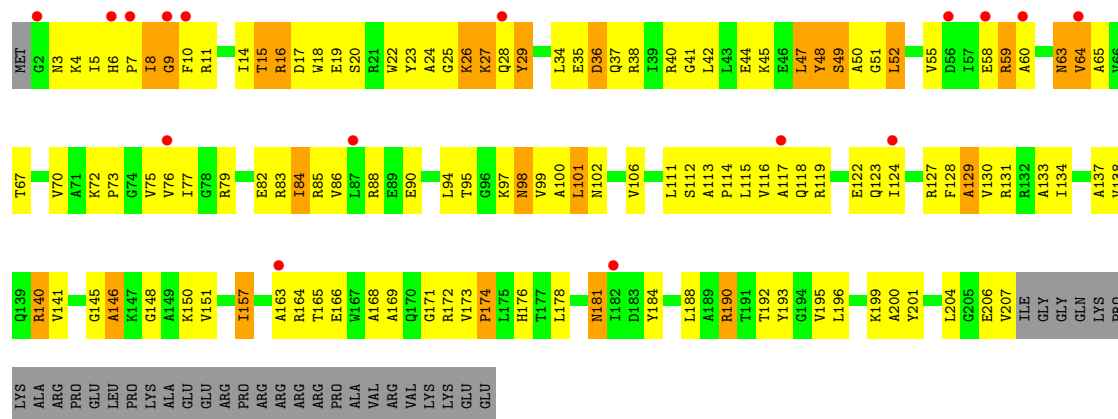




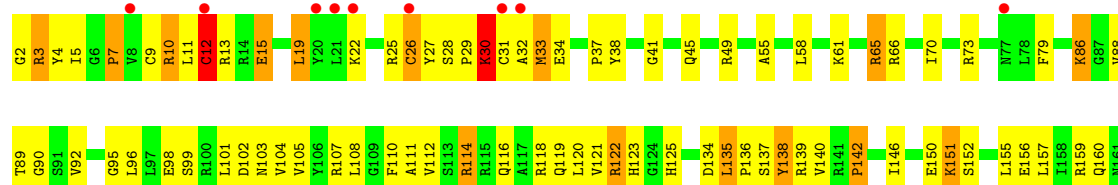
• Molecule 33: 30S RIBOSOMAL PROTEIN S3



• Molecule 33: 30S RIBOSOMAL PROTEIN S3

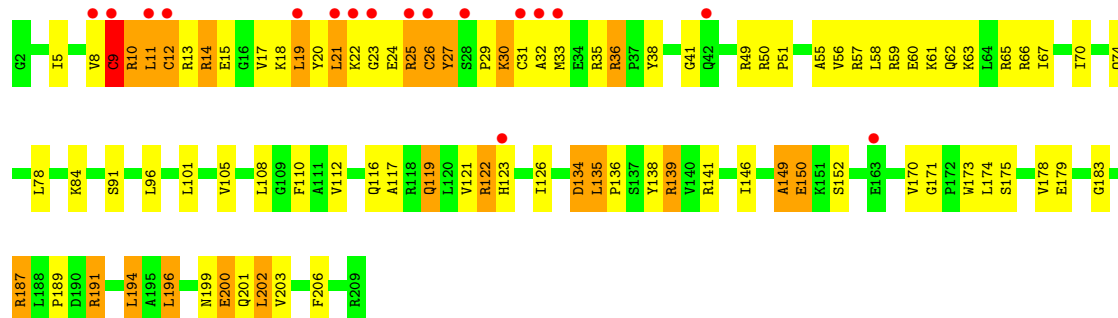


• Molecule 34: 30S RIBOSOMAL PROTEIN S4

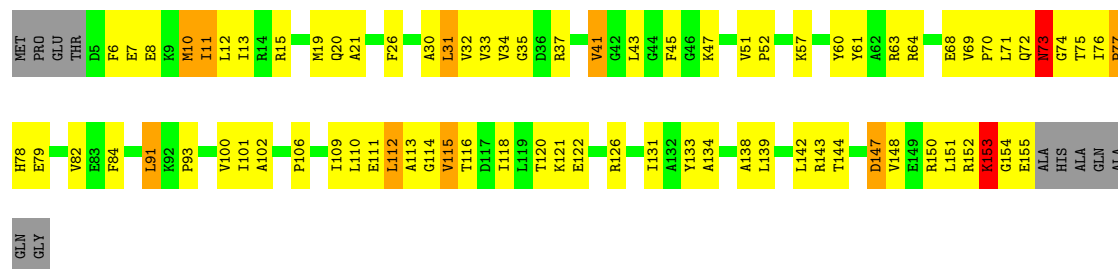




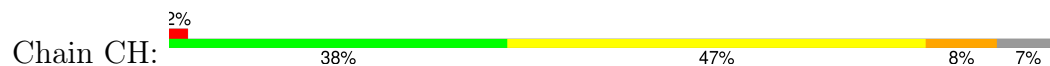
• Molecule 34: 30S RIBOSOMAL PROTEIN S4



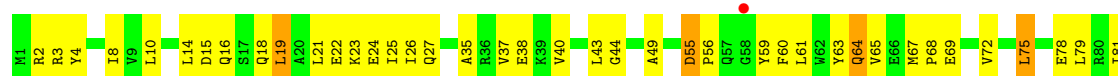
• Molecule 35: 30S RIBOSOMAL PROTEIN S5

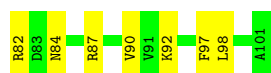


• Molecule 35: 30S RIBOSOMAL PROTEIN S5

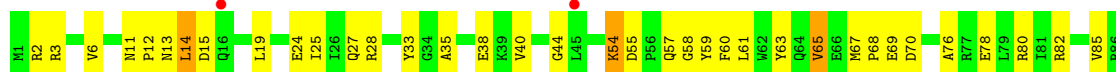


• Molecule 36: 30S RIBOSOMAL PROTEIN S6

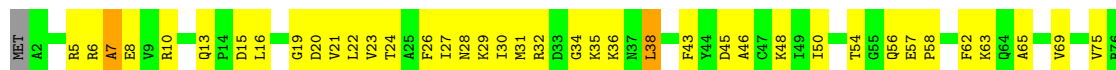




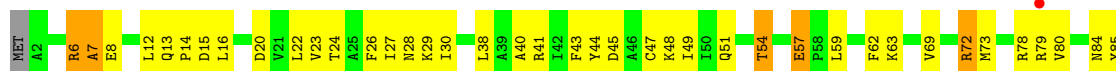
• Molecule 36: 30S RIBOSOMAL PROTEIN S6



• Molecule 37: 30S RIBOSOMAL PROTEIN S7



• Molecule 37: 30S RIBOSOMAL PROTEIN S7

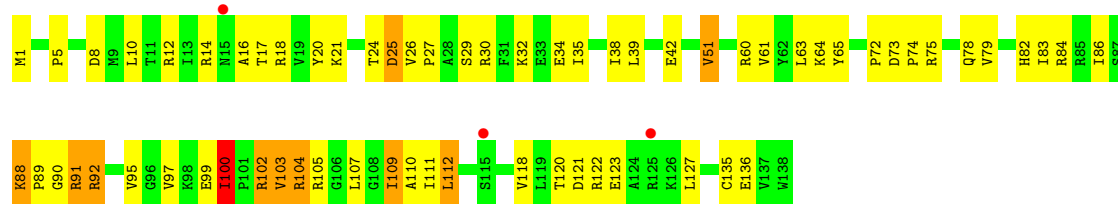


• Molecule 38: 30S RIBOSOMAL PROTEIN S8

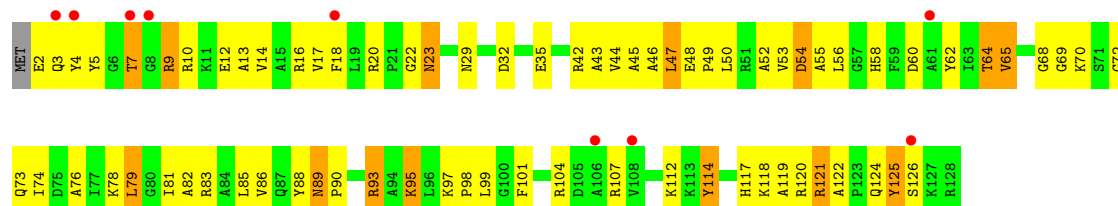


• Molecule 38: 30S RIBOSOMAL PROTEIN S8

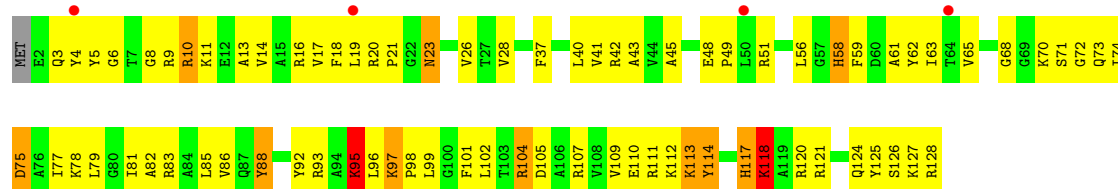




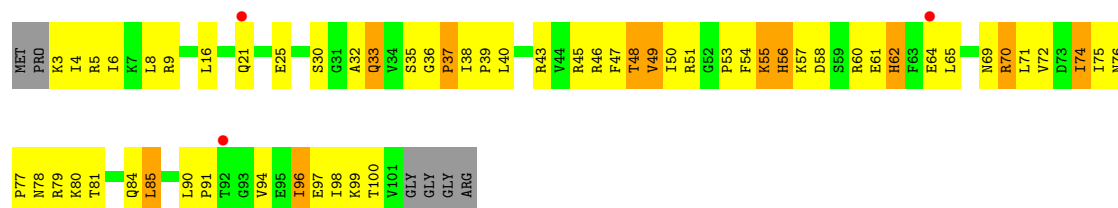
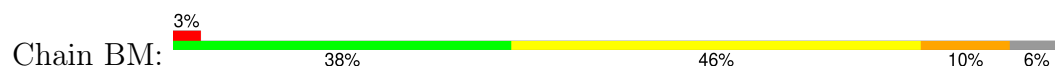
• Molecule 39: 30S RIBOSOMAL PROTEIN S9



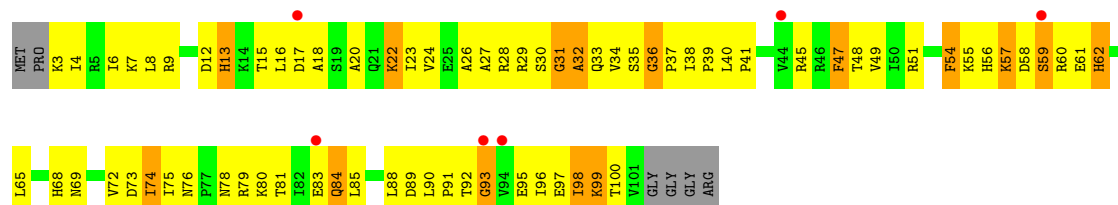
• Molecule 39: 30S RIBOSOMAL PROTEIN S9



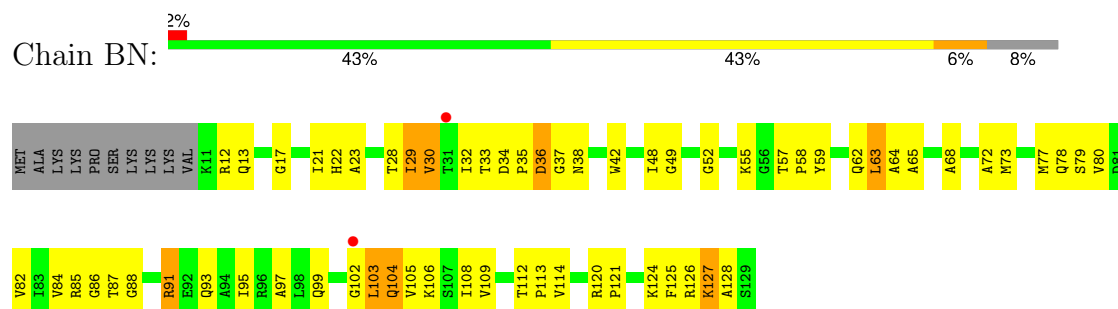
• Molecule 40: 30S RIBOSOMAL PROTEIN S10



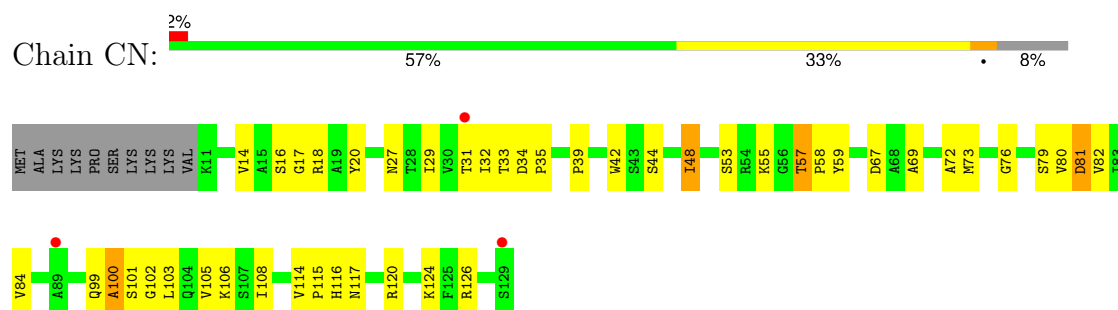
• Molecule 40: 30S RIBOSOMAL PROTEIN S10



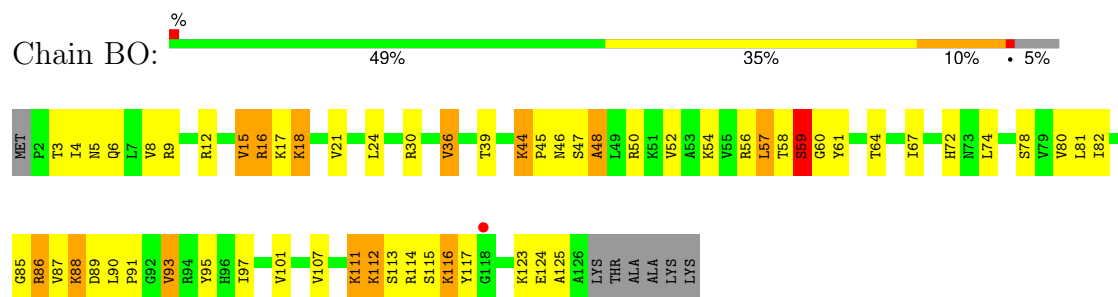
- Molecule 41: 30S RIBOSOMAL PROTEIN S11



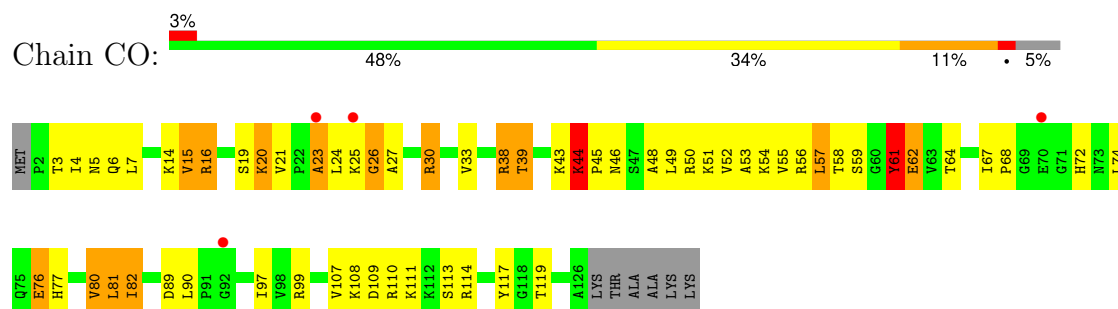
- Molecule 41: 30S RIBOSOMAL PROTEIN S11



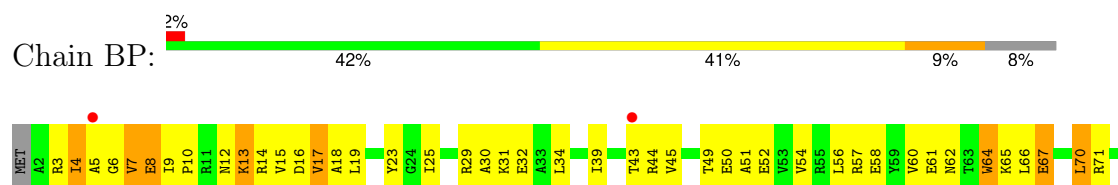
- Molecule 42: 30S RIBOSOMAL PROTEIN S12

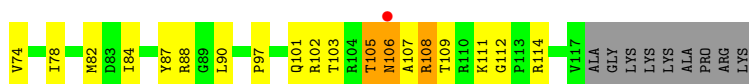


- Molecule 42: 30S RIBOSOMAL PROTEIN S12



- Molecule 43: 30S RIBOSOMAL PROTEIN S13

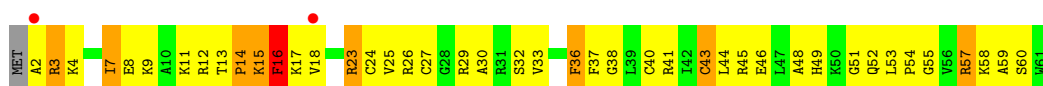




• Molecule 43: 30S RIBOSOMAL PROTEIN S13



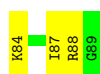
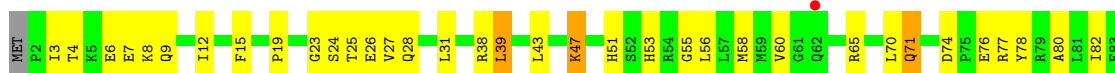
• Molecule 44: 30S RIBOSOMAL PROTEIN S14



• Molecule 44: 30S RIBOSOMAL PROTEIN S14



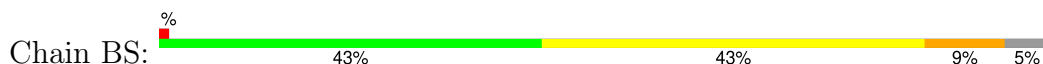
• Molecule 45: 30S RIBOSOMAL PROTEIN S15

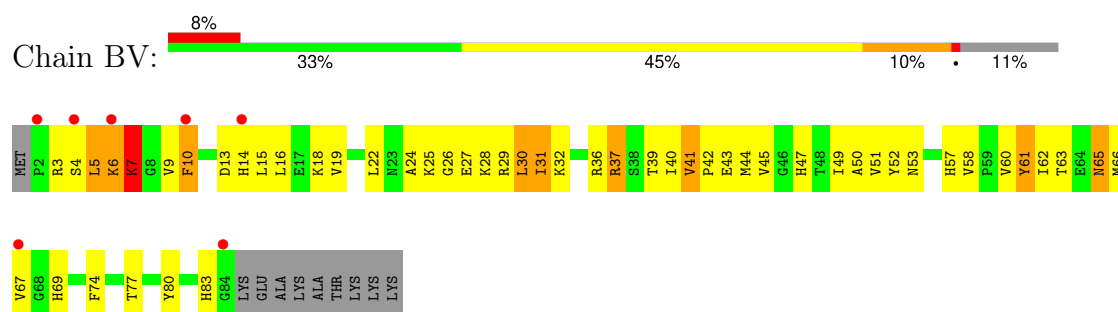


• Molecule 45: 30S RIBOSOMAL PROTEIN S15

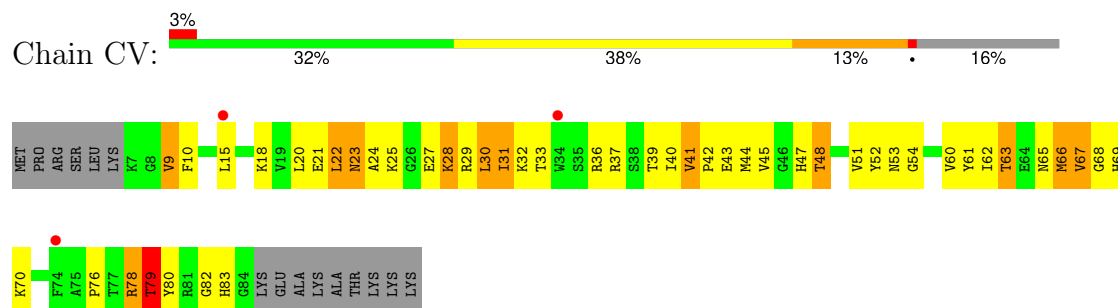


• Molecule 46: 30S RIBOSOMAL PROTEIN S16

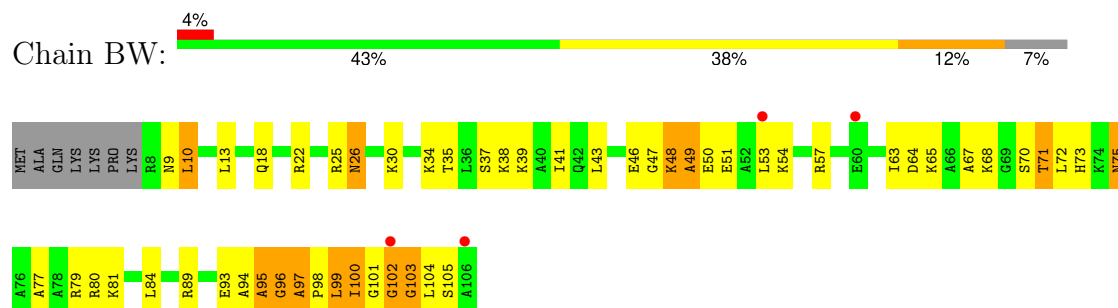




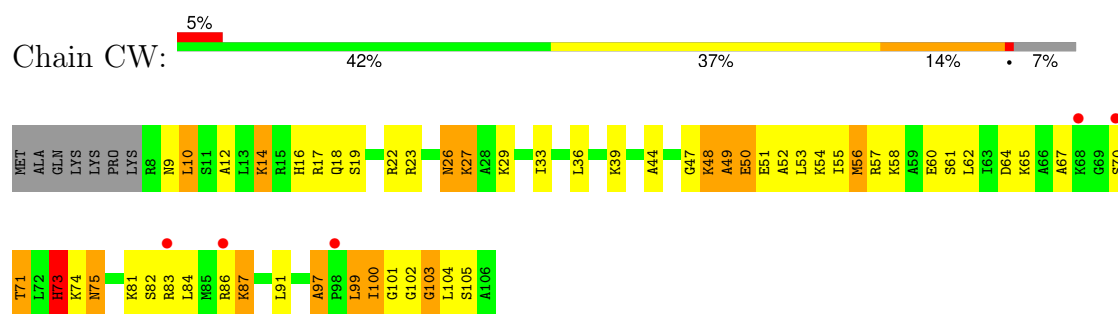
• Molecule 49: 30S RIBOSOMAL PROTEIN S19



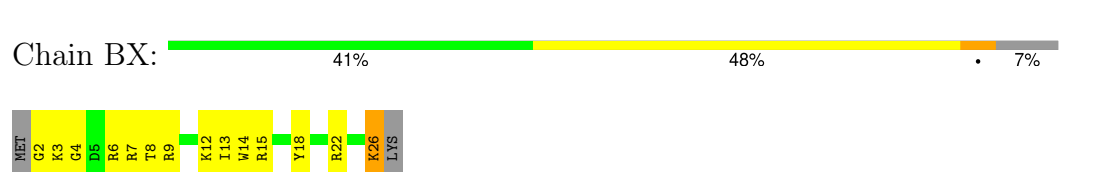
• Molecule 50: 30S RIBOSOMAL PROTEIN S20



• Molecule 50: 30S RIBOSOMAL PROTEIN S20



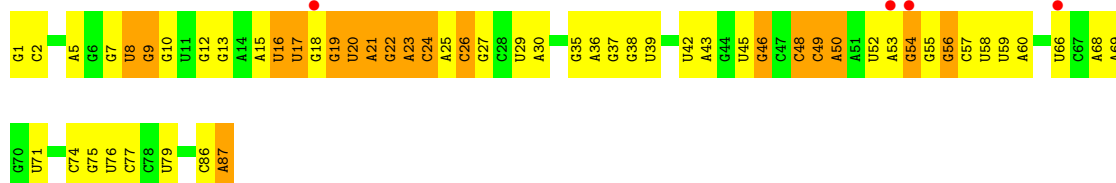
• Molecule 51: 30S RIBOSOMAL PROTEIN THX



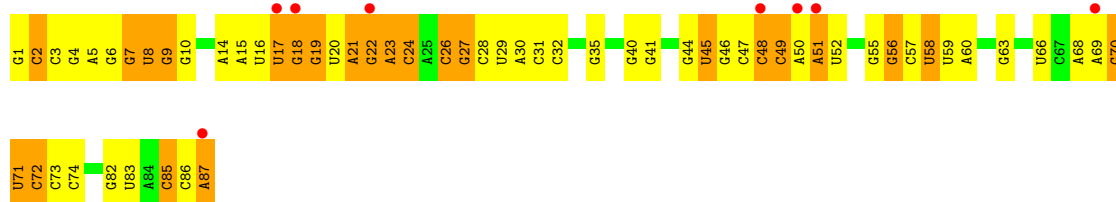
• Molecule 51: 30S RIBOSOMAL PROTEIN THX



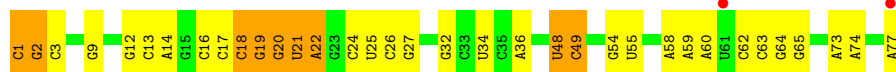
● Molecule 52: TRNA-LEU



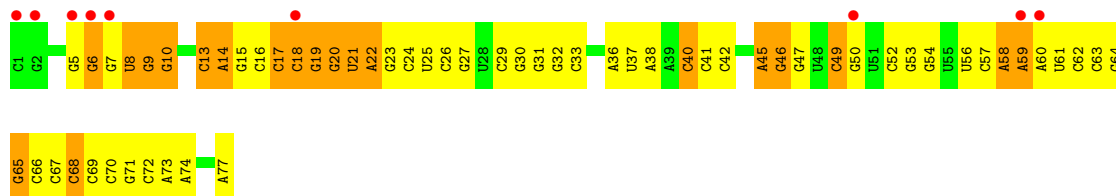
● Molecule 52: TRNA-LEU



● Molecule 53: TRNA-FMET

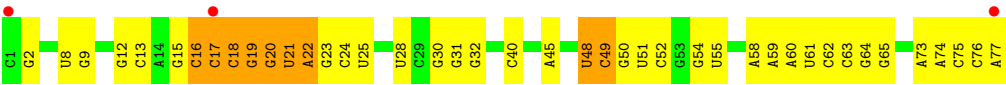


● Molecule 53: TRNA-FMET

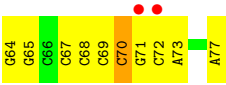
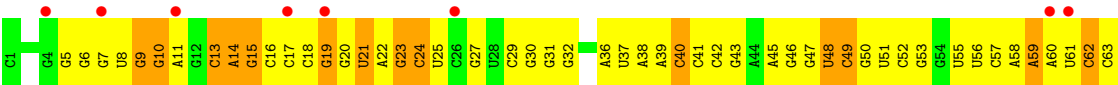


● Molecule 53: TRNA-FMET





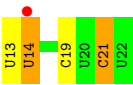
● Molecule 53: TRNA-FMET



● Molecule 54: MRNA



● Molecule 54: MRNA



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.19Å 451.05Å 621.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	153.76 – 3.10 153.76 – 3.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (153.76-3.10) 93.2 (153.76-3.10)	Depositor EDS
R_{merge}	0.33	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.90 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_810)	Depositor
R, R_{free}	0.201 , 0.240 0.202 , 0.237	Depositor DCC
R_{free} test set	1814 reflections (0.17%)	wwPDB-VP
Wilson B-factor (Å ²)	76.3	Xtriage
Anisotropy	0.156	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 99.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	299628	wwPDB-VP
Average B, all atoms (Å ²)	104.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.45% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	AA	0.37	0/70233	0.74	48/109643 (0.0%)
1	DA	0.33	1/70122 (0.0%)	0.71	58/109469 (0.1%)
2	AB	0.31	0/2928	0.72	6/4568 (0.1%)
2	DB	0.27	0/2928	0.71	2/4568 (0.0%)
3	AD	0.31	0/2166	0.55	0/2919
3	DD	0.29	0/2165	0.52	0/2919
4	AE	0.27	0/1602	0.53	0/2160
4	DE	0.27	0/1601	0.54	0/2160
5	AF	0.31	1/1621 (0.1%)	0.50	0/2196
5	DF	0.25	0/1662	0.50	0/2249
6	AG	0.24	0/1499	0.42	0/2016
6	DG	0.22	0/1499	0.41	0/2016
7	AH	0.25	0/1333	0.50	0/1802
7	DH	0.21	0/1332	0.48	0/1802
8	AK	0.24	0/1152	0.49	0/1558
8	DK	0.23	0/1151	0.49	0/1558
9	AM	0.26	0/1132	0.47	0/1525
9	DM	0.23	0/1131	0.45	0/1525
10	AN	0.27	0/943	0.46	0/1269
10	DN	0.26	0/943	0.46	0/1269
11	AO	0.29	0/1162	0.57	0/1544
11	DO	0.26	0/1162	0.56	0/1544
12	AP	0.26	0/1143	0.41	0/1527
12	DP	0.58	1/1143 (0.1%)	0.40	0/1527
13	A0	0.26	0/982	0.50	0/1312
13	D0	0.25	0/974	0.45	0/1302
14	AQ	0.27	0/892	0.53	0/1187
14	DQ	0.23	0/892	0.46	0/1187
15	AR	0.28	0/1156	0.51	0/1542
15	DR	0.26	0/1155	0.45	0/1542
16	A1	0.29	0/982	0.48	0/1306
16	D1	0.24	0/982	0.43	0/1306

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	A2	0.27	0/790	0.52	0/1057
17	D2	0.28	0/790	0.51	0/1057
18	AS	0.26	0/911	0.48	0/1220
18	DS	0.26	0/911	0.46	0/1220
19	AT	0.32	0/740	0.48	0/993
19	DT	0.31	0/739	0.46	0/993
20	AU	0.30	0/799	0.52	0/1064
20	DU	0.27	0/798	0.49	0/1064
21	AV	0.22	0/1427	0.48	0/1935
21	DV	0.21	0/1460	0.43	0/1982
22	A3	0.29	0/615	0.49	0/819
22	D3	0.26	0/621	0.43	0/827
23	AZ	0.28	0/770	0.52	0/1022
23	DZ	0.27	0/770	0.49	0/1022
24	AW	0.30	0/560	0.54	0/741
24	DW	0.25	0/583	0.48	0/771
25	AX	0.25	0/474	0.44	0/635
25	DX	0.22	0/474	0.42	0/635
26	A4	0.24	0/545	0.48	0/733
26	D4	0.24	0/527	0.48	0/709
27	A5	0.29	0/473	0.55	0/639
27	D5	0.27	0/473	0.57	0/639
28	A6	0.28	0/397	0.52	0/529
28	D6	0.25	0/396	0.51	0/529
29	A7	0.31	0/438	0.44	0/575
29	D7	0.26	0/438	0.43	0/575
30	A8	0.33	0/494	0.60	0/649
30	D8	0.34	0/494	0.68	0/649
31	BA	0.28	0/36234	0.65	19/56554 (0.0%)
31	CA	0.28	0/36237	0.65	15/56558 (0.0%)
32	BE	0.22	0/1959	0.42	0/2642
32	CE	0.22	0/1959	0.43	0/2642
33	BF	0.22	0/1629	0.41	0/2195
33	CF	0.21	0/1636	0.40	0/2205
34	BG	0.28	0/1733	0.45	0/2318
34	CG	0.26	0/1733	0.45	0/2318
35	BH	0.24	0/1171	0.44	0/1576
35	CH	0.24	0/1171	0.44	0/1576
36	BI	0.23	0/856	0.43	0/1154
36	CI	0.24	0/856	0.43	0/1154
37	BJ	0.22	0/1276	0.39	0/1709
37	CJ	0.22	0/1276	0.38	0/1709
38	BK	0.23	0/1136	0.44	0/1527

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	CK	0.22	0/1136	0.43	0/1527
39	BL	0.22	0/1029	0.42	0/1379
39	CL	0.22	0/1029	0.41	0/1379
40	BM	0.22	0/814	0.45	0/1095
40	CM	0.21	0/814	0.43	0/1095
41	BN	0.24	0/900	0.45	0/1213
41	CN	0.23	0/900	0.42	0/1213
42	BO	0.27	0/991	0.49	0/1327
42	CO	0.25	0/991	0.46	0/1327
43	BP	0.22	0/938	0.44	0/1258
43	CP	0.21	0/943	0.43	0/1265
44	BQ	0.26	0/501	0.49	0/664
44	CQ	0.23	0/501	0.43	0/664
45	BR	0.24	0/745	0.41	0/992
45	CR	0.23	0/745	0.40	0/992
46	BS	0.22	0/721	0.43	0/970
46	CS	0.24	0/721	0.43	0/970
47	BT	0.24	0/847	0.43	0/1131
47	CT	0.24	0/847	0.42	0/1131
48	BU	0.24	0/596	0.44	0/790
48	CU	0.24	0/596	0.43	0/790
49	BV	0.23	0/680	0.47	0/915
49	CV	0.22	0/638	0.44	0/860
50	BW	0.22	0/765	0.43	0/1007
50	CW	0.24	0/765	0.45	0/1007
51	BX	0.22	0/221	0.40	0/288
51	CX	0.21	0/221	0.41	0/288
52	BB	0.21	0/2080	0.51	0/3242
52	CB	0.20	0/2080	0.49	0/3242
53	BC	0.25	0/1835	0.56	0/2859
53	BD	0.16	0/1835	0.46	0/2859
53	CC	0.24	0/1835	0.57	0/2859
53	CD	0.16	0/1835	0.47	0/2859
54	B1	0.27	0/226	0.50	0/348
54	C1	0.37	0/226	0.73	1/348 (0.3%)
All	All	0.30	3/324084 (0.0%)	0.64	149/485290 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
7	AH	0	1
42	BO	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	DP	141	GLN	C-OXT	17.97	1.57	1.23
1	DA	1342	A	N7-C5	-5.40	1.36	1.39
5	AF	207	GLY	C-N	-5.12	1.23	1.33

The worst 5 of 149 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	DA	933	A	C4-N9-C1'	10.03	144.35	126.30
1	DA	933	A	C6-C5-N7	-10.02	125.28	132.30
1	AA	673	C	C2-N3-C4	-9.52	115.14	119.90
1	DA	933	A	C8-N9-C1'	-9.44	110.72	127.70
31	BA	1025	U	C5-C4-O4	-9.10	120.44	125.90

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	AH	153	LYS	Peptide
42	BO	44	LYS	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	62707	0	31614	1928	1
1	DA	62607	0	31565	1969	1
2	AB	2617	0	1328	93	0
2	DB	2617	0	1328	98	0
3	AD	2116	0	2195	197	0
3	DD	2115	0	2195	178	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	AE	1569	0	1634	163	0
4	DE	1568	0	1634	175	0
5	AF	1586	0	1632	111	0
5	DF	1627	0	1680	126	0
6	AG	1474	0	1535	127	0
6	DG	1474	0	1535	99	0
7	AH	1308	0	1382	143	0
7	DH	1307	0	1382	102	1
8	AK	1137	0	1223	93	0
8	DK	1136	0	1223	92	0
9	AM	1105	0	1180	98	0
9	DM	1104	0	1180	84	0
10	AN	933	0	996	40	0
10	DN	933	0	996	38	0
11	AO	1145	0	1228	157	0
11	DO	1145	0	1228	169	0
12	AP	1122	0	1179	184	0
12	DP	1122	0	1179	204	0
13	A0	968	0	1033	63	0
13	D0	960	0	1021	69	0
14	AQ	882	0	943	85	0
14	DQ	882	0	943	73	0
15	AR	1142	0	1202	92	0
15	DR	1141	0	1202	96	0
16	A1	964	0	1022	76	0
16	D1	964	0	1022	88	0
17	A2	779	0	852	75	0
17	D2	779	0	852	117	0
18	AS	900	0	964	61	0
18	DS	900	0	964	41	0
19	AT	726	0	778	52	0
19	DT	725	0	778	56	0
20	AU	786	0	878	77	0
20	DU	785	0	878	97	0
21	AV	1397	0	1430	120	0
21	DV	1428	0	1454	100	0
22	A3	607	0	628	41	0
22	D3	613	0	633	45	0
23	AZ	763	0	848	40	0
23	DZ	763	0	848	50	0
24	AW	558	0	610	29	0
24	DW	581	0	629	49	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	AX	469	0	518	21	0
25	DX	469	0	518	22	0
26	A4	533	0	522	79	0
26	D4	515	0	510	83	0
27	A5	459	0	480	53	0
27	D5	459	0	480	43	0
28	A6	390	0	404	64	0
28	D6	389	0	404	50	0
29	A7	430	0	480	19	0
29	D7	430	0	480	28	0
30	A8	488	0	560	80	0
30	D8	488	0	560	86	0
31	BA	32369	0	16339	1082	1
31	CA	32372	0	16338	1075	2
32	BE	1924	0	1975	154	0
32	CE	1924	0	1975	162	0
33	BF	1605	0	1668	114	0
33	CF	1612	0	1677	115	0
34	BG	1703	0	1764	120	0
34	CG	1703	0	1763	94	1
35	BH	1155	0	1213	64	0
35	CH	1155	0	1213	75	0
36	BI	843	0	857	41	1
36	CI	843	0	857	38	0
37	BJ	1257	0	1296	65	0
37	CJ	1257	0	1296	62	0
38	BK	1116	0	1177	68	0
38	CK	1116	0	1177	50	0
39	BL	1010	0	1037	84	0
39	CL	1010	0	1037	96	0
40	BM	801	0	849	74	0
40	CM	801	0	849	70	0
41	BN	885	0	904	57	0
41	CN	885	0	904	34	0
42	BO	975	0	1062	52	0
42	CO	975	0	1062	67	0
43	BP	928	0	987	62	0
43	CP	933	0	992	71	0
44	BQ	492	0	529	46	0
44	CQ	492	0	530	38	0
45	BR	734	0	771	34	0
45	CR	734	0	771	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
46	BS	705	0	725	41	0
46	CS	705	0	725	32	0
47	BT	834	0	904	47	0
47	CT	834	0	904	31	0
48	BU	591	0	662	24	0
48	CU	591	0	662	18	0
49	BV	665	0	686	66	0
49	CV	624	0	636	65	0
50	BW	763	0	861	56	0
50	CW	763	0	861	47	0
51	BX	217	0	234	16	0
51	CX	217	0	234	20	0
52	BB	1861	0	938	50	0
52	CB	1861	0	938	62	0
53	BC	1643	0	837	48	0
53	BD	1643	0	837	65	0
53	CC	1643	0	837	50	0
53	CD	1643	0	837	79	0
54	B1	205	0	105	7	0
54	C1	205	0	105	5	0
55	A0	1	0	0	0	0
55	A1	1	0	0	0	0
55	A2	1	0	0	0	0
55	A3	1	0	0	0	0
55	A5	2	0	0	0	0
55	A6	1	0	0	0	0
55	A7	1	0	0	0	0
55	AA	630	0	0	0	0
55	AB	17	0	0	0	0
55	AD	2	0	0	0	0
55	AE	4	0	0	0	0
55	AF	3	0	0	0	0
55	AO	3	0	0	0	0
55	AU	1	0	0	0	0
55	B1	2	0	0	0	0
55	BA	244	0	0	0	0
55	BB	8	0	0	0	0
55	BC	9	0	0	0	0
55	BD	1	0	0	0	0
55	BG	1	0	0	0	0
55	BN	2	0	0	0	0
55	BQ	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	CA	209	0	0	0	0
55	CB	5	0	0	0	0
55	CC	8	0	0	0	0
55	CG	3	0	0	0	0
55	CH	1	0	0	0	0
55	CS	1	0	0	0	0
55	D0	1	0	0	0	0
55	D1	2	0	0	0	0
55	D3	1	0	0	0	0
55	D5	1	0	0	0	0
55	DA	528	0	0	0	0
55	DB	14	0	0	0	0
55	DE	3	0	0	0	0
55	DP	1	0	0	0	0
55	DU	1	0	0	0	0
56	BG	1	0	0	0	0
56	BQ	1	0	0	0	0
56	CG	1	0	0	0	0
56	CQ	1	0	0	0	0
All	All	299628	0	200976	12579	4

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 25.

The worst 5 of 12579 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)
6:AG:108:ASN:HA	26:A4:38:LYS:CG	1.41	1.51
6:AG:108:ASN:CA	26:A4:38:LYS:HG2	1.46	1.45
1:AA:1056:G:H21	1:AA:1103:A:N6	1.13	1.45
1:DA:226:G:H21	1:DA:228:A:N6	0.93	1.41
1:DA:226:G:N2	1:DA:228:A:H61	1.15	1.40

All (4) 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)
31:BA:85:U:O2'	7:DH:100:GLY:O[3_555]	1.87	0.33
1:AA:2137:C:OP1	31:CA:999:U:O2'[4_555]	1.89	0.31
36:BI:15:ASP:OD2	34:CG:27:TYR:OH[4_555]	2.05	0.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:CA:86:U:O2'	1:DA:276:A:OP2[3_545]	2.15	0.05

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	
3	AD	270/272 (99%)	226 (84%)	31 (12%)	13 (5%)	2	11
3	DD	270/272 (99%)	231 (86%)	25 (9%)	14 (5%)	1	10
4	AE	203/205 (99%)	152 (75%)	33 (16%)	18 (9%)	0	3
4	DE	203/205 (99%)	128 (63%)	41 (20%)	34 (17%)	0	0
5	AF	201/208 (97%)	177 (88%)	13 (6%)	11 (6%)	1	9
5	DF	206/208 (99%)	162 (79%)	25 (12%)	19 (9%)	0	3
6	AG	179/181 (99%)	147 (82%)	21 (12%)	11 (6%)	1	7
6	DG	179/181 (99%)	141 (79%)	27 (15%)	11 (6%)	1	7
7	AH	168/170 (99%)	116 (69%)	22 (13%)	30 (18%)	0	0
7	DH	168/170 (99%)	108 (64%)	37 (22%)	23 (14%)	0	1
8	AK	144/146 (99%)	97 (67%)	27 (19%)	20 (14%)	0	1
8	DK	144/146 (99%)	106 (74%)	26 (18%)	12 (8%)	0	4
9	AM	136/138 (99%)	105 (77%)	18 (13%)	13 (10%)	0	3
9	DM	136/138 (99%)	108 (79%)	20 (15%)	8 (6%)	1	8
10	AN	120/122 (98%)	111 (92%)	7 (6%)	2 (2%)	7	30
10	DN	120/122 (98%)	108 (90%)	11 (9%)	1 (1%)	16	48
11	AO	148/150 (99%)	106 (72%)	25 (17%)	17 (12%)	0	1
11	DO	148/150 (99%)	92 (62%)	28 (19%)	28 (19%)	0	0
12	AP	139/141 (99%)	95 (68%)	25 (18%)	19 (14%)	0	1
12	DP	139/141 (99%)	91 (66%)	20 (14%)	28 (20%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	A0	116/118 (98%)	93 (80%)	15 (13%)	8 (7%)	1	5
13	D0	115/118 (98%)	93 (81%)	17 (15%)	5 (4%)	2	13
14	AQ	109/111 (98%)	77 (71%)	24 (22%)	8 (7%)	1	5
14	DQ	109/111 (98%)	78 (72%)	21 (19%)	10 (9%)	0	3
15	AR	135/137 (98%)	100 (74%)	25 (18%)	10 (7%)	1	5
15	DR	135/137 (98%)	103 (76%)	23 (17%)	9 (7%)	1	6
16	A1	115/117 (98%)	101 (88%)	7 (6%)	7 (6%)	1	7
16	D1	115/117 (98%)	93 (81%)	15 (13%)	7 (6%)	1	7
17	A2	99/101 (98%)	83 (84%)	9 (9%)	7 (7%)	1	5
17	D2	99/101 (98%)	73 (74%)	14 (14%)	12 (12%)	0	1
18	AS	111/113 (98%)	92 (83%)	14 (13%)	5 (4%)	2	12
18	DS	111/113 (98%)	99 (89%)	10 (9%)	2 (2%)	7	29
19	AT	90/92 (98%)	83 (92%)	6 (7%)	1 (1%)	12	39
19	DT	90/92 (98%)	75 (83%)	12 (13%)	3 (3%)	3	17
20	AU	100/102 (98%)	68 (68%)	19 (19%)	13 (13%)	0	1
20	DU	100/102 (98%)	61 (61%)	22 (22%)	17 (17%)	0	0
21	AV	173/179 (97%)	112 (65%)	36 (21%)	25 (14%)	0	0
21	DV	177/179 (99%)	120 (68%)	27 (15%)	30 (17%)	0	0
22	A3	74/77 (96%)	57 (77%)	15 (20%)	2 (3%)	4	21
22	D3	75/77 (97%)	62 (83%)	13 (17%)	0	100	100
23	AZ	95/97 (98%)	78 (82%)	10 (10%)	7 (7%)	1	5
23	DZ	95/97 (98%)	77 (81%)	7 (7%)	11 (12%)	0	1
24	AW	64/69 (93%)	56 (88%)	3 (5%)	5 (8%)	1	4
24	DW	67/69 (97%)	56 (84%)	5 (8%)	6 (9%)	0	3
25	AX	57/59 (97%)	49 (86%)	8 (14%)	0	100	100
25	DX	57/59 (97%)	51 (90%)	5 (9%)	1 (2%)	7	29
26	A4	64/66 (97%)	38 (59%)	16 (25%)	10 (16%)	0	0
26	D4	61/66 (92%)	24 (39%)	25 (41%)	12 (20%)	0	0
27	A5	57/59 (97%)	40 (70%)	10 (18%)	7 (12%)	0	1
27	D5	57/59 (97%)	46 (81%)	7 (12%)	4 (7%)	1	5
28	A6	43/45 (96%)	25 (58%)	12 (28%)	6 (14%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	D6	43/45 (96%)	25 (58%)	12 (28%)	6 (14%)	0	1
29	A7	47/49 (96%)	43 (92%)	3 (6%)	1 (2%)	5	25
29	D7	47/49 (96%)	46 (98%)	1 (2%)	0	100	100
30	A8	59/61 (97%)	50 (85%)	5 (8%)	4 (7%)	1	6
30	D8	59/61 (97%)	39 (66%)	11 (19%)	9 (15%)	0	0
32	BE	235/256 (92%)	170 (72%)	47 (20%)	18 (8%)	1	4
32	CE	235/256 (92%)	188 (80%)	23 (10%)	24 (10%)	0	3
33	BF	203/239 (85%)	141 (70%)	46 (23%)	16 (8%)	1	4
33	CF	204/239 (85%)	152 (74%)	37 (18%)	15 (7%)	1	5
34	BG	206/208 (99%)	168 (82%)	27 (13%)	11 (5%)	1	10
34	CG	206/208 (99%)	171 (83%)	30 (15%)	5 (2%)	5	22
35	BH	149/162 (92%)	129 (87%)	14 (9%)	6 (4%)	2	14
35	CH	149/162 (92%)	134 (90%)	11 (7%)	4 (3%)	4	21
36	BI	99/101 (98%)	93 (94%)	4 (4%)	2 (2%)	6	26
36	CI	99/101 (98%)	94 (95%)	4 (4%)	1 (1%)	13	42
37	BJ	153/156 (98%)	137 (90%)	15 (10%)	1 (1%)	19	51
37	CJ	153/156 (98%)	137 (90%)	13 (8%)	3 (2%)	6	26
38	BK	136/138 (99%)	115 (85%)	14 (10%)	7 (5%)	1	10
38	CK	136/138 (99%)	122 (90%)	11 (8%)	3 (2%)	5	24
39	BL	125/128 (98%)	100 (80%)	22 (18%)	3 (2%)	5	22
39	CL	125/128 (98%)	102 (82%)	19 (15%)	4 (3%)	3	18
40	BM	97/105 (92%)	76 (78%)	19 (20%)	2 (2%)	5	25
40	CM	97/105 (92%)	75 (77%)	13 (13%)	9 (9%)	0	3
41	BN	117/129 (91%)	97 (83%)	15 (13%)	5 (4%)	2	13
41	CN	117/129 (91%)	100 (86%)	14 (12%)	3 (3%)	4	21
42	BO	123/132 (93%)	101 (82%)	13 (11%)	9 (7%)	1	5
42	CO	123/132 (93%)	96 (78%)	19 (15%)	8 (6%)	1	6
43	BP	114/126 (90%)	86 (75%)	20 (18%)	8 (7%)	1	5
43	CP	115/126 (91%)	83 (72%)	22 (19%)	10 (9%)	0	4
44	BQ	58/61 (95%)	42 (72%)	11 (19%)	5 (9%)	0	4
44	CQ	58/61 (95%)	41 (71%)	11 (19%)	6 (10%)	0	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
45	BR	86/89 (97%)	75 (87%)	9 (10%)	2 (2%)	5	23
45	CR	86/89 (97%)	76 (88%)	9 (10%)	1 (1%)	11	38
46	BS	82/88 (93%)	65 (79%)	14 (17%)	3 (4%)	2	16
46	CS	82/88 (93%)	69 (84%)	13 (16%)	0	100	100
47	BT	98/105 (93%)	85 (87%)	11 (11%)	2 (2%)	6	26
47	CT	98/105 (93%)	92 (94%)	4 (4%)	2 (2%)	6	26
48	BU	70/88 (80%)	60 (86%)	8 (11%)	2 (3%)	3	20
48	CU	70/88 (80%)	63 (90%)	7 (10%)	0	100	100
49	BV	81/93 (87%)	63 (78%)	11 (14%)	7 (9%)	0	4
49	CV	76/93 (82%)	53 (70%)	16 (21%)	7 (9%)	0	3
50	BW	97/106 (92%)	75 (77%)	12 (12%)	10 (10%)	0	3
50	CW	97/106 (92%)	73 (75%)	13 (13%)	11 (11%)	0	2
51	BX	23/27 (85%)	19 (83%)	3 (13%)	1 (4%)	2	13
51	CX	23/27 (85%)	19 (83%)	0	4 (17%)	0	0
All	All	11342/11844 (96%)	8910 (79%)	1590 (14%)	842 (7%)	1	5

5 of 842 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	AD	26	LYS
3	AD	28	GLU
3	AD	33	LEU
3	AD	122	ASP
3	AD	237	GLU

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	
3	AD	214/214 (100%)	182 (85%)	32 (15%)	2	10
3	DD	214/214 (100%)	179 (84%)	35 (16%)	2	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	AE	165/165 (100%)	133 (81%)	32 (19%)	1	5
4	DE	165/165 (100%)	138 (84%)	27 (16%)	2	8
5	AF	161/165 (98%)	139 (86%)	22 (14%)	3	13
5	DF	165/165 (100%)	142 (86%)	23 (14%)	3	12
6	AG	155/155 (100%)	134 (86%)	21 (14%)	3	13
6	DG	155/155 (100%)	135 (87%)	20 (13%)	3	15
7	AH	142/142 (100%)	118 (83%)	24 (17%)	1	7
7	DH	142/142 (100%)	130 (92%)	12 (8%)	8	32
8	AK	122/122 (100%)	106 (87%)	16 (13%)	3	14
8	DK	122/122 (100%)	103 (84%)	19 (16%)	2	9
9	AM	117/117 (100%)	99 (85%)	18 (15%)	2	9
9	DM	117/117 (100%)	98 (84%)	19 (16%)	2	8
10	AN	100/100 (100%)	91 (91%)	9 (9%)	8	29
10	DN	100/100 (100%)	89 (89%)	11 (11%)	5	21
11	AO	116/116 (100%)	87 (75%)	29 (25%)	0	1
11	DO	116/116 (100%)	84 (72%)	32 (28%)	0	1
12	AP	111/111 (100%)	87 (78%)	24 (22%)	1	4
12	DP	111/111 (100%)	85 (77%)	26 (23%)	0	2
13	A0	101/101 (100%)	82 (81%)	19 (19%)	1	5
13	D0	100/101 (99%)	85 (85%)	15 (15%)	2	10
14	AQ	87/87 (100%)	68 (78%)	19 (22%)	1	3
14	DQ	87/87 (100%)	76 (87%)	11 (13%)	3	15
15	AR	120/120 (100%)	100 (83%)	20 (17%)	2	7
15	DR	120/120 (100%)	91 (76%)	29 (24%)	0	2
16	A1	93/93 (100%)	82 (88%)	11 (12%)	4	17
16	D1	93/93 (100%)	88 (95%)	5 (5%)	18	47
17	A2	82/82 (100%)	71 (87%)	11 (13%)	3	13
17	D2	82/82 (100%)	68 (83%)	14 (17%)	1	7
18	AS	92/92 (100%)	74 (80%)	18 (20%)	1	5
18	DS	92/92 (100%)	77 (84%)	15 (16%)	2	8
19	AT	74/74 (100%)	62 (84%)	12 (16%)	2	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	DT	74/74 (100%)	63 (85%)	11 (15%)	2	10
20	AU	85/85 (100%)	70 (82%)	15 (18%)	1	7
20	DU	85/85 (100%)	67 (79%)	18 (21%)	1	4
21	AV	154/158 (98%)	130 (84%)	24 (16%)	2	9
21	DV	158/158 (100%)	146 (92%)	12 (8%)	11	36
22	A3	61/62 (98%)	57 (93%)	4 (7%)	14	41
22	D3	62/62 (100%)	58 (94%)	4 (6%)	14	41
23	AZ	82/82 (100%)	72 (88%)	10 (12%)	4	16
23	DZ	82/82 (100%)	71 (87%)	11 (13%)	3	13
24	AW	62/64 (97%)	50 (81%)	12 (19%)	1	5
24	DW	64/64 (100%)	56 (88%)	8 (12%)	3	15
25	AX	51/51 (100%)	46 (90%)	5 (10%)	6	25
25	DX	51/51 (100%)	48 (94%)	3 (6%)	16	44
26	A4	59/59 (100%)	49 (83%)	10 (17%)	1	7
26	D4	57/59 (97%)	50 (88%)	7 (12%)	4	16
27	A5	51/51 (100%)	39 (76%)	12 (24%)	0	2
27	D5	51/51 (100%)	41 (80%)	10 (20%)	1	5
28	A6	44/44 (100%)	37 (84%)	7 (16%)	2	9
28	D6	44/44 (100%)	34 (77%)	10 (23%)	0	3
29	A7	42/42 (100%)	35 (83%)	7 (17%)	2	7
29	D7	42/42 (100%)	34 (81%)	8 (19%)	1	5
30	A8	51/51 (100%)	40 (78%)	11 (22%)	1	4
30	D8	51/51 (100%)	44 (86%)	7 (14%)	3	13
32	BE	205/220 (93%)	174 (85%)	31 (15%)	2	10
32	CE	205/220 (93%)	174 (85%)	31 (15%)	2	10
33	BF	159/188 (85%)	137 (86%)	22 (14%)	3	13
33	CF	160/188 (85%)	139 (87%)	21 (13%)	3	14
34	BG	180/180 (100%)	161 (89%)	19 (11%)	5	21
34	CG	180/180 (100%)	152 (84%)	28 (16%)	2	9
35	BH	116/123 (94%)	101 (87%)	15 (13%)	3	15
35	CH	116/123 (94%)	101 (87%)	15 (13%)	3	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	BI	90/90 (100%)	82 (91%)	8 (9%)	8	29
36	CI	90/90 (100%)	85 (94%)	5 (6%)	17	46
37	BJ	126/127 (99%)	113 (90%)	13 (10%)	6	22
37	CJ	126/127 (99%)	107 (85%)	19 (15%)	2	10
38	BK	119/119 (100%)	109 (92%)	10 (8%)	9	32
38	CK	119/119 (100%)	109 (92%)	10 (8%)	9	32
39	BL	98/99 (99%)	81 (83%)	17 (17%)	1	7
39	CL	98/99 (99%)	85 (87%)	13 (13%)	3	13
40	BM	89/92 (97%)	79 (89%)	10 (11%)	5	20
40	CM	89/92 (97%)	78 (88%)	11 (12%)	4	16
41	BN	90/99 (91%)	81 (90%)	9 (10%)	6	24
41	CN	90/99 (91%)	82 (91%)	8 (9%)	8	29
42	BO	104/109 (95%)	87 (84%)	17 (16%)	2	8
42	CO	104/109 (95%)	92 (88%)	12 (12%)	4	19
43	BP	94/101 (93%)	85 (90%)	9 (10%)	7	26
43	CP	94/101 (93%)	80 (85%)	14 (15%)	2	10
44	BQ	49/50 (98%)	40 (82%)	9 (18%)	1	6
44	CQ	49/50 (98%)	47 (96%)	2 (4%)	26	57
45	BR	79/80 (99%)	76 (96%)	3 (4%)	28	59
45	CR	79/80 (99%)	72 (91%)	7 (9%)	8	29
46	BS	72/74 (97%)	64 (89%)	8 (11%)	5	20
46	CS	72/74 (97%)	63 (88%)	9 (12%)	3	15
47	BT	95/97 (98%)	86 (90%)	9 (10%)	7	26
47	CT	95/97 (98%)	91 (96%)	4 (4%)	25	56
48	BU	63/77 (82%)	58 (92%)	5 (8%)	10	34
48	CU	63/77 (82%)	56 (89%)	7 (11%)	5	20
49	BV	72/80 (90%)	60 (83%)	12 (17%)	2	7
49	CV	67/80 (84%)	55 (82%)	12 (18%)	1	6
50	BW	76/82 (93%)	67 (88%)	9 (12%)	4	17
50	CW	76/82 (93%)	66 (87%)	10 (13%)	3	14
51	BX	20/22 (91%)	19 (95%)	1 (5%)	20	50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
51	CX	20/22 (91%)	20 (100%)	0	100	100
All	All	9584/9828 (98%)	8234 (86%)	1350 (14%)	3	12

5 of 1350 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
50	CW	84	LEU
12	DP	103	MET
3	DD	176	ARG
50	CW	83	ARG
7	DH	89	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 259 such sidechains are listed below:

Mol	Chain	Res	Type
19	DT	31	HIS
21	DV	50	GLN
34	BG	201	GLN
34	BG	45	GLN
22	D3	50	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	2911/2912 (99%)	555 (19%)	51 (1%)
1	DA	2905/2912 (99%)	601 (20%)	50 (1%)
2	AB	121/122 (99%)	24 (19%)	0
2	DB	121/122 (99%)	28 (23%)	0
31	BA	1506/1506 (100%)	291 (19%)	32 (2%)
31	CA	1505/1506 (99%)	315 (20%)	42 (2%)
52	BB	86/87 (98%)	26 (30%)	4 (4%)
52	CB	86/87 (98%)	30 (34%)	3 (3%)
53	BC	77/77 (100%)	12 (15%)	3 (3%)
53	BD	76/77 (98%)	25 (32%)	2 (2%)
53	CC	76/77 (98%)	14 (18%)	3 (3%)
53	CD	76/77 (98%)	16 (21%)	2 (2%)
54	B1	9/10 (90%)	2 (22%)	0
54	C1	9/10 (90%)	2 (22%)	0
All	All	9564/9582 (99%)	1941 (20%)	192 (2%)

5 of 1941 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	10	G
1	AA	15	G
1	AA	23	G
1	AA	34	C
1	AA	35	G

5 of 192 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
31	CA	993	G
1	DA	71	A
31	CA	1128	C
31	CA	1442	G
1	DA	654(S)	G

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 1720 ligands modelled in this entry, 1720 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 ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	2912/2912 (100%)	-0.10	41 (1%) 73 56	38, 71, 209, 243	0
1	DA	2907/2912 (99%)	0.07	44 (1%) 71 54	49, 82, 229, 246	0
2	AB	122/122 (100%)	0.33	1 (0%) 82 68	73, 98, 119, 180	0
2	DB	122/122 (100%)	0.72	0 100 100	87, 121, 145, 200	0
3	AD	272/272 (100%)	-0.36	2 (0%) 84 70	38, 61, 83, 107	0
3	DD	272/272 (100%)	-0.15	3 (1%) 77 61	45, 69, 94, 125	0
4	AE	205/205 (100%)	0.11	5 (2%) 59 41	44, 82, 133, 147	0
4	DE	205/205 (100%)	0.21	13 (6%) 27 16	51, 90, 144, 167	0
5	AF	203/208 (97%)	-0.20	2 (0%) 79 64	40, 74, 116, 133	0
5	DF	208/208 (100%)	0.17	7 (3%) 48 28	54, 96, 161, 183	0
6	AG	181/181 (100%)	0.17	3 (1%) 69 50	91, 110, 140, 149	0
6	DG	181/181 (100%)	0.46	9 (4%) 35 21	112, 138, 161, 171	0
7	AH	170/170 (100%)	0.41	9 (5%) 33 20	80, 110, 129, 154	0
7	DH	170/170 (100%)	0.85	17 (10%) 14 8	150, 196, 217, 230	0
8	AK	146/146 (100%)	0.43	7 (4%) 36 21	75, 124, 142, 149	0
8	DK	146/146 (100%)	0.44	11 (7%) 22 12	76, 127, 150, 154	0
9	AM	138/138 (100%)	0.14	5 (3%) 46 27	63, 86, 124, 137	0
9	DM	138/138 (100%)	0.22	5 (3%) 46 27	74, 105, 136, 148	0
10	AN	122/122 (100%)	-0.33	0 100 100	54, 74, 92, 103	0
10	DN	122/122 (100%)	-0.13	1 (0%) 82 68	62, 84, 106, 123	0
11	AO	150/150 (100%)	0.31	9 (6%) 29 17	45, 82, 112, 166	0
11	DO	150/150 (100%)	0.36	7 (4%) 37 22	50, 100, 140, 180	0
12	AP	141/141 (100%)	0.34	10 (7%) 23 14	58, 85, 110, 134	0
12	DP	141/141 (100%)	0.59	14 (9%) 14 8	58, 101, 131, 154	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	A0	118/118 (100%)	-0.12	1 (0%) 82 68	55, 80, 102, 114	0
13	D0	117/118 (99%)	0.02	1 (0%) 81 66	58, 78, 100, 119	0
14	AQ	111/111 (100%)	0.22	4 (3%) 46 27	75, 96, 120, 136	0
14	DQ	111/111 (100%)	0.48	6 (5%) 32 19	80, 118, 143, 165	0
15	AR	137/137 (100%)	0.12	4 (2%) 54 34	69, 89, 140, 171	0
15	DR	137/137 (100%)	0.21	6 (4%) 39 23	70, 94, 158, 186	0
16	A1	117/117 (100%)	-0.00	4 (3%) 48 28	46, 74, 108, 149	0
16	D1	117/117 (100%)	0.11	0 100 100	59, 95, 138, 157	0
17	A2	101/101 (100%)	0.14	3 (2%) 52 33	47, 96, 125, 142	0
17	D2	101/101 (100%)	0.52	3 (2%) 52 33	57, 121, 140, 151	0
18	AS	113/113 (100%)	-0.38	0 100 100	46, 70, 106, 155	0
18	DS	113/113 (100%)	-0.18	0 100 100	61, 74, 107, 155	0
19	AT	92/92 (100%)	-0.21	1 (1%) 77 61	54, 68, 98, 112	0
19	DT	92/92 (100%)	0.12	3 (3%) 49 30	64, 86, 112, 128	0
20	AU	102/102 (100%)	0.49	9 (8%) 17 10	70, 97, 148, 168	0
20	DU	102/102 (100%)	0.72	13 (12%) 9 5	85, 113, 163, 184	0
21	AV	175/179 (97%)	0.47	7 (4%) 43 25	87, 125, 190, 195	0
21	DV	179/179 (100%)	0.64	15 (8%) 18 10	112, 156, 209, 216	0
22	A3	76/77 (98%)	-0.17	0 100 100	56, 75, 95, 135	0
22	D3	77/77 (100%)	0.07	2 (2%) 57 38	66, 88, 113, 152	0
23	AZ	97/97 (100%)	-0.05	4 (4%) 42 24	50, 69, 126, 161	0
23	DZ	97/97 (100%)	0.15	5 (5%) 34 20	52, 78, 131, 156	0
24	AW	66/69 (95%)	-0.02	2 (3%) 52 33	60, 77, 97, 134	0
24	DW	69/69 (100%)	0.25	3 (4%) 40 24	79, 105, 134, 172	0
25	AX	59/59 (100%)	-0.13	0 100 100	63, 80, 112, 127	0
25	DX	59/59 (100%)	0.03	1 (1%) 69 50	74, 100, 138, 162	0
26	A4	66/66 (100%)	0.93	5 (7%) 21 12	117, 153, 177, 184	0
26	D4	63/66 (95%)	0.88	8 (12%) 9 5	143, 184, 193, 201	0
27	A5	59/59 (100%)	0.48	3 (5%) 34 20	43, 85, 167, 172	0
27	D5	59/59 (100%)	0.17	2 (3%) 48 28	55, 83, 177, 186	0
28	A6	45/45 (100%)	1.34	10 (22%) 3 1	107, 136, 159, 163	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	D6	45/45 (100%)	1.40	9 (20%) 3 2	121, 158, 176, 182	0
29	A7	49/49 (100%)	-0.52	0 100 100	38, 47, 95, 123	0
29	D7	49/49 (100%)	-0.50	0 100 100	49, 58, 115, 133	0
30	A8	61/61 (100%)	0.07	0 100 100	55, 68, 85, 108	0
30	D8	61/61 (100%)	0.53	8 (13%) 8 5	65, 81, 103, 120	0
31	BA	1506/1506 (100%)	0.40	49 (3%) 49 30	54, 103, 187, 244	0
31	CA	1506/1506 (100%)	0.50	69 (4%) 38 22	59, 109, 187, 245	0
32	BE	237/256 (92%)	0.63	14 (5%) 29 18	107, 142, 181, 191	0
32	CE	237/256 (92%)	0.81	23 (9%) 15 8	117, 158, 190, 208	0
33	BF	205/239 (85%)	0.20	3 (1%) 71 54	88, 118, 150, 162	0
33	CF	206/239 (86%)	0.83	16 (7%) 20 11	119, 143, 172, 183	0
34	BG	208/208 (100%)	0.48	10 (4%) 36 21	84, 110, 135, 149	0
34	CG	208/208 (100%)	0.37	17 (8%) 19 11	74, 101, 128, 142	0
35	BH	151/162 (93%)	0.02	0 100 100	79, 101, 129, 159	0
35	CH	151/162 (93%)	0.44	4 (2%) 57 38	90, 114, 139, 162	0
36	BI	101/101 (100%)	0.13	1 (0%) 79 64	77, 102, 122, 143	0
36	CI	101/101 (100%)	0.06	2 (1%) 64 45	73, 98, 121, 149	0
37	BJ	155/156 (99%)	0.29	1 (0%) 85 72	101, 122, 156, 167	0
37	CJ	155/156 (99%)	0.49	5 (3%) 50 31	105, 127, 158, 166	0
38	BK	138/138 (100%)	0.25	0 100 100	84, 108, 123, 132	0
38	CK	138/138 (100%)	0.29	3 (2%) 62 42	93, 118, 131, 141	0
39	BL	127/128 (99%)	0.62	9 (7%) 23 14	91, 141, 160, 169	0
39	CL	127/128 (99%)	0.63	4 (3%) 51 32	107, 151, 168, 172	0
40	BM	99/105 (94%)	0.54	3 (3%) 52 33	87, 140, 171, 176	0
40	CM	99/105 (94%)	0.74	6 (6%) 28 17	113, 154, 173, 176	0
41	BN	119/129 (92%)	0.11	2 (1%) 69 50	63, 101, 133, 162	0
41	CN	119/129 (92%)	0.28	3 (2%) 58 39	77, 103, 141, 166	0
42	BO	125/132 (94%)	-0.21	1 (0%) 82 68	61, 78, 116, 162	0
42	CO	125/132 (94%)	0.24	4 (3%) 50 31	70, 97, 130, 168	0
43	BP	116/126 (92%)	0.37	3 (2%) 57 38	87, 124, 144, 158	0
43	CP	117/126 (92%)	0.67	6 (5%) 34 20	105, 152, 166, 174	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	BQ	60/61 (98%)	0.43	2 (3%) 49 30	84, 107, 124, 134	0
44	CQ	60/61 (98%)	0.82	4 (6%) 25 15	120, 136, 153, 161	0
45	BR	88/89 (98%)	0.08	1 (1%) 77 61	73, 97, 120, 126	0
45	CR	88/89 (98%)	0.21	1 (1%) 77 61	75, 105, 129, 135	0
46	BS	84/88 (95%)	0.28	1 (1%) 76 60	98, 113, 141, 173	0
46	CS	84/88 (95%)	0.10	2 (2%) 59 41	79, 96, 122, 161	0
47	BT	100/105 (95%)	0.05	0 100 100	85, 105, 123, 137	0
47	CT	100/105 (95%)	0.18	2 (2%) 64 45	81, 104, 126, 143	0
48	BU	72/88 (81%)	0.08	0 100 100	75, 102, 140, 169	0
48	CU	72/88 (81%)	0.05	0 100 100	86, 109, 150, 165	0
49	BV	83/93 (89%)	0.62	7 (8%) 18 10	103, 129, 145, 156	0
49	CV	78/93 (83%)	0.66	3 (3%) 44 26	137, 160, 180, 183	0
50	BW	99/106 (93%)	0.50	4 (4%) 43 25	101, 123, 152, 162	0
50	CW	99/106 (93%)	0.32	5 (5%) 34 20	79, 110, 149, 164	0
51	BX	25/27 (92%)	0.28	0 100 100	93, 114, 133, 155	0
51	CX	25/27 (92%)	0.82	1 (4%) 43 25	110, 134, 152, 170	0
52	BB	87/87 (100%)	0.87	4 (4%) 38 22	83, 164, 192, 209	0
52	CB	87/87 (100%)	0.99	8 (9%) 16 9	99, 167, 196, 209	0
53	BC	77/77 (100%)	0.30	2 (2%) 57 38	66, 101, 139, 152	0
53	BD	77/77 (100%)	1.07	9 (11%) 10 7	75, 226, 239, 242	0
53	CC	77/77 (100%)	0.56	3 (3%) 44 26	77, 110, 148, 162	0
53	CD	77/77 (100%)	1.28	10 (12%) 9 5	78, 227, 239, 242	0
54	B1	10/10 (100%)	0.04	1 (10%) 14 8	73, 80, 132, 141	0
54	C1	10/10 (100%)	0.35	1 (10%) 14 8	81, 98, 145, 150	0
All	All	21111/21426 (98%)	0.24	696 (3%) 49 30	38, 99, 184, 246	0

The worst 5 of 696 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
34	BG	12	CYS	7.8
31	BA	1129	C	7.4
27	A5	2	ALA	7.3
12	AP	23	GLY	6.9
34	BG	26	CYS	6.8

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

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

6.3 Carbohydrates [i](#)

There are no 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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	CA	1667	1/1	-0.03	0.22	144,144,144,144	0
55	MG	BA	1692	1/1	0.20	0.20	132,132,132,132	0
55	MG	DA	3124	1/1	0.28	0.26	111,111,111,111	0
55	MG	BA	1742	1/1	0.29	0.22	133,133,133,133	0
55	MG	CA	1704	1/1	0.32	0.30	129,129,129,129	0
55	MG	BA	1784	1/1	0.35	0.51	106,106,106,106	0
55	MG	CA	1753	1/1	0.36	0.27	129,129,129,129	0
55	MG	BA	1638	1/1	0.40	0.37	123,123,123,123	0
55	MG	BA	1758	1/1	0.41	0.15	110,110,110,110	0
55	MG	DA	3010	1/1	0.43	0.26	121,121,121,121	0
55	MG	CA	1730	1/1	0.43	0.35	118,118,118,118	0
55	MG	DA	3272	1/1	0.46	0.50	117,117,117,117	0
55	MG	CA	1719	1/1	0.47	0.31	157,157,157,157	0
55	MG	BA	1714	1/1	0.49	0.17	127,127,127,127	0
55	MG	BA	1787	1/1	0.51	0.37	107,107,107,107	0
55	MG	BA	1712	1/1	0.53	0.46	125,125,125,125	0
55	MG	CA	1626	1/1	0.54	0.28	103,103,103,103	0
55	MG	CA	1748	1/1	0.54	0.38	91,91,91,91	0
55	MG	AA	3406	1/1	0.54	0.33	99,99,99,99	0
55	MG	CA	1802	1/1	0.56	0.28	107,107,107,107	0
55	MG	CA	1759	1/1	0.57	0.40	100,100,100,100	0
55	MG	BA	1713	1/1	0.58	0.29	107,107,107,107	0
55	MG	BA	1831	1/1	0.58	0.41	116,116,116,116	0
55	MG	DA	3526	1/1	0.58	0.22	92,92,92,92	0
55	MG	BB	105	1/1	0.59	0.28	115,115,115,115	0
55	MG	AA	3076	1/1	0.60	0.25	109,109,109,109	0
55	MG	DA	3497	1/1	0.61	0.17	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	CA	1789	1/1	0.61	0.25	117,117,117,117	0
55	MG	CA	1659	1/1	0.62	0.34	111,111,111,111	0
55	MG	CA	1800	1/1	0.62	0.14	102,102,102,102	0
55	MG	BD	101	1/1	0.63	0.17	108,108,108,108	0
55	MG	DA	3444	1/1	0.63	0.23	82,82,82,82	0
55	MG	BA	1751	1/1	0.63	0.40	122,122,122,122	0
55	MG	AA	3318	1/1	0.63	0.34	120,120,120,120	0
55	MG	DB	206	1/1	0.63	0.36	122,122,122,122	0
55	MG	DB	214	1/1	0.63	0.11	99,99,99,99	0
55	MG	BA	1609	1/1	0.64	0.32	84,84,84,84	0
55	MG	AA	3370	1/1	0.64	0.29	103,103,103,103	0
55	MG	DA	3357	1/1	0.64	0.74	89,89,89,89	0
55	MG	AA	3431	1/1	0.64	0.45	197,197,197,197	0
55	MG	CB	101	1/1	0.65	0.24	102,102,102,102	0
55	MG	CA	1699	1/1	0.65	0.12	106,106,106,106	0
55	MG	DA	3433	1/1	0.65	0.23	110,110,110,110	0
55	MG	AA	3230	1/1	0.65	0.31	112,112,112,112	0
55	MG	DA	3343	1/1	0.66	0.25	145,145,145,145	0
55	MG	BA	1686	1/1	0.66	0.36	94,94,94,94	0
55	MG	AA	3443	1/1	0.67	0.31	95,95,95,95	0
55	MG	BA	1834	1/1	0.67	0.24	86,86,86,86	0
55	MG	BA	1778	1/1	0.67	0.76	93,93,93,93	0
55	MG	CA	1762	1/1	0.67	0.22	105,105,105,105	0
55	MG	DA	3163	1/1	0.67	0.12	97,97,97,97	0
55	MG	BB	106	1/1	0.67	0.23	120,120,120,120	0
55	MG	CA	1747	1/1	0.67	0.49	114,114,114,114	0
55	MG	BG	301	1/1	0.68	0.27	110,110,110,110	0
55	MG	DA	3377	1/1	0.68	0.32	92,92,92,92	0
55	MG	DA	3060	1/1	0.68	0.44	85,85,85,85	0
55	MG	CA	1795	1/1	0.68	0.34	110,110,110,110	0
55	MG	BA	1828	1/1	0.68	0.38	85,85,85,85	0
55	MG	AA	3521	1/1	0.68	0.48	87,87,87,87	0
55	MG	AA	3419	1/1	0.68	0.29	102,102,102,102	0
55	MG	DA	3352	1/1	0.68	0.28	77,77,77,77	0
55	MG	DA	3065	1/1	0.69	0.29	95,95,95,95	0
55	MG	DA	3472	1/1	0.69	0.18	85,85,85,85	0
55	MG	BA	1678	1/1	0.69	0.63	75,75,75,75	0
55	MG	DA	3498	1/1	0.69	0.29	90,90,90,90	0
55	MG	BA	1829	1/1	0.69	0.29	102,102,102,102	0
55	MG	BA	1647	1/1	0.69	0.21	93,93,93,93	0
55	MG	DA	3332	1/1	0.69	0.70	90,90,90,90	0
55	MG	CA	1723	1/1	0.70	0.22	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	BA	1674	1/1	0.70	0.40	113,113,113,113	0
55	MG	CA	1734	1/1	0.70	0.29	92,92,92,92	0
55	MG	BA	1753	1/1	0.70	0.14	91,91,91,91	0
55	MG	BA	1636	1/1	0.70	0.43	92,92,92,92	0
55	MG	CA	1806	1/1	0.70	0.30	115,115,115,115	0
55	MG	AA	3573	1/1	0.70	0.22	47,47,47,47	0
55	MG	AA	3353	1/1	0.70	0.41	105,105,105,105	0
55	MG	DA	3045	1/1	0.70	0.38	79,79,79,79	0
55	MG	DA	3109	1/1	0.71	0.35	97,97,97,97	0
55	MG	AA	3058	1/1	0.71	0.52	85,85,85,85	0
55	MG	BA	1621	1/1	0.71	0.26	116,116,116,116	0
55	MG	BA	1718	1/1	0.71	0.24	104,104,104,104	0
55	MG	DA	3312	1/1	0.71	0.20	101,101,101,101	0
55	MG	DA	3038	1/1	0.71	0.16	102,102,102,102	0
55	MG	AA	3451	1/1	0.71	0.29	85,85,85,85	0
55	MG	AA	3055	1/1	0.71	0.30	100,100,100,100	0
55	MG	AA	3378	1/1	0.71	0.25	86,86,86,86	0
55	MG	CA	1657	1/1	0.72	0.32	94,94,94,94	0
55	MG	AA	3241	1/1	0.72	0.15	101,101,101,101	0
55	MG	BA	1804	1/1	0.72	0.27	80,80,80,80	0
55	MG	DA	3438	1/1	0.72	0.81	102,102,102,102	0
55	MG	BA	1810	1/1	0.72	0.30	110,110,110,110	0
55	MG	AA	3460	1/1	0.72	0.40	89,89,89,89	0
55	MG	CB	104	1/1	0.72	0.22	114,114,114,114	0
55	MG	DA	3004	1/1	0.72	0.49	91,91,91,91	0
55	MG	CA	1713	1/1	0.72	0.17	109,109,109,109	0
55	MG	AA	3508	1/1	0.72	0.30	96,96,96,96	0
55	MG	AA	3426	1/1	0.72	0.28	123,123,123,123	0
55	MG	AE	304	1/1	0.73	0.55	85,85,85,85	0
55	MG	CA	1727	1/1	0.73	0.28	84,84,84,84	0
55	MG	DA	3340	1/1	0.73	0.26	107,107,107,107	0
55	MG	BA	1765	1/1	0.73	0.31	99,99,99,99	0
55	MG	AA	3411	1/1	0.73	0.35	84,84,84,84	0
55	MG	BA	1611	1/1	0.73	0.33	97,97,97,97	0
55	MG	AA	3465	1/1	0.73	0.28	88,88,88,88	0
55	MG	DA	3429	1/1	0.73	0.14	94,94,94,94	0
55	MG	AA	3505	1/1	0.73	0.27	103,103,103,103	0
55	MG	DA	3059	1/1	0.73	0.31	104,104,104,104	0
55	MG	AA	3251	1/1	0.73	0.23	97,97,97,97	0
55	MG	DA	3447	1/1	0.73	0.62	86,86,86,86	0
55	MG	BA	1823	1/1	0.73	0.15	93,93,93,93	0
55	MG	DA	3473	1/1	0.73	0.26	103,103,103,103	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	BA	1735	1/1	0.73	0.35	80,80,80,80	0
55	MG	AA	3518	1/1	0.73	0.59	71,71,71,71	0
55	MG	AA	3450	1/1	0.73	0.36	84,84,84,84	0
55	MG	AA	3236	1/1	0.73	0.62	93,93,93,93	0
55	MG	DA	3278	1/1	0.73	0.21	116,116,116,116	0
55	MG	BC	102	1/1	0.74	0.20	100,100,100,100	0
55	MG	DA	3248	1/1	0.74	0.22	98,98,98,98	0
55	MG	AF	303	1/1	0.74	0.23	77,77,77,77	0
55	MG	BA	1841	1/1	0.74	0.22	105,105,105,105	0
55	MG	DA	3054	1/1	0.74	0.20	105,105,105,105	0
55	MG	DA	3455	1/1	0.74	0.30	95,95,95,95	0
55	MG	CA	1630	1/1	0.74	0.13	76,76,76,76	0
55	MG	AA	3102	1/1	0.74	0.21	108,108,108,108	0
55	MG	DA	3063	1/1	0.74	0.20	86,86,86,86	0
55	MG	BA	1747	1/1	0.74	0.14	97,97,97,97	0
55	MG	CC	101	1/1	0.74	0.25	110,110,110,110	0
55	MG	AA	3262	1/1	0.74	0.21	71,71,71,71	0
55	MG	DA	3412	1/1	0.74	0.30	97,97,97,97	0
55	MG	DA	3372	1/1	0.75	0.50	108,108,108,108	0
55	MG	DA	3076	1/1	0.75	0.16	96,96,96,96	0
55	MG	CC	107	1/1	0.75	0.48	102,102,102,102	0
55	MG	CC	108	1/1	0.75	0.26	110,110,110,110	0
55	MG	AD	301	1/1	0.75	0.12	100,100,100,100	0
55	MG	DA	3244	1/1	0.75	0.27	106,106,106,106	0
55	MG	CA	1634	1/1	0.75	0.47	90,90,90,90	0
55	MG	CA	1635	1/1	0.75	0.26	87,87,87,87	0
55	MG	AA	3346	1/1	0.75	0.10	98,98,98,98	0
55	MG	BA	1785	1/1	0.75	0.32	91,91,91,91	0
55	MG	DA	3315	1/1	0.75	0.21	82,82,82,82	0
55	MG	AA	3132	1/1	0.75	0.46	89,89,89,89	0
55	MG	BA	1798	1/1	0.75	0.38	89,89,89,89	0
55	MG	AA	3393	1/1	0.75	0.25	91,91,91,91	0
55	MG	BA	1838	1/1	0.75	0.47	101,101,101,101	0
55	MG	DA	3068	1/1	0.75	0.35	100,100,100,100	0
55	MG	DA	3249	1/1	0.76	0.21	87,87,87,87	0
55	MG	CA	1769	1/1	0.76	0.27	109,109,109,109	0
55	MG	CA	1773	1/1	0.76	0.15	115,115,115,115	0
55	MG	CA	1720	1/1	0.76	0.22	108,108,108,108	0
55	MG	DA	3398	1/1	0.76	0.33	107,107,107,107	0
55	MG	AA	3560	1/1	0.76	0.24	84,84,84,84	0
55	MG	DA	3422	1/1	0.76	0.16	96,96,96,96	0
55	MG	BA	1746	1/1	0.76	0.38	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	CA	1661	1/1	0.76	0.28	105,105,105,105	0
55	MG	AA	3430	1/1	0.76	0.15	88,88,88,88	0
55	MG	BA	1723	1/1	0.77	0.29	95,95,95,95	0
55	MG	BA	1637	1/1	0.77	0.20	93,93,93,93	0
55	MG	DA	3324	1/1	0.77	0.60	89,89,89,89	0
55	MG	DA	3025	1/1	0.77	0.17	111,111,111,111	0
55	MG	CA	1631	1/1	0.77	0.37	95,95,95,95	0
55	MG	DA	3453	1/1	0.77	0.47	94,94,94,94	0
55	MG	AA	3333	1/1	0.77	0.29	80,80,80,80	0
55	MG	AA	3108	1/1	0.77	0.50	79,79,79,79	0
55	MG	BA	1649	1/1	0.77	0.23	85,85,85,85	0
55	MG	AA	3495	1/1	0.77	0.26	98,98,98,98	0
55	MG	AA	3077	1/1	0.77	0.42	94,94,94,94	0
55	MG	DA	3504	1/1	0.77	0.32	119,119,119,119	0
55	MG	DA	3520	1/1	0.77	0.19	99,99,99,99	0
55	MG	CA	1662	1/1	0.77	0.39	102,102,102,102	0
55	MG	DA	3285	1/1	0.77	0.21	109,109,109,109	0
55	MG	DB	208	1/1	0.77	0.18	114,114,114,114	0
55	MG	DA	3299	1/1	0.77	0.21	92,92,92,92	0
55	MG	CA	1665	1/1	0.78	0.29	101,101,101,101	0
55	MG	BA	1745	1/1	0.78	0.22	90,90,90,90	0
55	MG	BA	1690	1/1	0.78	0.18	109,109,109,109	0
55	MG	DA	3261	1/1	0.78	0.23	89,89,89,89	0
55	MG	CA	1763	1/1	0.78	0.30	96,96,96,96	0
55	MG	AA	3478	1/1	0.78	0.15	93,93,93,93	0
55	MG	CA	1710	1/1	0.78	0.24	105,105,105,105	0
55	MG	CA	1777	1/1	0.78	0.44	95,95,95,95	0
55	MG	DA	3301	1/1	0.78	0.41	91,91,91,91	0
55	MG	BA	1749	1/1	0.78	0.26	95,95,95,95	0
55	MG	BA	1709	1/1	0.78	0.46	101,101,101,101	0
55	MG	AA	3249	1/1	0.78	0.18	92,92,92,92	0
55	MG	DA	3478	1/1	0.78	0.20	99,99,99,99	0
55	MG	AA	3446	1/1	0.78	0.28	93,93,93,93	0
55	MG	AA	3223	1/1	0.78	0.19	72,72,72,72	0
55	MG	AA	3388	1/1	0.78	0.33	119,119,119,119	0
55	MG	AA	3145	1/1	0.78	0.27	98,98,98,98	0
55	MG	AA	3288	1/1	0.78	0.22	73,73,73,73	0
55	MG	BA	1628	1/1	0.78	0.50	86,86,86,86	0
55	MG	DA	3225	1/1	0.78	0.26	64,64,64,64	0
55	MG	DB	212	1/1	0.78	0.14	94,94,94,94	0
55	MG	DA	3382	1/1	0.78	0.16	84,84,84,84	0
55	MG	DA	3404	1/1	0.79	0.45	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	DA	3410	1/1	0.79	0.34	99,99,99,99	0
55	MG	AA	3188	1/1	0.79	0.26	72,72,72,72	0
55	MG	BA	1698	1/1	0.79	0.21	73,73,73,73	0
55	MG	AA	3461	1/1	0.79	0.29	78,78,78,78	0
55	MG	AA	3202	1/1	0.79	0.34	55,55,55,55	0
55	MG	AA	3317	1/1	0.79	0.44	95,95,95,95	0
55	MG	BQ	101	1/1	0.79	0.32	99,99,99,99	0
55	MG	AA	3558	1/1	0.79	0.40	110,110,110,110	0
55	MG	DA	3066	1/1	0.79	0.17	83,83,83,83	0
55	MG	CA	1742	1/1	0.79	0.28	93,93,93,93	0
55	MG	AA	3486	1/1	0.79	0.35	96,96,96,96	0
55	MG	DA	3334	1/1	0.79	0.33	95,95,95,95	0
55	MG	DA	3477	1/1	0.79	0.27	125,125,125,125	0
55	MG	AA	3380	1/1	0.79	0.33	84,84,84,84	0
55	MG	CA	1749	1/1	0.79	0.17	106,106,106,106	0
55	MG	AB	216	1/1	0.79	0.34	112,112,112,112	0
55	MG	DA	3500	1/1	0.79	0.18	100,100,100,100	0
55	MG	DA	3502	1/1	0.79	0.15	96,96,96,96	0
55	MG	CA	1612	1/1	0.79	0.20	91,91,91,91	0
55	MG	CA	1761	1/1	0.79	0.32	96,96,96,96	0
55	MG	CA	1621	1/1	0.79	0.31	84,84,84,84	0
55	MG	BA	1775	1/1	0.79	0.20	100,100,100,100	0
55	MG	DA	3393	1/1	0.79	0.19	93,93,93,93	0
55	MG	DA	3397	1/1	0.79	0.60	150,150,150,150	0
55	MG	DA	3253	1/1	0.79	0.20	83,83,83,83	0
55	MG	AA	3387	1/1	0.80	0.26	102,102,102,102	0
55	MG	BA	1681	1/1	0.80	0.25	79,79,79,79	0
55	MG	DA	3425	1/1	0.80	0.16	88,88,88,88	0
55	MG	BA	1683	1/1	0.80	0.12	112,112,112,112	0
55	MG	AA	3435	1/1	0.80	0.18	137,137,137,137	0
55	MG	BA	1833	1/1	0.80	0.19	88,88,88,88	0
55	MG	DA	3440	1/1	0.80	0.15	92,92,92,92	0
55	MG	BA	1726	1/1	0.80	0.41	98,98,98,98	0
55	MG	AA	3496	1/1	0.80	0.36	91,91,91,91	0
55	MG	DA	3449	1/1	0.80	0.26	96,96,96,96	0
55	MG	CA	1637	1/1	0.80	0.21	97,97,97,97	0
55	MG	CH	201	1/1	0.80	0.30	96,96,96,96	0
55	MG	DA	3077	1/1	0.80	0.38	82,82,82,82	0
55	MG	CA	1643	1/1	0.80	0.24	97,97,97,97	0
55	MG	BA	1741	1/1	0.80	0.25	124,124,124,124	0
55	MG	DA	3132	1/1	0.80	0.28	56,56,56,56	0
55	MG	AA	3326	1/1	0.80	0.57	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	BA	1648	1/1	0.80	0.23	77,77,77,77	0
55	MG	DA	3236	1/1	0.80	0.27	57,57,57,57	0
55	MG	BA	1788	1/1	0.80	0.29	108,108,108,108	0
55	MG	DA	3388	1/1	0.80	0.14	85,85,85,85	0
55	MG	BA	1707	1/1	0.80	0.33	94,94,94,94	0
55	MG	BB	107	1/1	0.80	0.19	97,97,97,97	0
55	MG	DB	204	1/1	0.80	0.28	102,102,102,102	0
55	MG	AA	3349	1/1	0.80	0.17	79,79,79,79	0
55	MG	AA	3120	1/1	0.80	0.12	92,92,92,92	0
55	MG	DA	3405	1/1	0.80	0.39	97,97,97,97	0
55	MG	DA	3263	1/1	0.80	0.27	88,88,88,88	0
55	MG	AA	3444	1/1	0.81	0.22	87,87,87,87	0
55	MG	DA	3342	1/1	0.81	0.29	96,96,96,96	0
55	MG	CA	1614	1/1	0.81	0.42	95,95,95,95	0
55	MG	AA	3148	1/1	0.81	0.26	70,70,70,70	0
55	MG	AA	3343	1/1	0.81	0.40	94,94,94,94	0
55	MG	DA	3360	1/1	0.81	0.36	96,96,96,96	0
55	MG	DA	3366	1/1	0.81	0.18	97,97,97,97	0
55	MG	AA	3556	1/1	0.81	0.39	85,85,85,85	0
55	MG	AA	3257	1/1	0.81	0.16	84,84,84,84	0
55	MG	AA	3458	1/1	0.81	0.57	105,105,105,105	0
55	MG	BA	1819	1/1	0.81	0.29	107,107,107,107	0
55	MG	AA	3224	1/1	0.81	0.29	77,77,77,77	0
55	MG	DA	3396	1/1	0.81	0.21	89,89,89,89	0
55	MG	AA	3600	1/1	0.81	0.45	79,79,79,79	0
55	MG	DA	3084	1/1	0.81	0.20	87,87,87,87	0
55	MG	BA	1744	1/1	0.81	0.27	93,93,93,93	0
55	MG	DA	3116	1/1	0.81	0.38	96,96,96,96	0
55	MG	DA	3123	1/1	0.81	0.36	73,73,73,73	0
55	MG	CA	1770	1/1	0.81	0.15	75,75,75,75	0
55	MG	DA	3128	1/1	0.81	0.30	66,66,66,66	0
55	MG	AB	201	1/1	0.81	0.16	91,91,91,91	0
55	MG	DA	3426	1/1	0.81	0.21	94,94,94,94	0
55	MG	AB	203	1/1	0.81	0.35	70,70,70,70	0
55	MG	CA	1786	1/1	0.81	0.30	97,97,97,97	0
55	MG	AB	215	1/1	0.81	0.18	92,92,92,92	0
55	MG	CA	1664	1/1	0.81	0.27	97,97,97,97	0
55	MG	DA	3247	1/1	0.81	0.38	71,71,71,71	0
55	MG	AA	3164	1/1	0.81	0.19	102,102,102,102	0
55	MG	AA	3420	1/1	0.81	0.28	107,107,107,107	0
55	MG	CA	1803	1/1	0.81	0.24	87,87,87,87	0
55	MG	CA	1685	1/1	0.81	0.33	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	CA	1687	1/1	0.81	0.12	99,99,99,99	0
55	MG	DA	3271	1/1	0.81	0.24	76,76,76,76	0
55	MG	BA	1752	1/1	0.81	0.23	116,116,116,116	0
55	MG	BN	202	1/1	0.81	0.18	104,104,104,104	0
55	MG	AA	3366	1/1	0.81	0.35	78,78,78,78	0
55	MG	DA	3294	1/1	0.81	0.33	93,93,93,93	0
55	MG	AA	3301	1/1	0.81	0.26	113,113,113,113	0
55	MG	AA	3101	1/1	0.81	0.09	69,69,69,69	0
55	MG	DA	3309	1/1	0.81	0.30	69,69,69,69	0
55	MG	AA	3131	1/1	0.81	0.13	88,88,88,88	0
55	MG	DA	3525	1/1	0.81	0.32	88,88,88,88	0
55	MG	BA	1710	1/1	0.81	0.40	99,99,99,99	0
55	MG	DA	3318	1/1	0.81	0.53	93,93,93,93	0
55	MG	DA	3021	1/1	0.81	0.23	61,61,61,61	0
55	MG	DA	3326	1/1	0.81	0.31	63,63,63,63	0
55	MG	AA	3213	1/1	0.81	0.55	50,50,50,50	0
55	MG	CA	1606	1/1	0.81	0.23	96,96,96,96	0
55	MG	BA	1684	1/1	0.82	0.19	100,100,100,100	0
55	MG	DA	3431	1/1	0.82	0.26	93,93,93,93	0
55	MG	DA	3432	1/1	0.82	0.23	89,89,89,89	0
55	MG	AA	3619	1/1	0.82	0.26	94,94,94,94	0
55	MG	DA	3437	1/1	0.82	0.26	140,140,140,140	0
55	MG	DA	3185	1/1	0.82	0.25	64,64,64,64	0
55	MG	DA	3439	1/1	0.82	0.07	92,92,92,92	0
55	MG	BA	1639	1/1	0.82	0.43	94,94,94,94	0
55	MG	CA	1782	1/1	0.82	0.27	104,104,104,104	0
55	MG	DA	3446	1/1	0.82	0.39	98,98,98,98	0
55	MG	AA	3629	1/1	0.82	0.17	107,107,107,107	0
55	MG	BA	1695	1/1	0.82	0.20	101,101,101,101	0
55	MG	DA	3056	1/1	0.82	0.22	100,100,100,100	0
55	MG	AA	3398	1/1	0.82	0.23	91,91,91,91	0
55	MG	AA	3285	1/1	0.82	0.27	77,77,77,77	0
55	MG	BA	1654	1/1	0.82	0.33	74,74,74,74	0
55	MG	CA	1616	1/1	0.82	0.22	90,90,90,90	0
55	MG	AB	207	1/1	0.82	0.13	97,97,97,97	0
55	MG	CA	1809	1/1	0.82	0.22	100,100,100,100	0
55	MG	DA	3390	1/1	0.82	0.13	81,81,81,81	0
55	MG	CA	1623	1/1	0.82	0.14	98,98,98,98	0
55	MG	CA	1754	1/1	0.82	0.18	84,84,84,84	0
55	MG	AA	3534	1/1	0.82	0.16	100,100,100,100	0
55	MG	DA	3518	1/1	0.82	0.18	63,63,63,63	0
55	MG	DA	3091	1/1	0.82	0.39	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	CA	1627	1/1	0.82	0.28	102,102,102,102	0
55	MG	BA	1791	1/1	0.82	0.22	89,89,89,89	0
55	MG	DA	3311	1/1	0.82	0.13	80,80,80,80	0
55	MG	AA	3394	1/1	0.82	0.16	85,85,85,85	0
55	MG	AA	3618	1/1	0.82	0.28	76,76,76,76	0
55	MG	DB	210	1/1	0.82	0.41	76,76,76,76	0
55	MG	DA	3125	1/1	0.82	0.23	86,86,86,86	0
55	MG	DA	3007	1/1	0.82	0.15	75,75,75,75	0
55	MG	AA	3391	1/1	0.83	0.16	90,90,90,90	0
55	MG	DA	3003	1/1	0.83	0.23	70,70,70,70	0
55	MG	CA	1744	1/1	0.83	0.19	70,70,70,70	0
55	MG	CA	1745	1/1	0.83	0.20	87,87,87,87	0
55	MG	AA	3103	1/1	0.83	0.21	75,75,75,75	0
55	MG	AA	3532	1/1	0.83	0.12	89,89,89,89	0
55	MG	AA	3231	1/1	0.83	0.36	120,120,120,120	0
55	MG	AO	202	1/1	0.83	0.26	74,74,74,74	0
55	MG	BA	1605	1/1	0.83	0.34	69,69,69,69	0
55	MG	DA	3046	1/1	0.83	0.27	60,60,60,60	0
55	MG	AA	3095	1/1	0.83	0.21	75,75,75,75	0
55	MG	AA	3294	1/1	0.83	0.46	99,99,99,99	0
55	MG	BA	1844	1/1	0.83	0.18	95,95,95,95	0
55	MG	DA	3302	1/1	0.83	0.40	91,91,91,91	0
55	MG	DA	3308	1/1	0.83	0.29	95,95,95,95	0
55	MG	AA	3355	1/1	0.83	0.39	87,87,87,87	0
55	MG	BA	1626	1/1	0.83	0.32	76,76,76,76	0
55	MG	AA	3297	1/1	0.83	0.25	63,63,63,63	0
55	MG	AA	3367	1/1	0.83	0.27	101,101,101,101	0
55	MG	AA	3422	1/1	0.83	0.48	73,73,73,73	0
55	MG	AA	3005	1/1	0.83	0.33	38,38,38,38	0
55	MG	AA	3215	1/1	0.83	0.30	55,55,55,55	0
55	MG	CA	1689	1/1	0.83	0.17	87,87,87,87	0
55	MG	BC	104	1/1	0.83	0.26	106,106,106,106	0
55	MG	CA	1797	1/1	0.83	0.22	94,94,94,94	0
55	MG	DA	3481	1/1	0.83	0.31	45,45,45,45	0
55	MG	DA	3115	1/1	0.83	0.32	76,76,76,76	0
55	MG	AA	3049	1/1	0.83	0.22	106,106,106,106	0
55	MG	AA	3497	1/1	0.83	0.25	105,105,105,105	0
55	MG	AA	3254	1/1	0.83	0.31	97,97,97,97	0
55	MG	CA	1715	1/1	0.83	0.35	99,99,99,99	0
55	MG	AA	3165	1/1	0.83	0.37	71,71,71,71	0
55	MG	BA	1800	1/1	0.83	0.17	101,101,101,101	0
55	MG	DA	3521	1/1	0.83	0.23	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	DA	3135	1/1	0.83	0.25	64,64,64,64	0
55	MG	BA	1669	1/1	0.83	0.36	76,76,76,76	0
55	MG	DA	3176	1/1	0.83	0.15	78,78,78,78	0
55	MG	CB	102	1/1	0.83	0.15	94,94,94,94	0
55	MG	DA	3215	1/1	0.83	0.28	50,50,50,50	0
55	MG	CA	1622	1/1	0.83	0.33	74,74,74,74	0
55	MG	BA	1736	1/1	0.83	0.24	89,89,89,89	0
55	MG	BA	1672	1/1	0.83	0.24	104,104,104,104	0
55	MG	DA	3392	1/1	0.84	0.18	106,106,106,106	0
55	MG	BA	1824	1/1	0.84	0.56	97,97,97,97	0
55	MG	DA	3241	1/1	0.84	0.30	85,85,85,85	0
55	MG	DA	3243	1/1	0.84	0.20	83,83,83,83	0
55	MG	BA	1702	1/1	0.84	0.32	98,98,98,98	0
55	MG	AA	3032	1/1	0.84	0.21	60,60,60,60	0
55	MG	AA	3623	1/1	0.84	0.28	107,107,107,107	0
55	MG	CA	1638	1/1	0.84	0.36	93,93,93,93	0
55	MG	AA	3399	1/1	0.84	0.13	71,71,71,71	0
55	MG	BA	1670	1/1	0.84	0.22	62,62,62,62	0
55	MG	DA	3423	1/1	0.84	0.39	102,102,102,102	0
55	MG	BA	1754	1/1	0.84	0.16	80,80,80,80	0
55	MG	DA	3267	1/1	0.84	0.36	74,74,74,74	0
55	MG	BA	1616	1/1	0.84	0.16	92,92,92,92	0
55	MG	BA	1763	1/1	0.84	0.16	93,93,93,93	0
55	MG	DA	3276	1/1	0.84	0.17	86,86,86,86	0
55	MG	AA	3352	1/1	0.84	0.15	91,91,91,91	0
55	MG	DA	3279	1/1	0.84	0.28	66,66,66,66	0
55	MG	DA	3283	1/1	0.84	0.49	78,78,78,78	0
55	MG	BA	1766	1/1	0.84	0.21	116,116,116,116	0
55	MG	BA	1770	1/1	0.84	0.29	106,106,106,106	0
55	MG	BB	104	1/1	0.84	0.12	103,103,103,103	0
55	MG	BA	1677	1/1	0.84	0.35	92,92,92,92	0
55	MG	AA	3477	1/1	0.84	0.11	65,65,65,65	0
55	MG	CA	1694	1/1	0.84	0.40	94,94,94,94	0
55	MG	DA	3085	1/1	0.84	0.14	89,89,89,89	0
55	MG	DA	3086	1/1	0.84	0.18	98,98,98,98	0
55	MG	DA	3466	1/1	0.84	0.28	78,78,78,78	0
55	MG	AA	3190	1/1	0.84	0.53	83,83,83,83	0
55	MG	BA	1728	1/1	0.84	0.09	90,90,90,90	0
55	MG	BA	1732	1/1	0.84	0.14	94,94,94,94	0
55	MG	AA	3418	1/1	0.84	0.52	85,85,85,85	0
55	MG	AA	3193	1/1	0.84	0.22	94,94,94,94	0
55	MG	DA	3328	1/1	0.84	0.24	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	BA	1739	1/1	0.84	0.20	79,79,79,79	0
55	MG	AA	3066	1/1	0.84	0.30	103,103,103,103	0
55	MG	BA	1802	1/1	0.84	0.24	69,69,69,69	0
55	MG	DA	3131	1/1	0.84	0.18	93,93,93,93	0
55	MG	DA	3505	1/1	0.84	0.12	87,87,87,87	0
55	MG	AA	3179	1/1	0.84	0.47	70,70,70,70	0
55	MG	DA	3133	1/1	0.84	0.40	77,77,77,77	0
55	MG	BA	1640	1/1	0.84	0.30	80,80,80,80	0
55	MG	DA	3136	1/1	0.84	0.18	97,97,97,97	0
55	MG	DA	3362	1/1	0.84	0.19	86,86,86,86	0
55	MG	BA	1814	1/1	0.84	0.25	86,86,86,86	0
55	MG	CA	1625	1/1	0.84	0.23	85,85,85,85	0
55	MG	AA	3500	1/1	0.84	0.22	32,32,32,32	0
55	MG	BA	1822	1/1	0.84	0.22	107,107,107,107	0
55	MG	AA	3235	1/1	0.84	0.22	86,86,86,86	0
55	MG	DA	3227	1/1	0.84	0.28	81,81,81,81	0
55	MG	DU	201	1/1	0.84	0.24	72,72,72,72	0
55	MG	D3	101	1/1	0.84	0.27	68,68,68,68	0
55	MG	AA	3259	1/1	0.85	0.10	91,91,91,91	0
55	MG	AA	3490	1/1	0.85	0.17	88,88,88,88	0
55	MG	DA	3184	1/1	0.85	0.23	71,71,71,71	0
55	MG	BA	1737	1/1	0.85	0.13	102,102,102,102	0
55	MG	BA	1825	1/1	0.85	0.21	104,104,104,104	0
55	MG	AA	3298	1/1	0.85	0.28	80,80,80,80	0
55	MG	AA	3434	1/1	0.85	0.17	65,65,65,65	0
55	MG	AB	202	1/1	0.85	0.26	86,86,86,86	0
55	MG	DA	3403	1/1	0.85	0.13	78,78,78,78	0
55	MG	AA	3192	1/1	0.85	0.27	90,90,90,90	0
55	MG	AA	3307	1/1	0.85	0.52	75,75,75,75	0
55	MG	DA	3408	1/1	0.85	0.16	61,61,61,61	0
55	MG	CC	106	1/1	0.85	0.27	115,115,115,115	0
55	MG	AB	211	1/1	0.85	0.23	105,105,105,105	0
55	MG	AA	3364	1/1	0.85	0.35	89,89,89,89	0
55	MG	CA	1702	1/1	0.85	0.29	74,74,74,74	0
55	MG	AA	3310	1/1	0.85	0.18	74,74,74,74	0
55	MG	CA	1707	1/1	0.85	0.57	88,88,88,88	0
55	MG	BA	1750	1/1	0.85	0.32	79,79,79,79	0
55	MG	DA	3430	1/1	0.85	0.28	102,102,102,102	0
55	MG	AA	3509	1/1	0.85	0.42	80,80,80,80	0
55	MG	DA	3023	1/1	0.85	0.57	107,107,107,107	0
55	MG	AA	3264	1/1	0.85	0.29	74,74,74,74	0
55	MG	AA	3415	1/1	0.85	0.22	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	AA	3274	1/1	0.85	0.27	77,77,77,77	0
55	MG	BA	1755	1/1	0.85	0.14	106,106,106,106	0
55	MG	BA	1604	1/1	0.85	0.31	77,77,77,77	0
55	MG	BA	1759	1/1	0.85	0.24	97,97,97,97	0
55	MG	AA	3277	1/1	0.85	0.34	98,98,98,98	0
55	MG	BC	105	1/1	0.85	0.27	95,95,95,95	0
55	MG	AA	3555	1/1	0.85	0.19	68,68,68,68	0
55	MG	AA	3186	1/1	0.85	0.17	77,77,77,77	0
55	MG	AA	3463	1/1	0.85	0.46	108,108,108,108	0
55	MG	AA	3559	1/1	0.85	0.11	93,93,93,93	0
55	MG	DA	3469	1/1	0.85	0.20	64,64,64,64	0
55	MG	DA	3070	1/1	0.85	0.32	73,73,73,73	0
55	MG	BA	1622	1/1	0.85	0.23	84,84,84,84	0
55	MG	CA	1617	1/1	0.85	0.33	91,91,91,91	0
55	MG	AA	3078	1/1	0.85	0.15	84,84,84,84	0
55	MG	AA	3466	1/1	0.85	0.42	106,106,106,106	0
55	MG	DA	3485	1/1	0.85	0.23	40,40,40,40	0
55	MG	DA	3325	1/1	0.85	0.24	70,70,70,70	0
55	MG	AA	3578	1/1	0.85	0.18	52,52,52,52	0
55	MG	AA	3596	1/1	0.85	0.29	87,87,87,87	0
55	MG	DA	3331	1/1	0.85	0.13	76,76,76,76	0
55	MG	BA	1790	1/1	0.85	0.15	83,83,83,83	0
55	MG	AA	3599	1/1	0.85	0.28	84,84,84,84	0
55	MG	BA	1724	1/1	0.85	0.21	100,100,100,100	0
55	MG	DA	3519	1/1	0.85	0.30	114,114,114,114	0
55	MG	AA	3184	1/1	0.85	0.46	90,90,90,90	0
55	MG	BA	1727	1/1	0.85	0.32	125,125,125,125	0
55	MG	CA	1780	1/1	0.85	0.18	124,124,124,124	0
55	MG	DA	3353	1/1	0.85	0.35	70,70,70,70	0
55	MG	DA	3355	1/1	0.85	0.30	93,93,93,93	0
55	MG	AA	3604	1/1	0.85	0.15	84,84,84,84	0
55	MG	DB	207	1/1	0.85	0.23	98,98,98,98	0
55	MG	BA	1729	1/1	0.85	0.16	85,85,85,85	0
55	MG	BA	1731	1/1	0.85	0.31	67,67,67,67	0
55	MG	CA	1640	1/1	0.85	0.26	78,78,78,78	0
55	MG	BA	1818	1/1	0.85	0.16	82,82,82,82	0
55	MG	DA	3376	1/1	0.85	0.13	88,88,88,88	0
55	MG	AA	3428	1/1	0.85	0.26	106,106,106,106	0
55	MG	DA	3183	1/1	0.86	0.24	59,59,59,59	0
55	MG	AA	3013	1/1	0.86	0.22	49,49,49,49	0
55	MG	AA	3630	1/1	0.86	0.21	92,92,92,92	0
55	MG	DA	3192	1/1	0.86	0.25	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	DA	3204	1/1	0.86	0.21	50,50,50,50	0
55	MG	DA	3213	1/1	0.86	0.22	94,94,94,94	0
55	MG	AA	3498	1/1	0.86	0.28	86,86,86,86	0
55	MG	AA	3379	1/1	0.86	0.14	88,88,88,88	0
55	MG	AA	3046	1/1	0.86	0.20	54,54,54,54	0
55	MG	AA	3506	1/1	0.86	0.20	73,73,73,73	0
55	MG	DA	3239	1/1	0.86	0.45	75,75,75,75	0
55	MG	AB	208	1/1	0.86	0.26	87,87,87,87	0
55	MG	AA	3323	1/1	0.86	0.56	93,93,93,93	0
55	MG	AA	3324	1/1	0.86	0.16	60,60,60,60	0
55	MG	DA	3246	1/1	0.86	0.33	66,66,66,66	0
55	MG	AA	3094	1/1	0.86	0.17	81,81,81,81	0
55	MG	AA	3237	1/1	0.86	0.15	81,81,81,81	0
55	MG	DA	3018	1/1	0.86	0.19	85,85,85,85	0
55	MG	DA	3019	1/1	0.86	0.31	66,66,66,66	0
55	MG	AD	302	1/1	0.86	0.15	44,44,44,44	0
55	MG	BA	1767	1/1	0.86	0.23	101,101,101,101	0
55	MG	AA	3523	1/1	0.86	0.21	87,87,87,87	0
55	MG	BA	1700	1/1	0.86	0.26	97,97,97,97	0
55	MG	AA	3529	1/1	0.86	0.29	78,78,78,78	0
55	MG	DA	3273	1/1	0.86	0.12	108,108,108,108	0
55	MG	DA	3274	1/1	0.86	0.58	80,80,80,80	0
55	MG	AA	3447	1/1	0.86	0.10	51,51,51,51	0
55	MG	AA	3176	1/1	0.86	0.34	38,38,38,38	0
55	MG	AA	3554	1/1	0.86	0.19	86,86,86,86	0
55	MG	DA	3442	1/1	0.86	0.38	96,96,96,96	0
55	MG	AA	3345	1/1	0.86	0.17	78,78,78,78	0
55	MG	AA	3126	1/1	0.86	0.18	63,63,63,63	0
55	MG	DA	3288	1/1	0.86	0.21	82,82,82,82	0
55	MG	DA	3062	1/1	0.86	0.11	85,85,85,85	0
55	MG	BA	1615	1/1	0.86	0.27	104,104,104,104	0
55	MG	CA	1755	1/1	0.86	0.53	94,94,94,94	0
55	MG	CA	1756	1/1	0.86	0.21	93,93,93,93	0
55	MG	DA	3305	1/1	0.86	0.13	83,83,83,83	0
55	MG	AA	3181	1/1	0.86	0.23	92,92,92,92	0
55	MG	AA	3219	1/1	0.86	0.29	60,60,60,60	0
55	MG	AA	3412	1/1	0.86	0.47	88,88,88,88	0
55	MG	BA	1624	1/1	0.86	0.24	92,92,92,92	0
55	MG	DA	3078	1/1	0.86	0.15	87,87,87,87	0
55	MG	BA	1625	1/1	0.86	0.20	61,61,61,61	0
55	MG	DA	3489	1/1	0.86	0.41	57,57,57,57	0
55	MG	AA	3561	1/1	0.86	0.18	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	AA	3047	1/1	0.86	0.22	87,87,87,87	0
55	MG	AA	3302	1/1	0.86	0.23	84,84,84,84	0
55	MG	AA	3363	1/1	0.86	0.19	80,80,80,80	0
55	MG	DA	3111	1/1	0.86	0.40	67,67,67,67	0
55	MG	AA	3071	1/1	0.86	0.26	99,99,99,99	0
55	MG	DA	3516	1/1	0.86	0.19	60,60,60,60	0
55	MG	CA	1785	1/1	0.86	0.25	81,81,81,81	0
55	MG	AA	3017	1/1	0.86	0.25	59,59,59,59	0
55	MG	AA	3424	1/1	0.86	0.27	77,77,77,77	0
55	MG	AA	3491	1/1	0.86	0.36	93,93,93,93	0
55	MG	DA	3344	1/1	0.86	0.47	93,93,93,93	0
55	MG	DA	3346	1/1	0.86	0.42	83,83,83,83	0
55	MG	AA	3312	1/1	0.86	0.14	88,88,88,88	0
55	MG	AA	3620	1/1	0.86	0.40	99,99,99,99	0
55	MG	AA	3314	1/1	0.86	0.16	82,82,82,82	0
55	MG	CA	1682	1/1	0.86	0.29	97,97,97,97	0
55	MG	BA	1664	1/1	0.86	0.22	52,52,52,52	0
55	MG	BA	1665	1/1	0.86	0.28	66,66,66,66	0
55	MG	DA	3365	1/1	0.86	0.35	89,89,89,89	0
55	MG	CG	303	1/1	0.86	0.17	100,100,100,100	0
55	MG	AA	3624	1/1	0.86	0.20	80,80,80,80	0
55	MG	CA	1680	1/1	0.87	0.31	68,68,68,68	0
55	MG	DA	3180	1/1	0.87	0.34	50,50,50,50	0
55	MG	BA	1835	1/1	0.87	0.43	82,82,82,82	0
55	MG	DA	3368	1/1	0.87	0.20	87,87,87,87	0
55	MG	AA	3303	1/1	0.87	0.20	91,91,91,91	0
55	MG	DA	3375	1/1	0.87	0.14	82,82,82,82	0
55	MG	AA	3526	1/1	0.87	0.21	57,57,57,57	0
55	MG	AA	3468	1/1	0.87	0.15	92,92,92,92	0
55	MG	DA	3198	1/1	0.87	0.28	68,68,68,68	0
55	MG	CA	1691	1/1	0.87	0.24	69,69,69,69	0
55	MG	BA	1631	1/1	0.87	0.11	67,67,67,67	0
55	MG	BA	1764	1/1	0.87	0.29	93,93,93,93	0
55	MG	AA	3530	1/1	0.87	0.11	65,65,65,65	0
55	MG	CA	1703	1/1	0.87	0.10	88,88,88,88	0
55	MG	BB	102	1/1	0.87	0.18	86,86,86,86	0
55	MG	AA	3471	1/1	0.87	0.16	69,69,69,69	0
55	MG	DA	3240	1/1	0.87	0.44	80,80,80,80	0
55	MG	AA	3334	1/1	0.87	0.18	73,73,73,73	0
55	MG	CA	1711	1/1	0.87	0.26	88,88,88,88	0
55	MG	DA	3407	1/1	0.87	0.13	80,80,80,80	0
55	MG	BA	1769	1/1	0.87	0.35	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	AA	3171	1/1	0.87	0.14	81,81,81,81	0
55	MG	CA	1717	1/1	0.87	0.23	106,106,106,106	0
55	MG	DA	3414	1/1	0.87	0.30	74,74,74,74	0
55	MG	AA	3483	1/1	0.87	0.23	70,70,70,70	0
55	MG	BA	1643	1/1	0.87	0.20	80,80,80,80	0
55	MG	BA	1783	1/1	0.87	0.18	91,91,91,91	0
55	MG	DA	3256	1/1	0.87	0.30	82,82,82,82	0
55	MG	DA	3033	1/1	0.87	0.25	94,94,94,94	0
55	MG	DA	3035	1/1	0.87	0.24	102,102,102,102	0
55	MG	DA	3036	1/1	0.87	0.50	87,87,87,87	0
55	MG	CA	1725	1/1	0.87	0.24	75,75,75,75	0
55	MG	AB	210	1/1	0.87	0.46	71,71,71,71	0
55	MG	DA	3435	1/1	0.87	0.23	104,104,104,104	0
55	MG	AA	3373	1/1	0.87	0.26	71,71,71,71	0
55	MG	CA	1609	1/1	0.87	0.25	108,108,108,108	0
55	MG	DA	3275	1/1	0.87	0.37	81,81,81,81	0
55	MG	DA	3055	1/1	0.87	0.43	80,80,80,80	0
55	MG	AA	3488	1/1	0.87	0.19	94,94,94,94	0
55	MG	CA	1613	1/1	0.87	0.39	84,84,84,84	0
55	MG	DA	3281	1/1	0.87	0.18	75,75,75,75	0
55	MG	AA	3441	1/1	0.87	0.09	76,76,76,76	0
55	MG	AA	3233	1/1	0.87	0.10	74,74,74,74	0
55	MG	AA	3414	1/1	0.87	0.15	68,68,68,68	0
55	MG	BA	1794	1/1	0.87	0.44	94,94,94,94	0
55	MG	BA	1734	1/1	0.87	0.30	96,96,96,96	0
55	MG	BA	1799	1/1	0.87	0.28	85,85,85,85	0
55	MG	AE	303	1/1	0.87	0.15	91,91,91,91	0
55	MG	AA	3570	1/1	0.87	0.17	49,49,49,49	0
55	MG	DA	3474	1/1	0.87	0.29	103,103,103,103	0
55	MG	AA	3044	1/1	0.87	0.43	54,54,54,54	0
55	MG	BA	1806	1/1	0.87	0.21	75,75,75,75	0
55	MG	DA	3480	1/1	0.87	0.32	56,56,56,56	0
55	MG	DA	3082	1/1	0.87	0.23	83,83,83,83	0
55	MG	BA	1808	1/1	0.87	0.31	69,69,69,69	0
55	MG	AA	3417	1/1	0.87	0.13	78,78,78,78	0
55	MG	DA	3496	1/1	0.87	0.31	85,85,85,85	0
55	MG	CA	1766	1/1	0.87	0.24	75,75,75,75	0
55	MG	DA	3319	1/1	0.87	0.33	68,68,68,68	0
55	MG	BA	1675	1/1	0.87	0.19	89,89,89,89	0
55	MG	AO	203	1/1	0.87	0.34	63,63,63,63	0
55	MG	AA	3091	1/1	0.87	0.30	69,69,69,69	0
55	MG	AA	3208	1/1	0.87	0.20	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	DA	3329	1/1	0.87	0.27	80,80,80,80	0
55	MG	CA	1779	1/1	0.87	0.26	82,82,82,82	0
55	MG	DA	3120	1/1	0.87	0.31	78,78,78,78	0
55	MG	BA	1607	1/1	0.87	0.12	87,87,87,87	0
55	MG	CA	1653	1/1	0.87	0.33	73,73,73,73	0
55	MG	DA	3522	1/1	0.87	0.36	85,85,85,85	0
55	MG	CA	1654	1/1	0.87	0.21	88,88,88,88	0
55	MG	AA	3452	1/1	0.87	0.34	95,95,95,95	0
55	MG	DA	3527	1/1	0.87	0.29	96,96,96,96	0
55	MG	AA	3260	1/1	0.87	0.17	70,70,70,70	0
55	MG	AA	3611	1/1	0.87	0.31	54,54,54,54	0
55	MG	AA	3390	1/1	0.87	0.20	73,73,73,73	0
55	MG	AA	3098	1/1	0.87	0.20	71,71,71,71	0
55	MG	DB	209	1/1	0.87	0.25	103,103,103,103	0
55	MG	DA	3354	1/1	0.87	0.38	92,92,92,92	0
55	MG	AA	3242	1/1	0.87	0.28	58,58,58,58	0
55	MG	DB	213	1/1	0.87	0.13	90,90,90,90	0
55	MG	DA	3137	1/1	0.87	0.18	78,78,78,78	0
55	MG	DA	3359	1/1	0.87	0.17	75,75,75,75	0
55	MG	AA	3272	1/1	0.87	0.24	86,86,86,86	0
55	MG	CA	1724	1/1	0.88	0.31	88,88,88,88	0
55	MG	AA	3287	1/1	0.88	0.23	88,88,88,88	0
55	MG	AA	3369	1/1	0.88	0.26	85,85,85,85	0
55	MG	DA	3218	1/1	0.88	0.47	75,75,75,75	0
55	MG	AA	3182	1/1	0.88	0.33	77,77,77,77	0
55	MG	CA	1731	1/1	0.88	0.43	85,85,85,85	0
55	MG	BA	1652	1/1	0.88	0.20	86,86,86,86	0
55	MG	DA	3391	1/1	0.88	0.26	86,86,86,86	0
55	MG	AA	3535	1/1	0.88	0.16	82,82,82,82	0
55	MG	AA	3541	1/1	0.88	0.12	94,94,94,94	0
55	MG	AA	3289	1/1	0.88	0.28	62,62,62,62	0
55	MG	AA	3374	1/1	0.88	0.32	96,96,96,96	0
55	MG	DA	3043	1/1	0.88	0.22	81,81,81,81	0
55	MG	AA	3292	1/1	0.88	0.24	80,80,80,80	0
55	MG	AA	3481	1/1	0.88	0.27	66,66,66,66	0
55	MG	BA	1815	1/1	0.88	0.49	81,81,81,81	0
55	MG	BA	1817	1/1	0.88	0.33	92,92,92,92	0
55	MG	AA	3122	1/1	0.88	0.23	87,87,87,87	0
55	MG	DA	3057	1/1	0.88	0.32	81,81,81,81	0
55	MG	DA	3257	1/1	0.88	0.16	75,75,75,75	0
55	MG	AA	3330	1/1	0.88	0.13	61,61,61,61	0
55	MG	DA	3417	1/1	0.88	0.26	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	AA	3384	1/1	0.88	0.38	79,79,79,79	0
55	MG	CA	1760	1/1	0.88	0.30	103,103,103,103	0
55	MG	AA	3568	1/1	0.88	0.25	29,29,29,29	0
55	MG	A3	101	1/1	0.88	0.48	80,80,80,80	0
55	MG	AA	3295	1/1	0.88	0.29	70,70,70,70	0
55	MG	AA	3069	1/1	0.88	0.36	64,64,64,64	0
55	MG	AA	3493	1/1	0.88	0.27	89,89,89,89	0
55	MG	BA	1830	1/1	0.88	0.25	96,96,96,96	0
55	MG	CA	1660	1/1	0.88	0.17	76,76,76,76	0
55	MG	BA	1608	1/1	0.88	0.31	63,63,63,63	0
55	MG	DA	3081	1/1	0.88	0.18	73,73,73,73	0
55	MG	AA	3593	1/1	0.88	0.29	90,90,90,90	0
55	MG	DA	3284	1/1	0.88	0.18	81,81,81,81	0
55	MG	AA	3437	1/1	0.88	0.20	105,105,105,105	0
55	MG	BA	1696	1/1	0.88	0.38	90,90,90,90	0
55	MG	DA	3443	1/1	0.88	0.27	94,94,94,94	0
55	MG	AA	3338	1/1	0.88	0.18	72,72,72,72	0
55	MG	DA	3297	1/1	0.88	0.29	70,70,70,70	0
55	MG	BA	1761	1/1	0.88	0.35	85,85,85,85	0
55	MG	DA	3103	1/1	0.88	0.14	82,82,82,82	0
55	MG	DA	3451	1/1	0.88	0.25	65,65,65,65	0
55	MG	DA	3107	1/1	0.88	0.35	89,89,89,89	0
55	MG	DA	3304	1/1	0.88	0.26	106,106,106,106	0
55	MG	DA	3108	1/1	0.88	0.23	69,69,69,69	0
55	MG	DA	3307	1/1	0.88	0.35	77,77,77,77	0
55	MG	DA	3471	1/1	0.88	0.44	89,89,89,89	0
55	MG	CA	1788	1/1	0.88	0.30	68,68,68,68	0
55	MG	BA	1762	1/1	0.88	0.25	85,85,85,85	0
55	MG	DA	3310	1/1	0.88	0.24	80,80,80,80	0
55	MG	DA	3114	1/1	0.88	0.53	70,70,70,70	0
55	MG	CA	1790	1/1	0.88	0.23	75,75,75,75	0
55	MG	AA	3261	1/1	0.88	0.16	30,30,30,30	0
55	MG	DA	3317	1/1	0.88	0.18	87,87,87,87	0
55	MG	AA	3299	1/1	0.88	0.23	94,94,94,94	0
55	MG	DA	3121	1/1	0.88	0.20	99,99,99,99	0
55	MG	DA	3494	1/1	0.88	0.43	81,81,81,81	0
55	MG	BA	1705	1/1	0.88	0.40	70,70,70,70	0
55	MG	BB	101	1/1	0.88	0.12	88,88,88,88	0
55	MG	AA	3203	1/1	0.88	0.32	53,53,53,53	0
55	MG	CA	1696	1/1	0.88	0.21	79,79,79,79	0
55	MG	AA	3226	1/1	0.88	0.31	85,85,85,85	0
55	MG	AA	3448	1/1	0.88	0.20	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	AA	3270	1/1	0.88	0.18	96,96,96,96	0
55	MG	DA	3507	1/1	0.88	0.26	88,88,88,88	0
55	MG	DA	3512	1/1	0.88	0.34	70,70,70,70	0
55	MG	CS	101	1/1	0.88	0.18	84,84,84,84	0
55	MG	DA	3339	1/1	0.88	0.38	77,77,77,77	0
55	MG	AA	3621	1/1	0.88	0.16	100,100,100,100	0
55	MG	AA	3306	1/1	0.88	0.33	63,63,63,63	0
55	MG	DA	3156	1/1	0.88	0.72	62,62,62,62	0
55	MG	DA	3158	1/1	0.88	0.19	77,77,77,77	0
55	MG	AA	3512	1/1	0.88	0.47	71,71,71,71	0
55	MG	DA	3348	1/1	0.88	0.24	77,77,77,77	0
55	MG	DA	3349	1/1	0.88	0.25	83,83,83,83	0
55	MG	DA	3164	1/1	0.88	0.20	65,65,65,65	0
55	MG	DA	3167	1/1	0.88	0.12	72,72,72,72	0
55	MG	BA	1721	1/1	0.88	0.26	109,109,109,109	0
55	MG	BC	108	1/1	0.88	0.24	101,101,101,101	0
55	MG	AA	3247	1/1	0.88	0.26	76,76,76,76	0
55	MG	AA	3360	1/1	0.88	0.27	89,89,89,89	0
55	MG	DB	211	1/1	0.88	0.27	104,104,104,104	0
55	MG	AA	3043	1/1	0.88	0.24	83,83,83,83	0
55	MG	DA	3191	1/1	0.88	0.28	47,47,47,47	0
55	MG	AA	3210	1/1	0.88	0.24	58,58,58,58	0
55	MG	D1	202	1/1	0.88	0.19	102,102,102,102	0
55	MG	AA	3121	1/1	0.88	0.39	93,93,93,93	0
55	MG	DA	3200	1/1	0.88	0.41	66,66,66,66	0
55	MG	DA	3379	1/1	0.89	0.52	99,99,99,99	0
55	MG	AA	3207	1/1	0.89	0.32	44,44,44,44	0
55	MG	DA	3237	1/1	0.89	0.42	84,84,84,84	0
55	MG	BA	1653	1/1	0.89	0.29	91,91,91,91	0
55	MG	BA	1730	1/1	0.89	0.25	97,97,97,97	0
55	MG	DA	3042	1/1	0.89	0.09	84,84,84,84	0
55	MG	CA	1732	1/1	0.89	0.18	93,93,93,93	0
55	MG	AA	3010	1/1	0.89	0.38	52,52,52,52	0
55	MG	AA	3449	1/1	0.89	0.14	76,76,76,76	0
55	MG	DA	3047	1/1	0.89	0.24	84,84,84,84	0
55	MG	DA	3399	1/1	0.89	0.24	97,97,97,97	0
55	MG	DA	3402	1/1	0.89	0.19	73,73,73,73	0
55	MG	DA	3051	1/1	0.89	0.24	81,81,81,81	0
55	MG	AA	3246	1/1	0.89	0.41	73,73,73,73	0
55	MG	DA	3251	1/1	0.89	0.15	50,50,50,50	0
55	MG	BA	1668	1/1	0.89	0.36	73,73,73,73	0
55	MG	DA	3254	1/1	0.89	0.33	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	AA	3610	1/1	0.89	0.26	34,34,34,34	0
55	MG	AA	3263	1/1	0.89	0.19	56,56,56,56	0
55	MG	A6	101	1/1	0.89	0.29	121,121,121,121	0
55	MG	CA	1752	1/1	0.89	0.09	70,70,70,70	0
55	MG	BA	1601	1/1	0.89	0.48	65,65,65,65	0
55	MG	DA	3268	1/1	0.89	0.20	82,82,82,82	0
55	MG	AA	3613	1/1	0.89	0.10	104,104,104,104	0
55	MG	CA	1633	1/1	0.89	0.40	79,79,79,79	0
55	MG	BA	1676	1/1	0.89	0.21	81,81,81,81	0
55	MG	AA	3533	1/1	0.89	0.16	89,89,89,89	0
55	MG	CA	1636	1/1	0.89	0.25	80,80,80,80	0
55	MG	AA	3147	1/1	0.89	0.37	77,77,77,77	0
55	MG	BA	1679	1/1	0.89	0.25	86,86,86,86	0
55	MG	AA	3061	1/1	0.89	0.18	75,75,75,75	0
55	MG	CA	1642	1/1	0.89	0.22	78,78,78,78	0
55	MG	AA	3372	1/1	0.89	0.22	77,77,77,77	0
55	MG	CA	1644	1/1	0.89	0.14	59,59,59,59	0
55	MG	CA	1772	1/1	0.89	0.17	76,76,76,76	0
55	MG	DA	3286	1/1	0.89	0.12	86,86,86,86	0
55	MG	AA	3543	1/1	0.89	0.30	61,61,61,61	0
55	MG	BA	1613	1/1	0.89	0.13	96,96,96,96	0
55	MG	DA	3096	1/1	0.89	0.22	47,47,47,47	0
55	MG	DA	3101	1/1	0.89	0.41	57,57,57,57	0
55	MG	DA	3448	1/1	0.89	0.20	75,75,75,75	0
55	MG	CA	1655	1/1	0.89	0.50	87,87,87,87	0
55	MG	BA	1687	1/1	0.89	0.34	74,74,74,74	0
55	MG	AA	3183	1/1	0.89	0.09	79,79,79,79	0
55	MG	AA	3626	1/1	0.89	0.34	63,63,63,63	0
55	MG	BA	1618	1/1	0.89	0.30	94,94,94,94	0
55	MG	CA	1787	1/1	0.89	0.28	84,84,84,84	0
55	MG	AA	3173	1/1	0.89	0.33	70,70,70,70	0
55	MG	AA	3322	1/1	0.89	0.15	83,83,83,83	0
55	MG	DA	3118	1/1	0.89	0.56	72,72,72,72	0
55	MG	AA	3222	1/1	0.89	0.17	59,59,59,59	0
55	MG	AA	3438	1/1	0.89	0.15	77,77,77,77	0
55	MG	CA	1679	1/1	0.89	0.17	84,84,84,84	0
55	MG	CA	1798	1/1	0.89	0.25	96,96,96,96	0
55	MG	BA	1843	1/1	0.89	0.14	87,87,87,87	0
55	MG	DA	3321	1/1	0.89	0.26	81,81,81,81	0
55	MG	DA	3323	1/1	0.89	0.38	85,85,85,85	0
55	MG	AA	3507	1/1	0.89	0.17	62,62,62,62	0
55	MG	AB	204	1/1	0.89	0.27	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	BA	1630	1/1	0.89	0.15	105,105,105,105	0
55	MG	AB	206	1/1	0.89	0.23	97,97,97,97	0
55	MG	CA	1690	1/1	0.89	0.34	74,74,74,74	0
55	MG	BA	1768	1/1	0.89	0.18	86,86,86,86	0
55	MG	BA	1711	1/1	0.89	0.40	86,86,86,86	0
55	MG	DA	3142	1/1	0.89	0.28	51,51,51,51	0
55	MG	DA	3151	1/1	0.89	0.28	75,75,75,75	0
55	MG	AA	3279	1/1	0.89	0.10	81,81,81,81	0
55	MG	DA	3513	1/1	0.89	0.23	103,103,103,103	0
55	MG	BA	1771	1/1	0.89	0.16	100,100,100,100	0
55	MG	DA	3162	1/1	0.89	0.42	70,70,70,70	0
55	MG	CB	103	1/1	0.89	0.20	110,110,110,110	0
55	MG	AA	3416	1/1	0.89	0.23	70,70,70,70	0
55	MG	BA	1776	1/1	0.89	0.15	84,84,84,84	0
55	MG	AA	3149	1/1	0.89	0.28	49,49,49,49	0
55	MG	AA	3480	1/1	0.89	0.14	77,77,77,77	0
55	MG	AB	214	1/1	0.89	0.05	88,88,88,88	0
55	MG	BC	106	1/1	0.89	0.18	80,80,80,80	0
55	MG	DB	201	1/1	0.89	0.20	77,77,77,77	0
55	MG	DB	202	1/1	0.89	0.25	101,101,101,101	0
55	MG	AA	3520	1/1	0.89	0.38	97,97,97,97	0
55	MG	BC	109	1/1	0.89	0.24	92,92,92,92	0
55	MG	BA	1786	1/1	0.89	0.24	72,72,72,72	0
55	MG	DA	3012	1/1	0.89	0.15	64,64,64,64	0
55	MG	DA	3015	1/1	0.89	0.12	83,83,83,83	0
55	MG	CA	1601	1/1	0.89	0.29	95,95,95,95	0
55	MG	AA	3591	1/1	0.89	0.51	80,80,80,80	0
55	MG	CA	1721	1/1	0.89	0.16	94,94,94,94	0
55	MG	DA	3370	1/1	0.89	0.29	85,85,85,85	0
55	MG	CA	1607	1/1	0.89	0.28	77,77,77,77	0
55	MG	DA	3221	1/1	0.89	0.48	66,66,66,66	0
55	MG	AA	3362	1/1	0.89	0.27	86,86,86,86	0
55	MG	AA	3594	1/1	0.89	0.23	97,97,97,97	0
55	MG	DA	3140	1/1	0.90	0.31	49,49,49,49	0
55	MG	AA	3064	1/1	0.90	0.21	77,77,77,77	0
55	MG	CA	1668	1/1	0.90	0.30	75,75,75,75	0
55	MG	CA	1673	1/1	0.90	0.22	65,65,65,65	0
55	MG	CA	1675	1/1	0.90	0.31	65,65,65,65	0
55	MG	AA	3036	1/1	0.90	0.20	34,34,34,34	0
55	MG	AA	3304	1/1	0.90	0.22	59,59,59,59	0
55	MG	BA	1837	1/1	0.90	0.27	88,88,88,88	0
55	MG	DA	3166	1/1	0.90	0.25	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	AA	3113	1/1	0.90	0.35	55,55,55,55	0
55	MG	DA	3170	1/1	0.90	0.30	66,66,66,66	0
55	MG	BA	1839	1/1	0.90	0.23	61,61,61,61	0
55	MG	BA	1666	1/1	0.90	0.31	74,74,74,74	0
55	MG	DA	3374	1/1	0.90	0.34	72,72,72,72	0
55	MG	BA	1667	1/1	0.90	0.34	78,78,78,78	0
55	MG	AB	209	1/1	0.90	0.22	103,103,103,103	0
55	MG	AA	3467	1/1	0.90	0.18	83,83,83,83	0
55	MG	DA	3188	1/1	0.90	0.32	48,48,48,48	0
55	MG	DA	3381	1/1	0.90	0.27	89,89,89,89	0
55	MG	DA	3190	1/1	0.90	0.17	46,46,46,46	0
55	MG	AA	3162	1/1	0.90	0.28	45,45,45,45	0
55	MG	DA	3389	1/1	0.90	0.33	85,85,85,85	0
55	MG	AB	212	1/1	0.90	0.22	76,76,76,76	0
55	MG	DA	3195	1/1	0.90	0.14	73,73,73,73	0
55	MG	AA	3269	1/1	0.90	0.34	72,72,72,72	0
55	MG	AA	3545	1/1	0.90	0.26	72,72,72,72	0
55	MG	AA	3093	1/1	0.90	0.15	55,55,55,55	0
55	MG	DA	3206	1/1	0.90	0.23	65,65,65,65	0
55	MG	DA	3207	1/1	0.90	0.20	61,61,61,61	0
55	MG	AA	3421	1/1	0.90	0.39	64,64,64,64	0
55	MG	CA	1708	1/1	0.90	0.22	91,91,91,91	0
55	MG	AA	3195	1/1	0.90	0.21	62,62,62,62	0
55	MG	AA	3557	1/1	0.90	0.27	68,68,68,68	0
55	MG	BB	108	1/1	0.90	0.24	106,106,106,106	0
55	MG	CA	1714	1/1	0.90	0.17	115,115,115,115	0
55	MG	DA	3232	1/1	0.90	0.12	75,75,75,75	0
55	MG	AA	3196	1/1	0.90	0.20	60,60,60,60	0
55	MG	DA	3024	1/1	0.90	0.17	100,100,100,100	0
55	MG	CA	1716	1/1	0.90	0.25	78,78,78,78	0
55	MG	DA	3027	1/1	0.90	0.24	93,93,93,93	0
55	MG	DA	3028	1/1	0.90	0.16	71,71,71,71	0
55	MG	DA	3242	1/1	0.90	0.44	61,61,61,61	0
55	MG	DA	3029	1/1	0.90	0.12	92,92,92,92	0
55	MG	AA	3276	1/1	0.90	0.25	59,59,59,59	0
55	MG	DA	3427	1/1	0.90	0.21	78,78,78,78	0
55	MG	AA	3484	1/1	0.90	0.12	86,86,86,86	0
55	MG	AA	3485	1/1	0.90	0.19	96,96,96,96	0
55	MG	DA	3037	1/1	0.90	0.12	84,84,84,84	0
55	MG	AA	3037	1/1	0.90	0.18	50,50,50,50	0
55	MG	DA	3039	1/1	0.90	0.30	82,82,82,82	0
55	MG	DA	3434	1/1	0.90	0.10	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	DA	3041	1/1	0.90	0.20	91,91,91,91	0
55	MG	BA	1689	1/1	0.90	0.17	110,110,110,110	0
55	MG	AA	3004	1/1	0.90	0.18	37,37,37,37	0
55	MG	AA	3489	1/1	0.90	0.16	93,93,93,93	0
55	MG	CA	1604	1/1	0.90	0.19	78,78,78,78	0
55	MG	AA	3282	1/1	0.90	0.42	87,87,87,87	0
55	MG	AA	3284	1/1	0.90	0.48	80,80,80,80	0
55	MG	AA	3205	1/1	0.90	0.29	43,43,43,43	0
55	MG	BA	1699	1/1	0.90	0.19	58,58,58,58	0
55	MG	CA	1736	1/1	0.90	0.24	90,90,90,90	0
55	MG	CA	1741	1/1	0.90	0.17	83,83,83,83	0
55	MG	AA	3494	1/1	0.90	0.31	88,88,88,88	0
55	MG	CA	1743	1/1	0.90	0.40	71,71,71,71	0
55	MG	AA	3245	1/1	0.90	0.25	81,81,81,81	0
55	MG	DA	3277	1/1	0.90	0.20	77,77,77,77	0
55	MG	BA	1610	1/1	0.90	0.30	53,53,53,53	0
55	MG	AA	3598	1/1	0.90	0.17	84,84,84,84	0
55	MG	AA	3123	1/1	0.90	0.30	47,47,47,47	0
55	MG	DA	3282	1/1	0.90	0.32	55,55,55,55	0
55	MG	AA	3439	1/1	0.90	0.09	93,93,93,93	0
55	MG	AA	3602	1/1	0.90	0.12	70,70,70,70	0
55	MG	DA	3074	1/1	0.90	0.34	89,89,89,89	0
55	MG	DA	3075	1/1	0.90	0.37	80,80,80,80	0
55	MG	AA	3337	1/1	0.90	0.40	88,88,88,88	0
55	MG	AA	3075	1/1	0.90	0.08	71,71,71,71	0
55	MG	AA	3178	1/1	0.90	0.26	49,49,49,49	0
55	MG	DA	3080	1/1	0.90	0.15	114,114,114,114	0
55	MG	DA	3491	1/1	0.90	0.16	43,43,43,43	0
55	MG	AA	3127	1/1	0.90	0.21	47,47,47,47	0
55	MG	CA	1757	1/1	0.90	0.18	83,83,83,83	0
55	MG	BA	1801	1/1	0.90	0.12	93,93,93,93	0
55	MG	AA	3129	1/1	0.90	0.31	75,75,75,75	0
55	MG	BA	1722	1/1	0.90	0.20	90,90,90,90	0
55	MG	AA	3100	1/1	0.90	0.14	79,79,79,79	0
55	MG	AA	3400	1/1	0.90	0.23	86,86,86,86	0
55	MG	DA	3097	1/1	0.90	0.25	42,42,42,42	0
55	MG	DA	3100	1/1	0.90	0.34	62,62,62,62	0
55	MG	CA	1765	1/1	0.90	0.34	97,97,97,97	0
55	MG	AA	3510	1/1	0.90	0.26	73,73,73,73	0
55	MG	CA	1768	1/1	0.90	0.38	115,115,115,115	0
55	MG	BA	1811	1/1	0.90	0.27	86,86,86,86	0
55	MG	AA	3511	1/1	0.90	0.23	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	BA	1633	1/1	0.90	0.31	75,75,75,75	0
55	MG	BA	1635	1/1	0.90	0.18	87,87,87,87	0
55	MG	AA	3404	1/1	0.90	0.13	89,89,89,89	0
55	MG	CA	1647	1/1	0.90	0.33	65,65,65,65	0
55	MG	DA	3117	1/1	0.90	0.24	68,68,68,68	0
55	MG	CA	1650	1/1	0.90	0.24	90,90,90,90	0
55	MG	AA	3625	1/1	0.90	0.30	70,70,70,70	0
55	MG	BA	1820	1/1	0.90	0.32	97,97,97,97	0
55	MG	AA	3258	1/1	0.90	0.21	80,80,80,80	0
55	MG	DB	205	1/1	0.90	0.34	90,90,90,90	0
55	MG	CA	1656	1/1	0.90	0.17	87,87,87,87	0
55	MG	AA	3627	1/1	0.90	0.26	108,108,108,108	0
55	MG	AA	3628	1/1	0.90	0.14	89,89,89,89	0
55	MG	DA	3341	1/1	0.90	0.33	62,62,62,62	0
55	MG	AA	3410	1/1	0.90	0.12	99,99,99,99	0
55	MG	AA	3453	1/1	0.90	0.20	47,47,47,47	0
55	MG	AA	3048	1/1	0.90	0.19	63,63,63,63	0
55	MG	DA	3345	1/1	0.90	0.17	75,75,75,75	0
55	MG	AA	3459	1/1	0.90	0.23	110,110,110,110	0
55	MG	DE	302	1/1	0.90	0.25	75,75,75,75	0
55	MG	CA	1799	1/1	0.90	0.25	95,95,95,95	0
55	MG	AA	3062	1/1	0.90	0.12	73,73,73,73	0
55	MG	DA	3351	1/1	0.90	0.29	70,70,70,70	0
55	MG	AA	3191	1/1	0.91	0.33	61,61,61,61	0
55	MG	AA	3227	1/1	0.91	0.35	66,66,66,66	0
55	MG	AA	3012	1/1	0.91	0.28	45,45,45,45	0
55	MG	AA	3168	1/1	0.91	0.24	64,64,64,64	0
55	MG	DA	3199	1/1	0.91	0.18	49,49,49,49	0
55	MG	DA	3371	1/1	0.91	0.63	82,82,82,82	0
55	MG	BA	1602	1/1	0.91	0.20	65,65,65,65	0
55	MG	DA	3373	1/1	0.91	0.17	90,90,90,90	0
55	MG	AA	3354	1/1	0.91	0.36	79,79,79,79	0
55	MG	AA	3603	1/1	0.91	0.18	65,65,65,65	0
55	MG	CA	1641	1/1	0.91	0.11	101,101,101,101	0
55	MG	AA	3405	1/1	0.91	0.25	86,86,86,86	0
55	MG	AA	3006	1/1	0.91	0.55	60,60,60,60	0
55	MG	AA	3407	1/1	0.91	0.21	84,84,84,84	0
55	MG	DA	3219	1/1	0.91	0.15	79,79,79,79	0
55	MG	BA	1832	1/1	0.91	0.18	100,100,100,100	0
55	MG	BA	1682	1/1	0.91	0.28	98,98,98,98	0
55	MG	CA	1651	1/1	0.91	0.21	79,79,79,79	0
55	MG	DA	3050	1/1	0.91	0.53	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	DA	3234	1/1	0.91	0.36	55,55,55,55	0
55	MG	AA	3234	1/1	0.91	0.16	83,83,83,83	0
55	MG	DA	3053	1/1	0.91	0.15	86,86,86,86	0
55	MG	DA	3238	1/1	0.91	0.34	80,80,80,80	0
55	MG	AA	3361	1/1	0.91	0.21	88,88,88,88	0
55	MG	BA	1756	1/1	0.91	0.22	96,96,96,96	0
55	MG	BA	1612	1/1	0.91	0.23	90,90,90,90	0
55	MG	AA	3516	1/1	0.91	0.21	57,57,57,57	0
55	MG	BA	1614	1/1	0.91	0.28	93,93,93,93	0
55	MG	AA	3172	1/1	0.91	0.22	102,102,102,102	0
55	MG	DA	3061	1/1	0.91	0.28	67,67,67,67	0
55	MG	AA	3413	1/1	0.91	0.24	82,82,82,82	0
55	MG	CA	1767	1/1	0.91	0.20	94,94,94,94	0
55	MG	BA	1694	1/1	0.91	0.11	99,99,99,99	0
55	MG	BN	201	1/1	0.91	0.22	67,67,67,67	0
55	MG	DA	3415	1/1	0.91	0.15	84,84,84,84	0
55	MG	AA	3079	1/1	0.91	0.22	100,100,100,100	0
55	MG	DA	3420	1/1	0.91	0.34	73,73,73,73	0
55	MG	CA	1771	1/1	0.91	0.26	64,64,64,64	0
55	MG	DA	3255	1/1	0.91	0.27	83,83,83,83	0
55	MG	CA	1666	1/1	0.91	0.31	76,76,76,76	0
55	MG	AA	3311	1/1	0.91	0.29	58,58,58,58	0
55	MG	DA	3260	1/1	0.91	0.16	82,82,82,82	0
55	MG	CA	1775	1/1	0.91	0.31	66,66,66,66	0
55	MG	CA	1776	1/1	0.91	0.13	91,91,91,91	0
55	MG	DA	3266	1/1	0.91	0.28	97,97,97,97	0
55	MG	AA	3525	1/1	0.91	0.20	67,67,67,67	0
55	MG	CA	1669	1/1	0.91	0.17	67,67,67,67	0
55	MG	CA	1672	1/1	0.91	0.36	76,76,76,76	0
55	MG	CA	1781	1/1	0.91	0.31	92,92,92,92	0
55	MG	DA	3083	1/1	0.91	0.36	108,108,108,108	0
55	MG	AA	3175	1/1	0.91	0.27	70,70,70,70	0
55	MG	CA	1783	1/1	0.91	0.20	72,72,72,72	0
55	MG	CA	1784	1/1	0.91	0.45	102,102,102,102	0
55	MG	DA	3088	1/1	0.91	0.35	49,49,49,49	0
55	MG	BB	103	1/1	0.91	0.33	87,87,87,87	0
55	MG	AA	3086	1/1	0.91	0.31	70,70,70,70	0
55	MG	DA	3445	1/1	0.91	0.18	72,72,72,72	0
55	MG	AA	3315	1/1	0.91	0.19	68,68,68,68	0
55	MG	DA	3099	1/1	0.91	0.22	51,51,51,51	0
55	MG	BA	1703	1/1	0.91	0.23	118,118,118,118	0
55	MG	CA	1684	1/1	0.91	0.37	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	DA	3450	1/1	0.91	0.30	86,86,86,86	0
55	MG	DA	3102	1/1	0.91	0.36	72,72,72,72	0
55	MG	BA	1772	1/1	0.91	0.10	89,89,89,89	0
55	MG	DA	3454	1/1	0.91	0.25	108,108,108,108	0
55	MG	CA	1793	1/1	0.91	0.26	78,78,78,78	0
55	MG	DA	3458	1/1	0.91	0.22	88,88,88,88	0
55	MG	DA	3462	1/1	0.91	0.26	67,67,67,67	0
55	MG	AA	3135	1/1	0.91	0.24	66,66,66,66	0
55	MG	BA	1629	1/1	0.91	0.10	100,100,100,100	0
55	MG	DA	3298	1/1	0.91	0.13	95,95,95,95	0
55	MG	AA	3475	1/1	0.91	0.24	67,67,67,67	0
55	MG	AA	3476	1/1	0.91	0.18	94,94,94,94	0
55	MG	AA	3141	1/1	0.91	0.33	37,37,37,37	0
55	MG	CA	1695	1/1	0.91	0.34	77,77,77,77	0
55	MG	BC	107	1/1	0.91	0.12	88,88,88,88	0
55	MG	CA	1698	1/1	0.91	0.15	104,104,104,104	0
55	MG	CA	1807	1/1	0.91	0.31	121,121,121,121	0
55	MG	AA	3283	1/1	0.91	0.30	74,74,74,74	0
55	MG	AA	3479	1/1	0.91	0.20	97,97,97,97	0
55	MG	AA	3011	1/1	0.91	0.28	38,38,38,38	0
55	MG	AA	3377	1/1	0.91	0.17	85,85,85,85	0
55	MG	DA	3314	1/1	0.91	0.15	78,78,78,78	0
55	MG	CA	1705	1/1	0.91	0.21	86,86,86,86	0
55	MG	DA	3316	1/1	0.91	0.14	87,87,87,87	0
55	MG	BA	1719	1/1	0.91	0.28	91,91,91,91	0
55	MG	CA	1605	1/1	0.91	0.36	72,72,72,72	0
55	MG	AA	3482	1/1	0.91	0.16	82,82,82,82	0
55	MG	DA	3134	1/1	0.91	0.34	56,56,56,56	0
55	MG	DA	3506	1/1	0.91	0.41	80,80,80,80	0
55	MG	AA	3041	1/1	0.91	0.30	62,62,62,62	0
55	MG	DA	3511	1/1	0.91	0.27	65,65,65,65	0
55	MG	CC	104	1/1	0.91	0.18	90,90,90,90	0
55	MG	CC	105	1/1	0.91	0.24	74,74,74,74	0
55	MG	DA	3138	1/1	0.91	0.41	71,71,71,71	0
55	MG	DA	3517	1/1	0.91	0.29	62,62,62,62	0
55	MG	BA	1642	1/1	0.91	0.29	69,69,69,69	0
55	MG	DA	3141	1/1	0.91	0.24	44,44,44,44	0
55	MG	CA	1611	1/1	0.91	0.16	76,76,76,76	0
55	MG	AA	3248	1/1	0.91	0.26	53,53,53,53	0
55	MG	AA	3429	1/1	0.91	0.38	85,85,85,85	0
55	MG	DA	3524	1/1	0.91	0.25	99,99,99,99	0
55	MG	DA	3157	1/1	0.91	0.18	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	AA	3051	1/1	0.91	0.21	51,51,51,51	0
55	MG	DA	3161	1/1	0.91	0.41	73,73,73,73	0
55	MG	DA	3528	1/1	0.91	0.14	87,87,87,87	0
55	MG	AA	3381	1/1	0.91	0.36	88,88,88,88	0
55	MG	AA	3382	1/1	0.91	0.21	83,83,83,83	0
55	MG	CA	1620	1/1	0.91	0.35	70,70,70,70	0
55	MG	AA	3383	1/1	0.91	0.12	70,70,70,70	0
55	MG	DA	3017	1/1	0.91	0.26	88,88,88,88	0
55	MG	DA	3347	1/1	0.91	0.39	66,66,66,66	0
55	MG	AA	3053	1/1	0.91	0.27	59,59,59,59	0
55	MG	DA	3171	1/1	0.91	0.26	81,81,81,81	0
55	MG	BA	1658	1/1	0.91	0.30	54,54,54,54	0
55	MG	AA	3220	1/1	0.91	0.16	44,44,44,44	0
55	MG	DA	3022	1/1	0.91	0.11	66,66,66,66	0
55	MG	AA	3221	1/1	0.91	0.25	51,51,51,51	0
55	MG	AA	3150	1/1	0.91	0.44	58,58,58,58	0
55	MG	DA	3186	1/1	0.91	0.38	56,56,56,56	0
55	MG	DA	3358	1/1	0.91	0.26	90,90,90,90	0
55	MG	AA	3023	1/1	0.91	0.33	52,52,52,52	0
55	MG	AA	3026	1/1	0.91	0.17	35,35,35,35	0
55	MG	DA	3383	1/1	0.92	0.27	79,79,79,79	0
55	MG	CA	1686	1/1	0.92	0.43	68,68,68,68	0
55	MG	AA	3319	1/1	0.92	0.17	61,61,61,61	0
55	MG	BC	101	1/1	0.92	0.24	58,58,58,58	0
55	MG	AA	3081	1/1	0.92	0.25	41,41,41,41	0
55	MG	DA	3089	1/1	0.92	0.18	46,46,46,46	0
55	MG	BC	103	1/1	0.92	0.23	65,65,65,65	0
55	MG	DA	3093	1/1	0.92	0.17	51,51,51,51	0
55	MG	AA	3001	1/1	0.92	0.32	49,49,49,49	0
55	MG	AA	3087	1/1	0.92	0.17	45,45,45,45	0
55	MG	BA	1627	1/1	0.92	0.19	62,62,62,62	0
55	MG	CA	1801	1/1	0.92	0.32	71,71,71,71	0
55	MG	BA	1777	1/1	0.92	0.12	88,88,88,88	0
55	MG	DA	3264	1/1	0.92	0.18	76,76,76,76	0
55	MG	BA	1704	1/1	0.92	0.22	87,87,87,87	0
55	MG	CA	1805	1/1	0.92	0.22	81,81,81,81	0
55	MG	CA	1700	1/1	0.92	0.28	60,60,60,60	0
55	MG	DA	3409	1/1	0.92	0.11	70,70,70,70	0
55	MG	DA	3269	1/1	0.92	0.27	86,86,86,86	0
55	MG	BA	1781	1/1	0.92	0.43	57,57,57,57	0
55	MG	BA	1782	1/1	0.92	0.35	88,88,88,88	0
55	MG	B1	102	1/1	0.92	0.08	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	AA	3531	1/1	0.92	0.22	53,53,53,53	0
55	MG	CA	1603	1/1	0.92	0.26	75,75,75,75	0
55	MG	DA	3421	1/1	0.92	0.09	76,76,76,76	0
55	MG	AA	3204	1/1	0.92	0.37	56,56,56,56	0
55	MG	AA	3244	1/1	0.92	0.20	69,69,69,69	0
55	MG	AA	3169	1/1	0.92	0.09	74,74,74,74	0
55	MG	BA	1632	1/1	0.92	0.20	72,72,72,72	0
55	MG	DA	3280	1/1	0.92	0.15	80,80,80,80	0
55	MG	DA	3428	1/1	0.92	0.22	79,79,79,79	0
55	MG	AA	3038	1/1	0.92	0.29	70,70,70,70	0
55	MG	CC	102	1/1	0.92	0.23	69,69,69,69	0
55	MG	AA	3050	1/1	0.92	0.21	69,69,69,69	0
55	MG	AA	3027	1/1	0.92	0.28	49,49,49,49	0
55	MG	BA	1716	1/1	0.92	0.16	90,90,90,90	0
55	MG	BA	1717	1/1	0.92	0.19	79,79,79,79	0
55	MG	CA	1615	1/1	0.92	0.18	92,92,92,92	0
55	MG	DA	3291	1/1	0.92	0.43	70,70,70,70	0
55	MG	AA	3339	1/1	0.92	0.18	95,95,95,95	0
55	MG	AA	3546	1/1	0.92	0.13	33,33,33,33	0
55	MG	AA	3551	1/1	0.92	0.26	73,73,73,73	0
55	MG	DA	3441	1/1	0.92	0.19	67,67,67,67	0
55	MG	AA	3553	1/1	0.92	0.23	100,100,100,100	0
55	MG	AA	3072	1/1	0.92	0.21	75,75,75,75	0
55	MG	CA	1729	1/1	0.92	0.34	81,81,81,81	0
55	MG	DA	3303	1/1	0.92	0.37	61,61,61,61	0
55	MG	AA	3250	1/1	0.92	0.19	73,73,73,73	0
55	MG	BA	1644	1/1	0.92	0.20	78,78,78,78	0
55	MG	DA	3306	1/1	0.92	0.24	73,73,73,73	0
55	MG	AA	3214	1/1	0.92	0.38	66,66,66,66	0
55	MG	AA	3347	1/1	0.92	0.12	92,92,92,92	0
55	MG	DA	3153	1/1	0.92	0.21	54,54,54,54	0
55	MG	DA	3452	1/1	0.92	0.21	91,91,91,91	0
55	MG	DA	3155	1/1	0.92	0.29	49,49,49,49	0
55	MG	BA	1812	1/1	0.92	0.46	76,76,76,76	0
55	MG	CA	1737	1/1	0.92	0.20	109,109,109,109	0
55	MG	DA	3313	1/1	0.92	0.40	75,75,75,75	0
55	MG	BA	1813	1/1	0.92	0.24	80,80,80,80	0
55	MG	DA	3159	1/1	0.92	0.23	52,52,52,52	0
55	MG	DA	3468	1/1	0.92	0.14	53,53,53,53	0
55	MG	DA	3160	1/1	0.92	0.31	65,65,65,65	0
55	MG	AA	3074	1/1	0.92	0.43	81,81,81,81	0
55	MG	BA	1650	1/1	0.92	0.28	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	BA	1816	1/1	0.92	0.17	87,87,87,87	0
55	MG	AA	3351	1/1	0.92	0.31	84,84,84,84	0
55	MG	DA	3475	1/1	0.92	0.22	81,81,81,81	0
55	MG	DA	3476	1/1	0.92	0.16	76,76,76,76	0
55	MG	DA	3322	1/1	0.92	0.34	83,83,83,83	0
55	MG	AA	3256	1/1	0.92	0.15	65,65,65,65	0
55	MG	AA	3402	1/1	0.92	0.54	94,94,94,94	0
55	MG	DA	3169	1/1	0.92	0.28	68,68,68,68	0
55	MG	AA	3562	1/1	0.92	0.12	96,96,96,96	0
55	MG	DA	3487	1/1	0.92	0.17	59,59,59,59	0
55	MG	BA	1661	1/1	0.92	0.20	49,49,49,49	0
55	MG	DA	3490	1/1	0.92	0.13	49,49,49,49	0
55	MG	AA	3029	1/1	0.92	0.26	50,50,50,50	0
55	MG	AA	3133	1/1	0.92	0.19	38,38,38,38	0
55	MG	AA	3134	1/1	0.92	0.22	59,59,59,59	0
55	MG	BA	1826	1/1	0.92	0.26	73,73,73,73	0
55	MG	DA	3335	1/1	0.92	0.28	72,72,72,72	0
55	MG	AF	302	1/1	0.92	0.15	80,80,80,80	0
55	MG	AA	3575	1/1	0.92	0.23	40,40,40,40	0
55	MG	AA	3030	1/1	0.92	0.21	51,51,51,51	0
55	MG	AA	3581	1/1	0.92	0.16	67,67,67,67	0
55	MG	A0	201	1/1	0.92	0.22	46,46,46,46	0
55	MG	AA	3584	1/1	0.92	0.30	94,94,94,94	0
55	MG	DA	3508	1/1	0.92	0.30	77,77,77,77	0
55	MG	CA	1764	1/1	0.92	0.32	67,67,67,67	0
55	MG	DA	3196	1/1	0.92	0.33	82,82,82,82	0
55	MG	AA	3588	1/1	0.92	0.28	63,63,63,63	0
55	MG	AA	3502	1/1	0.92	0.17	81,81,81,81	0
55	MG	AA	3504	1/1	0.92	0.37	103,103,103,103	0
55	MG	DA	3350	1/1	0.92	0.21	79,79,79,79	0
55	MG	AA	3045	1/1	0.92	0.17	50,50,50,50	0
55	MG	DA	3058	1/1	0.92	0.49	75,75,75,75	0
55	MG	AA	3024	1/1	0.92	0.28	35,35,35,35	0
55	MG	CA	1663	1/1	0.92	0.28	72,72,72,72	0
55	MG	AA	3025	1/1	0.92	0.31	46,46,46,46	0
55	MG	DA	3356	1/1	0.92	0.10	80,80,80,80	0
55	MG	AA	3109	1/1	0.92	0.12	33,33,33,33	0
55	MG	BA	1757	1/1	0.92	0.23	88,88,88,88	0
55	MG	AA	3080	1/1	0.92	0.36	52,52,52,52	0
55	MG	DA	3222	1/1	0.92	0.27	57,57,57,57	0
55	MG	DA	3361	1/1	0.92	0.49	102,102,102,102	0
55	MG	AA	3114	1/1	0.92	0.24	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	DA	3226	1/1	0.92	0.24	57,57,57,57	0
55	MG	DA	3067	1/1	0.92	0.28	75,75,75,75	0
55	MG	AA	3464	1/1	0.92	0.19	83,83,83,83	0
55	MG	DA	3069	1/1	0.92	0.31	82,82,82,82	0
55	MG	AA	3271	1/1	0.92	0.28	68,68,68,68	0
55	MG	AA	3151	1/1	0.92	0.34	61,61,61,61	0
55	MG	AA	3371	1/1	0.92	0.19	69,69,69,69	0
55	MG	CA	1677	1/1	0.92	0.24	68,68,68,68	0
55	MG	CA	1678	1/1	0.92	0.19	67,67,67,67	0
55	MG	AA	3155	1/1	0.92	0.27	61,61,61,61	0
55	MG	BA	1693	1/1	0.92	0.11	80,80,80,80	0
55	MG	AA	3117	1/1	0.92	0.27	62,62,62,62	0
55	MG	AA	3472	1/1	0.92	0.14	81,81,81,81	0
55	MG	AA	3524	1/1	0.92	0.09	72,72,72,72	0
55	MG	DA	3205	1/1	0.93	0.36	60,60,60,60	0
55	MG	CA	1728	1/1	0.93	0.23	58,58,58,58	0
55	MG	AA	3018	1/1	0.93	0.29	38,38,38,38	0
55	MG	DA	3209	1/1	0.93	0.36	54,54,54,54	0
55	MG	AA	3115	1/1	0.93	0.31	56,56,56,56	0
55	MG	AA	3368	1/1	0.93	0.25	83,83,83,83	0
55	MG	BA	1779	1/1	0.93	0.08	105,105,105,105	0
55	MG	CA	1733	1/1	0.93	0.45	66,66,66,66	0
55	MG	BA	1688	1/1	0.93	0.20	76,76,76,76	0
55	MG	CA	1735	1/1	0.93	0.18	86,86,86,86	0
55	MG	AA	3267	1/1	0.93	0.26	80,80,80,80	0
55	MG	DA	3384	1/1	0.93	0.23	64,64,64,64	0
55	MG	DA	3385	1/1	0.93	0.17	90,90,90,90	0
55	MG	DA	3387	1/1	0.93	0.30	45,45,45,45	0
55	MG	AA	3423	1/1	0.93	0.24	69,69,69,69	0
55	MG	CA	1739	1/1	0.93	0.36	69,69,69,69	0
55	MG	DA	3228	1/1	0.93	0.25	71,71,71,71	0
55	MG	CA	1740	1/1	0.93	0.15	75,75,75,75	0
55	MG	DA	3233	1/1	0.93	0.50	84,84,84,84	0
55	MG	BA	1691	1/1	0.93	0.42	60,60,60,60	0
55	MG	DA	3395	1/1	0.93	0.17	80,80,80,80	0
55	MG	A5	102	1/1	0.93	0.18	75,75,75,75	0
55	MG	AA	3487	1/1	0.93	0.09	78,78,78,78	0
55	MG	AA	3563	1/1	0.93	0.15	75,75,75,75	0
55	MG	CA	1624	1/1	0.93	0.27	83,83,83,83	0
55	MG	AA	3313	1/1	0.93	0.40	62,62,62,62	0
55	MG	BA	1789	1/1	0.93	0.19	69,69,69,69	0
55	MG	AA	3187	1/1	0.93	0.67	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	CA	1750	1/1	0.93	0.28	91,91,91,91	0
55	MG	DA	3406	1/1	0.93	0.14	72,72,72,72	0
55	MG	CA	1629	1/1	0.93	0.12	82,82,82,82	0
55	MG	DA	3064	1/1	0.93	0.26	54,54,54,54	0
55	MG	AA	3572	1/1	0.93	0.21	40,40,40,40	0
55	MG	AA	3056	1/1	0.93	0.27	64,64,64,64	0
55	MG	BA	1797	1/1	0.93	0.26	89,89,89,89	0
55	MG	DA	3413	1/1	0.93	0.14	96,96,96,96	0
55	MG	DA	3250	1/1	0.93	0.28	54,54,54,54	0
55	MG	AA	3118	1/1	0.93	0.22	74,74,74,74	0
55	MG	DA	3416	1/1	0.93	0.19	75,75,75,75	0
55	MG	AA	3577	1/1	0.93	0.23	42,42,42,42	0
55	MG	DA	3419	1/1	0.93	0.28	90,90,90,90	0
55	MG	AA	3119	1/1	0.93	0.29	64,64,64,64	0
55	MG	DA	3073	1/1	0.93	0.18	69,69,69,69	0
55	MG	AA	3376	1/1	0.93	0.33	67,67,67,67	0
55	MG	AA	3433	1/1	0.93	0.31	77,77,77,77	0
55	MG	AA	3587	1/1	0.93	0.09	28,28,28,28	0
55	MG	AA	3273	1/1	0.93	0.24	63,63,63,63	0
55	MG	DA	3262	1/1	0.93	0.14	39,39,39,39	0
55	MG	AA	3589	1/1	0.93	0.20	72,72,72,72	0
55	MG	DA	3079	1/1	0.93	0.19	83,83,83,83	0
55	MG	AA	3154	1/1	0.93	0.36	55,55,55,55	0
55	MG	AA	3592	1/1	0.93	0.18	69,69,69,69	0
55	MG	CA	1645	1/1	0.93	0.54	71,71,71,71	0
55	MG	BA	1619	1/1	0.93	0.27	67,67,67,67	0
55	MG	CA	1648	1/1	0.93	0.22	65,65,65,65	0
55	MG	CA	1649	1/1	0.93	0.17	70,70,70,70	0
55	MG	BA	1620	1/1	0.93	0.22	58,58,58,58	0
55	MG	DA	3087	1/1	0.93	0.35	48,48,48,48	0
55	MG	AA	3275	1/1	0.93	0.28	65,65,65,65	0
55	MG	AA	3092	1/1	0.93	0.31	59,59,59,59	0
55	MG	DA	3090	1/1	0.93	0.16	47,47,47,47	0
55	MG	AA	3501	1/1	0.93	0.25	73,73,73,73	0
55	MG	AA	3597	1/1	0.93	0.12	67,67,67,67	0
55	MG	BA	1720	1/1	0.93	0.37	71,71,71,71	0
55	MG	CA	1778	1/1	0.93	0.11	69,69,69,69	0
55	MG	AA	3161	1/1	0.93	0.26	41,41,41,41	0
55	MG	AA	3503	1/1	0.93	0.08	72,72,72,72	0
55	MG	AA	3240	1/1	0.93	0.44	76,76,76,76	0
55	MG	AA	3442	1/1	0.93	0.22	49,49,49,49	0
55	MG	BA	1725	1/1	0.93	0.28	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	DA	3106	1/1	0.93	0.25	46,46,46,46	0
55	MG	AA	3057	1/1	0.93	0.16	52,52,52,52	0
55	MG	DA	3293	1/1	0.93	0.17	67,67,67,67	0
55	MG	AA	3022	1/1	0.93	0.20	43,43,43,43	0
55	MG	AA	3606	1/1	0.93	0.14	77,77,77,77	0
55	MG	DA	3457	1/1	0.93	0.24	62,62,62,62	0
55	MG	DA	3110	1/1	0.93	0.21	84,84,84,84	0
55	MG	AA	3386	1/1	0.93	0.28	74,74,74,74	0
55	MG	AA	3059	1/1	0.93	0.15	84,84,84,84	0
55	MG	DA	3467	1/1	0.93	0.24	49,49,49,49	0
55	MG	AA	3166	1/1	0.93	0.35	63,63,63,63	0
55	MG	AA	3617	1/1	0.93	0.12	92,92,92,92	0
55	MG	BA	1733	1/1	0.93	0.31	88,88,88,88	0
55	MG	CA	1794	1/1	0.93	0.25	72,72,72,72	0
55	MG	AA	3389	1/1	0.93	0.22	89,89,89,89	0
55	MG	AA	3167	1/1	0.93	0.27	51,51,51,51	0
55	MG	AA	3514	1/1	0.93	0.10	59,59,59,59	0
55	MG	AA	3340	1/1	0.93	0.24	61,61,61,61	0
55	MG	AA	3342	1/1	0.93	0.39	65,65,65,65	0
55	MG	BA	1840	1/1	0.93	0.27	80,80,80,80	0
55	MG	DA	3479	1/1	0.93	0.36	87,87,87,87	0
55	MG	DA	3130	1/1	0.93	0.34	64,64,64,64	0
55	MG	CA	1681	1/1	0.93	0.21	71,71,71,71	0
55	MG	BA	1740	1/1	0.93	0.21	72,72,72,72	0
55	MG	BA	1842	1/1	0.93	0.20	88,88,88,88	0
55	MG	AA	3519	1/1	0.93	0.14	91,91,91,91	0
55	MG	AA	3124	1/1	0.93	0.47	56,56,56,56	0
55	MG	BA	1743	1/1	0.93	0.32	58,58,58,58	0
55	MG	DA	3492	1/1	0.93	0.31	48,48,48,48	0
55	MG	CG	302	1/1	0.93	0.20	83,83,83,83	0
55	MG	DA	3495	1/1	0.93	0.18	65,65,65,65	0
55	MG	DA	3320	1/1	0.93	0.23	73,73,73,73	0
55	MG	CA	1688	1/1	0.93	0.40	75,75,75,75	0
55	MG	DA	3139	1/1	0.93	0.27	51,51,51,51	0
55	MG	AA	3454	1/1	0.93	0.16	78,78,78,78	0
55	MG	AA	3522	1/1	0.93	0.16	67,67,67,67	0
55	MG	DA	3503	1/1	0.93	0.09	52,52,52,52	0
55	MG	AA	3455	1/1	0.93	0.32	61,61,61,61	0
55	MG	DA	3144	1/1	0.93	0.35	68,68,68,68	0
55	MG	CA	1693	1/1	0.93	0.28	73,73,73,73	0
55	MG	BA	1651	1/1	0.93	0.48	73,73,73,73	0
55	MG	AA	3395	1/1	0.93	0.07	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	DA	3509	1/1	0.93	0.34	65,65,65,65	0
55	MG	CB	105	1/1	0.93	0.16	80,80,80,80	0
55	MG	AA	3344	1/1	0.93	0.11	71,71,71,71	0
55	MG	CA	1697	1/1	0.93	0.29	56,56,56,56	0
55	MG	DA	3514	1/1	0.93	0.35	49,49,49,49	0
55	MG	AA	3097	1/1	0.93	0.19	65,65,65,65	0
55	MG	AA	3291	1/1	0.93	0.25	70,70,70,70	0
55	MG	AA	3209	1/1	0.93	0.24	71,71,71,71	0
55	MG	BA	1662	1/1	0.93	0.27	80,80,80,80	0
55	MG	AA	3403	1/1	0.93	0.07	74,74,74,74	0
55	MG	AA	3348	1/1	0.93	0.12	92,92,92,92	0
55	MG	AA	3033	1/1	0.93	0.27	46,46,46,46	0
55	MG	DA	3005	1/1	0.93	0.36	83,83,83,83	0
55	MG	DA	3168	1/1	0.93	0.27	49,49,49,49	0
55	MG	CA	1706	1/1	0.93	0.30	77,77,77,77	0
55	MG	AA	3034	1/1	0.93	0.45	61,61,61,61	0
55	MG	AA	3252	1/1	0.93	0.23	68,68,68,68	0
55	MG	CA	1709	1/1	0.93	0.39	81,81,81,81	0
55	MG	AA	3539	1/1	0.93	0.52	54,54,54,54	0
55	MG	AA	3130	1/1	0.93	0.12	59,59,59,59	0
55	MG	AA	3015	1/1	0.93	0.21	30,30,30,30	0
55	MG	BA	1673	1/1	0.93	0.34	80,80,80,80	0
55	MG	AA	3002	1/1	0.93	0.27	40,40,40,40	0
55	MG	AA	3054	1/1	0.93	0.20	52,52,52,52	0
55	MG	AA	3547	1/1	0.93	0.21	45,45,45,45	0
55	MG	AA	3083	1/1	0.93	0.18	47,47,47,47	0
55	MG	DA	3026	1/1	0.93	0.22	82,82,82,82	0
55	MG	AA	3085	1/1	0.93	0.28	62,62,62,62	0
55	MG	AA	3111	1/1	0.93	0.34	43,43,43,43	0
55	MG	DA	3364	1/1	0.93	0.10	85,85,85,85	0
55	MG	AA	3070	1/1	0.93	0.29	66,66,66,66	0
55	MG	DE	303	1/1	0.93	0.25	52,52,52,52	0
55	MG	D0	201	1/1	0.93	0.15	78,78,78,78	0
55	MG	D1	201	1/1	0.93	0.33	73,73,73,73	0
55	MG	AF	301	1/1	0.93	0.19	75,75,75,75	0
55	MG	BA	1773	1/1	0.93	0.14	79,79,79,79	0
55	MG	AA	3365	1/1	0.93	0.20	83,83,83,83	0
55	MG	DA	3394	1/1	0.94	0.20	70,70,70,70	0
55	MG	CA	1792	1/1	0.94	0.32	91,91,91,91	0
55	MG	AA	3052	1/1	0.94	0.60	74,74,74,74	0
55	MG	AA	3445	1/1	0.94	0.22	69,69,69,69	0
55	MG	BA	1685	1/1	0.94	0.10	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	DA	3252	1/1	0.94	0.15	45,45,45,45	0
55	MG	DA	3400	1/1	0.94	0.12	82,82,82,82	0
55	MG	DA	3401	1/1	0.94	0.27	75,75,75,75	0
55	MG	DA	3094	1/1	0.94	0.33	45,45,45,45	0
55	MG	DA	3095	1/1	0.94	0.35	45,45,45,45	0
55	MG	A7	101	1/1	0.94	0.17	69,69,69,69	0
55	MG	AA	3582	1/1	0.94	0.20	33,33,33,33	0
55	MG	AA	3583	1/1	0.94	0.22	44,44,44,44	0
55	MG	DA	3258	1/1	0.94	0.24	56,56,56,56	0
55	MG	BA	1603	1/1	0.94	0.26	63,63,63,63	0
55	MG	AA	3392	1/1	0.94	0.25	94,94,94,94	0
55	MG	AA	3300	1/1	0.94	0.14	77,77,77,77	0
55	MG	DA	3411	1/1	0.94	0.26	77,77,77,77	0
55	MG	B1	101	1/1	0.94	0.28	64,64,64,64	0
55	MG	DA	3104	1/1	0.94	0.26	38,38,38,38	0
55	MG	DA	3105	1/1	0.94	0.28	72,72,72,72	0
55	MG	CA	1701	1/1	0.94	0.29	77,77,77,77	0
55	MG	AA	3028	1/1	0.94	0.23	51,51,51,51	0
55	MG	AA	3228	1/1	0.94	0.15	89,89,89,89	0
55	MG	CA	1808	1/1	0.94	0.25	73,73,73,73	0
55	MG	CA	1602	1/1	0.94	0.30	81,81,81,81	0
55	MG	CG	301	1/1	0.94	0.26	86,86,86,86	0
55	MG	DA	3113	1/1	0.94	0.20	44,44,44,44	0
55	MG	AA	3199	1/1	0.94	0.26	66,66,66,66	0
55	MG	BA	1780	1/1	0.94	0.30	58,58,58,58	0
55	MG	AA	3177	1/1	0.94	0.15	45,45,45,45	0
55	MG	AA	3232	1/1	0.94	0.14	47,47,47,47	0
55	MG	AA	3073	1/1	0.94	0.41	76,76,76,76	0
55	MG	CA	1608	1/1	0.94	0.19	81,81,81,81	0
55	MG	AA	3084	1/1	0.94	0.16	40,40,40,40	0
55	MG	DA	3122	1/1	0.94	0.12	71,71,71,71	0
55	MG	CA	1712	1/1	0.94	0.20	86,86,86,86	0
55	MG	AA	3513	1/1	0.94	0.13	73,73,73,73	0
55	MG	BA	1701	1/1	0.94	0.20	73,73,73,73	0
55	MG	AA	3356	1/1	0.94	0.09	72,72,72,72	0
55	MG	DA	3287	1/1	0.94	0.19	62,62,62,62	0
55	MG	AA	3357	1/1	0.94	0.28	61,61,61,61	0
55	MG	BA	1617	1/1	0.94	0.30	64,64,64,64	0
55	MG	CA	1718	1/1	0.94	0.14	78,78,78,78	0
55	MG	AA	3358	1/1	0.94	0.23	79,79,79,79	0
55	MG	AA	3359	1/1	0.94	0.17	60,60,60,60	0
55	MG	BA	1792	1/1	0.94	0.24	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	BA	1708	1/1	0.94	0.20	78,78,78,78	0
55	MG	BA	1796	1/1	0.94	0.23	78,78,78,78	0
55	MG	DA	3006	1/1	0.94	0.17	78,78,78,78	0
55	MG	AA	3409	1/1	0.94	0.20	98,98,98,98	0
55	MG	CA	1726	1/1	0.94	0.42	82,82,82,82	0
55	MG	AA	3462	1/1	0.94	0.10	69,69,69,69	0
55	MG	DA	3014	1/1	0.94	0.14	62,62,62,62	0
55	MG	DA	3143	1/1	0.94	0.34	69,69,69,69	0
55	MG	AA	3605	1/1	0.94	0.32	45,45,45,45	0
55	MG	DA	3145	1/1	0.94	0.36	54,54,54,54	0
55	MG	BA	1623	1/1	0.94	0.38	68,68,68,68	0
55	MG	AA	3180	1/1	0.94	0.22	56,56,56,56	0
55	MG	CA	1628	1/1	0.94	0.13	86,86,86,86	0
55	MG	AA	3608	1/1	0.94	0.34	69,69,69,69	0
55	MG	AA	3206	1/1	0.94	0.32	53,53,53,53	0
55	MG	AA	3099	1/1	0.94	0.27	64,64,64,64	0
55	MG	AA	3039	1/1	0.94	0.33	80,80,80,80	0
55	MG	BA	1809	1/1	0.94	0.30	88,88,88,88	0
55	MG	AA	3615	1/1	0.94	0.15	84,84,84,84	0
55	MG	AA	3008	1/1	0.94	0.25	42,42,42,42	0
55	MG	AA	3527	1/1	0.94	0.21	77,77,77,77	0
55	MG	AA	3316	1/1	0.94	0.28	87,87,87,87	0
55	MG	AA	3470	1/1	0.94	0.11	59,59,59,59	0
55	MG	BA	1634	1/1	0.94	0.23	68,68,68,68	0
55	MG	AA	3035	1/1	0.94	0.15	46,46,46,46	0
55	MG	AA	3622	1/1	0.94	0.11	71,71,71,71	0
55	MG	AA	3211	1/1	0.94	0.23	43,43,43,43	0
55	MG	DA	3327	1/1	0.94	0.37	85,85,85,85	0
55	MG	AA	3473	1/1	0.94	0.24	70,70,70,70	0
55	MG	DA	3172	1/1	0.94	0.21	59,59,59,59	0
55	MG	DA	3175	1/1	0.94	0.14	70,70,70,70	0
55	MG	AA	3212	1/1	0.94	0.34	56,56,56,56	0
55	MG	DA	3178	1/1	0.94	0.23	45,45,45,45	0
55	MG	AA	3320	1/1	0.94	0.29	70,70,70,70	0
55	MG	CA	1751	1/1	0.94	0.20	102,102,102,102	0
55	MG	DA	3044	1/1	0.94	0.16	66,66,66,66	0
55	MG	BA	1641	1/1	0.94	0.22	62,62,62,62	0
55	MG	AA	3321	1/1	0.94	0.35	68,68,68,68	0
55	MG	AA	3281	1/1	0.94	0.14	67,67,67,67	0
55	MG	CA	1652	1/1	0.94	0.27	70,70,70,70	0
55	MG	AA	3185	1/1	0.94	0.12	43,43,43,43	0
55	MG	DA	3499	1/1	0.94	0.30	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	AA	3544	1/1	0.94	0.23	67,67,67,67	0
55	MG	DA	3501	1/1	0.94	0.16	77,77,77,77	0
55	MG	CA	1758	1/1	0.94	0.28	64,64,64,64	0
55	MG	AA	3139	1/1	0.94	0.24	42,42,42,42	0
55	MG	AA	3325	1/1	0.94	0.23	78,78,78,78	0
55	MG	AA	3425	1/1	0.94	0.44	70,70,70,70	0
55	MG	CA	1658	1/1	0.94	0.29	78,78,78,78	0
55	MG	AA	3140	1/1	0.94	0.16	53,53,53,53	0
55	MG	AA	3552	1/1	0.94	0.33	75,75,75,75	0
55	MG	AA	3427	1/1	0.94	0.26	78,78,78,78	0
55	MG	DA	3510	1/1	0.94	0.25	67,67,67,67	0
55	MG	AA	3327	1/1	0.94	0.13	82,82,82,82	0
55	MG	AA	3216	1/1	0.94	0.34	56,56,56,56	0
55	MG	DA	3210	1/1	0.94	0.26	51,51,51,51	0
55	MG	DA	3211	1/1	0.94	0.26	49,49,49,49	0
55	MG	BA	1660	1/1	0.94	0.30	64,64,64,64	0
55	MG	DA	3214	1/1	0.94	0.54	70,70,70,70	0
55	MG	AA	3286	1/1	0.94	0.32	69,69,69,69	0
55	MG	DA	3216	1/1	0.94	0.27	47,47,47,47	0
55	MG	DA	3363	1/1	0.94	0.26	73,73,73,73	0
55	MG	AA	3217	1/1	0.94	0.28	58,58,58,58	0
55	MG	AA	3067	1/1	0.94	0.30	61,61,61,61	0
55	MG	DA	3220	1/1	0.94	0.34	67,67,67,67	0
55	MG	DA	3367	1/1	0.94	0.22	85,85,85,85	0
55	MG	AB	213	1/1	0.94	0.24	54,54,54,54	0
55	MG	AA	3189	1/1	0.94	0.23	57,57,57,57	0
55	MG	CA	1774	1/1	0.94	0.12	72,72,72,72	0
55	MG	DA	3072	1/1	0.94	0.26	98,98,98,98	0
55	MG	CA	1670	1/1	0.94	0.33	54,54,54,54	0
55	MG	DB	203	1/1	0.94	0.22	71,71,71,71	0
55	MG	AA	3105	1/1	0.94	0.34	64,64,64,64	0
55	MG	DA	3229	1/1	0.94	0.15	109,109,109,109	0
55	MG	DA	3231	1/1	0.94	0.23	55,55,55,55	0
55	MG	AA	3492	1/1	0.94	0.27	84,84,84,84	0
55	MG	AB	217	1/1	0.94	0.28	109,109,109,109	0
55	MG	AA	3436	1/1	0.94	0.18	82,82,82,82	0
55	MG	AA	3255	1/1	0.94	0.24	61,61,61,61	0
55	MG	BQ	102	1/1	0.94	0.09	89,89,89,89	0
55	MG	AA	3565	1/1	0.94	0.29	81,81,81,81	0
55	MG	AA	3566	1/1	0.94	0.32	73,73,73,73	0
55	MG	DA	3386	1/1	0.94	0.38	88,88,88,88	0
55	MG	DE	301	1/1	0.94	0.17	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	AA	3341	1/1	0.94	0.17	63,63,63,63	0
55	MG	AA	3107	1/1	0.94	0.17	56,56,56,56	0
55	MG	AA	3440	1/1	0.94	0.15	83,83,83,83	0
55	MG	AA	3009	1/1	0.94	0.32	48,48,48,48	0
55	MG	AA	3007	1/1	0.94	0.12	33,33,33,33	0
55	MG	AA	3576	1/1	0.94	0.14	36,36,36,36	0
55	MG	AA	3225	1/1	0.94	0.10	69,69,69,69	0
56	ZN	CG	304	1/1	0.94	0.23	112,112,112,112	0
55	MG	AA	3612	1/1	0.95	0.09	38,38,38,38	0
55	MG	AA	3014	1/1	0.95	0.37	41,41,41,41	0
55	MG	CA	1646	1/1	0.95	0.28	56,56,56,56	0
55	MG	DA	3001	1/1	0.95	0.20	58,58,58,58	0
55	MG	AA	3614	1/1	0.95	0.21	91,91,91,91	0
55	MG	BA	1697	1/1	0.95	0.13	84,84,84,84	0
55	MG	AA	3128	1/1	0.95	0.33	54,54,54,54	0
55	MG	AA	3616	1/1	0.95	0.25	69,69,69,69	0
55	MG	BA	1807	1/1	0.95	0.19	70,70,70,70	0
55	MG	DA	3009	1/1	0.95	0.14	88,88,88,88	0
55	MG	BA	1645	1/1	0.95	0.32	52,52,52,52	0
55	MG	AA	3385	1/1	0.95	0.20	75,75,75,75	0
55	MG	AA	3163	1/1	0.95	0.12	48,48,48,48	0
55	MG	DA	3456	1/1	0.95	0.14	83,83,83,83	0
55	MG	AA	3194	1/1	0.95	0.19	54,54,54,54	0
55	MG	AA	3328	1/1	0.95	0.29	71,71,71,71	0
55	MG	AA	3329	1/1	0.95	0.31	77,77,77,77	0
55	MG	DA	3465	1/1	0.95	0.36	51,51,51,51	0
55	MG	BA	1706	1/1	0.95	0.28	55,55,55,55	0
55	MG	DA	3020	1/1	0.95	0.24	51,51,51,51	0
55	MG	DA	3174	1/1	0.95	0.18	49,49,49,49	0
55	MG	DA	3092	1/1	0.95	0.31	47,47,47,47	0
55	MG	AA	3143	1/1	0.95	0.25	40,40,40,40	0
55	MG	DA	3177	1/1	0.95	0.23	51,51,51,51	0
55	MG	BA	1760	1/1	0.95	0.26	67,67,67,67	0
55	MG	BA	1606	1/1	0.95	0.09	88,88,88,88	0
55	MG	DA	3181	1/1	0.95	0.23	48,48,48,48	0
55	MG	AA	3457	1/1	0.95	0.20	73,73,73,73	0
55	MG	AA	3331	1/1	0.95	0.33	79,79,79,79	0
55	MG	AA	3144	1/1	0.95	0.32	51,51,51,51	0
55	MG	BA	1821	1/1	0.95	0.24	78,78,78,78	0
55	MG	DA	3378	1/1	0.95	0.17	56,56,56,56	0
55	MG	AA	3305	1/1	0.95	0.22	62,62,62,62	0
55	MG	DA	3482	1/1	0.95	0.18	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	DA	3484	1/1	0.95	0.25	46,46,46,46	0
55	MG	DA	3380	1/1	0.95	0.17	74,74,74,74	0
55	MG	DA	3486	1/1	0.95	0.36	46,46,46,46	0
55	MG	DA	3189	1/1	0.95	0.20	43,43,43,43	0
55	MG	AA	3198	1/1	0.95	0.32	57,57,57,57	0
55	MG	DA	3030	1/1	0.95	0.12	66,66,66,66	0
55	MG	AA	3003	1/1	0.95	0.21	43,43,43,43	0
55	MG	DA	3194	1/1	0.95	0.24	59,59,59,59	0
55	MG	DA	3034	1/1	0.95	0.09	72,72,72,72	0
55	MG	CA	1610	1/1	0.95	0.12	75,75,75,75	0
55	MG	DA	3197	1/1	0.95	0.32	52,52,52,52	0
55	MG	AA	3396	1/1	0.95	0.21	58,58,58,58	0
55	MG	DA	3295	1/1	0.95	0.15	66,66,66,66	0
55	MG	DA	3296	1/1	0.95	0.19	56,56,56,56	0
55	MG	AA	3308	1/1	0.95	0.15	58,58,58,58	0
55	MG	AA	3536	1/1	0.95	0.13	102,102,102,102	0
55	MG	DA	3203	1/1	0.95	0.40	52,52,52,52	0
55	MG	DA	3300	1/1	0.95	0.26	71,71,71,71	0
55	MG	AA	3586	1/1	0.95	0.23	80,80,80,80	0
55	MG	CA	1676	1/1	0.95	0.35	55,55,55,55	0
55	MG	CA	1796	1/1	0.95	0.20	81,81,81,81	0
55	MG	AA	3218	1/1	0.95	0.29	77,77,77,77	0
55	MG	AA	3540	1/1	0.95	0.18	44,44,44,44	0
55	MG	AA	3238	1/1	0.95	0.26	48,48,48,48	0
55	MG	AA	3542	1/1	0.95	0.28	40,40,40,40	0
55	MG	AA	3401	1/1	0.95	0.11	98,98,98,98	0
55	MG	DA	3049	1/1	0.95	0.28	72,72,72,72	0
55	MG	AA	3200	1/1	0.95	0.10	80,80,80,80	0
55	MG	CA	1683	1/1	0.95	0.26	84,84,84,84	0
55	MG	DA	3515	1/1	0.95	0.20	52,52,52,52	0
55	MG	DA	3217	1/1	0.95	0.29	51,51,51,51	0
55	MG	DA	3052	1/1	0.95	0.07	84,84,84,84	0
55	MG	CA	1804	1/1	0.95	0.13	81,81,81,81	0
55	MG	BA	1836	1/1	0.95	0.20	73,73,73,73	0
55	MG	DA	3127	1/1	0.95	0.28	44,44,44,44	0
55	MG	AA	3469	1/1	0.95	0.48	76,76,76,76	0
55	MG	DA	3223	1/1	0.95	0.10	83,83,83,83	0
55	MG	DA	3523	1/1	0.95	0.33	86,86,86,86	0
55	MG	DA	3224	1/1	0.95	0.32	59,59,59,59	0
55	MG	DA	3129	1/1	0.95	0.35	55,55,55,55	0
55	MG	AA	3595	1/1	0.95	0.11	90,90,90,90	0
55	MG	AA	3040	1/1	0.95	0.50	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	AA	3063	1/1	0.95	0.12	64,64,64,64	0
55	MG	BA	1680	1/1	0.95	0.28	71,71,71,71	0
55	MG	AA	3549	1/1	0.95	0.27	41,41,41,41	0
55	MG	AA	3021	1/1	0.95	0.28	38,38,38,38	0
55	MG	AA	3265	1/1	0.95	0.31	42,42,42,42	0
55	MG	DA	3424	1/1	0.95	0.08	79,79,79,79	0
55	MG	AA	3601	1/1	0.95	0.32	79,79,79,79	0
55	MG	AA	3375	1/1	0.95	0.21	74,74,74,74	0
55	MG	AA	3290	1/1	0.95	0.34	62,62,62,62	0
55	MG	AE	301	1/1	0.95	0.13	52,52,52,52	0
55	MG	AA	3266	1/1	0.95	0.14	47,47,47,47	0
55	MG	AA	3096	1/1	0.95	0.21	75,75,75,75	0
55	MG	DA	3337	1/1	0.95	0.31	75,75,75,75	0
55	MG	DA	3338	1/1	0.95	0.31	75,75,75,75	0
55	MG	AA	3090	1/1	0.95	0.28	68,68,68,68	0
55	MG	AA	3125	1/1	0.95	0.35	49,49,49,49	0
55	MG	AA	3106	1/1	0.95	0.25	65,65,65,65	0
55	MG	DA	3436	1/1	0.95	0.10	69,69,69,69	0
55	MG	DA	3146	1/1	0.95	0.27	38,38,38,38	0
55	MG	DA	3245	1/1	0.95	0.26	80,80,80,80	0
55	MG	DA	3148	1/1	0.95	0.22	42,42,42,42	0
55	MG	DA	3149	1/1	0.95	0.24	60,60,60,60	0
55	MG	DA	3150	1/1	0.95	0.26	76,76,76,76	0
56	ZN	BG	302	1/1	0.95	0.26	95,95,95,95	0
55	MG	AA	3159	1/1	0.95	0.15	30,30,30,30	0
55	MG	DA	3464	1/1	0.96	0.25	55,55,55,55	0
55	MG	DA	3290	1/1	0.96	0.24	59,59,59,59	0
55	MG	AA	3174	1/1	0.96	0.32	43,43,43,43	0
55	MG	DA	3292	1/1	0.96	0.31	56,56,56,56	0
55	MG	AA	3397	1/1	0.96	0.23	40,40,40,40	0
55	MG	DA	3208	1/1	0.96	0.24	40,40,40,40	0
55	MG	DA	3470	1/1	0.96	0.15	75,75,75,75	0
55	MG	AA	3585	1/1	0.96	0.10	46,46,46,46	0
55	MG	CA	1639	1/1	0.96	0.22	64,64,64,64	0
55	MG	AA	3157	1/1	0.96	0.27	41,41,41,41	0
55	MG	AA	3253	1/1	0.96	0.20	82,82,82,82	0
55	MG	BA	1803	1/1	0.96	0.08	81,81,81,81	0
55	MG	AA	3158	1/1	0.96	0.23	66,66,66,66	0
55	MG	BA	1805	1/1	0.96	0.28	62,62,62,62	0
55	MG	AA	3116	1/1	0.96	0.25	43,43,43,43	0
55	MG	BA	1655	1/1	0.96	0.33	89,89,89,89	0
55	MG	BA	1656	1/1	0.96	0.30	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	AA	3548	1/1	0.96	0.11	31,31,31,31	0
55	MG	AA	3515	1/1	0.96	0.29	67,67,67,67	0
55	MG	DA	3002	1/1	0.96	0.15	91,91,91,91	0
55	MG	AA	3160	1/1	0.96	0.21	31,31,31,31	0
55	MG	AA	3517	1/1	0.96	0.26	61,61,61,61	0
55	MG	BA	1663	1/1	0.96	0.12	47,47,47,47	0
55	MG	AA	3065	1/1	0.96	0.24	52,52,52,52	0
55	MG	AA	3280	1/1	0.96	0.23	65,65,65,65	0
55	MG	AA	3146	1/1	0.96	0.16	62,62,62,62	0
55	MG	AA	3137	1/1	0.96	0.13	43,43,43,43	0
55	MG	BA	1715	1/1	0.96	0.25	69,69,69,69	0
55	MG	DA	3013	1/1	0.96	0.18	55,55,55,55	0
55	MG	AA	3239	1/1	0.96	0.13	70,70,70,70	0
55	MG	AA	3408	1/1	0.96	0.18	70,70,70,70	0
55	MG	DA	3235	1/1	0.96	0.17	53,53,53,53	0
55	MG	DA	3016	1/1	0.96	0.20	105,105,105,105	0
55	MG	AA	3138	1/1	0.96	0.27	41,41,41,41	0
55	MG	BA	1671	1/1	0.96	0.09	74,74,74,74	0
55	MG	AA	3016	1/1	0.96	0.27	53,53,53,53	0
55	MG	AA	3332	1/1	0.96	0.42	82,82,82,82	0
55	MG	CA	1722	1/1	0.96	0.36	63,63,63,63	0
55	MG	AA	3309	1/1	0.96	0.33	64,64,64,64	0
55	MG	AA	3528	1/1	0.96	0.35	88,88,88,88	0
55	MG	BA	1827	1/1	0.96	0.20	85,85,85,85	0
55	MG	DA	3165	1/1	0.96	0.27	73,73,73,73	0
55	MG	DA	3330	1/1	0.96	0.10	74,74,74,74	0
55	MG	AA	3564	1/1	0.96	0.21	54,54,54,54	0
55	MG	AA	3020	1/1	0.96	0.19	31,31,31,31	0
55	MG	AA	3609	1/1	0.96	0.15	39,39,39,39	0
55	MG	AE	302	1/1	0.96	0.24	38,38,38,38	0
55	MG	AA	3335	1/1	0.96	0.28	90,90,90,90	0
55	MG	CA	1791	1/1	0.96	0.25	70,70,70,70	0
55	MG	AA	3567	1/1	0.96	0.30	38,38,38,38	0
55	MG	DA	3173	1/1	0.96	0.45	59,59,59,59	0
55	MG	CA	1674	1/1	0.96	0.14	76,76,76,76	0
55	MG	AA	3068	1/1	0.96	0.12	49,49,49,49	0
55	MG	CA	1618	1/1	0.96	0.23	89,89,89,89	0
55	MG	CA	1619	1/1	0.96	0.14	62,62,62,62	0
55	MG	AA	3152	1/1	0.96	0.31	53,53,53,53	0
55	MG	DA	3179	1/1	0.96	0.28	56,56,56,56	0
55	MG	AA	3571	1/1	0.96	0.19	48,48,48,48	0
55	MG	DA	3040	1/1	0.96	0.27	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	DA	3182	1/1	0.96	0.33	72,72,72,72	0
55	MG	CA	1738	1/1	0.96	0.44	75,75,75,75	0
55	MG	DA	3265	1/1	0.96	0.15	63,63,63,63	0
55	MG	AA	3153	1/1	0.96	0.18	33,33,33,33	0
55	MG	AA	3474	1/1	0.96	0.30	93,93,93,93	0
55	MG	AA	3170	1/1	0.96	0.22	34,34,34,34	0
55	MG	DA	3187	1/1	0.96	0.21	40,40,40,40	0
55	MG	DA	3270	1/1	0.96	0.34	73,73,73,73	0
55	MG	DA	3112	1/1	0.96	0.24	70,70,70,70	0
55	MG	A2	201	1/1	0.96	0.26	81,81,81,81	0
55	MG	AA	3142	1/1	0.96	0.14	61,61,61,61	0
55	MG	A5	101	1/1	0.96	0.16	49,49,49,49	0
55	MG	DA	3048	1/1	0.96	0.09	84,84,84,84	0
55	MG	DA	3193	1/1	0.96	0.17	49,49,49,49	0
55	MG	AA	3537	1/1	0.96	0.26	39,39,39,39	0
55	MG	AA	3042	1/1	0.96	0.15	67,67,67,67	0
55	MG	DA	3119	1/1	0.96	0.31	80,80,80,80	0
55	MG	AA	3579	1/1	0.96	0.20	35,35,35,35	0
55	MG	AA	3580	1/1	0.96	0.22	44,44,44,44	0
55	MG	BA	1795	1/1	0.96	0.18	66,66,66,66	0
55	MG	DP	201	1/1	0.96	0.11	63,63,63,63	0
55	MG	AA	3293	1/1	0.96	0.27	87,87,87,87	0
55	MG	DA	3201	1/1	0.96	0.27	75,75,75,75	0
55	MG	DA	3202	1/1	0.96	0.24	65,65,65,65	0
55	MG	CA	1692	1/1	0.96	0.23	75,75,75,75	0
55	MG	AA	3156	1/1	0.96	0.14	87,87,87,87	0
55	MG	DA	3459	1/1	0.96	0.18	49,49,49,49	0
56	ZN	BQ	103	1/1	0.96	0.08	129,129,129,129	0
55	MG	DA	3126	1/1	0.96	0.28	39,39,39,39	0
55	MG	DA	3212	1/1	0.97	0.15	70,70,70,70	0
55	MG	AA	3296	1/1	0.97	0.19	75,75,75,75	0
55	MG	BA	1793	1/1	0.97	0.15	82,82,82,82	0
55	MG	DA	3152	1/1	0.97	0.14	44,44,44,44	0
55	MG	AA	3336	1/1	0.97	0.20	48,48,48,48	0
55	MG	DA	3154	1/1	0.97	0.25	59,59,59,59	0
55	MG	AA	3201	1/1	0.97	0.16	42,42,42,42	0
55	MG	AA	3499	1/1	0.97	0.24	79,79,79,79	0
55	MG	AA	3229	1/1	0.97	0.04	18,18,18,18	0
55	MG	AU	201	1/1	0.97	0.16	74,74,74,74	0
55	MG	DA	3289	1/1	0.97	0.07	47,47,47,47	0
55	MG	DA	3098	1/1	0.97	0.20	41,41,41,41	0
55	MG	BA	1774	1/1	0.97	0.22	98,98,98,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	DA	3071	1/1	0.97	0.21	74,74,74,74	0
55	MG	BA	1657	1/1	0.97	0.25	44,44,44,44	0
55	MG	DA	3259	1/1	0.97	0.25	56,56,56,56	0
55	MG	DA	3483	1/1	0.97	0.33	45,45,45,45	0
55	MG	AA	3019	1/1	0.97	0.14	35,35,35,35	0
55	MG	BA	1659	1/1	0.97	0.27	70,70,70,70	0
55	MG	DA	3369	1/1	0.97	0.25	61,61,61,61	0
55	MG	AA	3104	1/1	0.97	0.25	54,54,54,54	0
55	MG	DA	3488	1/1	0.97	0.17	45,45,45,45	0
55	MG	DA	3333	1/1	0.97	0.13	85,85,85,85	0
55	MG	AA	3607	1/1	0.97	0.18	54,54,54,54	0
55	MG	DA	3230	1/1	0.97	0.14	68,68,68,68	0
55	MG	AA	3110	1/1	0.97	0.08	39,39,39,39	0
55	MG	DA	3493	1/1	0.97	0.30	46,46,46,46	0
55	MG	AA	3243	1/1	0.97	0.25	52,52,52,52	0
55	MG	AA	3278	1/1	0.97	0.20	81,81,81,81	0
55	MG	AA	3538	1/1	0.97	0.19	37,37,37,37	0
55	MG	AA	3088	1/1	0.97	0.26	60,60,60,60	0
55	MG	AA	3197	1/1	0.97	0.31	63,63,63,63	0
55	MG	AA	3112	1/1	0.97	0.33	48,48,48,48	0
55	MG	DA	3418	1/1	0.97	0.29	81,81,81,81	0
55	MG	BA	1646	1/1	0.97	0.17	70,70,70,70	0
55	MG	AA	3432	1/1	0.97	0.33	41,41,41,41	0
55	MG	CA	1671	1/1	0.97	0.28	51,51,51,51	0
55	MG	DA	3460	1/1	0.97	0.30	45,45,45,45	0
55	MG	DA	3461	1/1	0.97	0.21	50,50,50,50	0
55	MG	DA	3031	1/1	0.97	0.17	69,69,69,69	0
55	MG	DA	3463	1/1	0.97	0.27	44,44,44,44	0
55	MG	AA	3089	1/1	0.97	0.19	44,44,44,44	0
55	MG	AB	205	1/1	0.97	0.19	75,75,75,75	0
55	MG	AA	3082	1/1	0.97	0.21	39,39,39,39	0
55	MG	AA	3569	1/1	0.98	0.31	40,40,40,40	0
55	MG	DA	3032	1/1	0.98	0.20	73,73,73,73	0
55	MG	AA	3136	1/1	0.98	0.13	40,40,40,40	0
55	MG	AO	201	1/1	0.98	0.27	39,39,39,39	0
55	MG	AA	3456	1/1	0.98	0.16	70,70,70,70	0
55	MG	AA	3060	1/1	0.98	0.06	57,57,57,57	0
55	MG	AA	3268	1/1	0.98	0.32	47,47,47,47	0
55	MG	CA	1632	1/1	0.98	0.13	77,77,77,77	0
55	MG	A1	201	1/1	0.98	0.22	49,49,49,49	0
55	MG	BA	1748	1/1	0.98	0.27	61,61,61,61	0
55	MG	DA	3008	1/1	0.98	0.21	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	BA	1738	1/1	0.98	0.09	73,73,73,73	0
55	MG	CC	103	1/1	0.98	0.28	72,72,72,72	0
55	MG	DA	3011	1/1	0.98	0.08	68,68,68,68	0
55	MG	AA	3350	1/1	0.98	0.29	59,59,59,59	0
55	MG	D5	101	1/1	0.98	0.17	50,50,50,50	0
55	MG	DA	3336	1/1	0.98	0.15	68,68,68,68	0
55	MG	AA	3550	1/1	0.98	0.25	52,52,52,52	0
55	MG	CA	1746	1/1	0.98	0.36	59,59,59,59	0
55	MG	AA	3574	1/1	0.99	0.18	29,29,29,29	0
55	MG	AA	3031	1/1	0.99	0.28	44,44,44,44	0
55	MG	AA	3590	1/1	0.99	0.09	56,56,56,56	0
55	MG	DA	3147	1/1	0.99	0.05	16,16,16,16	0
56	ZN	CQ	101	1/1	0.99	0.09	113,113,113,113	0

6.5 Other polymers [i](#)

There are no such residues in this entry.