



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 13, 2018 – 01:16 pm GMT

PDB ID : 4V8B
Title : Crystal structure analysis of ribosomal decoding (near-cognate tRNA-leu complex).
Authors : Jenner, L.; Demeshkina, N.; Yusupov, M.; Yusupova, G.
Deposited on : 2011-12-06
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	trunk31020
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac	:	5.8.0158
CCP4	:	7.0 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk31020

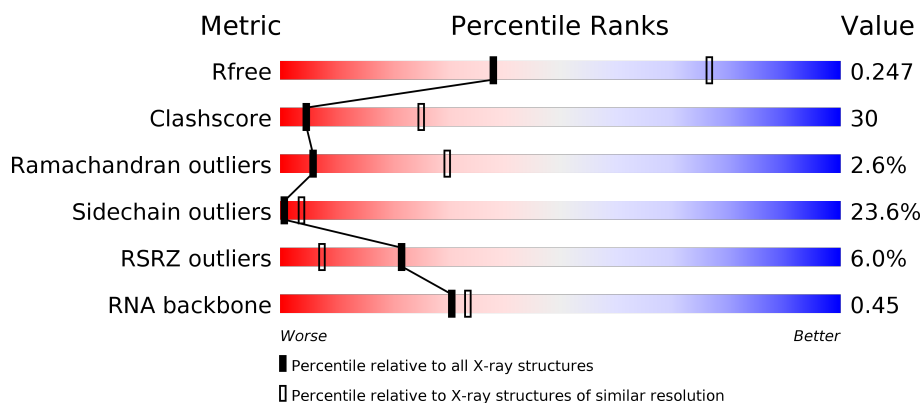
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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}	111664	1851 (3.00-3.00)
Clashscore	122126	2167 (3.00-3.00)
Ramachandran outliers	120053	2101 (3.00-3.00)
Sidechain outliers	120020	2104 (3.00-3.00)
RSRZ outliers	108989	1751 (3.00-3.00)
RNA backbone	2636	1017 (3.30-2.70)

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

Mol	Chain	Length	Quality of chain
1	AA	1506	<div> <div>32%</div> <div>48%</div> <div>19%</div> <div>•</div> </div>
1	CA	1506	<div> <div>30%</div> <div>47%</div> <div>22%</div> <div>•</div> </div>
2	AE	256	<div> <div>4%</div> <div>32%</div> <div>46%</div> <div>14%</div> <div>7%</div> <div>•</div> </div>
2	CE	256	<div> <div>10%</div> <div>34%</div> <div>41%</div> <div>16%</div> <div>7%</div> <div>•</div> </div>

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Mol	Chain	Length	Quality of chain
3	AF	239	
3	CF	239	
4	AG	208	
4	CG	208	
5	AH	162	
5	CH	162	
6	AI	101	
6	CI	101	
7	AJ	156	
7	CJ	156	
8	AK	138	
8	CK	138	
9	AL	128	
9	CL	128	
10	AM	105	
10	CM	105	
11	AN	129	
11	CN	129	
12	AO	132	
12	CO	132	
13	AP	126	
13	CP	126	
14	AQ	61	
14	CQ	61	
15	AR	89	

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Mol	Chain	Length	Quality of chain
15	CR	89	
16	AS	88	
16	CS	88	
17	AT	105	
17	CT	105	
18	AU	88	
18	CU	88	
19	AV	93	
19	CV	93	
20	AW	106	
20	CW	106	
21	AX	27	
21	CX	27	
22	AB	87	
22	CB	87	
23	AC	77	
23	AD	77	
23	CC	77	
23	CD	77	
24	A1	10	
24	C1	10	
25	BA	2912	
25	DA	2912	
26	BB	122	
26	DB	122	

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Mol	Chain	Length	Quality of chain
27	BD	276	
27	DD	276	
28	BE	206	
28	DE	206	
29	BF	210	
29	DF	210	
30	BG	182	
30	DG	182	
31	BH	180	
31	DH	180	
32	BK	148	
32	DK	148	
33	BM	140	
33	DM	140	
34	BN	122	
34	DN	122	
35	BO	150	
35	DO	150	
36	BP	141	
36	DP	141	
37	B0	118	
37	D0	118	
38	BQ	112	
38	DQ	112	
39	BR	146	




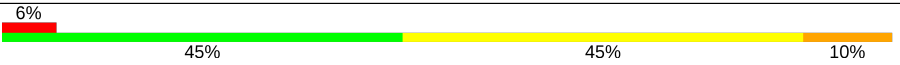
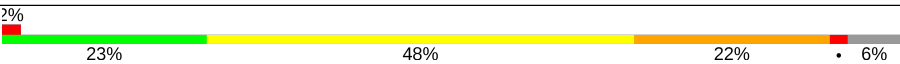
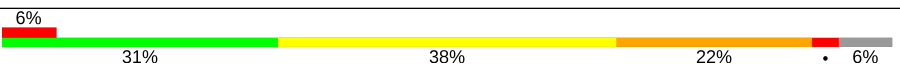
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Mol	Chain	Length	Quality of chain
39	DR	146	
40	B1	118	
40	D1	118	
41	B2	101	
41	D2	101	
42	BS	113	
42	DS	113	
43	BT	96	
43	DT	96	
44	BU	110	
44	DU	110	
45	BV	206	
45	DV	206	
46	B3	85	
46	D3	85	
47	BZ	98	
47	DZ	98	
48	BW	72	
48	DW	72	
49	BX	60	
49	DX	60	
50	B4	71	
50	D4	71	
51	B5	60	
51	D5	60	

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Mol	Chain	Length	Quality of chain
52	B6	54	
52	D6	54	
53	B7	49	
53	D7	49	
54	B8	65	
54	D8	65	

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	1625	-	-	-	X
55	MG	AA	1662	-	-	-	X
55	MG	AA	1706	-	-	-	X
55	MG	AA	1727	-	-	-	X
55	MG	AA	1735	-	-	-	X
55	MG	AA	1755	-	-	-	X
55	MG	AA	1761	-	-	-	X
55	MG	AA	1772	-	-	-	X
55	MG	AA	1781	-	-	-	X
55	MG	AA	1807	-	-	-	X
55	MG	AA	1836	-	-	-	X
55	MG	BA	3069	-	-	-	X
55	MG	BA	3073	-	-	-	X
55	MG	BA	3121	-	-	-	X
55	MG	BA	3247	-	-	-	X
55	MG	BA	3317	-	-	-	X
55	MG	BA	3324	-	-	-	X
55	MG	BA	3325	-	-	-	X
55	MG	BA	3328	-	-	-	X
55	MG	BA	3334	-	-	-	X
55	MG	BA	3339	-	-	-	X
55	MG	BA	3349	-	-	-	X
55	MG	BA	3379	-	-	-	X
55	MG	BA	3388	-	-	-	X
55	MG	BA	3399	-	-	-	X
55	MG	BA	3408	-	-	-	X
55	MG	BA	3418	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	BA	3431	-	-	-	X
55	MG	BA	3465	-	-	-	X
55	MG	BA	3466	-	-	-	X
55	MG	BA	3472	-	-	-	X
55	MG	BA	3473	-	-	-	X
55	MG	BA	3481	-	-	-	X
55	MG	BA	3505	-	-	-	X
55	MG	BA	3527	-	-	-	X
55	MG	BA	3533	-	-	-	X
55	MG	BA	3536	-	-	-	X
55	MG	BA	3547	-	-	-	X
55	MG	BA	3570	-	-	-	X
55	MG	BA	3573	-	-	-	X
55	MG	BA	3583	-	-	-	X
55	MG	BA	3591	-	-	-	X
55	MG	BA	3603	-	-	-	X
55	MG	BD	301	-	-	-	X
55	MG	CA	1612	-	-	-	X
55	MG	CA	1630	-	-	-	X
55	MG	CA	1683	-	-	-	X
55	MG	CA	1702	-	-	-	X
55	MG	CA	1709	-	-	-	X
55	MG	CA	1714	-	-	-	X
55	MG	CA	1729	-	-	-	X
55	MG	CA	1758	-	-	-	X
55	MG	CA	1763	-	-	-	X
55	MG	CA	1771	-	-	-	X
55	MG	CC	104	-	-	-	X
55	MG	CC	107	-	-	-	X
55	MG	D1	202	-	-	-	X
55	MG	DA	3010	-	-	-	X
55	MG	DA	3038	-	-	-	X
55	MG	DA	3042	-	-	-	X
55	MG	DA	3045	-	-	-	X
55	MG	DA	3059	-	-	-	X
55	MG	DA	3064	-	-	-	X
55	MG	DA	3080	-	-	-	X
55	MG	DA	3119	-	-	-	X
55	MG	DA	3146	-	-	-	X
55	MG	DA	3303	-	-	-	X
55	MG	DA	3346	-	-	-	X
55	MG	DA	3353	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	DA	3366	-	-	-	X
55	MG	DA	3371	-	-	-	X
55	MG	DA	3381	-	-	-	X
55	MG	DA	3393	-	-	-	X
55	MG	DA	3403	-	-	-	X
55	MG	DA	3406	-	-	-	X
55	MG	DA	3409	-	-	-	X
55	MG	DA	3415	-	-	-	X
55	MG	DA	3419	-	-	-	X
55	MG	DA	3424	-	-	-	X
55	MG	DA	3447	-	-	-	X
55	MG	DA	3462	-	-	-	X
55	MG	DA	3464	-	-	-	X
55	MG	DA	3480	-	-	-	X
55	MG	DA	3491	-	-	-	X
55	MG	DA	3493	-	-	-	X
55	MG	DA	3507	-	-	-	X
55	MG	DA	3508	-	-	-	X
55	MG	DA	3522	-	-	-	X
55	MG	DB	211	-	-	-	X

2 Entry composition

There are 56 unique types of molecules in this entry. The entry contains 299552 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

- Molecule 2 is a protein called 30S RIBOSOMAL PROTEIN S2.

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

- Molecule 3 is a protein called 30S RIBOSOMAL PROTEIN S3.

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

- Molecule 4 is a protein called 30S RIBOSOMAL PROTEIN S4.

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

- Molecule 5 is a protein called 30S RIBOSOMAL PROTEIN S5.

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

- Molecule 6 is a protein called 30S RIBOSOMAL PROTEIN S6.

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

- Molecule 7 is a protein called 30S RIBOSOMAL PROTEIN S7.

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

- Molecule 8 is a protein called 30S RIBOSOMAL PROTEIN S8.

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

- Molecule 9 is a protein called 30S RIBOSOMAL PROTEIN S9.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AV	78	Total	C	N	O	S	0	0	0
			624	398	115	109	2			
19	CV	78	Total	C	N	O	S	0	0	0
			624	398	115	109	2			

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

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

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

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

- Molecule 22 is a RNA chain called TRNA-LEU.

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

- Molecule 23 is a RNA chain called TRNA-FMET.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AC	77	Total	C	N	O	P	0	0	0
			1643	732	298	536	77			
23	AD	77	Total	C	N	O	P	0	0	0
			1643	732	298	536	77			
23	CC	77	Total	C	N	O	P	0	0	0
			1643	732	298	536	77			
23	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
AC	18	C	U	CONFLICT	GB AP012306.1
AD	18	C	U	CONFLICT	GB AP012306.1
CC	18	C	U	CONFLICT	GB AP012306.1
CD	18	C	U	CONFLICT	GB AP012306.1

- Molecule 24 is a RNA chain called MRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	A1	10	Total	C	N	O	P	0	0	0
			205	92	26	77	10			
24	C1	10	Total	C	N	O	P	0	0	0
			205	92	26	77	10			

- Molecule 25 is a RNA chain called RNA (2912-MER).

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

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BA	161	U	-	EXPRESSION TAG	GB AP008226.1
BA	654A	A	G	CONFLICT	GB AP008226.1
BA	654E	C	G	CONFLICT	GB AP008226.1
BA	654P	G	C	CONFLICT	GB AP008226.1
BA	654T	A	C	CONFLICT	GB AP008226.1
BA	1058	U	G	CONFLICT	GB AP008226.1
BA	1080	A	C	CONFLICT	GB AP008226.1
DA	168	U	-	INSERTION	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 26 is a RNA chain called 5S RIBOSOMAL RNA.

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

- Molecule 27 is a protein called 50S ribosomal protein L2.

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

- Molecule 28 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	BE	205	Total	C	N	O	S	0	0	0
			1568	991	300	271	6			
28	DE	205	Total	C	N	O	S	0	0	0
			1568	991	300	271	6			

- Molecule 29 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	BF	202	Total	C	N	O	S	0	0	0
			1585	1011	297	275	2			
29	DF	208	Total	C	N	O	S	0	0	0
			1627	1037	304	283	3			

- Molecule 30 is a protein called 50S ribosomal protein L5.

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

- Molecule 31 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	BH	170	Total	C	N	O	S	0	0	0
			1307	829	245	232	1			
31	DH	170	Total	C	N	O	S	0	0	0
			1307	829	245	232	1			

- Molecule 32 is a protein called 50S ribosomal protein L9.

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

- Molecule 33 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	BM	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			

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

- Molecule 34 is a protein called 50S ribosomal protein L14.

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

- Molecule 35 is a protein called 50S ribosomal protein L15.

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

- Molecule 36 is a protein called 50S ribosomal protein L16.

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

- Molecule 37 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	B0	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			
37	D0	117	Total	C	N	O		0	0	0
			960	599	202	159				

- Molecule 38 is a protein called 50S ribosomal protein L18.

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

- Molecule 39 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BR	137	Total	C	N	O	S	0	0	0
			1141	710	234	196	1			
39	DR	137	Total	C	N	O	S	0	0	0
			1141	710	234	196	1			

- Molecule 40 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	B1	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			
40	D1	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			

- Molecule 41 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	B2	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			
41	D2	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			

- Molecule 42 is a protein called 50S ribosomal protein L22.

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

- Molecule 43 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
43	BT	92	Total	C	N	O	0	0	0
			725	471	131	123			
43	DT	92	Total	C	N	O	0	0	0
			725	471	131	123			

- Molecule 44 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	BU	102	Total	C	N	O	S	0	0	0
			785	505	150	125	5			
44	DU	102	Total	C	N	O	S	0	0	0
			785	505	150	125	5			

- Molecule 45 is a protein called 50S ribosomal protein L25.

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

- Molecule 46 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	B3	76	Total	C	N	O	S	0	0	0
			607	376	128	102	1			
46	D3	77	Total	C	N	O	S	0	0	0
			613	379	129	104	1			

- Molecule 47 is a protein called 50S ribosomal protein L28.

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

- Molecule 48 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	BW	66	Total	C	N	O	S	0	0	0
			558	346	113	98	1			
48	DW	69	Total	C	N	O	S	0	0	0
			581	358	118	104	1			

- Molecule 49 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
49	BX	59	Total	C	N	O	0	0	0
			469	298	90	81			

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	B4	66	Total	C	N	O	S	0	0	0
			533	335	96	97	5			
50	D4	63	Total	C	N	O	S	0	0	0
			515	326	93	91	5			

- Molecule 51 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	B5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			
51	D5	58	Total	C	N	O	S	0	0	0
			454	285	89	75	5			

- Molecule 52 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	B6	45	Total	C	N	O	S	0	0	0
			389	241	79	65	4			
52	D6	45	Total	C	N	O	S	0	0	0
			389	241	79	65	4			

- Molecule 53 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	B7	49	Total	C	N	O	S	0	0	0
			430	263	108	57	2			
53	D7	49	Total	C	N	O	S	0	0	0
			430	263	108	57	2			

- Molecule 54 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	B8	61	Total	C	N	O	S	0	0	0
			488	312	99	75	2			
54	D8	61	Total	C	N	O	S	0	0	0
			488	312	99	75	2			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	BA	623	Total 623	Mg 623	0	0
55	CA	207	Total 207	Mg 207	0	0
55	AB	5	Total 5	Mg 5	0	0
55	B8	1	Total 1	Mg 1	0	0
55	BE	5	Total 5	Mg 5	0	0
55	DU	1	Total 1	Mg 1	0	0
55	B1	1	Total 1	Mg 1	0	0
55	AN	2	Total 2	Mg 2	0	0
55	CN	1	Total 1	Mg 1	0	0
55	B5	1	Total 1	Mg 1	0	0
55	BB	17	Total 17	Mg 17	0	0
55	D3	1	Total 1	Mg 1	0	0
55	BF	3	Total 3	Mg 3	0	0
55	DR	1	Total 1	Mg 1	0	0
55	B2	1	Total 1	Mg 1	0	0
55	AA	242	Total 242	Mg 242	0	0
55	CG	2	Total 2	Mg 2	0	0
55	BU	2	Total 2	Mg 2	0	0
55	A1	2	Total 2	Mg 2	0	0
55	AD	1	Total 1	Mg 1	0	0
55	CC	8	Total 8	Mg 8	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	DE	3	Total 3	Mg 3	0	0
55	B3	1	Total 1	Mg 1	0	0
55	DA	526	Total 526	Mg 526	0	0
55	B7	1	Total 1	Mg 1	0	0
55	AG	1	Total 1	Mg 1	0	0
55	BO	2	Total 2	Mg 2	0	0
55	AQ	1	Total 1	Mg 1	0	0
55	D1	2	Total 2	Mg 2	0	0
55	AH	1	Total 1	Mg 1	0	0
55	DP	1	Total 1	Mg 1	0	0
55	AC	9	Total 9	Mg 9	0	0
55	CB	3	Total 3	Mg 3	0	0
55	D5	1	Total 1	Mg 1	0	0
55	BD	1	Total 1	Mg 1	0	0
55	B0	1	Total 1	Mg 1	0	0
55	CS	1	Total 1	Mg 1	0	0
55	DB	14	Total 14	Mg 14	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	AG	1	Total 1	Zn 1	0	0
56	AQ	1	Total 1	Zn 1	0	0

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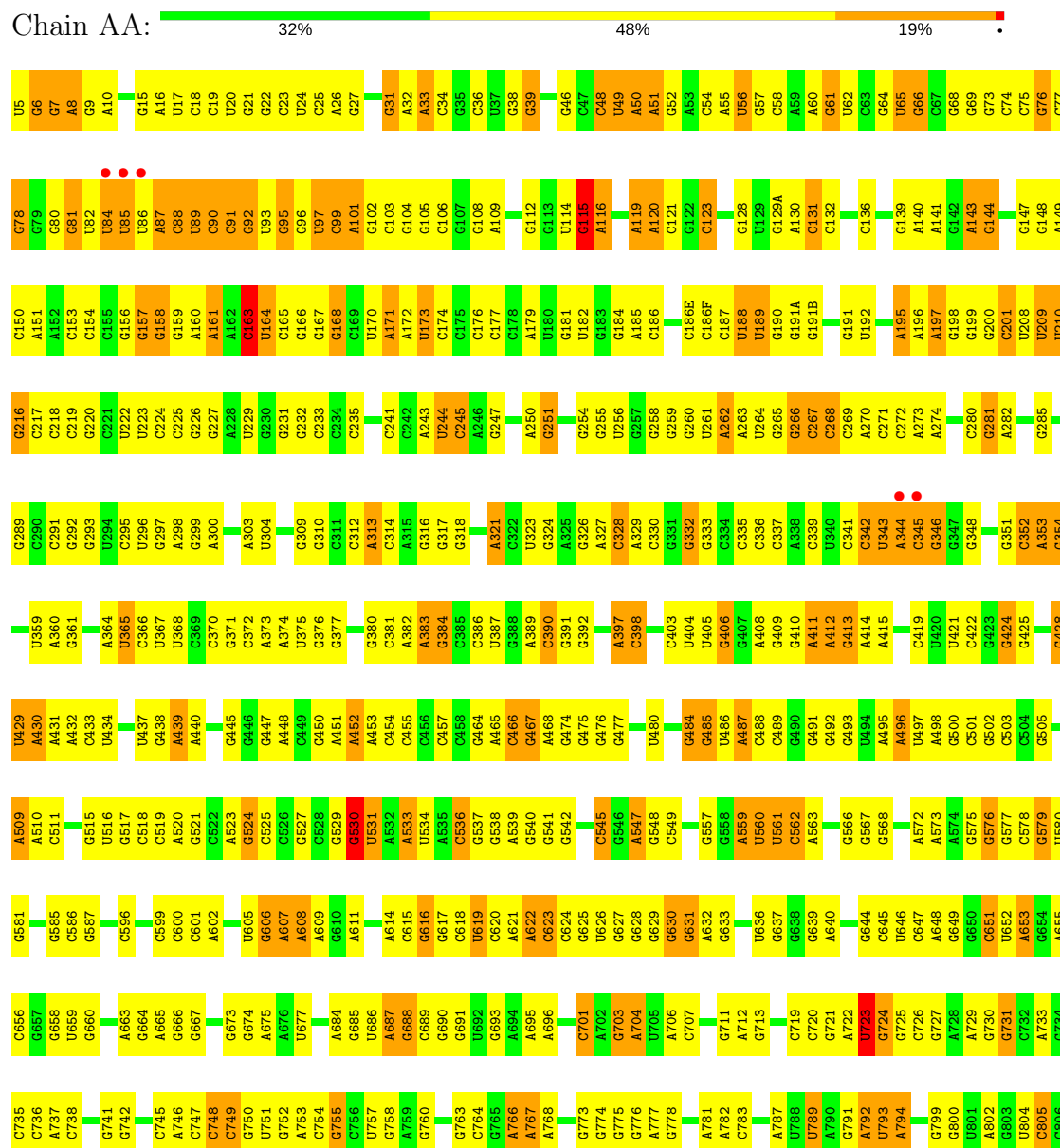
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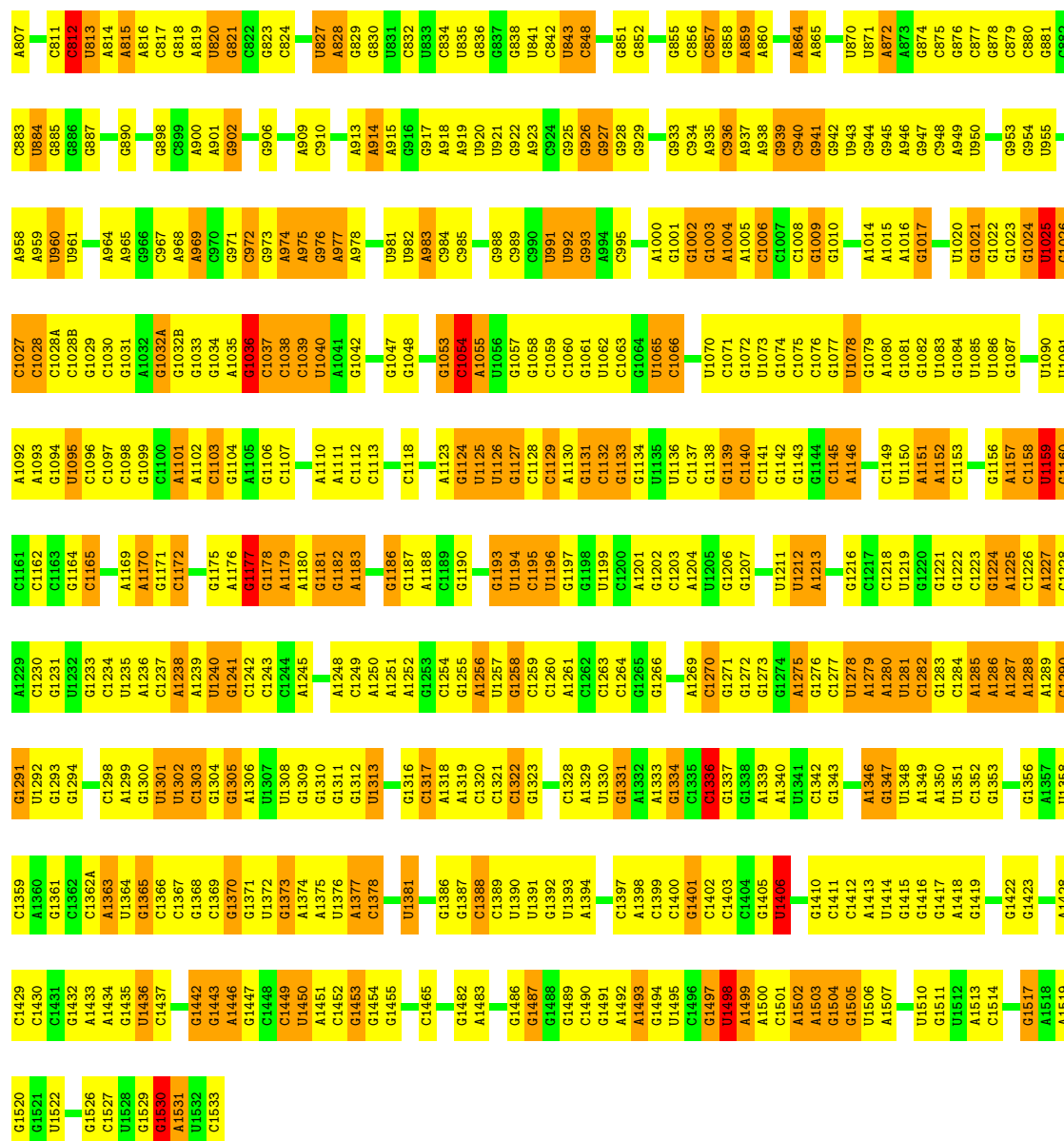
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	CQ	1	Total 1	Zn 1	0	0
56	CG	1	Total 1	Zn 1	0	0

3 Residue-property plots

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

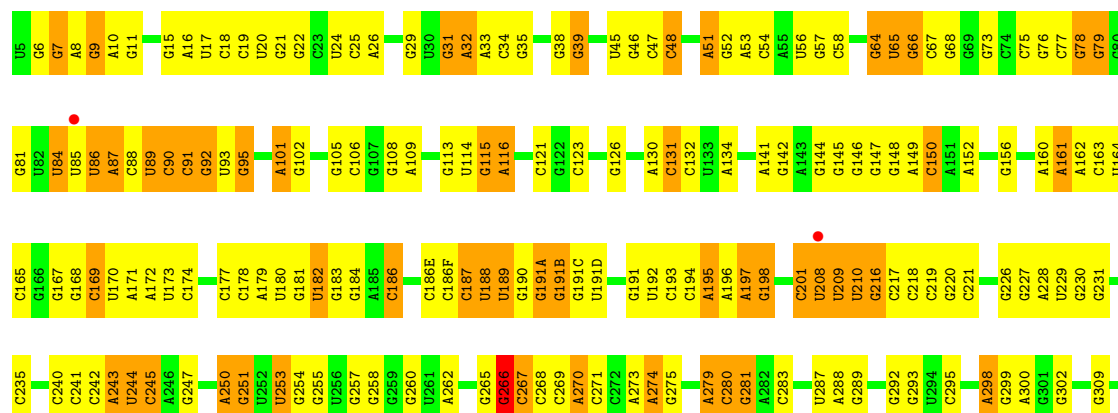
- Molecule 1: 16S ribosomal RNA



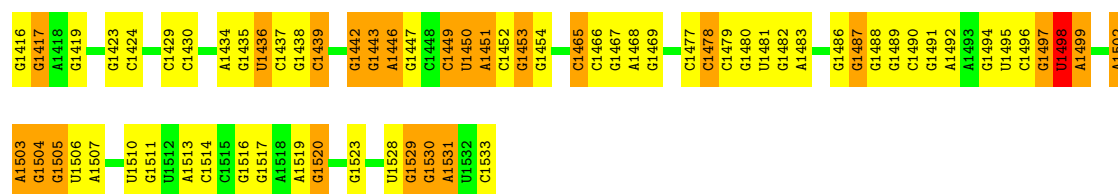


• Molecule 1: 16S ribosomal RNA

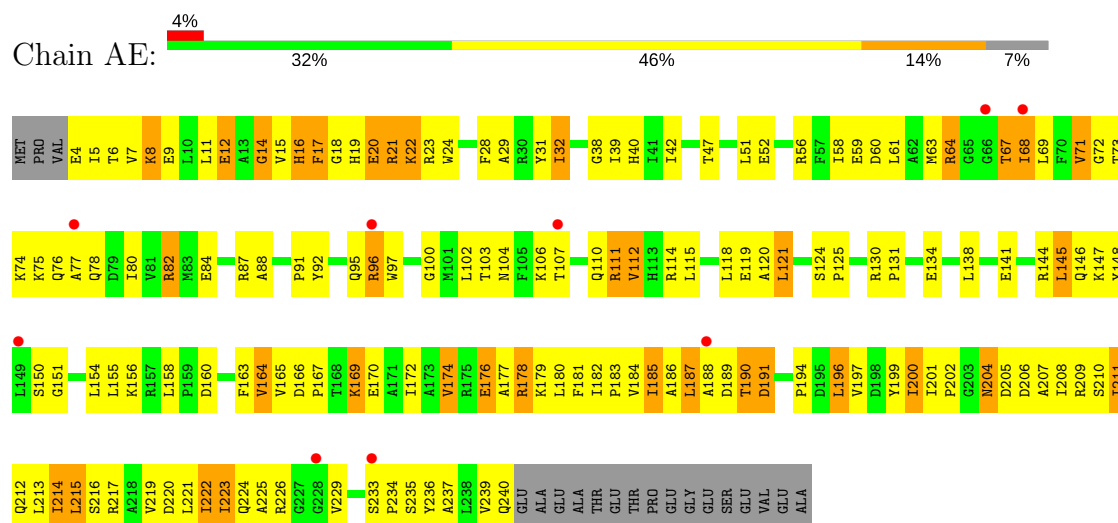
Chain CA: 30% 47% 22%



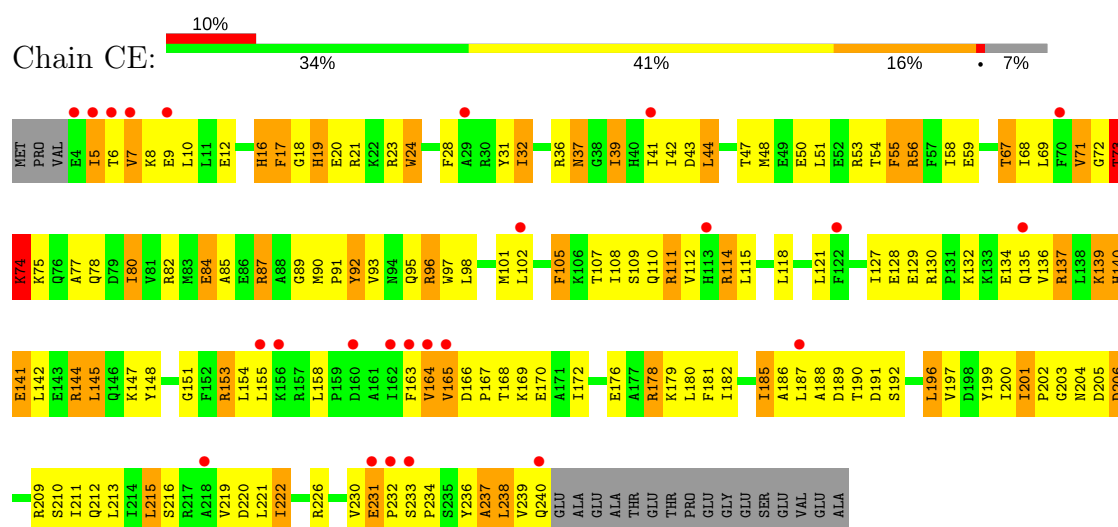
A1350	A1287	C1223	G1160	G1034	A978	G917	U833	G755	G692	G541	G467	C390	A313
U1351	A1288	G1224	C1161	A1035	C979	A918	C834	C756	G683	G542	A468	G391	C314
C1352	A1289	A1225	C1162	G1036	C980	A919	C835	U757	A694	C543	G474	G392	A315
G1353	G1290	C1163	C1102	C1037	U981	U920	U836	G758	G685	G544	G475	A393	G316
C1354	G1291	G1164	C1103	C1038	U982	U921	G837	G763	U686	C545	G476	G394	
G1355	U1292	C1165	G1104	C1039	A983	G922	G838	G764	G687	G546	G477	C395	A321
G1356	G1293	G1166	A1105	U1040	C984	A923	U839	G765	G688	A547	A478	G396	
A1357	G1294	G1167	G1106	A1041	C985		U841	C766	C689	G548		G397	G326
U1358	G1295	U1232	A1170	G1042	A986	G926	C842	A766	G690	C549	G481	A327	
	G1296	G1233	G1107	C1043	C987	G927	U843	G769	G691	G550	A482	C328	A329
G1361	C1297	C1172	C1108	A1044	C988	G928	C844		U692	U551	C483	U404	
C1362	U1298	G1173	C1109	C1045	C989	G929	C849	G773	G693	U552	G484	U405	
C1362A	A1299	G1174	A1110	A1046	C990	C930	U850	G774	A694	A553	G485	G407	
A1363	G1300	G1175	C1112	G1047	U991	C931	C851	G775	A695	C554	U486		
	U1301	A1176	C1113	G1048	U992	G932	G852	G776	A696	C555	A487	A408	
U1364	C1238	G1177			C993	G933	G853			C556	C488	G409	
G1365	A1239	G1178	U1052	U1053	A994	C934	G854	A777	G700	C559	C489	G410	
C1366	G1240	G1179	G1053	G1054	C995	A935	G858	G778	C701	A559		A411	
C1367	G1241	A1178	G1053	C1055	C996	C936	C936	C779	A702	U560		A412	
G1368	A1180	G1181	C1118	A1054	U997	A937	A859	A780	G703	U561		G413	
G1369	G1182	G1182	C1120	U1056	G998	A938	A860		A704	C562		A414	
	U1247	A1183	U1121	G1057	C998A	G939	C861	C783	U705	A563		U420	
G1371	G1310	G1184	U1122	G1058	U999	C940	C862	C784	A706	C564		U421	
G1372	G1311	G1185	A1123	C1059	A1000	G941	U863	G785	U707	U565		C422	
A1374	G1312	G1186	G1124	C1060	G1001	G942	U864	G786	C707	C566		G423	
U1375	U1313	G1187	U1125	G1061	G1002	U943		A787	G710	C567		G424	
U1376	C1314	A1188	U1126	U1062	G1003	G944	G869	U788	G711	C568		G425	
A1377	A1252	C1189	G1127	C1063	A1004	G945	U870	C791	A712	C569		G426	
G1378	G1253	G1190	C1128	G1064	A1005	A946	U871	A792	G713	C570		C427	
C1379	C1254	A1191	U1065	U1070	C1006	G947	A872	U793	U723	U571		U428	
U1380	G1255	C1192	A1130	C1066	C1007	C948	A873	C718	G719	A572		G429	
U1381	A1256	G1193	C1131	A1067	C1008	A949		C720	A510	A573		A430	
C1382	U1257	U1194	C1132	G1068	G1009	U950	C877	C795	U512	A574		A431	
	G1258	C1195	G1133	C1069	G1010	G951	G878	C796	G650	C575		A432	
G1386	C1259	U1196	G1134	C1071		G952	C879	A722	C513	C576		G433	
G1387	C1260	G1197	U1135	G1072	A1014	G953	C883	U723	C514	C577		U434	
A1324	A1261	G1198	U1136	U1073	A1015	U955	U884	G724	G515	C578		A360	
C1325	C1262	U1199	C1137	U1074	A1016	U956	C885		U516	C579		C435	
C1326	C1263	C1200	G1138	G1075	A1017	U957	C886	A728	G517	U580		C436	
U1391	G1266	A1201	G1139	C1076	C1018	A958	C887	G730	C518	U437		U437	
U1393	C1267	C1203	C1140	C1076	C1019	A959	C888	G731	C519	G438		G438	
A1394	U1268	A1204	G1142	U1077		U960	A889	C505	A520	A439		A440	
C1395	A1269	U1205	G1143	A1080	G1021	U961		C310	G521	C522		C444	
U1396	C1270	G1206	G1144	G1081	G1022	C962	A892	C912	C526			G444	
C1397	G1271	G1207	C1145	U1082	G1023	G963	C893	C912	G527	G446		G446	
A1398	C1272	C1208	A1146	U1083	G1024	A964	C897	U740	C528	G447		G447	
C1399	G1273	C1209	C1147	G1084	U1025	A965	C898	G741	G529	A448		A448	
G400	G1274		U1148	U1085	G1026	G966	C899	G742	G530	C449		G449	
C1401	A1275	U1212	C1149	U1086	C1027	C967	A900	C745	U531	A451		G450	
C1402	G1276	A1213	U1150		C1028	A968	A901	A746	A532	A452		A451	
C1403	C1277	G1215	A1151	G1089	C1028A	A969	C917	U672	A533	A453		A453	
U1406	U1278	G1216	C1152	U1090	C1028B	G970	C918	C747	U534				
	A1279	G1217	U1091	U1091	G1029	G971	A909	G673	G604	A535		C457	
	U1281	C1218	G1154	A1092	C1030	G972	C910	G674	U605	C536		C458	
	C1282	U1219	G1155	A1093	G1031	G973		A675	G606	G537		G459	
			A1157	G1094	A1032	A974	A913	U751	A607			G464	
			U1157	U1095	G1032A	A975	A914	G752	A608	A539		A465	
			C1096	C1096	G1032B	G976	A915	G754				A466	
			U1159	C1097	G1033	A977	G916						



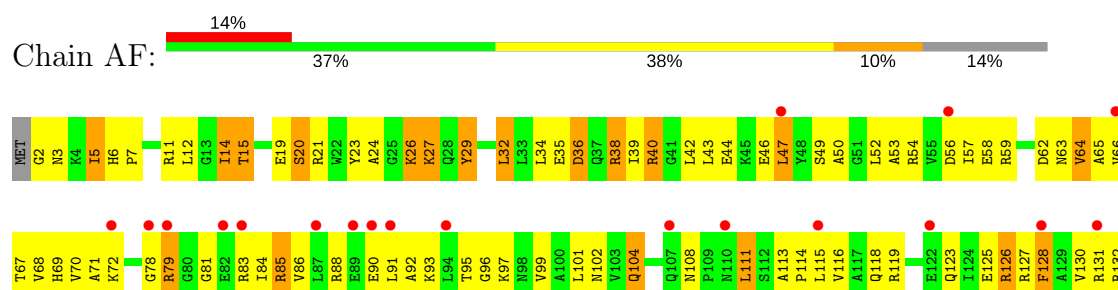
• Molecule 2: 30S RIBOSOMAL PROTEIN S2



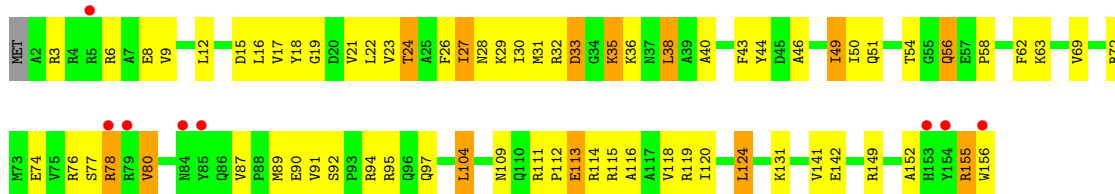
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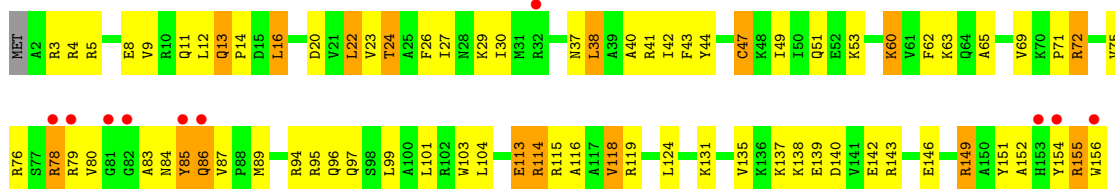
• Molecule 3: 30S RIBOSOMAL PROTEIN S3



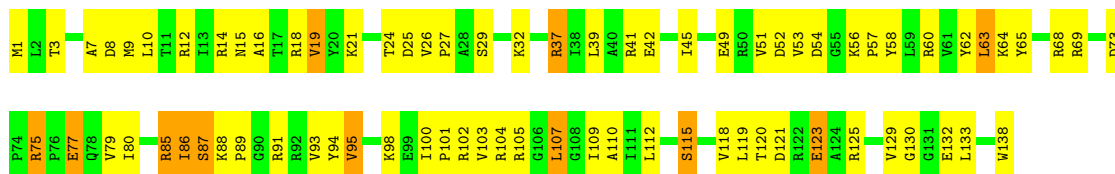




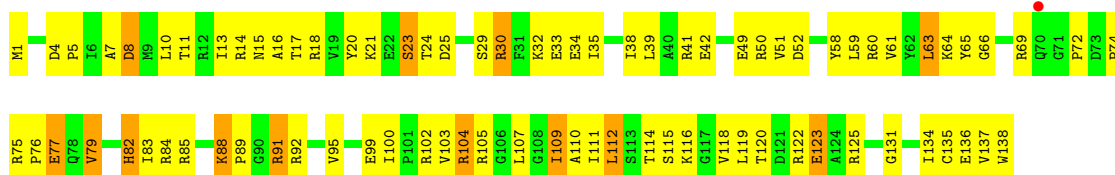
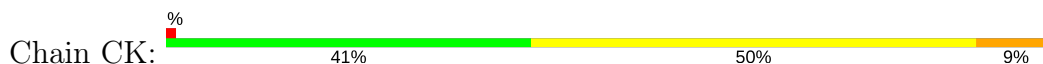
• Molecule 7: 30S RIBOSOMAL PROTEIN S7



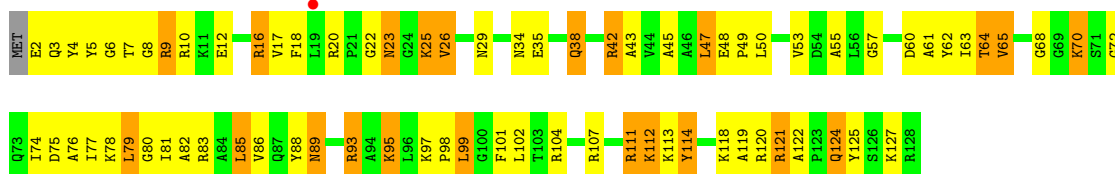
• Molecule 8: 30S RIBOSOMAL PROTEIN S8



• Molecule 8: 30S RIBOSOMAL PROTEIN S8

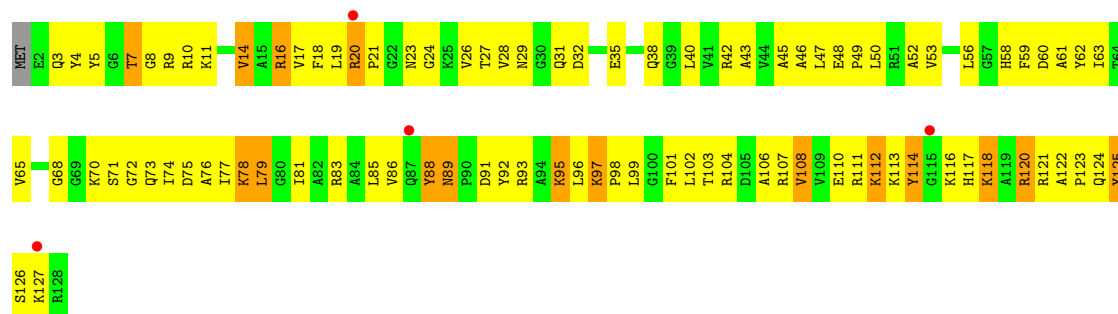


• Molecule 9: 30S RIBOSOMAL PROTEIN S9

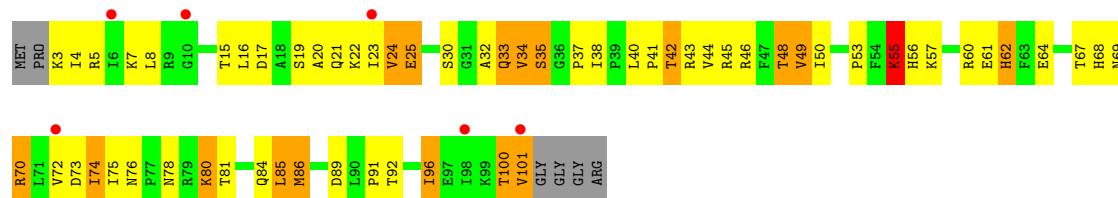


• Molecule 9: 30S RIBOSOMAL PROTEIN S9

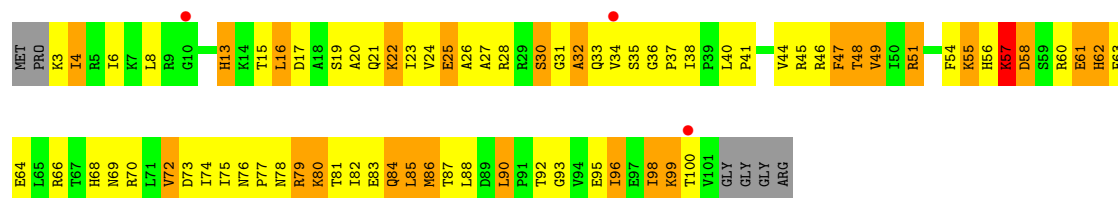




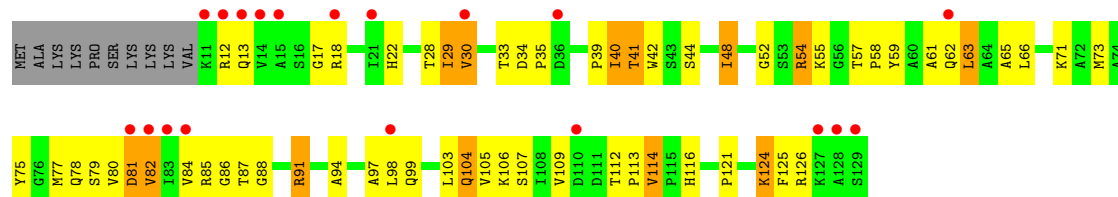
• Molecule 10: 30S RIBOSOMAL PROTEIN S10



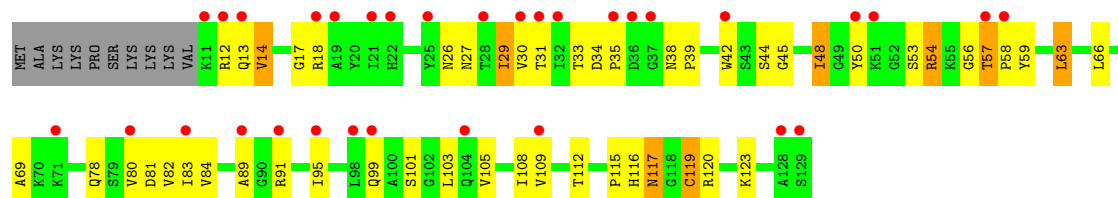
• Molecule 10: 30S RIBOSOMAL PROTEIN S10



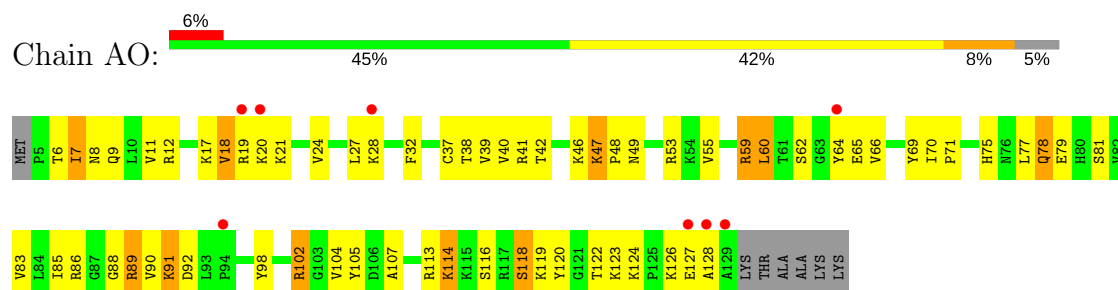
• Molecule 11: 30S RIBOSOMAL PROTEIN S11



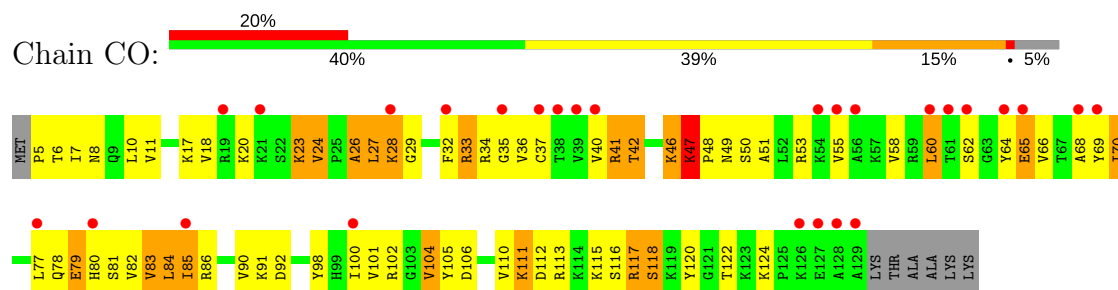
• Molecule 11: 30S RIBOSOMAL PROTEIN S11



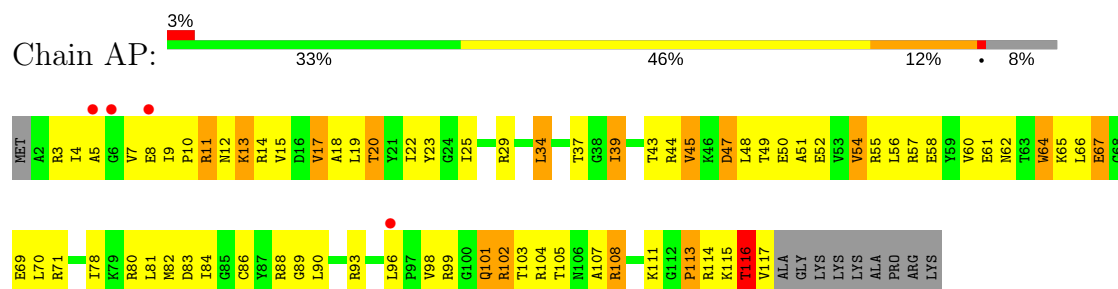
- Molecule 12: 30S RIBOSOMAL PROTEIN S12



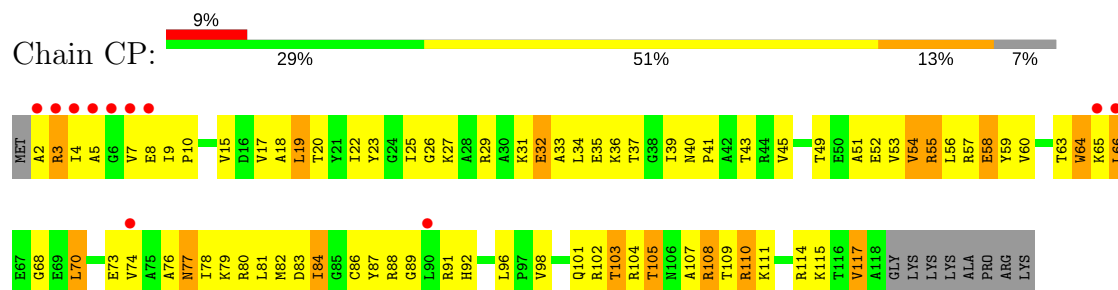
- Molecule 12: 30S RIBOSOMAL PROTEIN S12



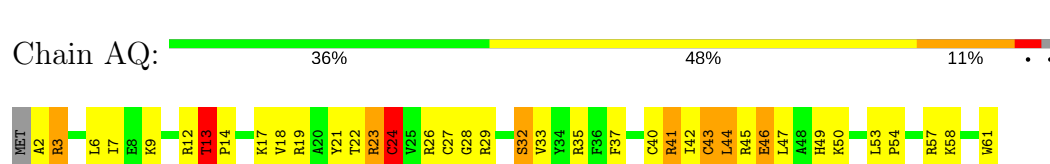
- Molecule 13: 30S RIBOSOMAL PROTEIN S13



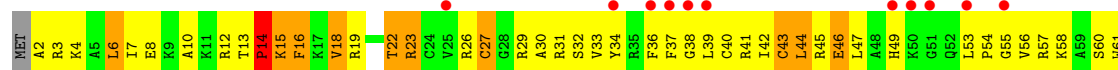
- Molecule 13: 30S RIBOSOMAL PROTEIN S13



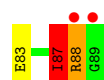
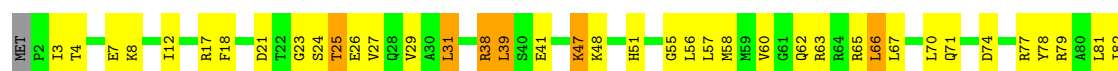
- Molecule 14: 30S RIBOSOMAL PROTEIN S14



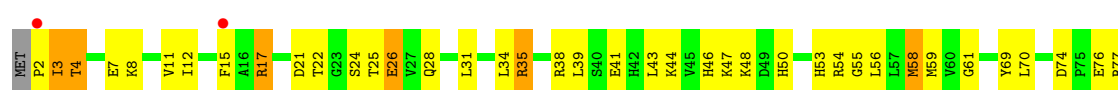
- Molecule 14: 30S RIBOSOMAL PROTEIN S14



• Molecule 15: 30S RIBOSOMAL PROTEIN S15



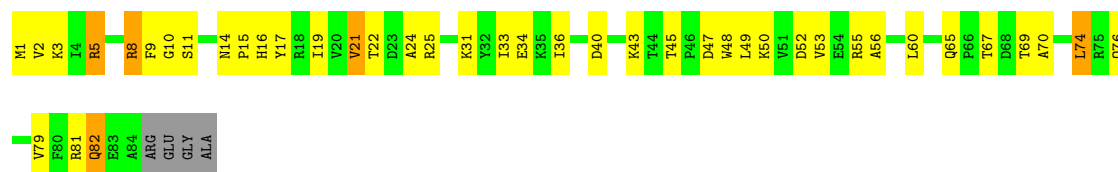
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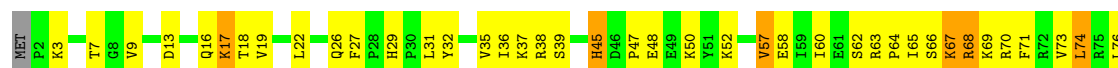
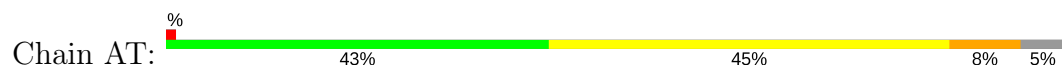
• Molecule 16: 30S RIBOSOMAL PROTEIN S16



• Molecule 16: 30S RIBOSOMAL PROTEIN S16



• Molecule 17: 30S RIBOSOMAL PROTEIN S17

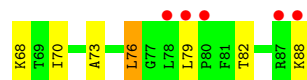
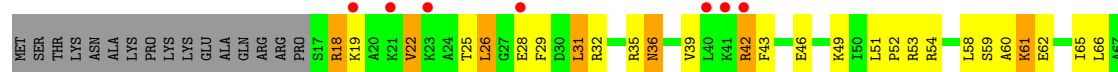
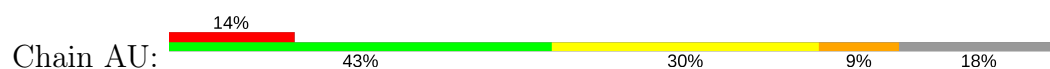




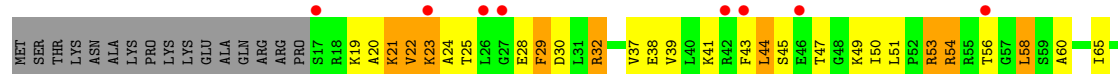
• Molecule 17: 30S RIBOSOMAL PROTEIN S17



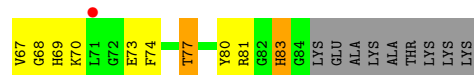
• Molecule 18: 30S RIBOSOMAL PROTEIN S18



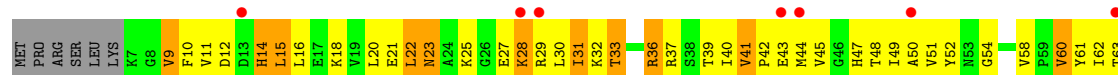
• Molecule 18: 30S RIBOSOMAL PROTEIN S18

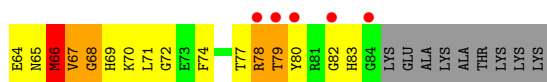


• Molecule 19: 30S RIBOSOMAL PROTEIN S19



• Molecule 19: 30S RIBOSOMAL PROTEIN S19





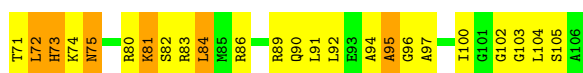
• Molecule 20: 30S RIBOSOMAL PROTEIN S20

Chain AW: 33% 52% 8% 7%



• Molecule 20: 30S RIBOSOMAL PROTEIN S20

Chain CW: 33% 47% 12% 7%



• Molecule 21: 30S RIBOSOMAL PROTEIN THX

Chain AX: 41% 41% 11% 7%



• Molecule 21: 30S RIBOSOMAL PROTEIN THX

Chain CX: 4% 37% 56% 7%



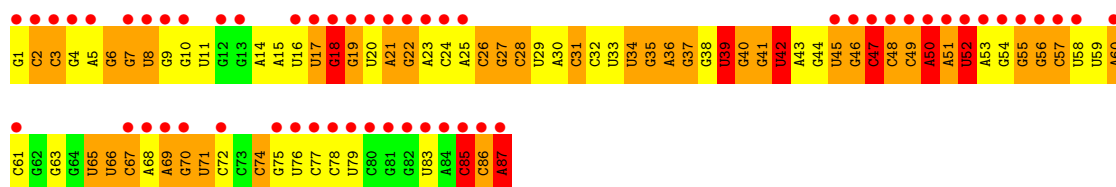
• Molecule 22: TRNA-LEU

Chain AB: 33% 26% 33% 36% 5%



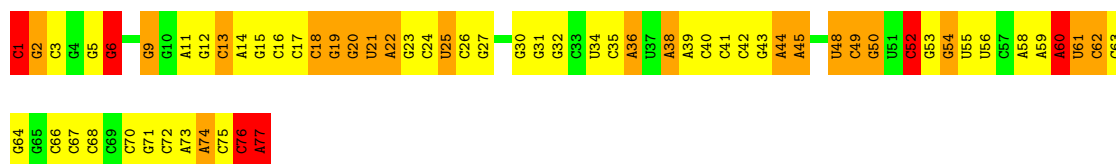
• Molecule 22: TRNA-LEU

Chain CB: 10% 63% 39% 41% 9%



● Molecule 23: TRNA-FMET

Chain AC: 18% 48% 26% 8%



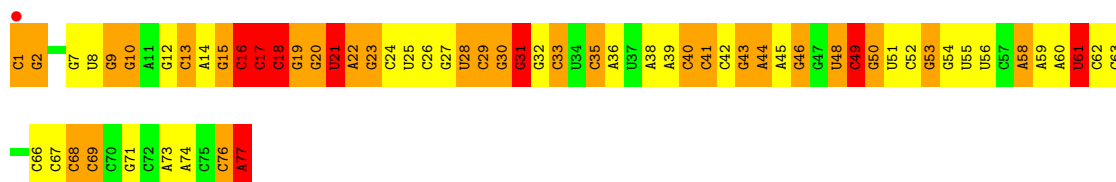
● Molecule 23: TRNA-FMET

Chain AD: 4% 16% 52% 32%



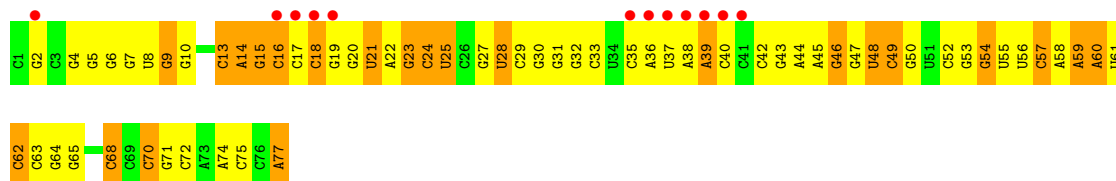
● Molecule 23: TRNA-FMET

Chain CC: % 18% 36% 35% 10%



● Molecule 23: TRNA-FMET

Chain CD: 16% 17% 53% 30%



● Molecule 24: MRNA

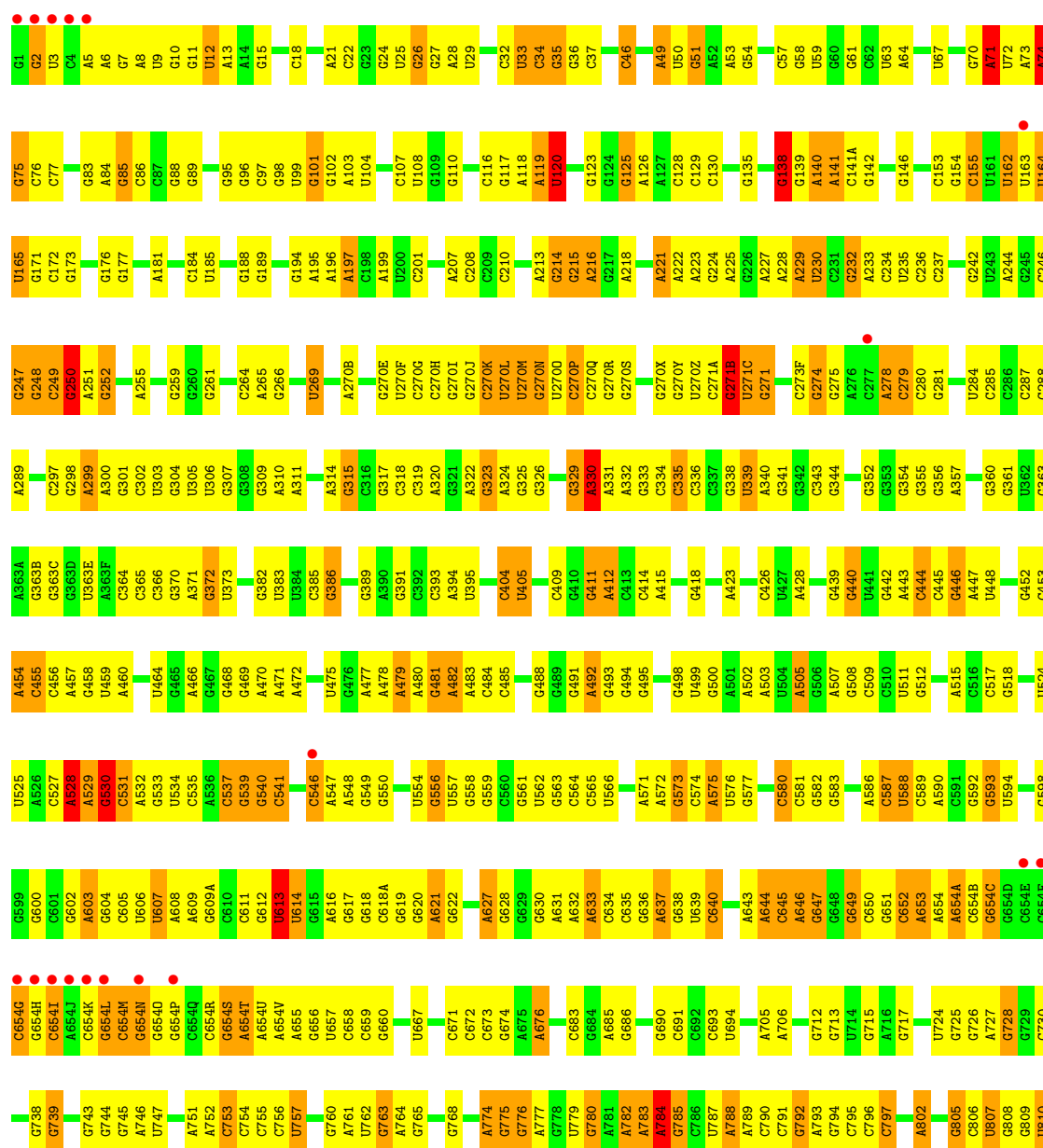
Chain A1: 20% 20% 40% 30% 10%



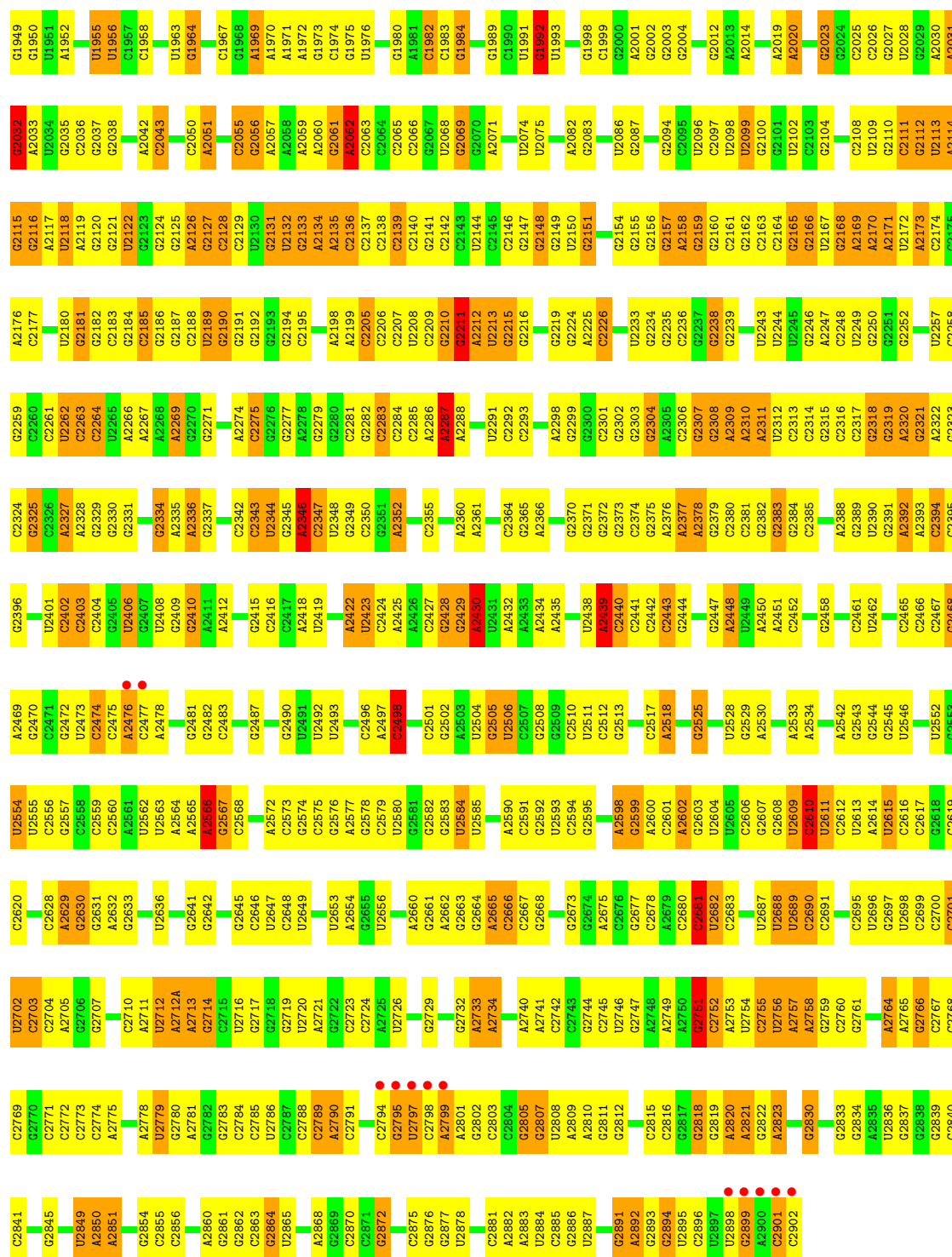
• Molecule 24: MRNA



• Molecule 25: RNA (2912-MER)





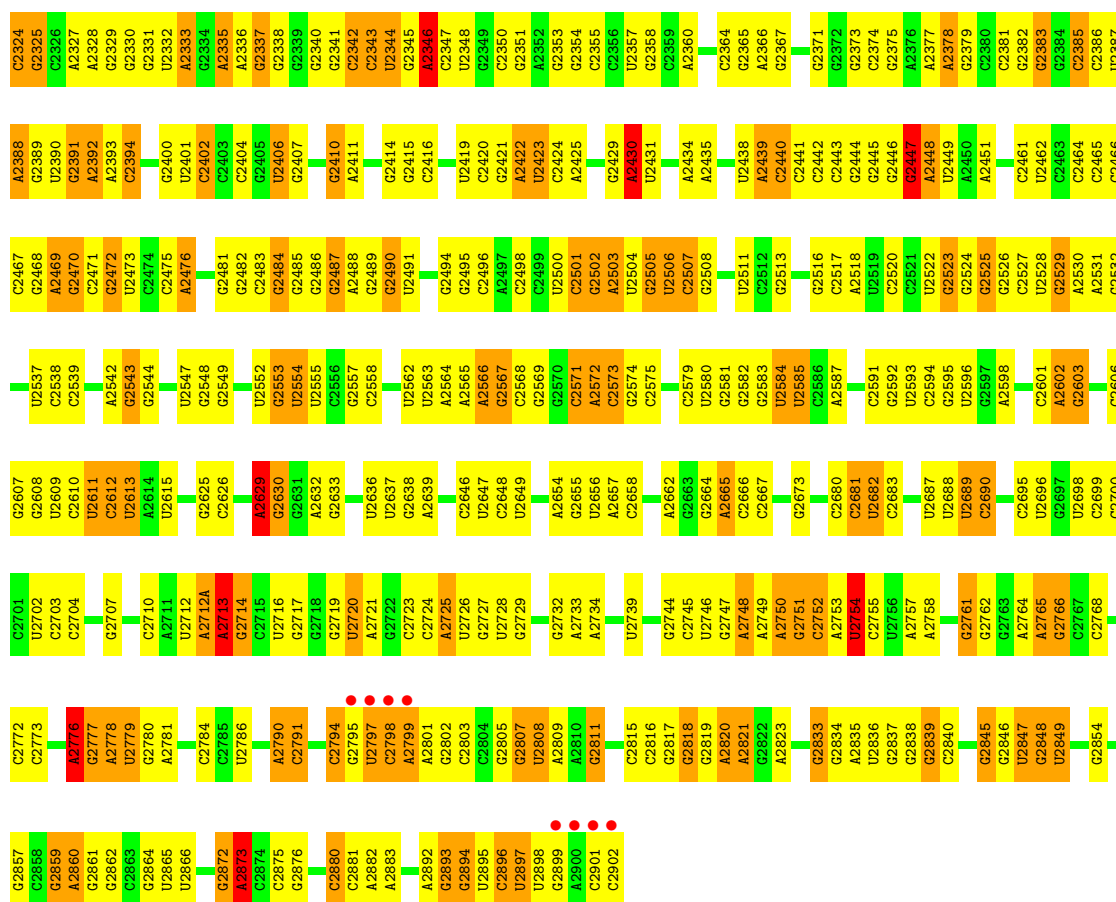


• Molecule 25: RNA (2912-MER)

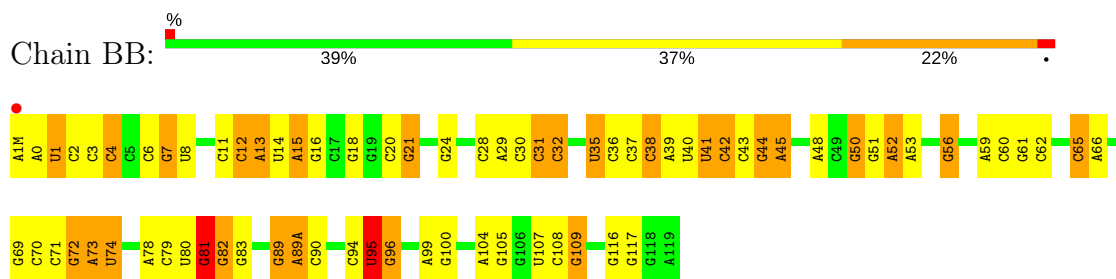


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C1104	C1042	C840	G978	C904	C840	G776	C708	C517	C443	G352	A278	G147	A71
U1105	C1043	A841	G979	U905	A841	A777	C708	U524	C444	G353	C279	U147	A72
G1106	G1044	G842	A980	G906	G842	G778	U709	U525	C445	G354	C280	C148	A73
G1107	G1045	G843	A981	U907	G843	U779	G710	U526	C446	G355			A74
U1108	A1046	C844	C982	C908	C844	G780		A526	A447	G356	U284	G152	G75
G1047	A1047	G845	A983	A909	G845	A781	G715	C527	U448	G240	C285	G153	C76
G1110	A1048	C846		A910	C846	A782	A716	A528	U448	G241	C286	G154	C77
A1111	C1049	U847	C986	A911	U847	A783	G717	A529	C453	G242	C287	C155	C78
A1112	A1050	A784	G987	A912	A784	A784	A718	G630	A454	U243	C288	U	A78
U1113	G1051	A849	A988	U913	A849	G785	C719	C531	C455	A244	U	U	A79
G1114	C1052	C850	C989	C914	C786	G786	C720	A532	C456	G245	A289	U	G80
G1115	C1053	U851	A990	C915	U787	U787	C721	A533	A457	C246	G290	U	G81
C1116	A1054	G854	C991	G916	C854	A788	A722	G534	A458	G247		U	G82
G1122	G1055	G855	C992	A917	C854F	A789	G723	U535	U459	G248	C296	U	G83
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		C888		A959	C678		U762	U576	A502	G412	G337	G216	A127
		C889		A960	C679		G763	G577	A503	G413	U271C	G217	A128
		A890		C961	C680		A764	G578	U504	G414	G271	A218	C129
		G892		G962	C681		G765	G579	A505	A415	C337	A221	
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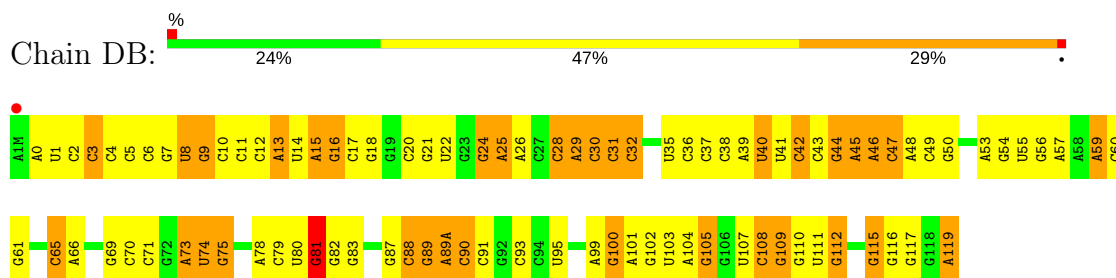
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G2279	G2136	G2136	G2061	G1973	G1907	A1820	C1742	C1651	A1570	C1493	G1425	G1346	A1269	U1199
C2280	C2137	A2062	A2062	C1974	C1908	A1821	G1743	G1651	A1571	U1494	G1426	G1347	C1271	U1199
C2281	C2138	C2063	C2063	A1977	C1909	G1826	G1750	G1652	A1572	A1496	A1427	G1348	C1271	C1200
G2282	C2140	C2064	C2064	A1978	A1913	G1827	C1751	A1654	C1575	C1499	C1428	A1349	U1272	C1201
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C2284	C2142	C2066	G2067	C1979	U1915	A1829	G1756	C1656	C1577	G1500	U1430	G1351	A1274	G1203
C2285	C2143	G2067	U2068	G1980	U1916	C1830	U1757	C1657	U1578	C1502	U1431	U1352	A1275	A1204
A2286	U2143	U2068	G2068	A1981	U1917	G1831	G1758	C1658	A1579	C1502	C1432	U1352	A1276	U1205
A2287	U2144	G2069	G2069	G1989	A1918	G1832	A1759	C1659	A1580	U1503	U1433	G1356	G1277	U1210
A2288	C2145	G2070	A2071	C1990	A1919	G1833	C1767	C1660	G1581	C1504	U1434	G1357	A1278	U1211
G2289	G2146	A2071	A2071	C1990	G1920	A1834	U1762	C1661	G1582	C1505	G1435	G1358	U1279	G1212
G2290	G2147	U2074	U2074	G1991	C1921	G1835	G1763	C1662	A1583	C1506	G1436	A1360	A1284	A1213
G2291	C2148	U2075	U2075	G1992	G1922	A1836	G1764	C1666	C1585	A1507	U1437	A1361	A1285	A1214
G2292	G2149	U2076	U2076	G1993	G1923	C1837	C1767	C1667	A1586	A1508	U1438	A1362	G1286	G1215
C2293	U2150	U2077	U2077	C1994	U1924	G1838	U1768	C1668	C1588	C1509	U1439	A1363	A1287	G1216
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G2295	C2152	G2087	G2087	C1999	U1926	G1844	G1770	C1670	C1515	C1515	G1444	G1371	U1288	G1218
G2296	G2153	G2087	G2087	G2010	A1927	C1844	G1771	C1671	G1593	G1519	A1444A	U1372	U1292	A1220
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G2298	G2155	G2087	G2087	G2012	G1929	A1847	G1773	C1673	G1595	G1521	C1446	A1378	C1298	G1222
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G2304	G2161	G2100	G2100	G2018	G1935	G1858	U1779	C1679	G1601	G1530	U1454	G1387	C1304	G1229
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G2306	C2163	G2104	G2104	G2024	A1937	A1860	C1781	C1681	G1606	C1532	G1459	G1389	G1309	G1235
G2307	C2164	G2105	G2105	G2025	A1938	G1861	C1782	C1682	C1607	C1533	A1460	U1391	G1310	G1236
G2308	U2167	G2106	G2106	C2026	U1939	G1862	A1783	C1683	A1608	G1534	G1461	U1392	G1311	A1237
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G2310	A2169	C2108	C2108	C1942	C1942	G1864	A1785	C1685	A1610	A1536	G1465	A1394	U1313	G1239
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G2312	A2171	A2031	A2031	U1944	U1944	A1870	A1791	C1687	C1612	G1538	G1467	U1396	A1241	A1241
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G2314	A2173	U2113	U2113	U1946	U1946	A1873	U1794	C1689	A1614	U1541	A1471	G1401	A1321	G1245
G2315	A2174	A2033	A2033	C1947	C1947	G1879	C1795	C1690	C1615	G1542	A1472	A1402	U1322	A1246
G2316	C2175	G2036	G2036	G1948	G1948	C1880	U1796	C1691	A1616	C1544	C1474	C1403	G1324	A1247
G2317	A2176	G2037	G2037	G1949	G1949	C1881	C1797	C1692	G1619					
G2318	C2177	U2118	U2118	U1951	U1951	C1882		G1702	G1619					



• Molecule 26: 5S RIBOSOMAL RNA

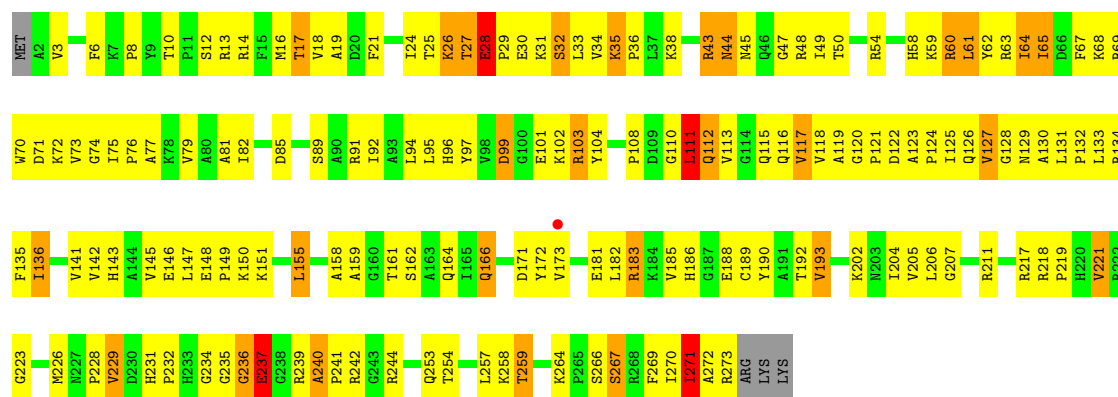


• Molecule 26: 5S RIBOSOMAL RNA

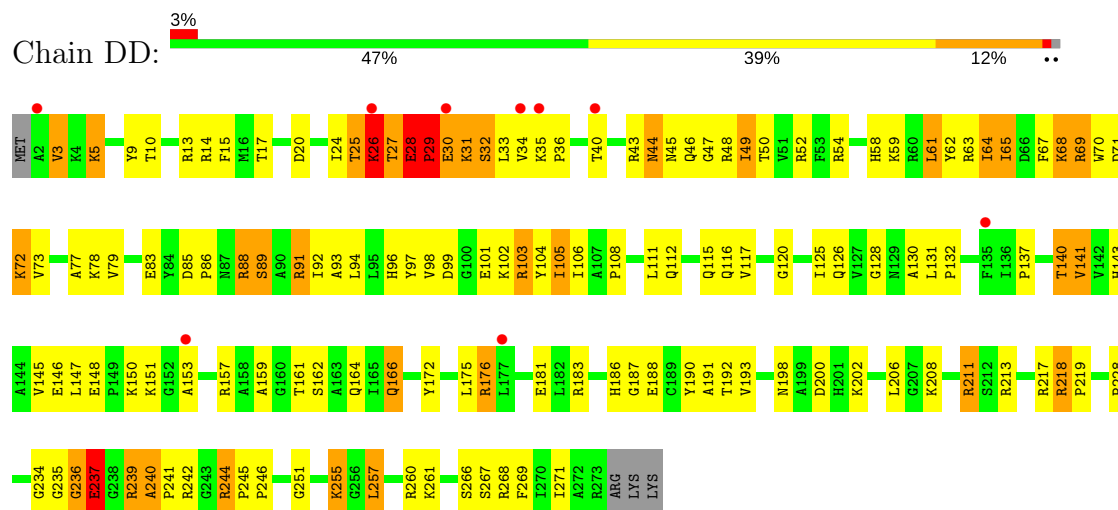


• Molecule 27: 50S ribosomal protein L2

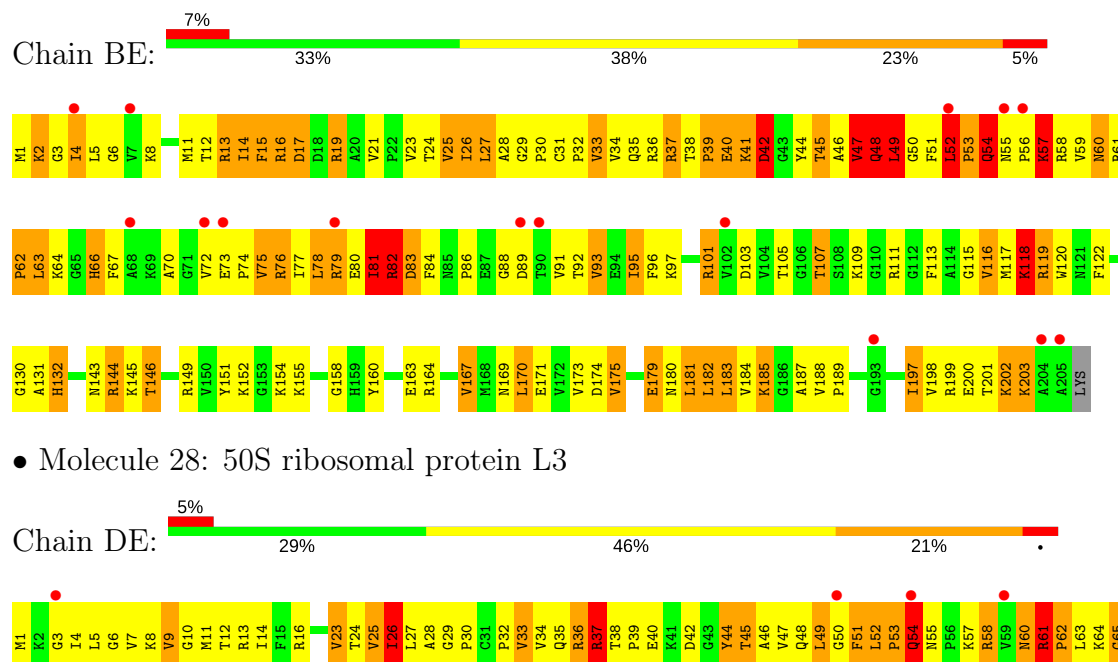




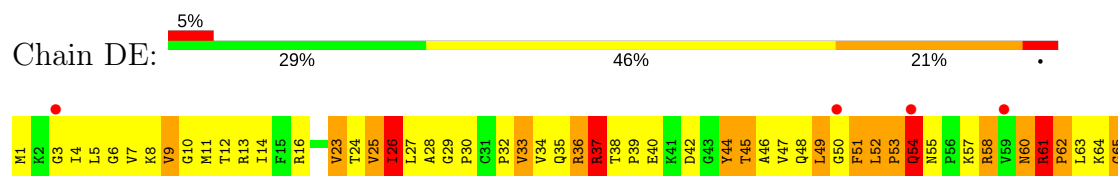
• Molecule 27: 50S ribosomal protein L2

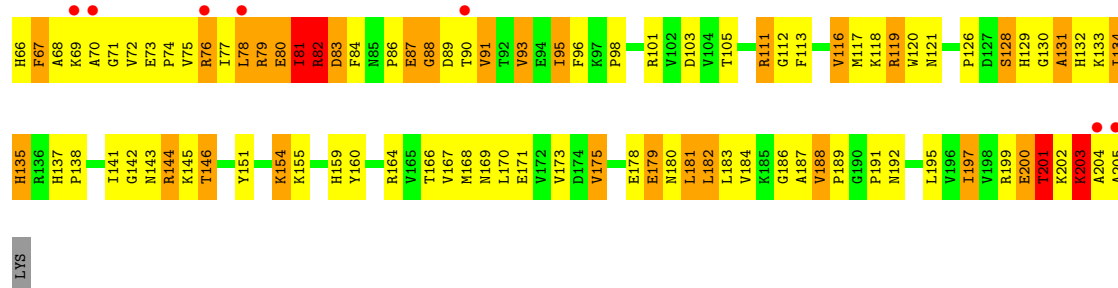


• Molecule 28: 50S ribosomal protein L3

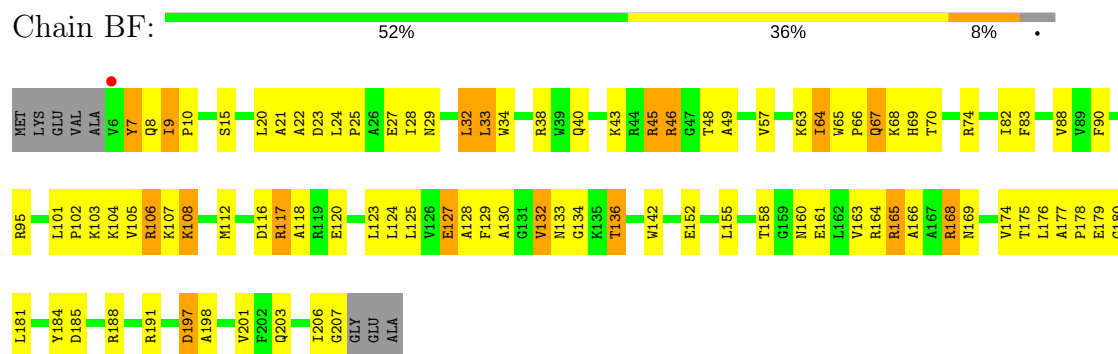


• Molecule 28: 50S ribosomal protein L3

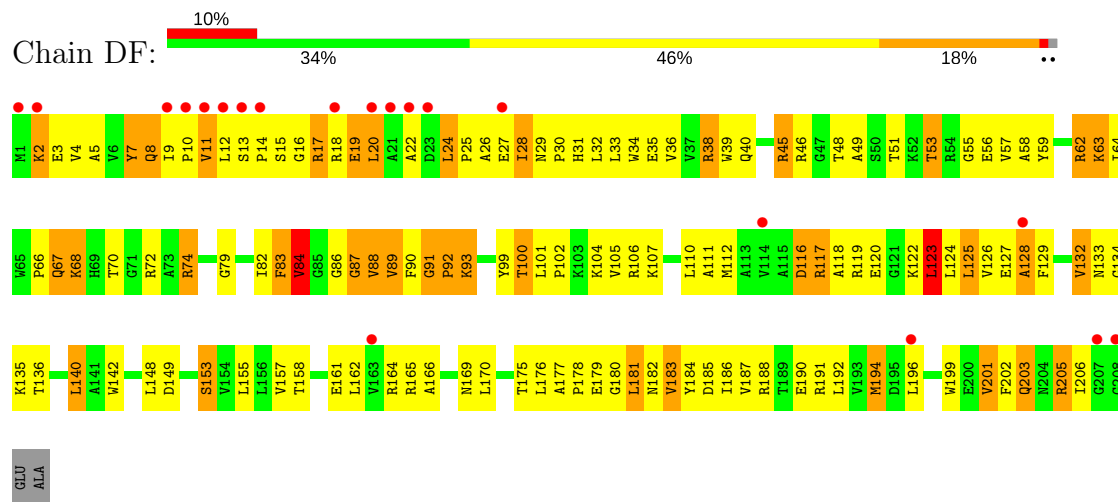




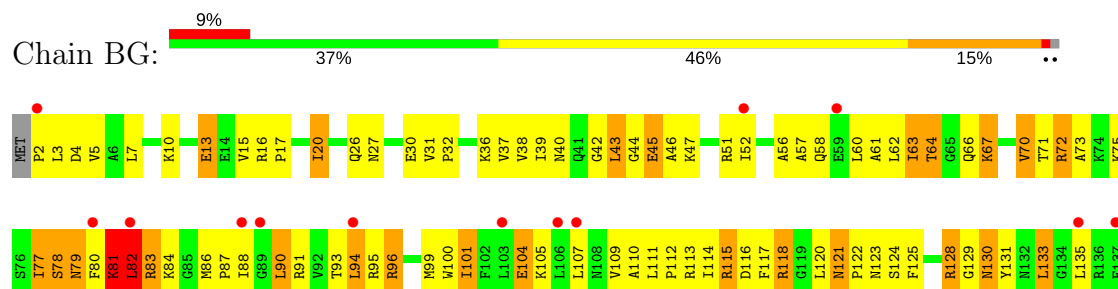
• Molecule 29: 50S ribosomal protein L4

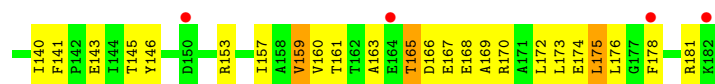


• Molecule 29: 50S ribosomal protein L4

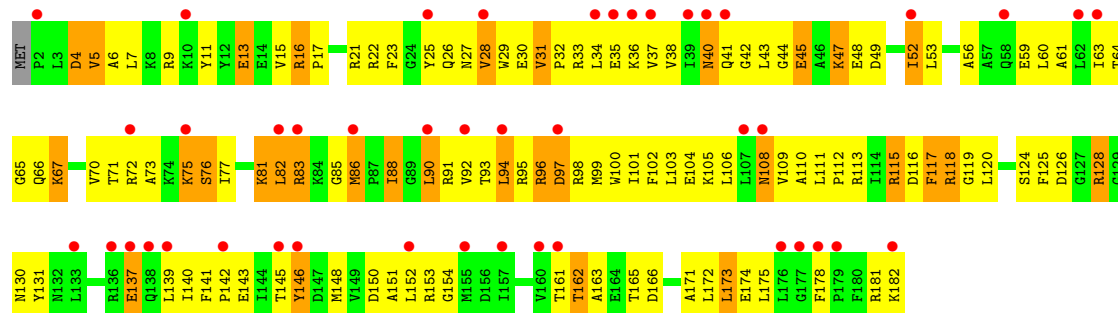


• Molecule 30: 50S ribosomal protein L5

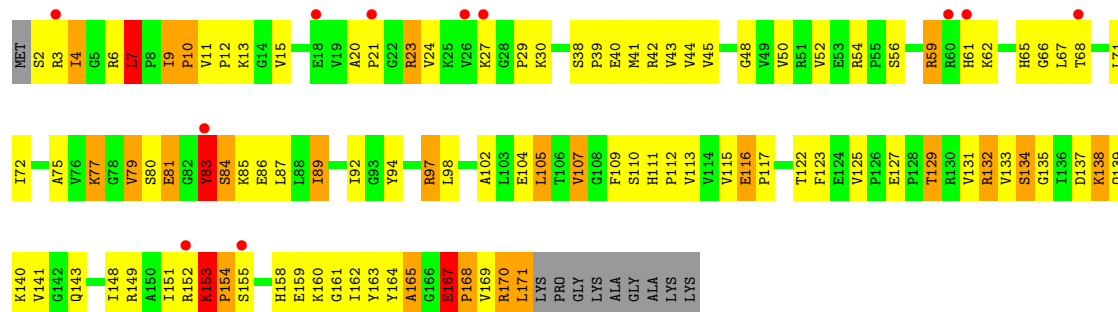




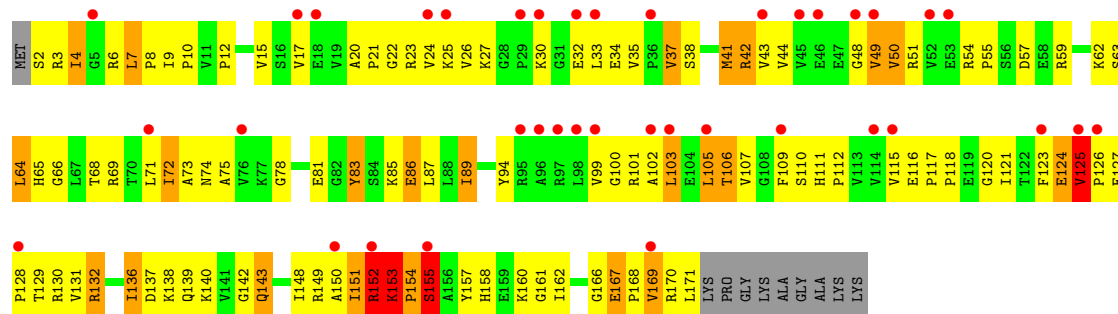
• Molecule 30: 50S ribosomal protein L5



• Molecule 31: 50S ribosomal protein L6

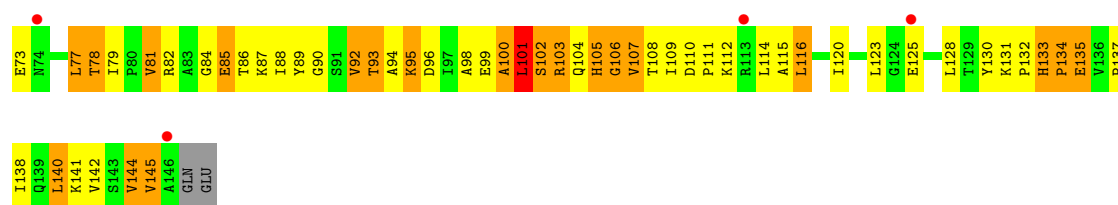


• Molecule 31: 50S ribosomal protein L6

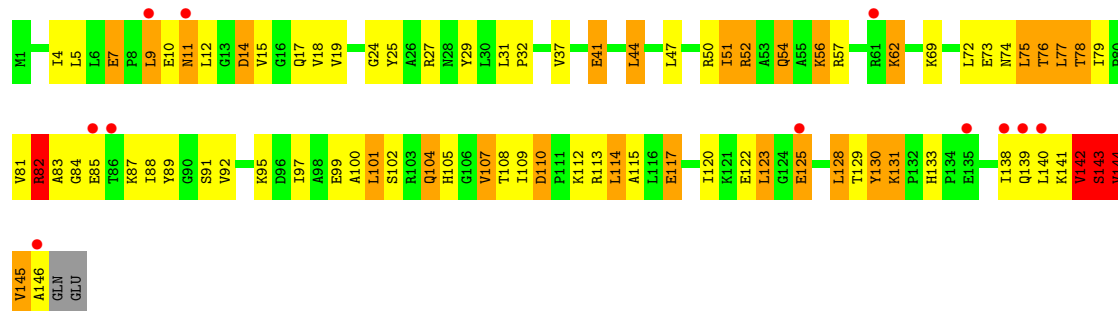
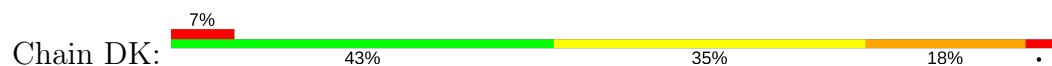


• Molecule 32: 50S ribosomal protein L9

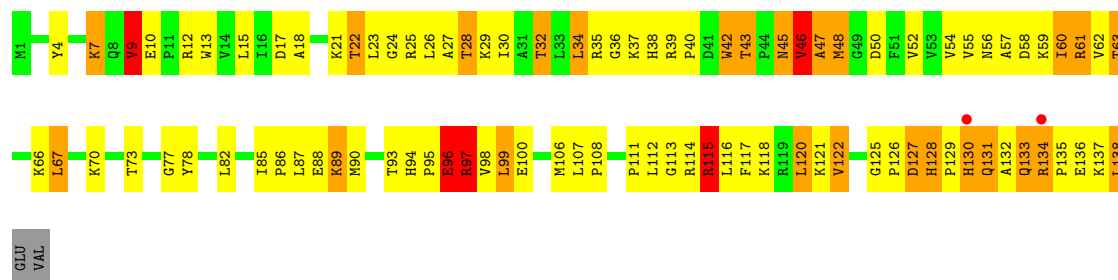




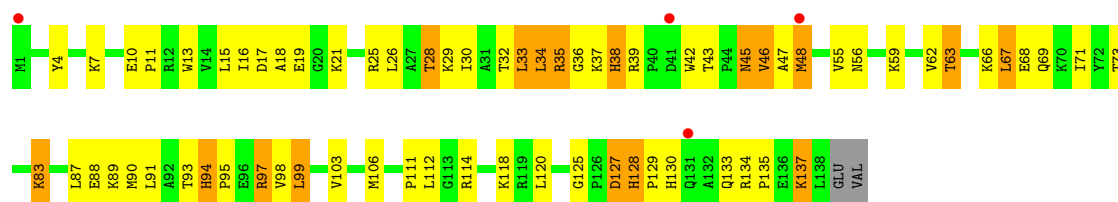
• Molecule 32: 50S ribosomal protein L9



• Molecule 33: 50S ribosomal protein L13

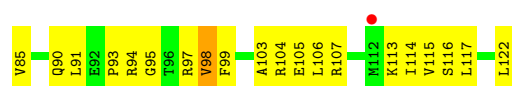


• Molecule 33: 50S ribosomal protein L13

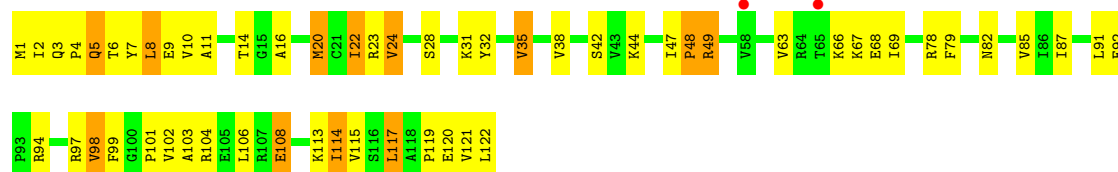


• Molecule 34: 50S ribosomal protein L14

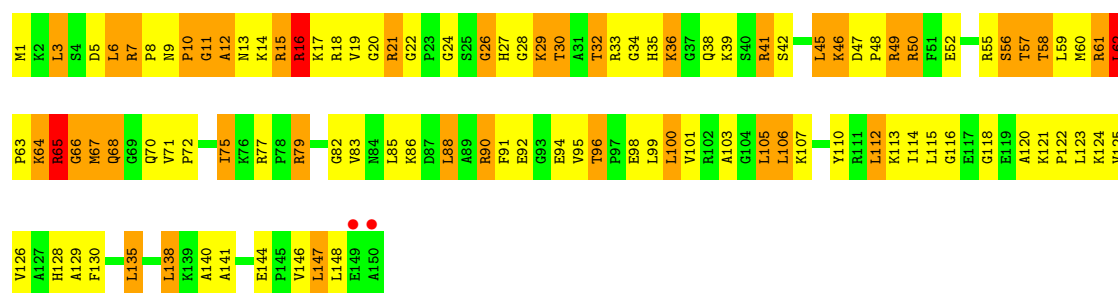




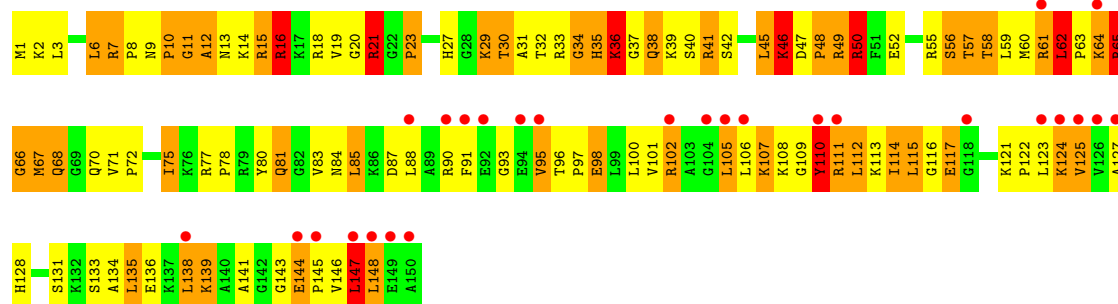
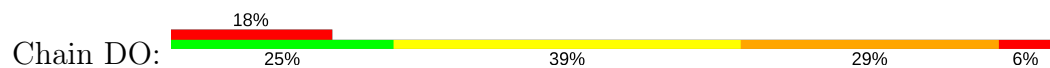
- Molecule 34: 50S ribosomal protein L14



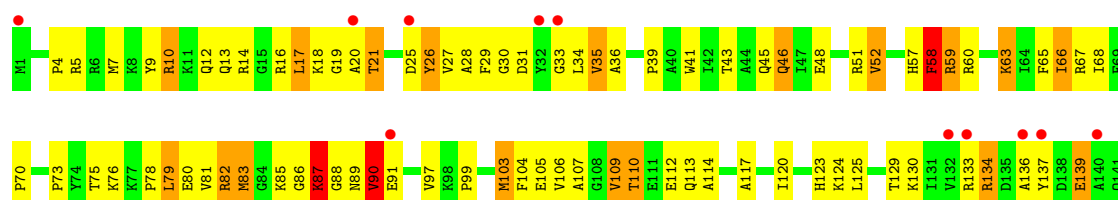
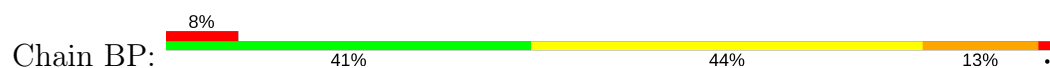
- Molecule 35: 50S ribosomal protein L15



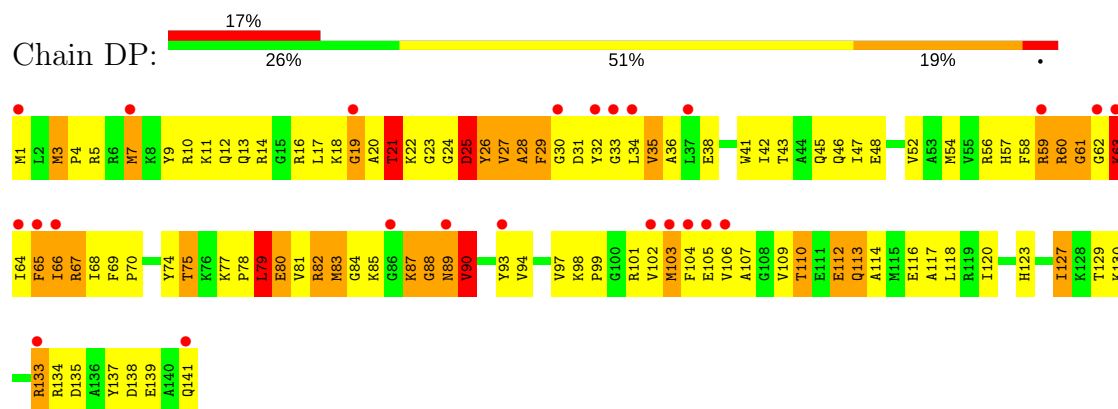
- Molecule 35: 50S ribosomal protein L15



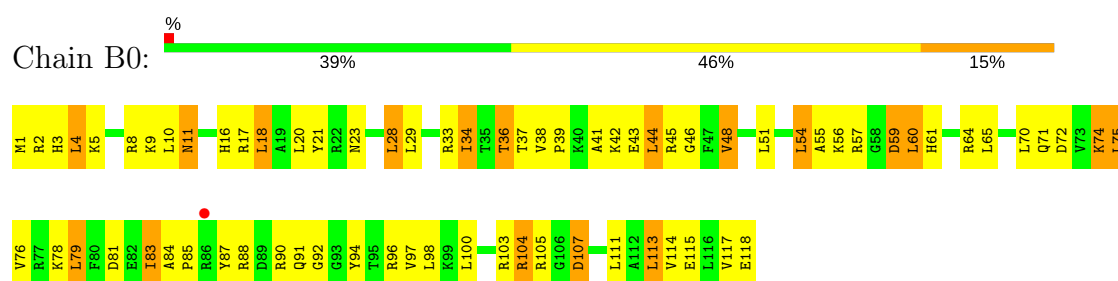
- Molecule 36: 50S ribosomal protein L16



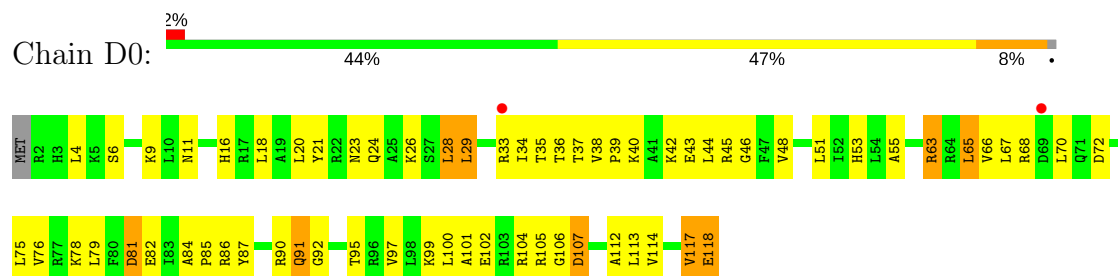
- Molecule 36: 50S ribosomal protein L16



- Molecule 37: 50S ribosomal protein L17



- Molecule 37: 50S ribosomal protein L17

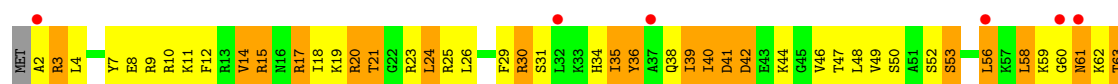


- Molecule 38: 50S ribosomal protein L18

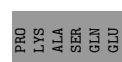


- Molecule 38: 50S ribosomal protein L18

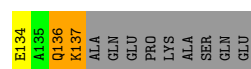
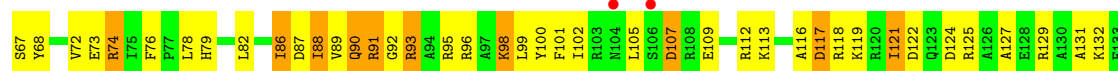




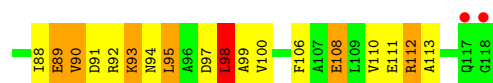
• Molecule 39: 50S ribosomal protein L19



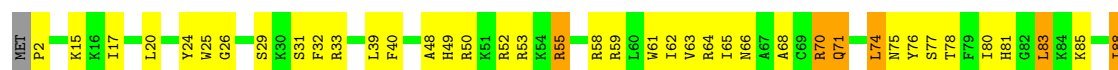
• Molecule 39: 50S ribosomal protein L19



• Molecule 40: 50S ribosomal protein L20



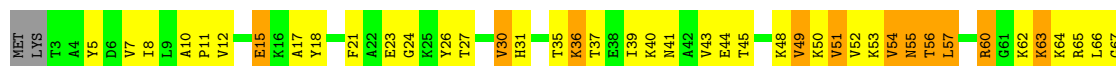
• Molecule 40: 50S ribosomal protein L20



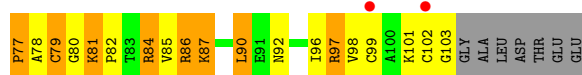
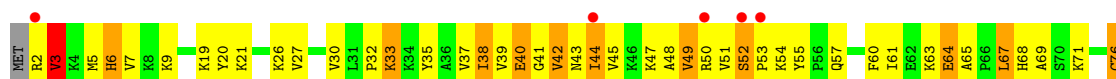




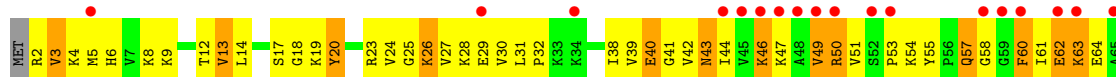
• Molecule 43: 50S ribosomal protein L23



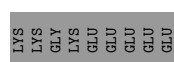
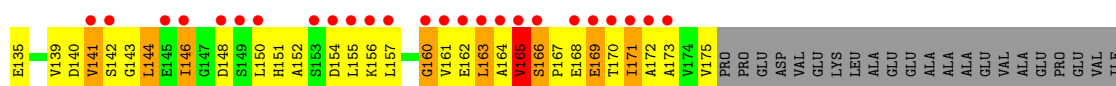
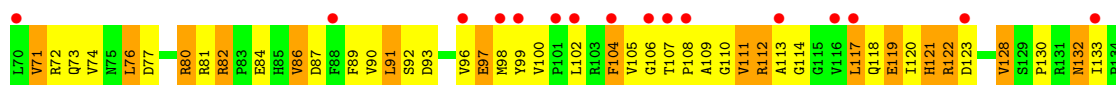
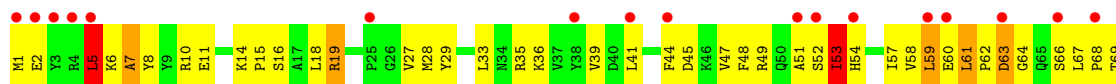
• Molecule 44: 50S ribosomal protein L24



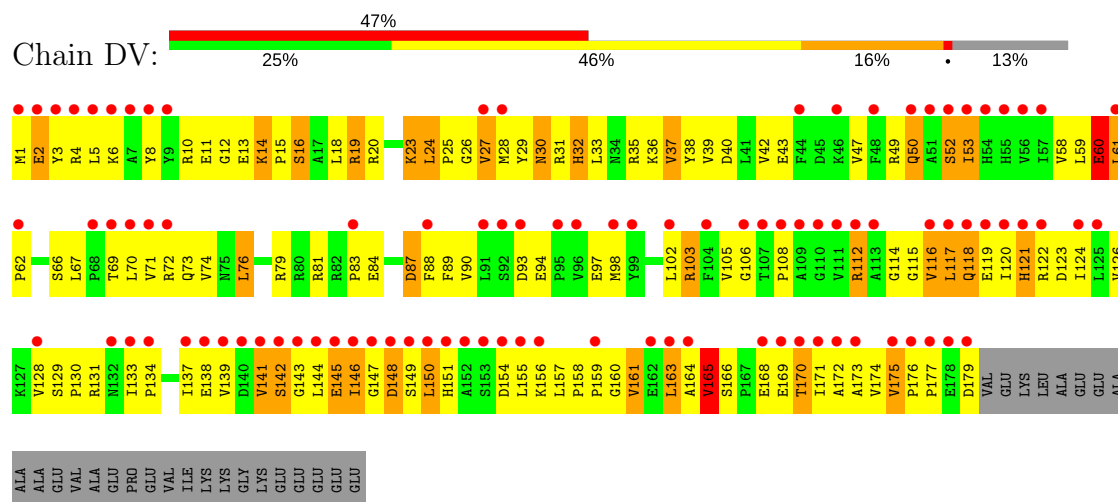
• Molecule 44: 50S ribosomal protein L24



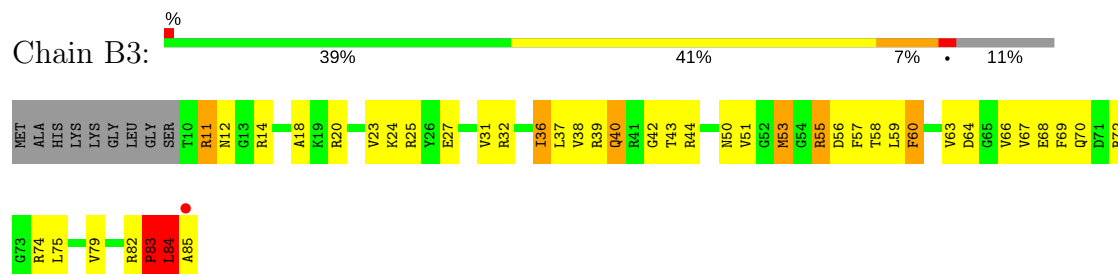
• Molecule 45: 50S ribosomal protein L25



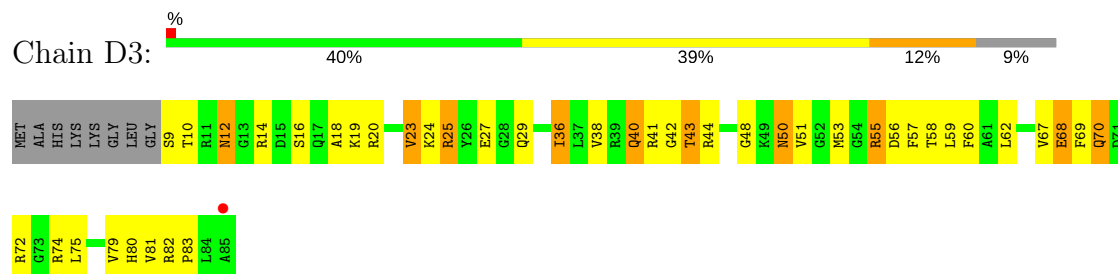
- Molecule 45: 50S ribosomal protein L25



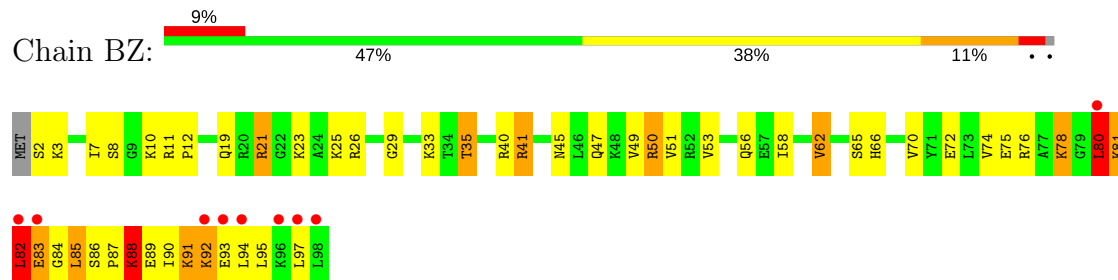
- Molecule 46: 50S ribosomal protein L27



- Molecule 46: 50S ribosomal protein L27

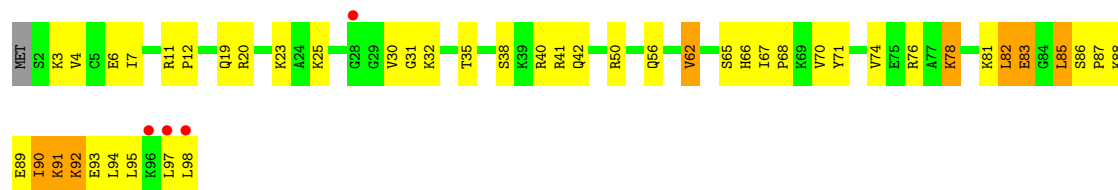


- Molecule 47: 50S ribosomal protein L28

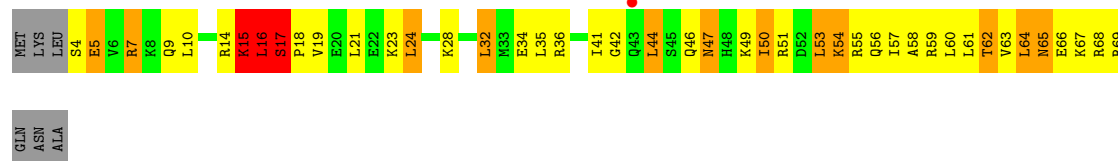


- Molecule 47: 50S ribosomal protein L28

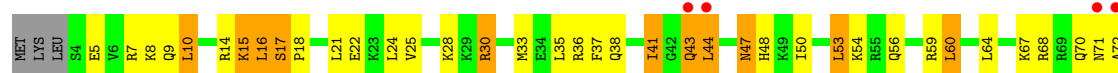




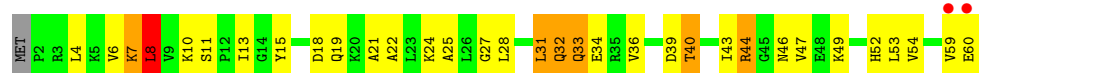
• Molecule 48: 50S ribosomal protein L29



• Molecule 48: 50S ribosomal protein L29



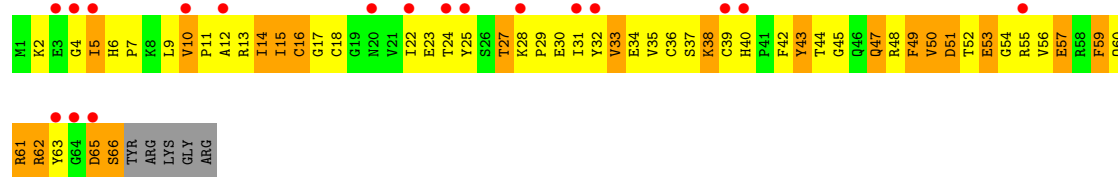
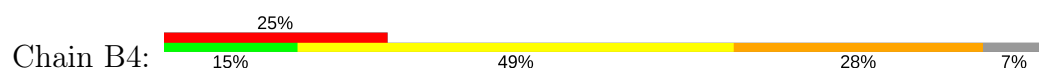
• Molecule 49: 50S ribosomal protein L30



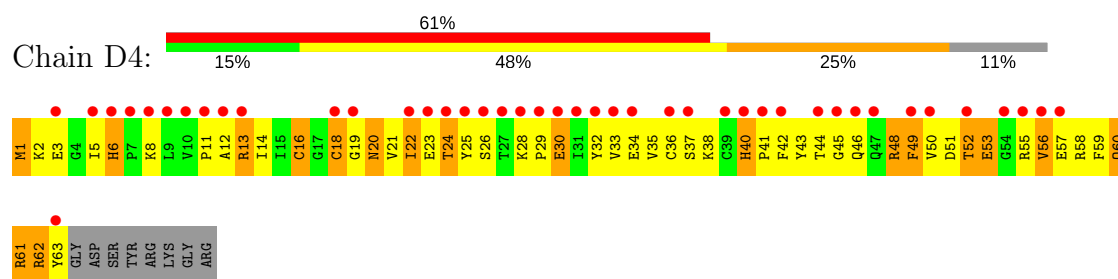
• Molecule 49: 50S ribosomal protein L30



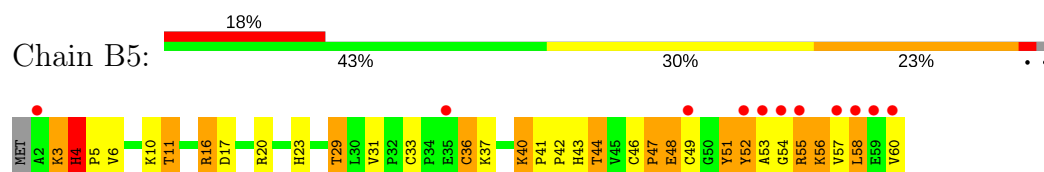
• Molecule 50: 50S ribosomal protein L31



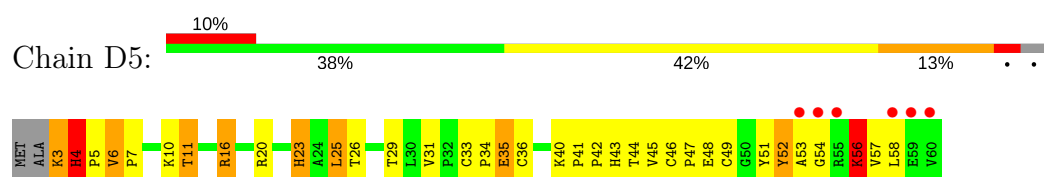
• Molecule 50: 50S ribosomal protein L31



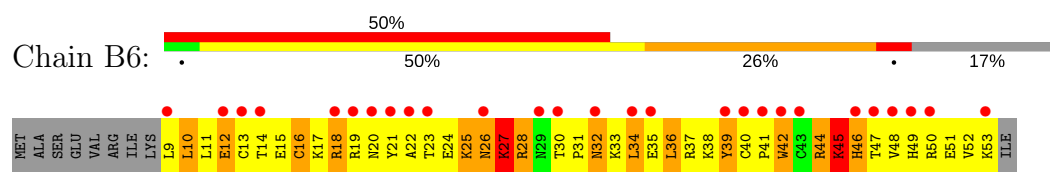
- Molecule 51: 50S ribosomal protein L32



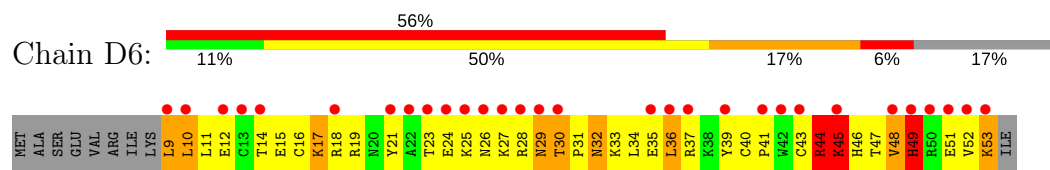
- Molecule 51: 50S ribosomal protein L32



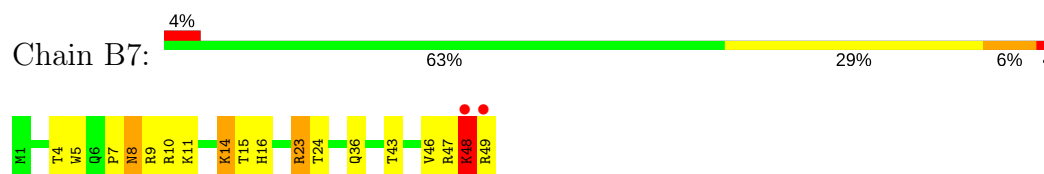
- Molecule 52: 50S ribosomal protein L33



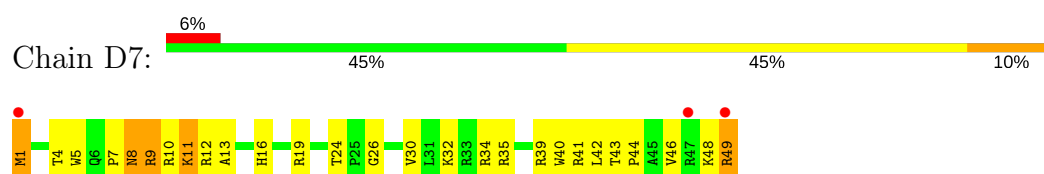
- Molecule 52: 50S ribosomal protein L33



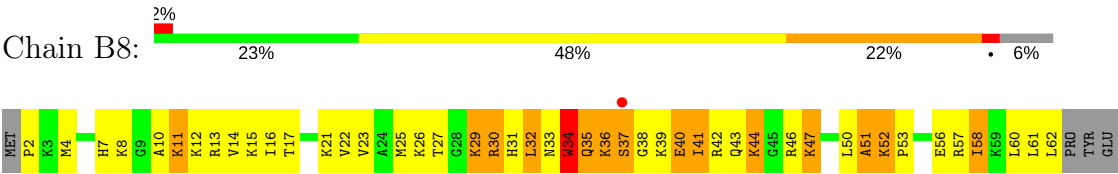
- Molecule 53: 50S ribosomal protein L34



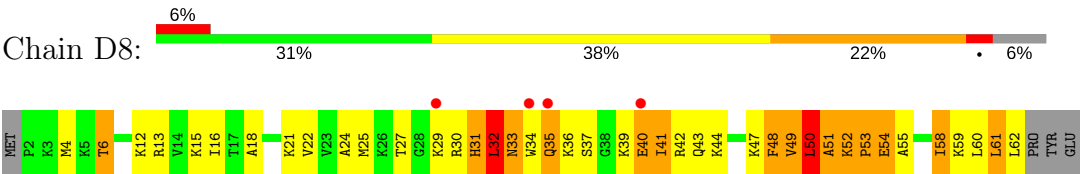
- Molecule 53: 50S ribosomal protein L34



● Molecule 54: 50S ribosomal protein L35



● Molecule 54: 50S ribosomal protein L35



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.00Å 450.05Å 621.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	153.53 – 3.00 153.53 – 3.00	Depositor EDS
% Data completeness (in resolution range)	94.1 (153.53-3.00) 93.7 (153.53-3.00)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.7.1 _743	Depositor
R, R_{free}	0.211 , 0.272 0.209 , 0.247	Depositor DCC
R_{free} test set	2000 reflections (0.17%)	wwPDB-VP
Wilson B-factor (Å ²)	77.4	Xtriage
Anisotropy	0.190	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 67.8	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	0.94	EDS
Total number of atoms	299552	wwPDB-VP
Average B, all atoms (Å ²)	100.0	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	0.44	5/36234 (0.0%)	0.91	68/56554 (0.1%)
1	CA	0.42	1/36237 (0.0%)	0.90	79/56558 (0.1%)
2	AE	0.29	0/1959	0.56	0/2642
2	CE	0.28	0/1959	0.53	0/2642
3	AF	0.33	0/1629	0.53	0/2195
3	CF	0.31	0/1636	0.54	0/2205
4	AG	0.49	2/1733 (0.1%)	0.62	1/2318 (0.0%)
4	CG	0.38	0/1733	0.61	0/2318
5	AH	0.35	0/1171	0.58	0/1576
5	CH	0.34	0/1171	0.56	0/1576
6	AI	0.33	0/856	0.55	0/1154
6	CI	0.32	0/856	0.54	0/1154
7	AJ	0.29	0/1276	0.50	0/1709
7	CJ	0.28	0/1276	0.45	0/1709
8	AK	0.33	0/1136	0.60	0/1527
8	CK	0.27	0/1136	0.51	0/1527
9	AL	0.29	0/1029	0.52	0/1379
9	CL	0.29	0/1029	0.53	0/1379
10	AM	0.31	0/814	0.59	1/1095 (0.1%)
10	CM	0.28	0/814	0.54	0/1095
11	AN	0.33	0/900	0.57	0/1213
11	CN	0.31	0/900	0.56	0/1213
12	AO	0.40	0/991	0.68	1/1327 (0.1%)
12	CO	0.35	0/991	0.60	0/1327
13	AP	0.30	0/938	0.57	0/1258
13	CP	0.28	0/943	0.52	0/1265
14	AQ	0.42	0/501	0.66	1/664 (0.2%)
14	CQ	0.29	0/501	0.58	0/664
15	AR	0.35	0/745	0.58	0/992
15	CR	0.30	0/745	0.51	0/992
16	AS	0.29	0/721	0.53	0/970
16	CS	0.31	0/721	0.58	0/970

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AT	0.35	0/847	0.54	0/1131
17	CT	0.31	0/847	0.51	0/1131
18	AU	0.34	0/596	0.64	0/790
18	CU	0.35	0/596	0.59	0/790
19	AV	0.33	0/638	0.59	0/860
19	CV	0.31	0/638	0.65	0/860
20	AW	0.29	0/765	0.52	0/1007
20	CW	0.32	0/765	0.63	0/1007
21	AX	0.28	0/221	0.55	0/288
21	CX	0.28	0/221	0.49	0/288
22	AB	1.15	2/2080 (0.1%)	1.41	25/3242 (0.8%)
22	CB	1.34	6/2080 (0.3%)	1.41	36/3242 (1.1%)
23	AC	1.12	3/1835 (0.2%)	1.69	56/2859 (2.0%)
23	AD	0.57	0/1835	0.97	7/2859 (0.2%)
23	CC	1.08	1/1835 (0.1%)	1.52	44/2859 (1.5%)
23	CD	0.61	0/1835	0.98	5/2859 (0.2%)
24	A1	1.43	2/226 (0.9%)	1.60	7/348 (2.0%)
24	C1	1.57	1/226 (0.4%)	1.73	5/348 (1.4%)
25	BA	0.59	15/70233 (0.0%)	1.07	285/109643 (0.3%)
25	DA	0.52	13/70122 (0.0%)	1.00	265/109469 (0.2%)
26	BB	0.49	0/2928	0.97	9/4568 (0.2%)
26	DB	0.44	0/2928	0.96	7/4568 (0.2%)
27	BD	0.50	0/2165	0.80	2/2919 (0.1%)
27	DD	0.46	0/2165	0.72	0/2919
28	BE	0.38	0/1601	0.67	2/2160 (0.1%)
28	DE	0.38	0/1601	0.69	0/2160
29	BF	0.43	0/1620	0.67	0/2194
29	DF	0.36	0/1662	0.65	0/2249
30	BG	0.36	0/1499	0.60	0/2016
30	DG	0.29	0/1499	0.54	0/2016
31	BH	0.36	0/1332	0.67	1/1802 (0.1%)
31	DH	0.28	0/1332	0.55	0/1802
32	BK	0.34	0/1151	0.68	1/1558 (0.1%)
32	DK	0.33	0/1151	0.66	1/1558 (0.1%)
33	BM	0.42	0/1131	0.69	0/1525
33	DM	0.29	0/1131	0.59	0/1525
34	BN	0.40	0/943	0.64	0/1269
34	DN	0.36	0/943	0.60	0/1269
35	BO	0.39	0/1162	0.76	0/1544
35	DO	0.32	0/1162	0.65	1/1544 (0.1%)
36	BP	0.52	0/1143	0.80	0/1527
36	DP	0.32	0/1143	0.54	0/1527
37	B0	0.39	0/982	0.69	0/1312

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
37	D0	0.37	0/974	0.64	0/1302
38	BQ	0.42	0/892	0.70	1/1187 (0.1%)
38	DQ	0.30	0/892	0.62	1/1187 (0.1%)
39	BR	0.40	0/1155	0.66	0/1542
39	DR	0.37	0/1155	0.59	0/1542
40	B1	0.42	0/982	0.67	1/1306 (0.1%)
40	D1	0.34	0/982	0.57	0/1306
41	B2	0.42	0/790	0.74	2/1057 (0.2%)
41	D2	0.32	0/790	0.59	0/1057
42	BS	0.37	0/911	0.62	0/1220
42	DS	0.38	0/911	0.64	0/1220
43	BT	0.50	0/739	0.68	0/993
43	DT	0.47	0/739	0.62	0/993
44	BU	0.45	0/798	0.68	0/1064
44	DU	0.41	0/798	0.72	0/1064
45	BV	0.32	0/1427	0.63	0/1935
45	DV	0.28	0/1460	0.56	0/1982
46	B3	0.44	0/615	0.67	0/819
46	D3	0.39	0/621	0.61	0/827
47	BZ	0.42	0/770	0.73	1/1022 (0.1%)
47	DZ	0.39	0/770	0.70	0/1022
48	BW	0.53	0/560	0.72	0/741
48	DW	0.37	0/583	0.63	0/771
49	BX	0.36	0/474	0.64	1/635 (0.2%)
49	DX	0.32	0/474	0.53	0/635
50	B4	0.34	0/545	0.72	1/733 (0.1%)
50	D4	0.32	0/527	0.67	0/709
51	B5	0.43	0/473	0.69	0/639
51	D5	0.34	0/468	0.70	0/632
52	B6	0.43	0/396	0.70	0/529
52	D6	0.33	0/396	0.63	0/529
53	B7	0.46	0/438	0.68	0/575
53	D7	0.40	0/438	0.59	0/575
54	B8	0.52	0/494	0.71	0/649
54	D8	0.38	0/494	0.71	1/649 (0.2%)
All	All	0.51	51/324027 (0.0%)	0.93	919/485226 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	AE	0	3
2	CE	0	5
3	CF	0	1
4	AG	0	1
8	AK	0	1
10	AM	0	1
12	AO	0	2
14	AQ	0	1
14	CQ	0	2
15	AR	0	1
19	CV	0	1
20	CW	0	1
27	BD	0	6
27	DD	0	3
28	BE	0	1
28	DE	0	6
29	DF	0	2
30	BG	0	1
30	DG	0	1
31	BH	0	2
31	DH	0	2
32	BK	0	3
32	DK	0	4
33	BM	0	1
35	BO	0	4
35	DO	0	3
36	BP	0	3
37	D0	0	2
38	BQ	0	1
38	DQ	0	2
39	BR	0	2
40	B1	0	1
40	D1	0	1
41	B2	0	1
43	BT	0	1
44	DU	0	2
45	BV	0	3
45	DV	0	2
46	B3	0	2
48	BW	0	2
48	DW	0	1
50	B4	0	4
50	D4	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
51	B5	0	1
51	D5	0	1
52	B6	0	1
52	D6	0	1
53	B7	0	1
54	B8	0	2
54	D8	0	1
All	All	0	99

The worst 5 of 51 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	DA	1143	A	N7-C5	-11.10	1.32	1.39
4	AG	12	CYS	CB-SG	10.86	2.00	1.82
25	DA	2873	A	N7-C5	-10.30	1.33	1.39
25	DA	1342	A	N7-C5	-9.87	1.33	1.39
25	BA	2430	A	N9-C4	-9.40	1.32	1.37

The worst 5 of 919 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	BA	1899	G	N3-C4-N9	-15.77	116.54	126.00
1	AA	1025	U	C5-C4-O4	-15.29	116.72	125.90
1	AA	1177	G	N9-C4-C5	14.63	111.25	105.40
1	AA	1177	G	C4-C5-N7	-14.21	105.12	110.80
25	DA	1899	G	N3-C4-N9	-13.25	118.05	126.00

There are no chirality outliers.

5 of 99 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	AE	14	GLY	Peptide
2	AE	194	PRO	Peptide
2	AE	71	VAL	Peptide
4	AG	29	PRO	Peptide
8	AK	102	ARG	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	32369	0	16339	1207	1
1	CA	32372	0	16338	1298	1
2	AE	1924	0	1975	158	0
2	CE	1924	0	1975	180	0
3	AF	1605	0	1668	111	0
3	CF	1612	0	1677	144	0
4	AG	1703	0	1764	146	0
4	CG	1703	0	1763	140	1
5	AH	1155	0	1213	74	0
5	CH	1155	0	1213	91	0
6	AI	843	0	857	39	1
6	CI	843	0	857	45	0
7	AJ	1257	0	1296	68	0
7	CJ	1257	0	1296	74	0
8	AK	1116	0	1177	75	0
8	CK	1116	0	1177	66	0
9	AL	1010	0	1037	99	0
9	CL	1010	0	1037	121	0
10	AM	801	0	849	78	0
10	CM	801	0	849	114	0
11	AN	885	0	904	65	0
11	CN	885	0	904	45	0
12	AO	975	0	1062	62	0
12	CO	975	0	1062	75	0
13	AP	928	0	987	66	0
13	CP	933	0	992	107	0
14	AQ	492	0	529	47	0
14	CQ	492	0	531	68	0
15	AR	734	0	771	38	0
15	CR	734	0	771	35	0
16	AS	705	0	725	79	0
16	CS	705	0	725	45	0
17	AT	834	0	904	55	0
17	CT	834	0	904	41	0
18	AU	591	0	662	30	0
18	CU	591	0	662	47	0
19	AV	624	0	636	71	0
19	CV	624	0	636	91	0
20	AW	763	0	859	73	0
20	CW	763	0	861	56	0
21	AX	217	0	234	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	CX	217	0	234	23	0
22	AB	1861	0	938	85	0
22	CB	1861	0	938	99	0
23	AC	1643	0	837	75	0
23	AD	1643	0	837	97	0
23	CC	1643	0	837	91	0
23	CD	1643	0	837	108	0
24	A1	205	0	103	12	0
24	C1	205	0	103	10	0
25	BA	62707	0	31613	2105	0
25	DA	62607	0	31565	2108	1
26	BB	2617	0	1328	94	0
26	DB	2617	0	1328	135	0
27	BD	2115	0	2195	238	0
27	DD	2115	0	2195	211	0
28	BE	1568	0	1634	334	0
28	DE	1568	0	1634	256	0
29	BF	1585	0	1632	119	0
29	DF	1627	0	1680	184	0
30	BG	1474	0	1535	171	0
30	DG	1474	0	1535	148	0
31	BH	1307	0	1382	135	0
31	DH	1307	0	1382	156	1
32	BK	1136	0	1223	99	0
32	DK	1136	0	1223	84	0
33	BM	1104	0	1180	142	0
33	DM	1104	0	1180	87	0
34	BN	933	0	996	63	0
34	DN	933	0	996	51	0
35	BO	1145	0	1228	200	0
35	DO	1145	0	1227	240	0
36	BP	1122	0	1179	95	0
36	DP	1122	0	1179	208	0
37	B0	968	0	1033	78	0
37	D0	960	0	1021	60	0
38	BQ	882	0	943	106	0
38	DQ	882	0	943	120	0
39	BR	1141	0	1202	116	0
39	DR	1141	0	1202	125	0
40	B1	964	0	1022	98	0
40	D1	964	0	1022	94	0
41	B2	779	0	852	80	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	D2	779	0	852	129	0
42	BS	900	0	964	71	0
42	DS	900	0	964	42	0
43	BT	725	0	778	53	0
43	DT	725	0	778	75	0
44	BU	785	0	878	75	0
44	DU	785	0	878	98	0
45	BV	1397	0	1430	120	0
45	DV	1428	0	1454	162	0
46	B3	607	0	628	50	0
46	D3	613	0	633	52	0
47	BZ	763	0	848	50	0
47	DZ	763	0	848	46	0
48	BW	558	0	610	44	0
48	DW	581	0	629	49	0
49	BX	469	0	518	35	0
49	DX	469	0	518	24	0
50	B4	533	0	522	84	0
50	D4	515	0	510	84	0
51	B5	459	0	480	54	0
51	D5	454	0	475	44	0
52	B6	389	0	404	80	0
52	D6	389	0	404	84	0
53	B7	430	0	480	30	0
53	D7	430	0	480	36	0
54	B8	488	0	558	110	0
54	D8	488	0	558	113	0
55	A1	2	0	0	0	0
55	AA	242	0	0	0	0
55	AB	5	0	0	0	0
55	AC	9	0	0	0	0
55	AD	1	0	0	0	0
55	AG	1	0	0	0	0
55	AH	1	0	0	0	0
55	AN	2	0	0	0	0
55	AQ	1	0	0	0	0
55	B0	1	0	0	0	0
55	B1	1	0	0	0	0
55	B2	1	0	0	0	0
55	B3	1	0	0	0	0
55	B5	1	0	0	0	0
55	B7	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	B8	1	0	0	0	0
55	BA	623	0	0	0	0
55	BB	17	0	0	0	0
55	BD	1	0	0	0	0
55	BE	5	0	0	0	0
55	BF	3	0	0	0	0
55	BO	2	0	0	0	0
55	BU	2	0	0	0	0
55	CA	207	0	0	0	0
55	CB	3	0	0	0	0
55	CC	8	0	0	0	0
55	CG	2	0	0	0	0
55	CN	1	0	0	0	0
55	CS	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	526	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	DR	1	0	0	0	0
55	DU	1	0	0	0	0
56	AG	1	0	0	0	0
56	AQ	1	0	0	0	0
56	CG	1	0	0	0	0
56	CQ	1	0	0	0	0
All	All	299552	0	200910	14872	3

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 30.

The worst 5 of 14872 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)
1:AA:625:G:H4'	16:AS:16:HIS:CD2	1.33	1.61
28:DE:46:ALA:CB	28:DE:82:ARG:HA	1.37	1.55
30:BG:83:ARG:H	30:BG:86:MET:CE	1.24	1.47
36:DP:26:TYR:CE1	36:DP:139:GLU:HB2	1.48	1.45
25:BA:1056:G:N2	25:BA:1103:A:H62	1.13	1.44

All (3) 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)
1:AA:85:U:O2'	31:DH:100:GLY:O[3_555]	1.90	0.30
1:CA:86:U:O2'	25:DA:276:A:OP2[3_545]	2.02	0.18
6:AI:15:ASP:OD2	4:CG:27:TYR:OH[4_555]	2.17	0.03

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AE	235/256 (92%)	190 (81%)	45 (19%)	0	100	100
2	CE	235/256 (92%)	190 (81%)	41 (17%)	4 (2%)	10	42
3	AF	203/239 (85%)	179 (88%)	24 (12%)	0	100	100
3	CF	204/239 (85%)	179 (88%)	23 (11%)	2 (1%)	17	56
4	AG	206/208 (99%)	179 (87%)	24 (12%)	3 (2%)	11	45
4	CG	206/208 (99%)	179 (87%)	25 (12%)	2 (1%)	17	56
5	AH	149/162 (92%)	137 (92%)	10 (7%)	2 (1%)	13	49
5	CH	149/162 (92%)	139 (93%)	10 (7%)	0	100	100
6	AI	99/101 (98%)	92 (93%)	7 (7%)	0	100	100
6	CI	99/101 (98%)	94 (95%)	5 (5%)	0	100	100
7	AJ	153/156 (98%)	142 (93%)	11 (7%)	0	100	100
7	CJ	153/156 (98%)	143 (94%)	10 (6%)	0	100	100
8	AK	136/138 (99%)	123 (90%)	12 (9%)	1 (1%)	24	64
8	CK	136/138 (99%)	123 (90%)	13 (10%)	0	100	100
9	AL	125/128 (98%)	110 (88%)	15 (12%)	0	100	100
9	CL	125/128 (98%)	114 (91%)	11 (9%)	0	100	100
10	AM	97/105 (92%)	86 (89%)	11 (11%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	CM	97/105 (92%)	84 (87%)	9 (9%)	4 (4%)	3	18
11	AN	117/129 (91%)	102 (87%)	14 (12%)	1 (1%)	19	59
11	CN	117/129 (91%)	104 (89%)	13 (11%)	0	100	100
12	AO	123/132 (93%)	105 (85%)	16 (13%)	2 (2%)	11	43
12	CO	123/132 (93%)	105 (85%)	15 (12%)	3 (2%)	6	32
13	AP	114/126 (90%)	89 (78%)	23 (20%)	2 (2%)	9	40
13	CP	115/126 (91%)	96 (84%)	17 (15%)	2 (2%)	10	42
14	AQ	58/61 (95%)	49 (84%)	9 (16%)	0	100	100
14	CQ	58/61 (95%)	49 (84%)	8 (14%)	1 (2%)	10	42
15	AR	86/89 (97%)	74 (86%)	11 (13%)	1 (1%)	14	51
15	CR	86/89 (97%)	76 (88%)	10 (12%)	0	100	100
16	AS	82/88 (93%)	71 (87%)	8 (10%)	3 (4%)	4	21
16	CS	82/88 (93%)	75 (92%)	7 (8%)	0	100	100
17	AT	98/105 (93%)	91 (93%)	7 (7%)	0	100	100
17	CT	98/105 (93%)	91 (93%)	7 (7%)	0	100	100
18	AU	70/88 (80%)	64 (91%)	5 (7%)	1 (1%)	12	47
18	CU	70/88 (80%)	61 (87%)	9 (13%)	0	100	100
19	AV	76/93 (82%)	68 (90%)	6 (8%)	2 (3%)	6	30
19	CV	76/93 (82%)	60 (79%)	12 (16%)	4 (5%)	2	13
20	AW	97/106 (92%)	84 (87%)	13 (13%)	0	100	100
20	CW	97/106 (92%)	80 (82%)	16 (16%)	1 (1%)	17	56
21	AX	23/27 (85%)	22 (96%)	1 (4%)	0	100	100
21	CX	23/27 (85%)	21 (91%)	2 (9%)	0	100	100
27	BD	270/276 (98%)	243 (90%)	22 (8%)	5 (2%)	9	39
27	DD	270/276 (98%)	248 (92%)	15 (6%)	7 (3%)	6	30
28	BE	203/206 (98%)	149 (73%)	30 (15%)	24 (12%)	0	2
28	DE	203/206 (98%)	144 (71%)	41 (20%)	18 (9%)	1	4
29	BF	200/210 (95%)	179 (90%)	21 (10%)	0	100	100
29	DF	206/210 (98%)	168 (82%)	30 (15%)	8 (4%)	3	19
30	BG	179/182 (98%)	154 (86%)	20 (11%)	5 (3%)	5	28
30	DG	179/182 (98%)	150 (84%)	28 (16%)	1 (1%)	27	67

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	BH	168/180 (93%)	133 (79%)	28 (17%)	7 (4%)	3	17
31	DH	168/180 (93%)	125 (74%)	35 (21%)	8 (5%)	2	15
32	BK	144/148 (97%)	102 (71%)	32 (22%)	10 (7%)	1	6
32	DK	144/148 (97%)	113 (78%)	28 (19%)	3 (2%)	8	36
33	BM	136/140 (97%)	113 (83%)	16 (12%)	7 (5%)	2	13
33	DM	136/140 (97%)	119 (88%)	15 (11%)	2 (2%)	11	45
34	BN	120/122 (98%)	111 (92%)	9 (8%)	0	100	100
34	DN	120/122 (98%)	113 (94%)	6 (5%)	1 (1%)	21	61
35	BO	148/150 (99%)	107 (72%)	27 (18%)	14 (10%)	1	3
35	DO	148/150 (99%)	102 (69%)	24 (16%)	22 (15%)	0	1
36	BP	139/141 (99%)	109 (78%)	27 (19%)	3 (2%)	7	34
36	DP	139/141 (99%)	93 (67%)	30 (22%)	16 (12%)	0	2
37	B0	116/118 (98%)	101 (87%)	13 (11%)	2 (2%)	10	42
37	D0	115/118 (98%)	109 (95%)	6 (5%)	0	100	100
38	BQ	109/112 (97%)	86 (79%)	20 (18%)	3 (3%)	5	28
38	DQ	109/112 (97%)	87 (80%)	19 (17%)	3 (3%)	5	28
39	BR	135/146 (92%)	114 (84%)	21 (16%)	0	100	100
39	DR	135/146 (92%)	119 (88%)	14 (10%)	2 (2%)	11	45
40	B1	115/118 (98%)	103 (90%)	11 (10%)	1 (1%)	19	59
40	D1	115/118 (98%)	101 (88%)	14 (12%)	0	100	100
41	B2	99/101 (98%)	92 (93%)	5 (5%)	2 (2%)	8	37
41	D2	99/101 (98%)	78 (79%)	14 (14%)	7 (7%)	1	6
42	BS	111/113 (98%)	97 (87%)	10 (9%)	4 (4%)	4	21
42	DS	111/113 (98%)	103 (93%)	8 (7%)	0	100	100
43	BT	90/96 (94%)	84 (93%)	4 (4%)	2 (2%)	7	34
43	DT	90/96 (94%)	78 (87%)	10 (11%)	2 (2%)	7	34
44	BU	100/110 (91%)	80 (80%)	15 (15%)	5 (5%)	2	14
44	DU	100/110 (91%)	70 (70%)	24 (24%)	6 (6%)	2	10
45	BV	173/206 (84%)	129 (75%)	37 (21%)	7 (4%)	3	18
45	DV	177/206 (86%)	132 (75%)	35 (20%)	10 (6%)	2	11
46	B3	74/85 (87%)	67 (90%)	5 (7%)	2 (3%)	5	29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
46	D3	75/85 (88%)	69 (92%)	6 (8%)	0	100	100
47	BZ	95/98 (97%)	85 (90%)	7 (7%)	3 (3%)	4	24
47	DZ	95/98 (97%)	84 (88%)	10 (10%)	1 (1%)	16	53
48	BW	64/72 (89%)	58 (91%)	4 (6%)	2 (3%)	4	25
48	DW	67/72 (93%)	60 (90%)	6 (9%)	1 (2%)	11	45
49	BX	57/60 (95%)	52 (91%)	5 (9%)	0	100	100
49	DX	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
50	B4	64/71 (90%)	41 (64%)	21 (33%)	2 (3%)	4	25
50	D4	61/71 (86%)	32 (52%)	28 (46%)	1 (2%)	11	43
51	B5	57/60 (95%)	49 (86%)	7 (12%)	1 (2%)	9	40
51	D5	56/60 (93%)	48 (86%)	7 (12%)	1 (2%)	9	40
52	B6	43/54 (80%)	27 (63%)	14 (33%)	2 (5%)	2	15
52	D6	43/54 (80%)	29 (67%)	10 (23%)	4 (9%)	1	3
53	B7	47/49 (96%)	44 (94%)	3 (6%)	0	100	100
53	D7	47/49 (96%)	45 (96%)	2 (4%)	0	100	100
54	B8	59/65 (91%)	47 (80%)	7 (12%)	5 (8%)	1	4
54	D8	59/65 (91%)	40 (68%)	12 (20%)	7 (12%)	0	2
All	All	11335/12052 (94%)	9588 (85%)	1457 (13%)	290 (3%)	6	30

5 of 290 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	AG	13	ARG
4	AG	14	ARG
11	AN	82	VAL
16	AS	17	TYR
18	AU	22	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AE	205/220 (93%)	155 (76%)	50 (24%)	1	3
2	CE	205/220 (93%)	159 (78%)	46 (22%)	1	4
3	AF	159/188 (85%)	120 (76%)	39 (24%)	1	3
3	CF	160/188 (85%)	124 (78%)	36 (22%)	1	4
4	AG	180/180 (100%)	144 (80%)	36 (20%)	1	7
4	CG	180/180 (100%)	140 (78%)	40 (22%)	1	5
5	AH	116/123 (94%)	88 (76%)	28 (24%)	1	3
5	CH	116/123 (94%)	89 (77%)	27 (23%)	1	4
6	AI	90/90 (100%)	76 (84%)	14 (16%)	3	14
6	CI	90/90 (100%)	74 (82%)	16 (18%)	2	10
7	AJ	126/127 (99%)	104 (82%)	22 (18%)	2	10
7	CJ	126/127 (99%)	89 (71%)	37 (29%)	0	2
8	AK	119/119 (100%)	100 (84%)	19 (16%)	2	13
8	CK	119/119 (100%)	94 (79%)	25 (21%)	1	6
9	AL	98/99 (99%)	70 (71%)	28 (29%)	0	2
9	CL	98/99 (99%)	69 (70%)	29 (30%)	0	2
10	AM	89/92 (97%)	66 (74%)	23 (26%)	0	3
10	CM	89/92 (97%)	60 (67%)	29 (33%)	0	1
11	AN	90/99 (91%)	74 (82%)	16 (18%)	2	10
11	CN	90/99 (91%)	73 (81%)	17 (19%)	1	9
12	AO	104/109 (95%)	88 (85%)	16 (15%)	3	14
12	CO	104/109 (95%)	80 (77%)	24 (23%)	1	4
13	AP	94/101 (93%)	71 (76%)	23 (24%)	1	3
13	CP	94/101 (93%)	75 (80%)	19 (20%)	1	7
14	AQ	49/50 (98%)	33 (67%)	16 (33%)	0	1
14	CQ	49/50 (98%)	39 (80%)	10 (20%)	1	6
15	AR	79/80 (99%)	68 (86%)	11 (14%)	4	18
15	CR	79/80 (99%)	66 (84%)	13 (16%)	2	12
16	AS	72/74 (97%)	53 (74%)	19 (26%)	0	3
16	CS	72/74 (97%)	62 (86%)	10 (14%)	4	18
17	AT	95/97 (98%)	82 (86%)	13 (14%)	4	18
17	CT	95/97 (98%)	89 (94%)	6 (6%)	20	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	AU	63/77 (82%)	50 (79%)	13 (21%)	1	6
18	CU	63/77 (82%)	48 (76%)	15 (24%)	1	3
19	AV	67/80 (84%)	47 (70%)	20 (30%)	0	2
19	CV	67/80 (84%)	53 (79%)	14 (21%)	1	6
20	AW	76/82 (93%)	60 (79%)	16 (21%)	1	6
20	CW	76/82 (93%)	55 (72%)	21 (28%)	0	2
21	AX	20/22 (91%)	17 (85%)	3 (15%)	3	15
21	CX	20/22 (91%)	20 (100%)	0	100	100
27	BD	214/218 (98%)	172 (80%)	42 (20%)	1	8
27	DD	214/218 (98%)	162 (76%)	52 (24%)	1	3
28	BE	165/166 (99%)	114 (69%)	51 (31%)	0	1
28	DE	165/166 (99%)	121 (73%)	44 (27%)	0	2
29	BF	161/166 (97%)	129 (80%)	32 (20%)	1	7
29	DF	165/166 (99%)	122 (74%)	43 (26%)	0	3
30	BG	155/156 (99%)	115 (74%)	40 (26%)	0	3
30	DG	155/156 (99%)	113 (73%)	42 (27%)	0	2
31	BH	142/148 (96%)	107 (75%)	35 (25%)	0	3
31	DH	142/148 (96%)	110 (78%)	32 (22%)	1	4
32	BK	122/124 (98%)	91 (75%)	31 (25%)	0	3
32	DK	122/124 (98%)	84 (69%)	38 (31%)	0	1
33	BM	117/119 (98%)	87 (74%)	30 (26%)	0	3
33	DM	117/119 (98%)	96 (82%)	21 (18%)	2	10
34	BN	100/100 (100%)	83 (83%)	17 (17%)	2	11
34	DN	100/100 (100%)	78 (78%)	22 (22%)	1	5
35	BO	116/116 (100%)	78 (67%)	38 (33%)	0	1
35	DO	116/116 (100%)	72 (62%)	44 (38%)	0	0
36	BP	111/111 (100%)	84 (76%)	27 (24%)	1	3
36	DP	111/111 (100%)	85 (77%)	26 (23%)	1	4
37	B0	101/101 (100%)	78 (77%)	23 (23%)	1	4
37	D0	100/101 (99%)	80 (80%)	20 (20%)	1	7
38	BQ	87/88 (99%)	65 (75%)	22 (25%)	0	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	DQ	87/88 (99%)	53 (61%)	34 (39%)	0	0
39	BR	120/127 (94%)	92 (77%)	28 (23%)	1	4
39	DR	120/127 (94%)	84 (70%)	36 (30%)	0	2
40	B1	93/94 (99%)	76 (82%)	17 (18%)	2	9
40	D1	93/94 (99%)	80 (86%)	13 (14%)	4	17
41	B2	82/82 (100%)	61 (74%)	21 (26%)	0	3
41	D2	82/82 (100%)	50 (61%)	32 (39%)	0	0
42	BS	92/92 (100%)	72 (78%)	20 (22%)	1	5
42	DS	92/92 (100%)	65 (71%)	27 (29%)	0	2
43	BT	74/78 (95%)	61 (82%)	13 (18%)	2	10
43	DT	74/78 (95%)	57 (77%)	17 (23%)	1	4
44	BU	85/91 (93%)	65 (76%)	20 (24%)	1	4
44	DU	85/91 (93%)	51 (60%)	34 (40%)	0	0
45	BV	154/179 (86%)	116 (75%)	38 (25%)	0	3
45	DV	158/179 (88%)	124 (78%)	34 (22%)	1	6
46	B3	61/67 (91%)	54 (88%)	7 (12%)	6	25
46	D3	62/67 (92%)	47 (76%)	15 (24%)	1	3
47	BZ	82/83 (99%)	64 (78%)	18 (22%)	1	5
47	DZ	82/83 (99%)	64 (78%)	18 (22%)	1	5
48	BW	62/67 (92%)	42 (68%)	20 (32%)	0	1
48	DW	64/67 (96%)	50 (78%)	14 (22%)	1	5
49	BX	51/52 (98%)	41 (80%)	10 (20%)	1	8
49	DX	51/52 (98%)	42 (82%)	9 (18%)	2	10
50	B4	59/63 (94%)	41 (70%)	18 (30%)	0	1
50	D4	57/63 (90%)	38 (67%)	19 (33%)	0	1
51	B5	51/52 (98%)	35 (69%)	16 (31%)	0	1
51	D5	51/52 (98%)	37 (72%)	14 (28%)	0	2
52	B6	44/52 (85%)	27 (61%)	17 (39%)	0	0
52	D6	44/52 (85%)	31 (70%)	13 (30%)	0	2
53	B7	42/42 (100%)	34 (81%)	8 (19%)	1	9
53	D7	42/42 (100%)	32 (76%)	10 (24%)	1	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
54	B8	51/55 (93%)	40 (78%)	11 (22%)	1	5
54	D8	51/55 (93%)	41 (80%)	10 (20%)	1	8
All	All	9579/9996 (96%)	7317 (76%)	2262 (24%)	1	4

5 of 2262 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
49	BX	53	LEU
7	CJ	13	GLN
44	DU	62	GLU
51	B5	48	GLU
3	CF	28	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 255 such sidechains are listed below:

Mol	Chain	Res	Type
48	BW	65	ASN
6	CI	32	ASN
46	D3	12	ASN
49	BX	46	ASN
2	CE	78	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1505/1506 (99%)	375 (24%)	32 (2%)
1	CA	1505/1506 (99%)	409 (27%)	41 (2%)
22	AB	86/87 (98%)	40 (46%)	5 (5%)
22	CB	86/87 (98%)	46 (53%)	2 (2%)
23	AC	77/77 (100%)	23 (29%)	6 (7%)
23	AD	76/77 (98%)	28 (36%)	1 (1%)
23	CC	77/77 (100%)	21 (27%)	5 (6%)
23	CD	76/77 (98%)	26 (34%)	1 (1%)
24	A1	9/10 (90%)	3 (33%)	1 (11%)
24	C1	9/10 (90%)	3 (33%)	0
25	BA	2911/2912 (99%)	713 (24%)	57 (1%)
25	DA	2905/2912 (99%)	763 (26%)	57 (1%)
26	BB	121/122 (99%)	30 (24%)	0
26	DB	121/122 (99%)	39 (32%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	9564/9582 (99%)	2519 (26%)	208 (2%)

5 of 2519 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	6	G
1	AA	7	G
1	AA	8	A
1	AA	32	A
1	AA	33	A

5 of 208 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	BA	2439	A
1	CA	412	A
25	DA	2275	C
25	BA	2610	C
1	CA	115	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 1700 ligands modelled in this entry, 1700 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	1506/1506 (100%)	-0.57	5 (0%) 93 83	50, 98, 179, 234	0
1	CA	1506/1506 (100%)	-0.56	4 (0%) 93 83	62, 109, 181, 235	0
2	AE	237/256 (92%)	0.27	9 (3%) 40 16	103, 136, 174, 185	0
2	CE	237/256 (92%)	0.59	25 (10%) 6 2	114, 151, 185, 201	0
3	AF	205/239 (85%)	0.91	34 (16%) 1 0	84, 111, 144, 153	0
3	CF	206/239 (86%)	1.40	59 (28%) 0 0	118, 138, 166, 174	0
4	AG	208/208 (100%)	0.47	13 (6%) 20 6	80, 105, 129, 142	0
4	CG	208/208 (100%)	0.39	14 (6%) 18 5	77, 102, 123, 136	0
5	AH	151/162 (93%)	0.52	8 (5%) 26 10	74, 97, 118, 152	0
5	CH	151/162 (93%)	0.22	7 (4%) 32 12	91, 112, 134, 153	0
6	AI	101/101 (100%)	0.93	14 (13%) 2 1	76, 99, 115, 137	0
6	CI	101/101 (100%)	0.95	19 (18%) 1 0	74, 95, 116, 141	0
7	AJ	155/156 (99%)	-0.08	8 (5%) 27 10	99, 114, 145, 155	0
7	CJ	155/156 (99%)	0.27	10 (6%) 19 6	102, 122, 149, 156	0
8	AK	138/138 (100%)	-0.02	0 100 100	84, 103, 117, 122	0
8	CK	138/138 (100%)	-0.21	1 (0%) 87 68	94, 116, 128, 136	0
9	AL	127/128 (99%)	-0.31	1 (0%) 86 64	85, 133, 153, 160	0
9	CL	127/128 (99%)	-0.03	4 (3%) 49 21	107, 145, 160, 164	0
10	AM	99/105 (94%)	0.38	6 (6%) 21 7	81, 132, 162, 165	0
10	CM	99/105 (94%)	0.49	3 (3%) 50 22	111, 149, 165, 170	0
11	AN	119/129 (92%)	1.10	19 (15%) 1 0	64, 97, 128, 154	0
11	CN	119/129 (92%)	1.48	32 (26%) 0 0	79, 101, 134, 158	0
12	AO	125/132 (94%)	0.41	8 (6%) 19 6	63, 73, 105, 151	0
12	CO	125/132 (94%)	1.07	27 (21%) 0 0	75, 98, 124, 160	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AP	116/126 (92%)	-0.14	4 (3%) 45 19	86, 117, 136, 145	0
13	CP	117/126 (92%)	0.44	11 (9%) 8 3	106, 146, 161, 164	0
14	AQ	60/61 (98%)	-0.12	0 100 100	86, 101, 115, 126	0
14	CQ	60/61 (98%)	0.94	11 (18%) 1 0	118, 132, 146, 153	0
15	AR	88/89 (98%)	0.04	2 (2%) 60 31	72, 93, 114, 117	0
15	CR	88/89 (98%)	0.03	2 (2%) 60 31	73, 104, 127, 133	0
16	AS	84/88 (95%)	-0.37	0 100 100	90, 107, 133, 165	0
16	CS	84/88 (95%)	-0.34	0 100 100	81, 96, 120, 153	0
17	AT	100/105 (95%)	-0.21	1 (1%) 82 59	82, 100, 118, 130	0
17	CT	100/105 (95%)	-0.24	1 (1%) 82 59	82, 102, 125, 137	0
18	AU	72/88 (81%)	1.10	12 (16%) 1 0	78, 99, 132, 159	0
18	CU	72/88 (81%)	1.08	12 (16%) 1 0	85, 106, 144, 157	0
19	AV	78/93 (83%)	0.19	2 (2%) 56 27	100, 122, 137, 144	0
19	CV	78/93 (83%)	0.78	12 (15%) 2 0	136, 154, 174, 177	0
20	AW	99/106 (93%)	-0.44	0 100 100	93, 115, 144, 155	0
20	CW	99/106 (93%)	-0.23	0 100 100	83, 109, 143, 157	0
21	AX	25/27 (92%)	-0.63	0 100 100	88, 109, 125, 147	0
21	CX	25/27 (92%)	0.03	1 (4%) 38 15	112, 133, 148, 160	0
22	AB	87/87 (100%)	1.67	29 (33%) 0 0	78, 145, 185, 196	0
22	CB	87/87 (100%)	4.00	55 (63%) 0 0	92, 148, 188, 200	0
23	AC	77/77 (100%)	-0.36	0 100 100	63, 100, 132, 147	0
23	AD	77/77 (100%)	0.15	3 (3%) 39 16	71, 218, 232, 234	0
23	CC	77/77 (100%)	-0.20	1 (1%) 77 51	73, 107, 141, 153	0
23	CD	77/77 (100%)	0.64	12 (15%) 2 0	77, 219, 231, 234	0
24	A1	10/10 (100%)	0.53	2 (20%) 1 0	67, 81, 112, 112	0
24	C1	10/10 (100%)	0.51	2 (20%) 1 0	81, 98, 118, 124	0
25	BA	2912/2912 (100%)	-0.30	36 (1%) 79 53	36, 66, 200, 234	0
25	DA	2907/2912 (99%)	-0.26	48 (1%) 70 41	45, 80, 220, 235	0
26	BB	122/122 (100%)	-0.60	1 (0%) 86 64	66, 91, 110, 169	0
26	DB	122/122 (100%)	-0.47	1 (0%) 86 64	84, 120, 141, 189	0
27	BD	272/276 (98%)	0.09	1 (0%) 92 78	35, 57, 79, 96	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
27	DD	272/276 (98%)	0.37	9 (3%) 46 20	42, 67, 88, 119	0
28	BE	205/206 (99%)	0.42	15 (7%) 15 4	43, 77, 123, 132	0
28	DE	205/206 (99%)	0.24	11 (5%) 26 9	52, 88, 137, 159	0
29	BF	202/210 (96%)	-0.13	1 (0%) 90 74	38, 70, 108, 123	0
29	DF	208/210 (99%)	0.59	20 (9%) 8 3	48, 94, 152, 175	0
30	BG	181/182 (99%)	0.69	17 (9%) 8 3	81, 101, 130, 142	0
30	DG	181/182 (99%)	1.21	44 (24%) 0 0	112, 135, 155, 162	0
31	BH	170/180 (94%)	0.45	11 (6%) 19 6	74, 104, 121, 146	0
31	DH	170/180 (94%)	1.06	38 (22%) 0 0	148, 188, 209, 218	0
32	BK	146/148 (98%)	0.22	4 (2%) 54 26	69, 121, 137, 142	0
32	DK	146/148 (98%)	0.38	11 (7%) 14 4	77, 120, 143, 150	0
33	BM	138/140 (98%)	0.09	2 (1%) 75 49	57, 81, 116, 129	0
33	DM	138/140 (98%)	0.11	4 (2%) 51 23	71, 102, 133, 143	0
34	BN	122/122 (100%)	0.35	1 (0%) 86 64	48, 67, 83, 97	0
34	DN	122/122 (100%)	0.42	2 (1%) 72 44	62, 82, 102, 118	0
35	BO	150/150 (100%)	-0.12	2 (1%) 77 51	42, 77, 106, 153	0
35	DO	150/150 (100%)	0.95	27 (18%) 1 0	44, 99, 135, 171	0
36	BP	141/141 (100%)	0.44	11 (7%) 13 4	52, 78, 99, 125	0
36	DP	141/141 (100%)	0.90	24 (17%) 1 0	58, 98, 129, 148	0
37	B0	118/118 (100%)	0.33	1 (0%) 86 64	50, 76, 94, 110	0
37	D0	117/118 (99%)	0.01	2 (1%) 70 41	50, 75, 97, 113	0
38	BQ	111/112 (99%)	0.36	4 (3%) 42 17	70, 88, 110, 127	0
38	DQ	111/112 (99%)	0.41	9 (8%) 12 4	83, 117, 139, 159	0
39	BR	137/146 (93%)	0.19	4 (2%) 51 23	60, 82, 134, 163	0
39	DR	137/146 (93%)	0.18	5 (3%) 42 17	69, 93, 154, 174	0
40	B1	117/118 (99%)	-0.19	2 (1%) 70 41	44, 70, 101, 132	0
40	D1	117/118 (99%)	0.23	2 (1%) 70 41	58, 89, 131, 152	0
41	B2	101/101 (100%)	0.08	3 (2%) 50 22	48, 92, 115, 132	0
41	D2	101/101 (100%)	0.78	13 (12%) 3 1	58, 115, 133, 142	0
42	BS	113/113 (100%)	0.05	4 (3%) 44 18	41, 65, 97, 147	0
42	DS	113/113 (100%)	0.06	2 (1%) 68 39	54, 69, 104, 148	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
43	BT	92/96 (95%)	0.10	2 (2%) 62 33	49, 63, 87, 104	0
43	DT	92/96 (95%)	0.21	5 (5%) 26 9	64, 80, 104, 121	0
44	BU	102/110 (92%)	0.37	7 (6%) 17 5	67, 92, 142, 159	0
44	DU	102/110 (92%)	1.12	24 (23%) 0 0	82, 109, 160, 176	0
45	BV	175/206 (84%)	1.67	58 (33%) 0 0	80, 117, 179, 183	0
45	DV	179/206 (86%)	2.69	96 (53%) 0 0	110, 151, 199, 206	0
46	B3	76/85 (89%)	-0.16	1 (1%) 77 51	52, 68, 83, 117	0
46	D3	77/85 (90%)	0.16	1 (1%) 77 51	65, 86, 108, 141	0
47	BZ	97/98 (98%)	0.27	9 (9%) 8 3	46, 64, 122, 151	0
47	DZ	97/98 (98%)	0.15	4 (4%) 37 15	54, 77, 126, 148	0
48	BW	66/72 (91%)	-0.00	1 (1%) 73 46	55, 73, 90, 120	0
48	DW	69/72 (95%)	0.27	4 (5%) 23 8	77, 100, 130, 167	0
49	BX	59/60 (98%)	0.11	2 (3%) 45 19	60, 75, 105, 120	0
49	DX	59/60 (98%)	0.62	2 (3%) 45 19	73, 98, 130, 153	0
50	B4	66/71 (92%)	1.49	18 (27%) 0 0	111, 146, 164, 173	0
50	D4	63/71 (88%)	3.03	43 (68%) 0 0	140, 176, 185, 191	0
51	B5	59/60 (98%)	0.93	11 (18%) 1 0	43, 80, 163, 168	0
51	D5	58/60 (96%)	0.43	6 (10%) 6 2	52, 78, 167, 178	0
52	B6	45/54 (83%)	2.85	27 (60%) 0 0	105, 134, 156, 160	0
52	D6	45/54 (83%)	3.12	30 (66%) 0 0	121, 156, 173, 176	0
53	B7	49/49 (100%)	-0.10	2 (4%) 37 15	35, 45, 88, 118	0
53	D7	49/49 (100%)	0.26	3 (6%) 21 7	44, 54, 112, 131	0
54	B8	61/65 (93%)	-0.04	1 (1%) 72 44	51, 64, 81, 102	0
54	D8	61/65 (93%)	0.60	4 (6%) 18 6	65, 79, 94, 123	0
All	All	21104/21634 (97%)	0.11	1258 (5%) 22 7	35, 96, 177, 235	0

The worst 5 of 1258 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
22	CB	54	G	18.7
22	CB	53	A	15.6
22	CB	55	G	14.7
45	DV	147	GLY	14.5
22	CB	52	U	14.5

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	CA	1714	1/1	0.18	0.60	92,92,92,92	0
55	MG	CA	1805	1/1	0.19	0.28	94,94,94,94	0
55	MG	DA	3315	1/1	0.23	0.28	108,108,108,108	0
55	MG	BA	3490	1/1	0.28	0.08	166,166,166,166	0
55	MG	CC	107	1/1	0.31	0.63	99,99,99,99	0
55	MG	DA	3487	1/1	0.37	0.39	95,95,95,95	0
55	MG	BA	3461	1/1	0.39	0.27	91,91,91,91	0
55	MG	BA	3547	1/1	0.41	0.41	77,77,77,77	0
55	MG	DA	3490	1/1	0.42	0.14	126,126,126,126	0
55	MG	BA	3334	1/1	0.43	0.56	96,96,96,96	0
55	MG	AD	101	1/1	0.45	0.39	101,101,101,101	0
55	MG	DB	213	1/1	0.45	0.16	94,94,94,94	0
55	MG	CA	1751	1/1	0.46	0.27	94,94,94,94	0
55	MG	DA	3491	1/1	0.46	0.61	103,103,103,103	0
55	MG	D1	202	1/1	0.46	0.46	89,89,89,89	0
55	MG	BA	3463	1/1	0.47	0.30	72,72,72,72	0
55	MG	CA	1689	1/1	0.48	0.29	89,89,89,89	0
55	MG	DA	3500	1/1	0.48	0.33	92,92,92,92	0
55	MG	DA	3464	1/1	0.49	0.49	98,98,98,98	0
55	MG	AH	201	1/1	0.49	0.39	99,99,99,99	0
55	MG	AA	1758	1/1	0.49	0.35	85,85,85,85	0
55	MG	BA	3580	1/1	0.50	0.21	71,71,71,71	0
55	MG	AA	1700	1/1	0.51	0.21	99,99,99,99	0
55	MG	DA	3357	1/1	0.51	0.29	96,96,96,96	0
55	MG	AA	1772	1/1	0.52	0.55	85,85,85,85	0
55	MG	BA	3325	1/1	0.52	0.43	76,76,76,76	0
55	MG	AQ	101	1/1	0.52	0.15	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	1755	1/1	0.53	0.55	104,104,104,104	0
55	MG	AA	1725	1/1	0.53	0.19	82,82,82,82	0
55	MG	DA	3441	1/1	0.53	0.10	137,137,137,137	0
55	MG	DA	3429	1/1	0.54	0.33	99,99,99,99	0
55	MG	AA	1751	1/1	0.54	0.29	98,98,98,98	0
55	MG	DA	3304	1/1	0.55	0.37	85,85,85,85	0
55	MG	DB	207	1/1	0.55	0.33	115,115,115,115	0
55	MG	BA	3465	1/1	0.55	0.46	93,93,93,93	0
55	MG	BA	3151	1/1	0.56	0.27	83,83,83,83	0
55	MG	AA	1715	1/1	0.57	0.27	115,115,115,115	0
55	MG	DA	3303	1/1	0.57	0.40	70,70,70,70	0
55	MG	BA	3075	1/1	0.58	0.27	110,110,110,110	0
55	MG	BA	3500	1/1	0.58	0.28	97,97,97,97	0
55	MG	DA	3380	1/1	0.59	0.18	139,139,139,139	0
55	MG	DA	3146	1/1	0.59	0.53	92,92,92,92	0
55	MG	BD	301	1/1	0.59	0.61	85,85,85,85	0
55	MG	BA	3379	1/1	0.59	0.45	82,82,82,82	0
55	MG	DA	3064	1/1	0.59	0.43	101,101,101,101	0
55	MG	CA	1763	1/1	0.59	0.47	91,91,91,91	0
55	MG	CA	1769	1/1	0.59	0.33	105,105,105,105	0
55	MG	CS	101	1/1	0.61	0.30	87,87,87,87	0
55	MG	AA	1753	1/1	0.61	0.10	108,108,108,108	0
55	MG	DA	3010	1/1	0.61	0.40	97,97,97,97	0
55	MG	DA	3492	1/1	0.61	0.34	88,88,88,88	0
55	MG	AA	1703	1/1	0.62	0.24	92,92,92,92	0
55	MG	AA	1777	1/1	0.62	0.39	90,90,90,90	0
55	MG	AA	1727	1/1	0.62	0.86	87,87,87,87	0
55	MG	DA	3151	1/1	0.62	0.25	85,85,85,85	0
55	MG	DA	3042	1/1	0.62	0.50	81,81,81,81	0
55	MG	AA	1731	1/1	0.63	0.30	103,103,103,103	0
55	MG	CA	1741	1/1	0.63	0.14	106,106,106,106	0
55	MG	BA	3603	1/1	0.64	0.61	63,63,63,63	0
55	MG	CA	1757	1/1	0.64	0.21	97,97,97,97	0
55	MG	DA	3522	1/1	0.64	0.48	78,78,78,78	0
55	MG	BA	3541	1/1	0.64	0.20	96,96,96,96	0
55	MG	DA	3447	1/1	0.64	0.46	82,82,82,82	0
55	MG	DA	3119	1/1	0.65	0.44	98,98,98,98	0
55	MG	DA	3517	1/1	0.66	0.40	84,84,84,84	0
55	MG	BA	3420	1/1	0.66	0.34	94,94,94,94	0
55	MG	CG	301	1/1	0.66	0.36	83,83,83,83	0
55	MG	CC	101	1/1	0.66	0.36	92,92,92,92	0
55	MG	CA	1664	1/1	0.66	0.29	99,99,99,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	DA	3273	1/1	0.66	0.19	99,99,99,99	0
55	MG	CA	1807	1/1	0.66	0.24	126,126,126,126	0
55	MG	DA	3461	1/1	0.66	0.23	84,84,84,84	0
55	MG	DA	3494	1/1	0.67	0.21	75,75,75,75	0
55	MG	DA	3402	1/1	0.67	0.32	101,101,101,101	0
55	MG	DA	3068	1/1	0.67	0.18	91,91,91,91	0
55	MG	BA	3272	1/1	0.67	0.17	94,94,94,94	0
55	MG	BA	3484	1/1	0.67	0.23	117,117,117,117	0
55	MG	CA	1762	1/1	0.67	0.31	96,96,96,96	0
55	MG	DA	3120	1/1	0.67	0.26	90,90,90,90	0
55	MG	CA	1759	1/1	0.67	0.37	103,103,103,103	0
55	MG	DA	3507	1/1	0.67	0.44	91,91,91,91	0
55	MG	DA	3350	1/1	0.67	0.25	91,91,91,91	0
55	MG	AA	1720	1/1	0.68	0.19	93,93,93,93	0
55	MG	DA	3371	1/1	0.68	0.49	82,82,82,82	0
55	MG	BA	3349	1/1	0.68	0.42	97,97,97,97	0
55	MG	CA	1696	1/1	0.68	0.37	91,91,91,91	0
55	MG	DA	3459	1/1	0.68	0.28	86,86,86,86	0
55	MG	AA	1680	1/1	0.68	0.29	80,80,80,80	0
55	MG	DA	3028	1/1	0.68	0.22	101,101,101,101	0
55	MG	BA	3086	1/1	0.68	0.31	95,95,95,95	0
55	MG	BA	3606	1/1	0.68	0.35	77,77,77,77	0
55	MG	BA	3570	1/1	0.68	0.41	87,87,87,87	0
55	MG	AA	1804	1/1	0.68	0.11	74,74,74,74	0
55	MG	AA	1769	1/1	0.68	0.14	104,104,104,104	0
55	MG	DA	3422	1/1	0.68	0.39	84,84,84,84	0
55	MG	AA	1630	1/1	0.68	0.16	101,101,101,101	0
55	MG	DA	3401	1/1	0.68	0.16	71,71,71,71	0
55	MG	AA	1836	1/1	0.69	0.60	79,79,79,79	0
55	MG	AB	103	1/1	0.69	0.30	111,111,111,111	0
55	MG	DA	3020	1/1	0.69	0.32	85,85,85,85	0
55	MG	BA	3227	1/1	0.69	0.40	91,91,91,91	0
55	MG	CA	1660	1/1	0.69	0.17	85,85,85,85	0
55	MG	DA	3480	1/1	0.69	0.41	63,63,63,63	0
55	MG	BA	3472	1/1	0.69	0.61	89,89,89,89	0
55	MG	DA	3059	1/1	0.70	0.77	106,106,106,106	0
55	MG	BA	3415	1/1	0.70	0.37	84,84,84,84	0
55	MG	CA	1638	1/1	0.70	0.33	101,101,101,101	0
55	MG	BA	3527	1/1	0.70	0.55	93,93,93,93	0
55	MG	AA	1621	1/1	0.70	0.19	108,108,108,108	0
55	MG	BA	3057	1/1	0.70	0.14	70,70,70,70	0
55	MG	AA	1770	1/1	0.70	0.25	102,102,102,102	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	DA	3335	1/1	0.70	0.21	61,61,61,61	0
55	MG	DA	3338	1/1	0.70	0.31	86,86,86,86	0
55	MG	CA	1758	1/1	0.71	0.46	78,78,78,78	0
55	MG	BA	3397	1/1	0.71	0.24	81,81,81,81	0
55	MG	BA	3087	1/1	0.71	0.38	77,77,77,77	0
55	MG	AA	1612	1/1	0.71	0.14	91,91,91,91	0
55	MG	DA	3465	1/1	0.71	0.34	74,74,74,74	0
55	MG	CA	1630	1/1	0.71	0.45	91,91,91,91	0
55	MG	AA	1690	1/1	0.71	0.17	96,96,96,96	0
55	MG	AA	1781	1/1	0.71	0.43	94,94,94,94	0
55	MG	BA	3399	1/1	0.72	0.58	90,90,90,90	0
55	MG	AA	1662	1/1	0.72	0.64	81,81,81,81	0
55	MG	CA	1709	1/1	0.72	0.50	108,108,108,108	0
55	MG	DA	3290	1/1	0.72	0.31	79,79,79,79	0
55	MG	BA	3402	1/1	0.72	0.27	91,91,91,91	0
55	MG	BA	3324	1/1	0.72	0.50	73,73,73,73	0
55	MG	AA	1635	1/1	0.72	0.24	86,86,86,86	0
55	MG	CA	1632	1/1	0.72	0.30	95,95,95,95	0
55	MG	DA	3353	1/1	0.72	0.75	93,93,93,93	0
55	MG	DA	3320	1/1	0.72	0.15	76,76,76,76	0
55	MG	CA	1644	1/1	0.72	0.29	120,120,120,120	0
55	MG	AA	1681	1/1	0.72	0.33	80,80,80,80	0
55	MG	DA	3396	1/1	0.73	0.25	82,82,82,82	0
55	MG	DA	3067	1/1	0.73	0.35	94,94,94,94	0
55	MG	DA	3277	1/1	0.73	0.28	89,89,89,89	0
55	MG	DA	3080	1/1	0.73	0.55	75,75,75,75	0
55	MG	AA	1782	1/1	0.73	0.19	96,96,96,96	0
55	MG	DA	3508	1/1	0.73	0.70	80,80,80,80	0
55	MG	BA	3505	1/1	0.73	0.48	96,96,96,96	0
55	MG	DA	3344	1/1	0.73	0.33	95,95,95,95	0
55	MG	BA	3573	1/1	0.73	0.46	83,83,83,83	0
55	MG	BA	3354	1/1	0.73	0.21	72,72,72,72	0
55	MG	DB	208	1/1	0.73	0.22	90,90,90,90	0
55	MG	BA	3481	1/1	0.73	0.55	69,69,69,69	0
55	MG	BA	3232	1/1	0.73	0.31	72,72,72,72	0
55	MG	AA	1826	1/1	0.73	0.12	101,101,101,101	0
55	MG	DA	3424	1/1	0.73	0.73	70,70,70,70	0
55	MG	BA	3598	1/1	0.73	0.38	77,77,77,77	0
55	MG	CA	1614	1/1	0.73	0.38	86,86,86,86	0
55	MG	BA	3417	1/1	0.73	0.27	99,99,99,99	0
55	MG	CA	1770	1/1	0.74	0.23	102,102,102,102	0
55	MG	BB	208	1/1	0.74	0.25	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	DA	3088	1/1	0.74	0.24	96,96,96,96	0
55	MG	BA	3467	1/1	0.74	0.32	78,78,78,78	0
55	MG	BA	3431	1/1	0.74	0.71	88,88,88,88	0
55	MG	BA	3121	1/1	0.74	0.48	57,57,57,57	0
55	MG	BA	3282	1/1	0.74	0.09	83,83,83,83	0
55	MG	DB	211	1/1	0.74	0.41	93,93,93,93	0
55	MG	BA	3106	1/1	0.74	0.36	75,75,75,75	0
55	MG	BA	3327	1/1	0.74	0.20	70,70,70,70	0
55	MG	DA	3485	1/1	0.74	0.20	81,81,81,81	0
55	MG	DA	3425	1/1	0.74	0.25	81,81,81,81	0
55	MG	BA	3290	1/1	0.74	0.39	97,97,97,97	0
55	MG	DA	3134	1/1	0.74	0.28	72,72,72,72	0
55	MG	AA	1807	1/1	0.74	0.60	98,98,98,98	0
55	MG	CA	1641	1/1	0.74	0.29	66,66,66,66	0
55	MG	CA	1645	1/1	0.74	0.22	86,86,86,86	0
55	MG	AA	1813	1/1	0.75	0.29	107,107,107,107	0
55	MG	CC	104	1/1	0.75	0.59	89,89,89,89	0
55	MG	DA	3404	1/1	0.75	0.30	61,61,61,61	0
55	MG	BA	3368	1/1	0.75	0.30	88,88,88,88	0
55	MG	BA	3591	1/1	0.75	0.47	64,64,64,64	0
55	MG	BA	3534	1/1	0.75	0.30	79,79,79,79	0
55	MG	BA	3342	1/1	0.75	0.30	66,66,66,66	0
55	MG	DA	3415	1/1	0.75	0.54	96,96,96,96	0
55	MG	BA	3466	1/1	0.75	0.44	97,97,97,97	0
55	MG	AA	1614	1/1	0.75	0.26	91,91,91,91	0
55	MG	CA	1729	1/1	0.75	0.84	77,77,77,77	0
55	MG	BA	3446	1/1	0.75	0.19	92,92,92,92	0
55	MG	CA	1637	1/1	0.75	0.34	79,79,79,79	0
55	MG	BB	216	1/1	0.75	0.15	94,94,94,94	0
55	MG	BA	3059	1/1	0.75	0.38	91,91,91,91	0
55	MG	DA	3236	1/1	0.76	0.32	55,55,55,55	0
55	MG	DA	3298	1/1	0.76	0.33	77,77,77,77	0
55	MG	CA	1699	1/1	0.76	0.27	97,97,97,97	0
55	MG	DA	3493	1/1	0.76	0.55	82,82,82,82	0
55	MG	BA	3072	1/1	0.76	0.29	77,77,77,77	0
55	MG	BA	3418	1/1	0.76	0.41	78,78,78,78	0
55	MG	BA	3098	1/1	0.76	0.25	48,48,48,48	0
55	MG	BA	3073	1/1	0.76	0.42	82,82,82,82	0
55	MG	BE	304	1/1	0.76	0.37	80,80,80,80	0
55	MG	DA	3394	1/1	0.76	0.20	90,90,90,90	0
55	MG	BA	3408	1/1	0.76	0.45	87,87,87,87	0
55	MG	BA	3583	1/1	0.76	0.50	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	BA	3341	1/1	0.76	0.25	81,81,81,81	0
55	MG	BA	3116	1/1	0.76	0.33	73,73,73,73	0
55	MG	DA	3366	1/1	0.76	0.43	83,83,83,83	0
55	MG	AA	1822	1/1	0.76	0.14	107,107,107,107	0
55	MG	DA	3340	1/1	0.76	0.20	85,85,85,85	0
55	MG	BA	3462	1/1	0.76	0.27	87,87,87,87	0
55	MG	AB	105	1/1	0.76	0.19	110,110,110,110	0
55	MG	DA	3038	1/1	0.77	0.47	97,97,97,97	0
55	MG	BA	3509	1/1	0.77	0.29	83,83,83,83	0
55	MG	AA	1820	1/1	0.77	0.30	75,75,75,75	0
55	MG	BA	3317	1/1	0.77	0.73	89,89,89,89	0
55	MG	AA	1706	1/1	0.77	0.46	74,74,74,74	0
55	MG	DA	3381	1/1	0.77	0.47	99,99,99,99	0
55	MG	DA	3137	1/1	0.77	0.18	82,82,82,82	0
55	MG	BA	3247	1/1	0.77	0.48	70,70,70,70	0
55	MG	AA	1647	1/1	0.77	0.36	88,88,88,88	0
55	MG	AA	1616	1/1	0.77	0.18	94,94,94,94	0
55	MG	DA	3011	1/1	0.77	0.21	65,65,65,65	0
55	MG	DA	3078	1/1	0.77	0.37	89,89,89,89	0
55	MG	DA	3312	1/1	0.77	0.29	85,85,85,85	0
55	MG	BA	3069	1/1	0.77	0.45	77,77,77,77	0
55	MG	CA	1616	1/1	0.77	0.28	88,88,88,88	0
55	MG	BA	3339	1/1	0.77	0.58	88,88,88,88	0
55	MG	DA	3058	1/1	0.78	0.31	76,76,76,76	0
55	MG	BA	3412	1/1	0.78	0.35	78,78,78,78	0
55	MG	BA	3133	1/1	0.78	0.29	66,66,66,66	0
55	MG	DA	3406	1/1	0.78	0.73	86,86,86,86	0
55	MG	CA	1683	1/1	0.78	0.41	87,87,87,87	0
55	MG	CA	1612	1/1	0.78	0.51	82,82,82,82	0
55	MG	CA	1702	1/1	0.78	0.41	78,78,78,78	0
55	MG	CA	1797	1/1	0.78	0.32	87,87,87,87	0
55	MG	BA	3536	1/1	0.78	0.68	73,73,73,73	0
55	MG	BA	3432	1/1	0.78	0.32	80,80,80,80	0
55	MG	BA	3054	1/1	0.78	0.25	80,80,80,80	0
55	MG	DA	3045	1/1	0.78	0.54	94,94,94,94	0
55	MG	DA	3524	1/1	0.78	0.28	105,105,105,105	0
55	MG	DA	3419	1/1	0.78	0.45	84,84,84,84	0
55	MG	BA	3332	1/1	0.78	0.32	61,61,61,61	0
55	MG	DA	3409	1/1	0.78	0.50	76,76,76,76	0
55	MG	DA	3186	1/1	0.78	0.31	60,60,60,60	0
55	MG	DA	3029	1/1	0.78	0.27	79,79,79,79	0
55	MG	CA	1749	1/1	0.78	0.20	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	BA	3530	1/1	0.78	0.30	81,81,81,81	0
55	MG	DA	3393	1/1	0.78	0.52	69,69,69,69	0
55	MG	BA	3367	1/1	0.78	0.26	82,82,82,82	0
55	MG	BA	3442	1/1	0.78	0.37	76,76,76,76	0
55	MG	DA	3274	1/1	0.78	0.30	87,87,87,87	0
55	MG	BA	3385	1/1	0.78	0.16	87,87,87,87	0
55	MG	AA	1611	1/1	0.79	0.18	92,92,92,92	0
55	MG	AA	1754	1/1	0.79	0.19	95,95,95,95	0
55	MG	DA	3346	1/1	0.79	0.58	75,75,75,75	0
55	MG	CA	1756	1/1	0.79	0.40	81,81,81,81	0
55	MG	AA	1710	1/1	0.79	0.29	92,92,92,92	0
55	MG	DA	3387	1/1	0.79	0.29	92,92,92,92	0
55	MG	CA	1734	1/1	0.79	0.25	93,93,93,93	0
55	MG	AA	1735	1/1	0.79	0.46	79,79,79,79	0
55	MG	BB	214	1/1	0.79	0.24	86,86,86,86	0
55	MG	BA	3533	1/1	0.79	0.57	72,72,72,72	0
55	MG	DR	201	1/1	0.79	0.22	71,71,71,71	0
55	MG	AB	102	1/1	0.79	0.26	86,86,86,86	0
55	MG	BA	3563	1/1	0.79	0.19	82,82,82,82	0
55	MG	AA	1679	1/1	0.79	0.28	86,86,86,86	0
55	MG	AA	1625	1/1	0.79	0.45	57,57,57,57	0
55	MG	BB	217	1/1	0.79	0.18	98,98,98,98	0
55	MG	CA	1766	1/1	0.79	0.30	85,85,85,85	0
55	MG	AA	1761	1/1	0.79	0.41	113,113,113,113	0
55	MG	AA	1786	1/1	0.79	0.19	86,86,86,86	0
55	MG	AA	1696	1/1	0.79	0.29	88,88,88,88	0
55	MG	AA	1708	1/1	0.79	0.40	91,91,91,91	0
55	MG	DA	3091	1/1	0.79	0.31	92,92,92,92	0
55	MG	BB	210	1/1	0.79	0.40	64,64,64,64	0
55	MG	BA	3388	1/1	0.79	0.49	88,88,88,88	0
55	MG	BA	3080	1/1	0.79	0.17	91,91,91,91	0
55	MG	DA	3057	1/1	0.79	0.35	83,83,83,83	0
55	MG	BA	3328	1/1	0.79	0.71	69,69,69,69	0
55	MG	DA	3123	1/1	0.79	0.25	83,83,83,83	0
55	MG	DA	3251	1/1	0.79	0.27	74,74,74,74	0
55	MG	BB	209	1/1	0.79	0.40	102,102,102,102	0
55	MG	BA	3404	1/1	0.79	0.17	60,60,60,60	0
55	MG	DA	3462	1/1	0.79	0.78	107,107,107,107	0
55	MG	AA	1652	1/1	0.80	0.44	81,81,81,81	0
55	MG	BA	3313	1/1	0.80	0.18	88,88,88,88	0
55	MG	DA	3297	1/1	0.80	0.23	83,83,83,83	0
55	MG	DA	3476	1/1	0.80	0.33	107,107,107,107	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	BA	3403	1/1	0.80	0.66	93,93,93,93	0
55	MG	BA	3084	1/1	0.80	0.52	82,82,82,82	0
55	MG	DA	3187	1/1	0.80	0.45	42,42,42,42	0
55	MG	DA	3070	1/1	0.80	0.28	78,78,78,78	0
55	MG	DA	3431	1/1	0.80	0.43	91,91,91,91	0
55	MG	BA	3571	1/1	0.80	0.36	92,92,92,92	0
55	MG	DA	3403	1/1	0.80	0.47	76,76,76,76	0
55	MG	BA	3104	1/1	0.80	0.20	57,57,57,57	0
55	MG	BA	3366	1/1	0.80	1.04	94,94,94,94	0
55	MG	CA	1623	1/1	0.80	0.10	90,90,90,90	0
55	MG	CA	1618	1/1	0.80	0.17	93,93,93,93	0
55	MG	AA	1785	1/1	0.80	0.40	96,96,96,96	0
55	MG	DA	3512	1/1	0.80	0.48	75,75,75,75	0
55	MG	CA	1604	1/1	0.80	0.17	81,81,81,81	0
55	MG	CA	1727	1/1	0.80	0.45	94,94,94,94	0
55	MG	DA	3479	1/1	0.80	0.11	99,99,99,99	0
55	MG	CA	1771	1/1	0.80	0.42	76,76,76,76	0
55	MG	AA	1812	1/1	0.80	0.59	73,73,73,73	0
55	MG	CA	1740	1/1	0.80	0.33	68,68,68,68	0
55	MG	CA	1669	1/1	0.80	0.19	60,60,60,60	0
55	MG	BA	3473	1/1	0.80	0.49	76,76,76,76	0
55	MG	DA	3043	1/1	0.80	0.23	82,82,82,82	0
55	MG	AA	1617	1/1	0.80	0.50	69,69,69,69	0
55	MG	BA	3304	1/1	0.80	0.28	56,56,56,56	0
55	MG	CA	1667	1/1	0.80	0.16	102,102,102,102	0
55	MG	CA	1626	1/1	0.81	0.18	93,93,93,93	0
55	MG	CA	1677	1/1	0.81	0.42	73,73,73,73	0
55	MG	AA	1719	1/1	0.81	0.60	79,79,79,79	0
55	MG	BA	3088	1/1	0.81	0.17	77,77,77,77	0
55	MG	DA	3072	1/1	0.81	0.44	112,112,112,112	0
55	MG	CA	1693	1/1	0.81	0.54	76,76,76,76	0
55	MG	AA	1730	1/1	0.81	0.43	78,78,78,78	0
55	MG	BA	3361	1/1	0.81	0.41	64,64,64,64	0
55	MG	AA	1806	1/1	0.81	0.28	81,81,81,81	0
55	MG	DA	3417	1/1	0.81	0.22	81,81,81,81	0
55	MG	BA	3579	1/1	0.81	0.13	92,92,92,92	0
55	MG	DA	3502	1/1	0.81	0.50	97,97,97,97	0
55	MG	DA	3139	1/1	0.81	0.44	80,80,80,80	0
55	MG	BA	3592	1/1	0.81	0.36	89,89,89,89	0
55	MG	DA	3341	1/1	0.81	0.52	84,84,84,84	0
55	MG	BA	3330	1/1	0.81	0.29	79,79,79,79	0
55	MG	DA	3478	1/1	0.81	0.32	80,80,80,80	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	0.81	0.22	87,87,87,87	0
55	MG	B3	101	1/1	0.81	0.55	71,71,71,71	0
55	MG	CA	1755	1/1	0.81	0.49	92,92,92,92	0
55	MG	AA	1702	1/1	0.81	0.19	93,93,93,93	0
55	MG	CA	1681	1/1	0.81	0.52	72,72,72,72	0
55	MG	BA	3546	1/1	0.81	0.16	87,87,87,87	0
55	MG	BA	3277	1/1	0.81	0.30	86,86,86,86	0
55	MG	BA	3301	1/1	0.81	0.32	76,76,76,76	0
55	MG	CA	1719	1/1	0.81	0.23	129,129,129,129	0
55	MG	AC	103	1/1	0.81	0.38	66,66,66,66	0
55	MG	AA	1840	1/1	0.81	0.47	87,87,87,87	0
55	MG	CA	1732	1/1	0.81	0.21	109,109,109,109	0
55	MG	CA	1777	1/1	0.81	0.30	88,88,88,88	0
55	MG	DA	3330	1/1	0.81	0.14	81,81,81,81	0
55	MG	DA	3007	1/1	0.81	0.25	74,74,74,74	0
55	MG	AA	1832	1/1	0.81	0.35	94,94,94,94	0
55	MG	DA	3448	1/1	0.81	0.71	79,79,79,79	0
55	MG	DA	3302	1/1	0.81	0.57	95,95,95,95	0
55	MG	DA	3440	1/1	0.81	0.36	86,86,86,86	0
55	MG	AA	1698	1/1	0.81	0.33	72,72,72,72	0
55	MG	AA	1790	1/1	0.81	0.24	98,98,98,98	0
55	MG	BA	3438	1/1	0.81	0.41	91,91,91,91	0
55	MG	DA	3333	1/1	0.81	0.52	87,87,87,87	0
55	MG	DU	201	1/1	0.81	0.15	72,72,72,72	0
55	MG	BA	3457	1/1	0.81	0.91	88,88,88,88	0
55	MG	AA	1705	1/1	0.81	0.31	83,83,83,83	0
55	MG	DA	3092	1/1	0.81	0.30	68,68,68,68	0
55	MG	BA	3614	1/1	0.81	0.17	69,69,69,69	0
55	MG	BA	3175	1/1	0.81	0.52	69,69,69,69	0
55	MG	BA	3409	1/1	0.81	0.20	68,68,68,68	0
55	MG	BA	3526	1/1	0.81	0.39	86,86,86,86	0
55	MG	DA	3025	1/1	0.82	1.38	84,84,84,84	0
55	MG	AA	1713	1/1	0.82	0.31	115,115,115,115	0
55	MG	CA	1798	1/1	0.82	0.21	85,85,85,85	0
55	MG	BA	3588	1/1	0.82	0.34	83,83,83,83	0
55	MG	DA	3075	1/1	0.82	0.35	79,79,79,79	0
55	MG	DA	3473	1/1	0.82	0.48	96,96,96,96	0
55	MG	CB	101	1/1	0.82	0.20	101,101,101,101	0
55	MG	AA	1728	1/1	0.82	0.13	108,108,108,108	0
55	MG	BA	3476	1/1	0.82	0.26	81,81,81,81	0
55	MG	AA	1688	1/1	0.82	0.21	72,72,72,72	0
55	MG	BA	3365	1/1	0.82	0.33	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	BA	3161	1/1	0.82	0.22	56,56,56,56	0
55	MG	CA	1787	1/1	0.82	0.13	87,87,87,87	0
55	MG	AA	1768	1/1	0.82	0.36	101,101,101,101	0
55	MG	CB	103	1/1	0.82	0.46	103,103,103,103	0
55	MG	DB	210	1/1	0.82	0.37	71,71,71,71	0
55	MG	AA	1677	1/1	0.82	0.32	87,87,87,87	0
55	MG	BA	3613	1/1	0.82	0.28	93,93,93,93	0
55	MG	DA	3505	1/1	0.82	0.48	81,81,81,81	0
55	MG	BA	3265	1/1	0.82	0.74	60,60,60,60	0
55	MG	DA	3281	1/1	0.82	0.88	76,76,76,76	0
55	MG	AA	1689	1/1	0.82	0.26	115,115,115,115	0
55	MG	AA	1791	1/1	0.82	0.11	109,109,109,109	0
55	MG	BA	3496	1/1	0.82	0.26	96,96,96,96	0
55	MG	CA	1624	1/1	0.82	0.36	88,88,88,88	0
55	MG	BA	3250	1/1	0.82	0.15	60,60,60,60	0
55	MG	BA	3586	1/1	0.82	0.35	63,63,63,63	0
55	MG	DA	3136	1/1	0.82	0.34	76,76,76,76	0
55	MG	BA	3370	1/1	0.82	0.46	56,56,56,56	0
55	MG	B7	101	1/1	0.82	0.46	67,67,67,67	0
55	MG	BA	3398	1/1	0.82	0.44	70,70,70,70	0
55	MG	AA	1637	1/1	0.82	0.18	98,98,98,98	0
55	MG	BA	3521	1/1	0.82	0.60	79,79,79,79	0
55	MG	DA	3327	1/1	0.82	0.34	61,61,61,61	0
55	MG	BA	3597	1/1	0.82	0.23	79,79,79,79	0
55	MG	DA	3337	1/1	0.82	0.46	89,89,89,89	0
55	MG	BA	3572	1/1	0.82	0.30	87,87,87,87	0
55	MG	CA	1801	1/1	0.83	0.28	89,89,89,89	0
55	MG	AC	106	1/1	0.83	0.56	89,89,89,89	0
55	MG	AA	1815	1/1	0.83	0.46	84,84,84,84	0
55	MG	DA	3449	1/1	0.83	0.38	87,87,87,87	0
55	MG	DA	3503	1/1	0.83	0.65	80,80,80,80	0
55	MG	DA	3519	1/1	0.83	0.47	85,85,85,85	0
55	MG	DA	3004	1/1	0.83	0.48	99,99,99,99	0
55	MG	DA	3364	1/1	0.83	0.27	71,71,71,71	0
55	MG	CA	1712	1/1	0.83	0.53	86,86,86,86	0
55	MG	AA	1797	1/1	0.83	0.11	99,99,99,99	0
55	MG	AA	1819	1/1	0.83	0.35	87,87,87,87	0
55	MG	BA	3309	1/1	0.83	0.19	68,68,68,68	0
55	MG	DB	205	1/1	0.83	0.35	69,69,69,69	0
55	MG	CA	1720	1/1	0.83	0.49	102,102,102,102	0
55	MG	BA	3595	1/1	0.83	0.18	65,65,65,65	0
55	MG	AA	1776	1/1	0.83	0.18	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	DB	206	1/1	0.83	0.28	90,90,90,90	0
55	MG	AA	1824	1/1	0.83	0.56	86,86,86,86	0
55	MG	BA	3193	1/1	0.83	0.51	85,85,85,85	0
55	MG	DA	3129	1/1	0.83	0.25	82,82,82,82	0
55	MG	CA	1636	1/1	0.83	0.27	78,78,78,78	0
55	MG	DA	3002	1/1	0.83	0.33	93,93,93,93	0
55	MG	DA	3484	1/1	0.83	0.40	83,83,83,83	0
55	MG	CA	1662	1/1	0.83	0.24	90,90,90,90	0
55	MG	AA	1823	1/1	0.83	0.44	77,77,77,77	0
55	MG	AA	1711	1/1	0.83	0.28	89,89,89,89	0
55	MG	DA	3513	1/1	0.83	0.76	67,67,67,67	0
55	MG	BA	3185	1/1	0.83	0.36	76,76,76,76	0
55	MG	BA	3441	1/1	0.83	0.20	86,86,86,86	0
55	MG	AA	1766	1/1	0.83	0.16	79,79,79,79	0
55	MG	DA	3085	1/1	0.83	0.32	91,91,91,91	0
55	MG	BA	3345	1/1	0.83	0.71	73,73,73,73	0
55	MG	DA	3432	1/1	0.83	0.29	69,69,69,69	0
55	MG	BB	212	1/1	0.83	0.50	81,81,81,81	0
55	MG	AA	1749	1/1	0.83	0.21	81,81,81,81	0
55	MG	CA	1773	1/1	0.83	0.73	92,92,92,92	0
55	MG	DA	3084	1/1	0.83	0.29	88,88,88,88	0
55	MG	BA	3252	1/1	0.83	0.43	67,67,67,67	0
55	MG	DA	3197	1/1	0.83	0.70	70,70,70,70	0
55	MG	BA	3359	1/1	0.83	0.43	79,79,79,79	0
55	MG	AA	1828	1/1	0.83	0.11	105,105,105,105	0
55	MG	AA	1729	1/1	0.84	0.36	113,113,113,113	0
55	MG	BA	3222	1/1	0.84	0.33	89,89,89,89	0
55	MG	DA	3389	1/1	0.84	0.79	64,64,64,64	0
55	MG	CA	1608	1/1	0.84	0.30	81,81,81,81	0
55	MG	CA	1790	1/1	0.84	0.19	110,110,110,110	0
55	MG	BA	3166	1/1	0.84	0.62	72,72,72,72	0
55	MG	BA	3110	1/1	0.84	0.52	59,59,59,59	0
55	MG	AA	1759	1/1	0.84	0.36	77,77,77,77	0
55	MG	CA	1625	1/1	0.84	0.21	90,90,90,90	0
55	MG	DA	3525	1/1	0.84	0.78	79,79,79,79	0
55	MG	DA	3384	1/1	0.84	0.42	65,65,65,65	0
55	MG	AA	1724	1/1	0.84	0.20	84,84,84,84	0
55	MG	DA	3342	1/1	0.84	0.42	82,82,82,82	0
55	MG	DA	3347	1/1	0.84	0.12	75,75,75,75	0
55	MG	DA	3309	1/1	0.84	0.21	94,94,94,94	0
55	MG	AA	1618	1/1	0.84	0.27	82,82,82,82	0
55	MG	DA	3497	1/1	0.84	0.36	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	CA	1629	1/1	0.84	0.16	98,98,98,98	0
55	MG	DA	3051	1/1	0.84	0.27	85,85,85,85	0
55	MG	CB	102	1/1	0.84	0.28	87,87,87,87	0
55	MG	BA	3256	1/1	0.84	0.41	61,61,61,61	0
55	MG	BA	3517	1/1	0.84	0.54	70,70,70,70	0
55	MG	BA	3295	1/1	0.84	0.44	81,81,81,81	0
55	MG	CA	1737	1/1	0.84	0.28	99,99,99,99	0
55	MG	BA	3350	1/1	0.84	0.32	55,55,55,55	0
55	MG	DA	3483	1/1	0.84	0.15	90,90,90,90	0
55	MG	DA	3287	1/1	0.84	0.64	65,65,65,65	0
55	MG	DA	3468	1/1	0.84	0.42	92,92,92,92	0
55	MG	AB	101	1/1	0.84	0.28	90,90,90,90	0
55	MG	BA	3300	1/1	0.84	0.35	88,88,88,88	0
55	MG	BA	3052	1/1	0.84	0.20	64,64,64,64	0
55	MG	CA	1772	1/1	0.84	0.29	72,72,72,72	0
55	MG	DA	3475	1/1	0.84	0.35	88,88,88,88	0
55	MG	DA	3427	1/1	0.84	0.28	76,76,76,76	0
55	MG	BA	3400	1/1	0.84	0.52	80,80,80,80	0
55	MG	DA	3356	1/1	0.84	0.29	67,67,67,67	0
55	MG	CA	1791	1/1	0.84	0.30	79,79,79,79	0
55	MG	DA	3247	1/1	0.84	0.20	87,87,87,87	0
55	MG	BA	3401	1/1	0.84	0.45	62,62,62,62	0
55	MG	BA	3537	1/1	0.84	0.42	89,89,89,89	0
55	MG	AA	1803	1/1	0.84	0.29	91,91,91,91	0
55	MG	AA	1684	1/1	0.84	0.18	90,90,90,90	0
55	MG	AA	1683	1/1	0.84	0.20	87,87,87,87	0
55	MG	BA	3191	1/1	0.84	0.21	81,81,81,81	0
55	MG	BA	3607	1/1	0.84	0.34	96,96,96,96	0
55	MG	BA	3120	1/1	0.84	0.42	56,56,56,56	0
55	MG	DA	3477	1/1	0.84	0.60	89,89,89,89	0
55	MG	CA	1656	1/1	0.84	0.30	92,92,92,92	0
55	MG	AA	1757	1/1	0.84	0.06	110,110,110,110	0
55	MG	AA	1816	1/1	0.84	0.24	81,81,81,81	0
55	MG	DA	3501	1/1	0.84	0.92	88,88,88,88	0
55	MG	CA	1802	1/1	0.84	0.45	74,74,74,74	0
55	MG	AA	1723	1/1	0.84	0.32	84,84,84,84	0
55	MG	DA	3283	1/1	0.84	0.44	61,61,61,61	0
55	MG	DB	209	1/1	0.85	0.20	92,92,92,92	0
55	MG	BA	3514	1/1	0.85	0.31	71,71,71,71	0
55	MG	DA	3467	1/1	0.85	0.40	61,61,61,61	0
55	MG	BA	3495	1/1	0.85	0.25	123,123,123,123	0
55	MG	AA	1709	1/1	0.85	0.19	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	BA	3391	1/1	0.85	0.46	86,86,86,86	0
55	MG	BA	3392	1/1	0.85	0.39	70,70,70,70	0
55	MG	BA	3154	1/1	0.85	0.30	55,55,55,55	0
55	MG	AA	1839	1/1	0.85	0.37	74,74,74,74	0
55	MG	DA	3131	1/1	0.85	0.25	79,79,79,79	0
55	MG	BB	201	1/1	0.85	0.43	92,92,92,92	0
55	MG	BA	3089	1/1	0.85	0.33	88,88,88,88	0
55	MG	DA	3400	1/1	0.85	0.40	89,89,89,89	0
55	MG	CA	1711	1/1	0.85	0.38	90,90,90,90	0
55	MG	BA	3215	1/1	0.85	0.48	74,74,74,74	0
55	MG	CA	1659	1/1	0.85	0.20	110,110,110,110	0
55	MG	CA	1783	1/1	0.85	0.47	100,100,100,100	0
55	MG	DA	3292	1/1	0.85	0.24	89,89,89,89	0
55	MG	AC	105	1/1	0.85	0.50	93,93,93,93	0
55	MG	DA	3094	1/1	0.85	0.94	94,94,94,94	0
55	MG	DA	3237	1/1	0.85	0.27	83,83,83,83	0
55	MG	DA	3140	1/1	0.85	0.28	78,78,78,78	0
55	MG	BA	3134	1/1	0.85	0.18	81,81,81,81	0
55	MG	DA	3061	1/1	0.85	0.56	74,74,74,74	0
55	MG	DA	3117	1/1	0.85	0.38	78,78,78,78	0
55	MG	AA	1802	1/1	0.85	0.45	85,85,85,85	0
55	MG	DA	3509	1/1	0.85	0.41	64,64,64,64	0
55	MG	AA	1793	1/1	0.85	0.39	73,73,73,73	0
55	MG	CA	1753	1/1	0.85	0.26	123,123,123,123	0
55	MG	BA	3112	1/1	0.85	0.28	77,77,77,77	0
55	MG	BA	3164	1/1	0.85	0.68	86,86,86,86	0
55	MG	B8	101	1/1	0.85	0.19	97,97,97,97	0
55	MG	DA	3460	1/1	0.85	0.46	72,72,72,72	0
55	MG	AA	1651	1/1	0.85	0.56	71,71,71,71	0
55	MG	BA	3206	1/1	0.85	0.38	75,75,75,75	0
55	MG	CA	1780	1/1	0.85	0.32	88,88,88,88	0
55	MG	AA	1640	1/1	0.85	0.33	90,90,90,90	0
55	MG	BA	3411	1/1	0.85	0.30	68,68,68,68	0
55	MG	BA	3485	1/1	0.85	0.26	80,80,80,80	0
55	MG	DA	3361	1/1	0.85	0.71	79,79,79,79	0
55	MG	AA	1626	1/1	0.86	0.46	69,69,69,69	0
55	MG	BA	3140	1/1	0.86	0.25	58,58,58,58	0
55	MG	AA	1795	1/1	0.86	0.23	73,73,73,73	0
55	MG	BA	3622	1/1	0.86	0.47	59,59,59,59	0
55	MG	BA	3371	1/1	0.86	0.31	70,70,70,70	0
55	MG	AA	1834	1/1	0.86	0.48	97,97,97,97	0
55	MG	BA	3356	1/1	0.86	0.51	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	CA	1796	1/1	0.86	0.40	102,102,102,102	0
55	MG	BA	3291	1/1	0.86	0.39	72,72,72,72	0
55	MG	CA	1672	1/1	0.86	0.75	75,75,75,75	0
55	MG	DA	3466	1/1	0.86	0.63	78,78,78,78	0
55	MG	DA	3041	1/1	0.86	0.41	86,86,86,86	0
55	MG	CA	1804	1/1	0.86	0.30	75,75,75,75	0
55	MG	BA	3348	1/1	0.86	0.29	61,61,61,61	0
55	MG	BA	3358	1/1	0.86	0.37	74,74,74,74	0
55	MG	AC	107	1/1	0.86	0.28	94,94,94,94	0
55	MG	CA	1723	1/1	0.86	0.07	86,86,86,86	0
55	MG	DA	3005	1/1	0.86	0.48	77,77,77,77	0
55	MG	CG	302	1/1	0.86	0.14	101,101,101,101	0
55	MG	DA	3077	1/1	0.86	0.11	64,64,64,64	0
55	MG	DA	3183	1/1	0.86	0.51	57,57,57,57	0
55	MG	BA	3285	1/1	0.86	0.35	72,72,72,72	0
55	MG	DA	3164	1/1	0.86	0.45	47,47,47,47	0
55	MG	DA	3370	1/1	0.86	0.10	67,67,67,67	0
55	MG	DA	3486	1/1	0.86	0.32	68,68,68,68	0
55	MG	BA	3357	1/1	0.86	0.56	81,81,81,81	0
55	MG	B2	201	1/1	0.86	0.42	85,85,85,85	0
55	MG	AA	1638	1/1	0.86	0.31	104,104,104,104	0
55	MG	BA	3310	1/1	0.86	0.37	57,57,57,57	0
55	MG	AA	1674	1/1	0.86	0.33	98,98,98,98	0
55	MG	BA	3362	1/1	0.86	0.24	48,48,48,48	0
55	MG	DA	3430	1/1	0.86	0.58	62,62,62,62	0
55	MG	DA	3098	1/1	0.86	0.46	68,68,68,68	0
55	MG	BA	3083	1/1	0.86	0.12	62,62,62,62	0
55	MG	BA	3394	1/1	0.86	0.19	81,81,81,81	0
55	MG	AA	1682	1/1	0.86	0.16	91,91,91,91	0
55	MG	AA	1716	1/1	0.86	0.22	92,92,92,92	0
55	MG	BA	3551	1/1	0.86	0.40	87,87,87,87	0
55	MG	BA	3565	1/1	0.86	0.28	77,77,77,77	0
55	MG	DA	3062	1/1	0.86	0.27	72,72,72,72	0
55	MG	BA	3240	1/1	0.86	0.54	88,88,88,88	0
55	MG	DA	3367	1/1	0.86	0.43	82,82,82,82	0
55	MG	DB	212	1/1	0.86	0.26	88,88,88,88	0
55	MG	DA	3413	1/1	0.86	0.29	94,94,94,94	0
55	MG	DA	3363	1/1	0.86	0.79	79,79,79,79	0
55	MG	BA	3396	1/1	0.86	0.19	82,82,82,82	0
55	MG	CA	1745	1/1	0.86	0.12	91,91,91,91	0
55	MG	BA	3523	1/1	0.86	0.60	70,70,70,70	0
55	MG	CA	1761	1/1	0.86	0.40	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	3049	1/1	0.86	0.28	74,74,74,74	0
55	MG	CA	1698	1/1	0.86	0.09	107,107,107,107	0
55	MG	DA	3306	1/1	0.86	0.54	65,65,65,65	0
55	MG	AA	1817	1/1	0.87	0.21	85,85,85,85	0
55	MG	AA	1835	1/1	0.87	0.29	87,87,87,87	0
55	MG	DA	3319	1/1	0.87	0.40	74,74,74,74	0
55	MG	BA	3455	1/1	0.87	0.24	76,76,76,76	0
55	MG	BA	3364	1/1	0.87	0.45	82,82,82,82	0
55	MG	DA	3291	1/1	0.87	0.59	65,65,65,65	0
55	MG	CA	1784	1/1	0.87	0.23	81,81,81,81	0
55	MG	AA	1639	1/1	0.87	0.31	91,91,91,91	0
55	MG	BA	3506	1/1	0.87	0.37	78,78,78,78	0
55	MG	BA	3471	1/1	0.87	0.31	72,72,72,72	0
55	MG	DA	3455	1/1	0.87	0.29	69,69,69,69	0
55	MG	DA	3026	1/1	0.87	0.43	95,95,95,95	0
55	MG	CA	1601	1/1	0.87	0.31	96,96,96,96	0
55	MG	BA	3203	1/1	0.87	0.33	85,85,85,85	0
55	MG	AA	1742	1/1	0.87	0.17	78,78,78,78	0
55	MG	AA	1752	1/1	0.87	0.27	78,78,78,78	0
55	MG	AA	1778	1/1	0.87	0.14	106,106,106,106	0
55	MG	BA	3479	1/1	0.87	0.46	82,82,82,82	0
55	MG	DA	3168	1/1	0.87	0.29	49,49,49,49	0
55	MG	DA	3515	1/1	0.87	0.63	82,82,82,82	0
55	MG	BA	3584	1/1	0.87	0.18	72,72,72,72	0
55	MG	BA	3497	1/1	0.87	0.21	71,71,71,71	0
55	MG	BA	3375	1/1	0.87	0.25	50,50,50,50	0
55	MG	DA	3523	1/1	0.87	0.91	81,81,81,81	0
55	MG	CA	1774	1/1	0.87	0.13	104,104,104,104	0
55	MG	CA	1768	1/1	0.87	0.41	84,84,84,84	0
55	MG	DA	3438	1/1	0.87	0.25	87,87,87,87	0
55	MG	DA	3520	1/1	0.87	0.83	76,76,76,76	0
55	MG	BA	3378	1/1	0.87	0.56	76,76,76,76	0
55	MG	BA	3319	1/1	0.87	0.28	65,65,65,65	0
55	MG	DA	3482	1/1	0.87	0.45	81,81,81,81	0
55	MG	AA	1656	1/1	0.87	0.43	87,87,87,87	0
55	MG	BA	3266	1/1	0.87	0.41	77,77,77,77	0
55	MG	CA	1691	1/1	0.87	0.33	78,78,78,78	0
55	MG	BA	3387	1/1	0.87	0.40	73,73,73,73	0
55	MG	AA	1830	1/1	0.87	0.30	73,73,73,73	0
55	MG	BA	3578	1/1	0.87	0.35	81,81,81,81	0
55	MG	BA	3475	1/1	0.87	0.31	83,83,83,83	0
55	MG	DB	204	1/1	0.87	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	BA	3090	1/1	0.87	0.47	49,49,49,49	0
55	MG	DA	3023	1/1	0.87	0.44	57,57,57,57	0
55	MG	CA	1611	1/1	0.87	0.89	93,93,93,93	0
55	MG	CA	1725	1/1	0.87	0.24	86,86,86,86	0
55	MG	AA	1633	1/1	0.87	0.25	74,74,74,74	0
55	MG	DA	3434	1/1	0.87	0.15	74,74,74,74	0
55	MG	DA	3471	1/1	0.88	0.43	80,80,80,80	0
55	MG	CA	1686	1/1	0.88	0.42	73,73,73,73	0
55	MG	AA	1675	1/1	0.88	0.45	80,80,80,80	0
55	MG	DA	3034	1/1	0.88	0.33	62,62,62,62	0
55	MG	CA	1697	1/1	0.88	0.30	65,65,65,65	0
55	MG	CA	1679	1/1	0.88	0.37	85,85,85,85	0
55	MG	CA	1713	1/1	0.88	0.57	102,102,102,102	0
55	MG	DA	3439	1/1	0.88	0.33	62,62,62,62	0
55	MG	DA	3015	1/1	0.88	0.69	89,89,89,89	0
55	MG	BE	305	1/1	0.88	0.42	71,71,71,71	0
55	MG	CA	1747	1/1	0.88	0.26	94,94,94,94	0
55	MG	BA	3444	1/1	0.88	0.50	78,78,78,78	0
55	MG	AA	1821	1/1	0.88	0.23	75,75,75,75	0
55	MG	AA	1744	1/1	0.88	0.13	117,117,117,117	0
55	MG	BA	3267	1/1	0.88	0.30	61,61,61,61	0
55	MG	DA	3040	1/1	0.88	0.14	81,81,81,81	0
55	MG	DA	3435	1/1	0.88	0.11	72,72,72,72	0
55	MG	BA	3448	1/1	0.88	0.43	100,100,100,100	0
55	MG	DA	3368	1/1	0.88	0.72	73,73,73,73	0
55	MG	CC	105	1/1	0.88	0.59	82,82,82,82	0
55	MG	CA	1700	1/1	0.88	0.47	77,77,77,77	0
55	MG	DA	3436	1/1	0.88	0.30	98,98,98,98	0
55	MG	DA	3405	1/1	0.88	0.47	79,79,79,79	0
55	MG	BA	3510	1/1	0.88	0.15	108,108,108,108	0
55	MG	DA	3090	1/1	0.88	0.33	86,86,86,86	0
55	MG	BA	3094	1/1	0.88	0.56	78,78,78,78	0
55	MG	DA	3504	1/1	0.88	0.34	65,65,65,65	0
55	MG	DA	3442	1/1	0.88	0.22	91,91,91,91	0
55	MG	DA	3377	1/1	0.88	0.22	98,98,98,98	0
55	MG	CA	1657	1/1	0.88	0.27	95,95,95,95	0
55	MG	BA	3445	1/1	0.88	0.35	79,79,79,79	0
55	MG	AA	1613	1/1	0.88	0.07	85,85,85,85	0
55	MG	CA	1803	1/1	0.88	0.30	96,96,96,96	0
55	MG	BA	3569	1/1	0.88	0.54	85,85,85,85	0
55	MG	CA	1760	1/1	0.88	0.27	91,91,91,91	0
55	MG	BA	3623	1/1	0.88	0.40	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	DE	302	1/1	0.88	0.27	65,65,65,65	0
55	MG	BA	3231	1/1	0.88	0.50	73,73,73,73	0
55	MG	DA	3175	1/1	0.88	0.34	83,83,83,83	0
55	MG	DA	3526	1/1	0.88	0.31	68,68,68,68	0
55	MG	CA	1742	1/1	0.88	0.15	97,97,97,97	0
55	MG	CA	1643	1/1	0.88	0.49	82,82,82,82	0
55	MG	CA	1673	1/1	0.88	0.53	64,64,64,64	0
55	MG	BA	3574	1/1	0.88	0.53	78,78,78,78	0
55	MG	CA	1615	1/1	0.88	0.22	81,81,81,81	0
55	MG	DA	3454	1/1	0.88	0.37	92,92,92,92	0
55	MG	DA	3263	1/1	0.88	0.86	82,82,82,82	0
55	MG	CA	1609	1/1	0.88	0.16	115,115,115,115	0
55	MG	BA	3532	1/1	0.88	0.22	85,85,85,85	0
55	MG	BA	3575	1/1	0.88	0.35	71,71,71,71	0
55	MG	DA	3125	1/1	0.88	0.43	45,45,45,45	0
55	MG	CA	1707	1/1	0.88	0.57	98,98,98,98	0
55	MG	AA	1743	1/1	0.88	0.11	107,107,107,107	0
55	MG	DA	3376	1/1	0.88	0.53	82,82,82,82	0
55	MG	AA	1745	1/1	0.88	0.56	67,67,67,67	0
55	MG	DB	214	1/1	0.88	0.19	96,96,96,96	0
55	MG	BA	3482	1/1	0.88	0.39	57,57,57,57	0
55	MG	BA	3489	1/1	0.88	0.24	70,70,70,70	0
55	MG	DB	203	1/1	0.88	0.33	66,66,66,66	0
55	MG	DA	3395	1/1	0.88	0.47	69,69,69,69	0
55	MG	AC	109	1/1	0.88	0.41	82,82,82,82	0
55	MG	DA	3383	1/1	0.88	0.47	87,87,87,87	0
55	MG	BA	3621	1/1	0.88	0.15	63,63,63,63	0
55	MG	BA	3204	1/1	0.88	0.34	78,78,78,78	0
55	MG	BA	3503	1/1	0.88	0.20	65,65,65,65	0
55	MG	DA	3220	1/1	0.88	0.36	66,66,66,66	0
55	MG	AA	1739	1/1	0.88	0.07	93,93,93,93	0
55	MG	AA	1737	1/1	0.88	0.55	83,83,83,83	0
55	MG	BA	3507	1/1	0.88	0.30	89,89,89,89	0
55	MG	AC	102	1/1	0.88	0.67	93,93,93,93	0
55	MG	BA	3531	1/1	0.88	0.36	53,53,53,53	0
55	MG	BA	3424	1/1	0.88	0.65	72,72,72,72	0
55	MG	BA	3211	1/1	0.88	0.46	39,39,39,39	0
55	MG	DA	3428	1/1	0.88	0.58	84,84,84,84	0
55	MG	BA	3118	1/1	0.88	0.42	61,61,61,61	0
55	MG	AA	1693	1/1	0.88	0.16	87,87,87,87	0
55	MG	CA	1767	1/1	0.88	0.46	77,77,77,77	0
55	MG	DA	3399	1/1	0.88	0.45	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	3395	1/1	0.88	0.31	72,72,72,72	0
55	MG	AA	1694	1/1	0.88	0.12	91,91,91,91	0
55	MG	BF	302	1/1	0.88	0.22	72,72,72,72	0
55	MG	BA	3114	1/1	0.88	0.20	74,74,74,74	0
55	MG	CA	1800	1/1	0.88	0.32	78,78,78,78	0
55	MG	BA	3511	1/1	0.88	0.15	89,89,89,89	0
55	MG	BB	204	1/1	0.88	0.31	78,78,78,78	0
55	MG	DA	3481	1/1	0.88	0.41	96,96,96,96	0
55	MG	CA	1634	1/1	0.88	0.45	77,77,77,77	0
55	MG	CA	1648	1/1	0.88	0.42	65,65,65,65	0
55	MG	DA	3352	1/1	0.89	0.65	64,64,64,64	0
55	MG	BA	3425	1/1	0.89	0.51	91,91,91,91	0
55	MG	AA	1773	1/1	0.89	0.26	87,87,87,87	0
55	MG	AA	1631	1/1	0.89	0.21	66,66,66,66	0
55	MG	BA	3502	1/1	0.89	0.26	67,67,67,67	0
55	MG	CA	1704	1/1	0.89	0.28	99,99,99,99	0
55	MG	CA	1687	1/1	0.89	0.17	89,89,89,89	0
55	MG	DA	3412	1/1	0.89	0.33	89,89,89,89	0
55	MG	BA	3167	1/1	0.89	0.38	73,73,73,73	0
55	MG	BA	3416	1/1	0.89	0.18	87,87,87,87	0
55	MG	D1	201	1/1	0.89	0.39	71,71,71,71	0
55	MG	DA	3511	1/1	0.89	0.43	76,76,76,76	0
55	MG	BA	3223	1/1	0.89	0.27	92,92,92,92	0
55	MG	BA	3494	1/1	0.89	0.77	76,76,76,76	0
55	MG	DA	3391	1/1	0.89	0.23	78,78,78,78	0
55	MG	DA	3351	1/1	0.89	0.28	79,79,79,79	0
55	MG	DB	201	1/1	0.89	0.37	81,81,81,81	0
55	MG	BA	3381	1/1	0.89	0.44	90,90,90,90	0
55	MG	BA	3589	1/1	0.89	0.31	41,41,41,41	0
55	MG	CA	1781	1/1	0.89	0.05	117,117,117,117	0
55	MG	AA	1722	1/1	0.89	0.46	68,68,68,68	0
55	MG	CA	1647	1/1	0.89	0.51	61,61,61,61	0
55	MG	DA	3053	1/1	0.89	0.62	62,62,62,62	0
55	MG	AA	1643	1/1	0.89	0.62	85,85,85,85	0
55	MG	CA	1715	1/1	0.89	0.25	104,104,104,104	0
55	MG	DA	3048	1/1	0.89	0.49	75,75,75,75	0
55	MG	BA	3331	1/1	0.89	0.42	65,65,65,65	0
55	MG	DA	3112	1/1	0.89	0.35	81,81,81,81	0
55	MG	BA	3061	1/1	0.89	0.54	61,61,61,61	0
55	MG	DA	3055	1/1	0.89	0.54	68,68,68,68	0
55	MG	A1	102	1/1	0.89	0.42	86,86,86,86	0
55	MG	BA	3447	1/1	0.89	0.49	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	BF	303	1/1	0.89	0.48	66,66,66,66	0
55	MG	BA	3034	1/1	0.89	0.34	41,41,41,41	0
55	MG	AA	1615	1/1	0.89	0.55	105,105,105,105	0
55	MG	DA	3019	1/1	0.89	0.92	90,90,90,90	0
55	MG	DA	3150	1/1	0.89	0.34	68,68,68,68	0
55	MG	CA	1639	1/1	0.89	0.36	95,95,95,95	0
55	MG	DA	3408	1/1	0.89	0.11	73,73,73,73	0
55	MG	BA	3539	1/1	0.89	0.26	74,74,74,74	0
55	MG	BA	3060	1/1	0.89	0.17	64,64,64,64	0
55	MG	BA	3270	1/1	0.89	0.22	76,76,76,76	0
55	MG	AA	1787	1/1	0.89	0.47	96,96,96,96	0
55	MG	AA	1673	1/1	0.89	0.47	78,78,78,78	0
55	MG	AA	1734	1/1	0.89	0.19	96,96,96,96	0
55	MG	BA	3323	1/1	0.89	0.32	66,66,66,66	0
55	MG	BA	3289	1/1	0.89	0.56	60,60,60,60	0
55	MG	BA	3552	1/1	0.89	0.30	102,102,102,102	0
55	MG	BA	3435	1/1	0.89	0.28	65,65,65,65	0
55	MG	BA	3314	1/1	0.89	0.58	64,64,64,64	0
55	MG	AA	1718	1/1	0.89	0.58	82,82,82,82	0
55	MG	BO	202	1/1	0.89	0.23	37,37,37,37	0
55	MG	BA	3543	1/1	0.89	0.41	80,80,80,80	0
55	MG	AA	1712	1/1	0.89	0.38	78,78,78,78	0
55	MG	BA	3225	1/1	0.89	0.17	65,65,65,65	0
55	MG	BA	3210	1/1	0.89	0.20	74,74,74,74	0
55	MG	AB	104	1/1	0.89	0.35	82,82,82,82	0
55	MG	DA	3369	1/1	0.89	0.27	74,74,74,74	0
55	MG	BA	3053	1/1	0.89	0.28	95,95,95,95	0
55	MG	DA	3328	1/1	0.89	0.34	47,47,47,47	0
55	MG	DA	3307	1/1	0.89	0.26	77,77,77,77	0
55	MG	BA	3619	1/1	0.89	0.33	69,69,69,69	0
55	MG	DA	3037	1/1	0.89	0.33	98,98,98,98	0
55	MG	BA	3548	1/1	0.89	0.48	76,76,76,76	0
55	MG	DA	3018	1/1	0.89	0.28	77,77,77,77	0
55	MG	CA	1665	1/1	0.89	0.17	83,83,83,83	0
55	MG	DA	3027	1/1	0.89	0.23	77,77,77,77	0
55	MG	CA	1684	1/1	0.89	0.61	85,85,85,85	0
55	MG	DA	3488	1/1	0.89	0.58	86,86,86,86	0
55	MG	DA	3154	1/1	0.89	0.32	69,69,69,69	0
55	MG	BA	3273	1/1	0.89	0.41	94,94,94,94	0
55	MG	CA	1663	1/1	0.89	0.35	81,81,81,81	0
55	MG	BA	3103	1/1	0.89	0.49	52,52,52,52	0
55	MG	AN	202	1/1	0.89	0.32	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	BA	3260	1/1	0.89	0.42	47,47,47,47	0
55	MG	BA	3249	1/1	0.89	0.29	30,30,30,30	0
55	MG	CA	1668	1/1	0.89	0.42	79,79,79,79	0
55	MG	DA	3173	1/1	0.89	0.22	60,60,60,60	0
55	MG	DA	3047	1/1	0.89	0.42	76,76,76,76	0
55	MG	CA	1785	1/1	0.90	0.24	105,105,105,105	0
55	MG	DA	3358	1/1	0.90	0.53	88,88,88,88	0
55	MG	DA	3373	1/1	0.90	0.43	79,79,79,79	0
55	MG	AA	1774	1/1	0.90	0.13	91,91,91,91	0
55	MG	DA	3076	1/1	0.90	0.37	86,86,86,86	0
55	MG	CA	1655	1/1	0.90	0.37	87,87,87,87	0
55	MG	DA	3398	1/1	0.90	0.40	74,74,74,74	0
55	MG	BA	3144	1/1	0.90	0.29	48,48,48,48	0
55	MG	BA	3360	1/1	0.90	0.14	84,84,84,84	0
55	MG	BA	3257	1/1	0.90	0.25	64,64,64,64	0
55	MG	AA	1809	1/1	0.90	0.36	63,63,63,63	0
55	MG	DA	3230	1/1	0.90	0.16	59,59,59,59	0
55	MG	BB	202	1/1	0.90	0.14	79,79,79,79	0
55	MG	BA	3217	1/1	0.90	0.31	52,52,52,52	0
55	MG	AA	1678	1/1	0.90	0.35	74,74,74,74	0
55	MG	AA	1668	1/1	0.90	0.63	76,76,76,76	0
55	MG	BA	3281	1/1	0.90	0.54	72,72,72,72	0
55	MG	BA	3451	1/1	0.90	0.48	65,65,65,65	0
55	MG	BA	3587	1/1	0.90	0.32	64,64,64,64	0
55	MG	DA	3498	1/1	0.90	0.24	85,85,85,85	0
55	MG	BA	3593	1/1	0.90	0.26	80,80,80,80	0
55	MG	AA	1692	1/1	0.90	0.13	115,115,115,115	0
55	MG	CA	1606	1/1	0.90	0.35	87,87,87,87	0
55	MG	DA	3269	1/1	0.90	0.42	84,84,84,84	0
55	MG	AA	1653	1/1	0.90	0.53	81,81,81,81	0
55	MG	BA	3321	1/1	0.90	0.41	77,77,77,77	0
55	MG	DA	3060	1/1	0.90	0.85	73,73,73,73	0
55	MG	DA	3225	1/1	0.90	0.59	73,73,73,73	0
55	MG	BA	3439	1/1	0.90	0.36	71,71,71,71	0
55	MG	AA	1624	1/1	0.90	0.28	79,79,79,79	0
55	MG	DA	3496	1/1	0.90	0.24	83,83,83,83	0
55	MG	DB	202	1/1	0.90	0.18	98,98,98,98	0
55	MG	DA	3279	1/1	0.90	0.24	84,84,84,84	0
55	MG	BA	3423	1/1	0.90	0.56	61,61,61,61	0
55	MG	DA	3253	1/1	0.90	0.17	87,87,87,87	0
55	MG	CA	1628	1/1	0.90	0.21	101,101,101,101	0
55	MG	DA	3385	1/1	0.90	0.70	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	BA	3132	1/1	0.90	0.41	71,71,71,71	0
55	MG	BA	3292	1/1	0.90	0.40	85,85,85,85	0
55	MG	CA	1778	1/1	0.90	0.40	96,96,96,96	0
55	MG	CA	1633	1/1	0.90	0.28	91,91,91,91	0
55	MG	BA	3393	1/1	0.90	0.51	81,81,81,81	0
55	MG	DA	3348	1/1	0.90	0.60	73,73,73,73	0
55	MG	DA	3032	1/1	0.90	0.12	76,76,76,76	0
55	MG	CA	1688	1/1	0.90	0.34	71,71,71,71	0
55	MG	BA	3581	1/1	0.90	0.33	69,69,69,69	0
55	MG	DA	3437	1/1	0.90	0.20	87,87,87,87	0
55	MG	BA	3421	1/1	0.90	0.35	62,62,62,62	0
55	MG	AA	1664	1/1	0.90	0.20	45,45,45,45	0
55	MG	DA	3514	1/1	0.90	0.68	59,59,59,59	0
55	MG	BA	3449	1/1	0.90	0.36	80,80,80,80	0
55	MG	DA	3332	1/1	0.90	0.39	76,76,76,76	0
55	MG	BA	3544	1/1	0.90	0.40	72,72,72,72	0
55	MG	AA	1808	1/1	0.90	0.54	76,76,76,76	0
55	MG	BA	3336	1/1	0.90	0.47	66,66,66,66	0
55	MG	BA	3038	1/1	0.90	0.40	56,56,56,56	0
55	MG	BA	3516	1/1	0.90	0.86	78,78,78,78	0
55	MG	BA	3535	1/1	0.90	0.44	80,80,80,80	0
55	MG	BA	3322	1/1	0.90	0.63	64,64,64,64	0
55	MG	DA	3336	1/1	0.90	0.41	87,87,87,87	0
55	MG	DA	3179	1/1	0.90	0.32	70,70,70,70	0
55	MG	BA	3437	1/1	0.90	0.42	67,67,67,67	0
55	MG	CA	1654	1/1	0.90	0.31	99,99,99,99	0
55	MG	CA	1635	1/1	0.90	0.78	86,86,86,86	0
55	MG	DA	3003	1/1	0.91	0.29	64,64,64,64	0
55	MG	BA	3596	1/1	0.91	0.46	55,55,55,55	0
55	MG	DA	3294	1/1	0.91	0.23	64,64,64,64	0
55	MG	BA	3609	1/1	0.91	0.65	70,70,70,70	0
55	MG	DA	3506	1/1	0.91	0.40	78,78,78,78	0
55	MG	DA	3518	1/1	0.91	0.41	83,83,83,83	0
55	MG	DA	3073	1/1	0.91	0.52	80,80,80,80	0
55	MG	BA	3617	1/1	0.91	0.72	71,71,71,71	0
55	MG	BA	3474	1/1	0.91	0.43	80,80,80,80	0
55	MG	BU	202	1/1	0.91	0.12	55,55,55,55	0
55	MG	DA	3349	1/1	0.91	0.29	63,63,63,63	0
55	MG	DA	3489	1/1	0.91	0.16	71,71,71,71	0
55	MG	BA	3187	1/1	0.91	0.48	73,73,73,73	0
55	MG	DA	3093	1/1	0.91	0.20	80,80,80,80	0
55	MG	DA	3266	1/1	0.91	0.50	55,55,55,55	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	0.91	0.31	88,88,88,88	0
55	MG	BA	3065	1/1	0.91	0.34	91,91,91,91	0
55	MG	CA	1652	1/1	0.91	0.33	71,71,71,71	0
55	MG	DA	3343	1/1	0.91	0.36	95,95,95,95	0
55	MG	BA	3305	1/1	0.91	0.42	70,70,70,70	0
55	MG	BA	3205	1/1	0.91	0.33	80,80,80,80	0
55	MG	BA	3179	1/1	0.91	0.44	64,64,64,64	0
55	MG	DA	3318	1/1	0.91	0.22	63,63,63,63	0
55	MG	AA	1663	1/1	0.91	0.27	47,47,47,47	0
55	MG	BA	3513	1/1	0.91	0.41	90,90,90,90	0
55	MG	AA	1644	1/1	0.91	0.16	62,62,62,62	0
55	MG	DA	3359	1/1	0.91	0.36	76,76,76,76	0
55	MG	BA	3219	1/1	0.91	0.43	76,76,76,76	0
55	MG	AA	1829	1/1	0.91	0.55	77,77,77,77	0
55	MG	CA	1640	1/1	0.91	0.33	81,81,81,81	0
55	MG	DA	3451	1/1	0.91	0.47	75,75,75,75	0
55	MG	CA	1718	1/1	0.91	0.07	92,92,92,92	0
55	MG	BA	3459	1/1	0.91	0.42	70,70,70,70	0
55	MG	BA	3556	1/1	0.91	0.51	58,58,58,58	0
55	MG	DA	3188	1/1	0.91	0.60	56,56,56,56	0
55	MG	DA	3407	1/1	0.91	0.42	73,73,73,73	0
55	MG	DA	3044	1/1	0.91	0.29	73,73,73,73	0
55	MG	BA	3127	1/1	0.91	0.59	53,53,53,53	0
55	MG	AA	1801	1/1	0.91	0.49	84,84,84,84	0
55	MG	DA	3152	1/1	0.91	0.07	67,67,67,67	0
55	MG	DA	3314	1/1	0.91	0.47	76,76,76,76	0
55	MG	BA	3145	1/1	0.91	0.35	74,74,74,74	0
55	MG	BA	3553	1/1	0.91	0.21	78,78,78,78	0
55	MG	DA	3293	1/1	0.91	0.48	75,75,75,75	0
55	MG	BA	3469	1/1	0.91	0.30	60,60,60,60	0
55	MG	DA	3242	1/1	0.91	0.58	63,63,63,63	0
55	MG	BA	3618	1/1	0.91	0.47	73,73,73,73	0
55	MG	BA	3071	1/1	0.91	0.23	70,70,70,70	0
55	MG	CA	1786	1/1	0.91	0.26	73,73,73,73	0
55	MG	BA	3488	1/1	0.91	0.36	80,80,80,80	0
55	MG	BA	3470	1/1	0.91	0.31	88,88,88,88	0
55	MG	BA	3344	1/1	0.91	0.36	55,55,55,55	0
55	MG	BA	3234	1/1	0.91	0.43	86,86,86,86	0
55	MG	CA	1794	1/1	0.91	0.34	74,74,74,74	0
55	MG	AA	1764	1/1	0.91	0.17	79,79,79,79	0
55	MG	AA	1607	1/1	0.91	0.22	89,89,89,89	0
55	MG	BA	3611	1/1	0.91	0.52	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	DA	3259	1/1	0.91	0.26	72,72,72,72	0
55	MG	AA	1697	1/1	0.91	0.41	84,84,84,84	0
55	MG	BA	3146	1/1	0.91	0.38	59,59,59,59	0
55	MG	DA	3285	1/1	0.91	0.25	50,50,50,50	0
55	MG	AA	1771	1/1	0.91	0.11	70,70,70,70	0
55	MG	BA	3542	1/1	0.91	0.48	72,72,72,72	0
55	MG	AA	1767	1/1	0.91	0.22	96,96,96,96	0
55	MG	BA	3460	1/1	0.91	0.13	83,83,83,83	0
55	MG	BA	3582	1/1	0.91	0.42	86,86,86,86	0
55	MG	DA	3056	1/1	0.91	0.44	81,81,81,81	0
55	MG	BA	3302	1/1	0.91	0.41	26,26,26,26	0
55	MG	CC	108	1/1	0.91	0.56	106,106,106,106	0
55	MG	BA	3318	1/1	0.91	0.53	75,75,75,75	0
55	MG	AA	1831	1/1	0.91	0.45	90,90,90,90	0
55	MG	BA	3293	1/1	0.91	0.26	65,65,65,65	0
55	MG	DA	3226	1/1	0.91	0.41	62,62,62,62	0
55	MG	BA	3246	1/1	0.91	0.40	68,68,68,68	0
55	MG	BA	3335	1/1	0.91	0.35	58,58,58,58	0
55	MG	CA	1631	1/1	0.91	0.11	81,81,81,81	0
55	MG	DA	3128	1/1	0.91	0.34	77,77,77,77	0
55	MG	AA	1810	1/1	0.91	0.45	67,67,67,67	0
55	MG	BA	3566	1/1	0.91	0.29	88,88,88,88	0
55	MG	DA	3050	1/1	0.91	0.68	66,66,66,66	0
55	MG	BA	3303	1/1	0.91	0.38	72,72,72,72	0
55	MG	BA	3524	1/1	0.91	0.19	66,66,66,66	0
55	MG	BA	3487	1/1	0.91	0.10	94,94,94,94	0
55	MG	BA	3278	1/1	0.91	0.42	81,81,81,81	0
55	MG	BA	3540	1/1	0.91	0.30	61,61,61,61	0
55	MG	AA	1704	1/1	0.91	0.11	83,83,83,83	0
55	MG	DA	3355	1/1	0.91	0.50	77,77,77,77	0
55	MG	BA	3601	1/1	0.91	0.20	85,85,85,85	0
55	MG	CA	1733	1/1	0.91	0.43	69,69,69,69	0
55	MG	BA	3122	1/1	0.91	0.30	37,37,37,37	0
55	MG	DA	3017	1/1	0.91	0.37	75,75,75,75	0
55	MG	BA	3501	1/1	0.92	0.24	55,55,55,55	0
55	MG	BA	3194	1/1	0.92	0.42	68,68,68,68	0
55	MG	CA	1708	1/1	0.92	0.09	97,97,97,97	0
55	MG	BA	3414	1/1	0.92	0.13	72,72,72,72	0
55	MG	BA	3195	1/1	0.92	0.49	47,47,47,47	0
55	MG	DA	3086	1/1	0.92	0.20	114,114,114,114	0
55	MG	BA	3311	1/1	0.92	0.30	83,83,83,83	0
55	MG	BA	3343	1/1	0.92	0.30	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	CA	1649	1/1	0.92	0.29	64,64,64,64	0
55	MG	DA	3410	1/1	0.92	0.39	78,78,78,78	0
55	MG	DA	3313	1/1	0.92	0.29	85,85,85,85	0
55	MG	BA	3271	1/1	0.92	0.20	35,35,35,35	0
55	MG	BA	3070	1/1	0.92	0.13	63,63,63,63	0
55	MG	AA	1701	1/1	0.92	0.19	70,70,70,70	0
55	MG	CA	1682	1/1	0.92	0.38	86,86,86,86	0
55	MG	BA	3296	1/1	0.92	0.40	53,53,53,53	0
55	MG	BA	3105	1/1	0.92	0.32	75,75,75,75	0
55	MG	BA	3518	1/1	0.92	0.23	70,70,70,70	0
55	MG	DA	3322	1/1	0.92	0.54	70,70,70,70	0
55	MG	BA	3130	1/1	0.92	0.43	44,44,44,44	0
55	MG	CA	1765	1/1	0.92	0.25	101,101,101,101	0
55	MG	BA	3101	1/1	0.92	0.64	63,63,63,63	0
55	MG	DA	3030	1/1	0.92	0.40	74,74,74,74	0
55	MG	BA	3559	1/1	0.92	0.17	81,81,81,81	0
55	MG	AA	1756	1/1	0.92	0.22	69,69,69,69	0
55	MG	DA	3009	1/1	0.92	0.53	68,68,68,68	0
55	MG	DA	3130	1/1	0.92	0.18	60,60,60,60	0
55	MG	BA	3468	1/1	0.92	0.32	77,77,77,77	0
55	MG	DA	3231	1/1	0.92	0.43	72,72,72,72	0
55	MG	AA	1760	1/1	0.92	0.69	78,78,78,78	0
55	MG	DA	3300	1/1	0.92	0.27	81,81,81,81	0
55	MG	BA	3214	1/1	0.92	0.56	67,67,67,67	0
55	MG	BA	3434	1/1	0.92	0.51	75,75,75,75	0
55	MG	BA	3483	1/1	0.92	0.34	68,68,68,68	0
55	MG	AA	1732	1/1	0.92	0.33	92,92,92,92	0
55	MG	AA	1628	1/1	0.92	0.35	69,69,69,69	0
55	MG	CA	1607	1/1	0.92	0.43	85,85,85,85	0
55	MG	BA	3458	1/1	0.92	0.12	82,82,82,82	0
55	MG	BE	301	1/1	0.92	0.39	59,59,59,59	0
55	MG	BA	3363	1/1	0.92	0.56	67,67,67,67	0
55	MG	BA	3081	1/1	0.92	0.30	75,75,75,75	0
55	MG	DA	3458	1/1	0.92	0.60	92,92,92,92	0
55	MG	DA	3074	1/1	0.92	0.18	70,70,70,70	0
55	MG	DA	3444	1/1	0.92	0.17	73,73,73,73	0
55	MG	AA	1717	1/1	0.92	0.40	74,74,74,74	0
55	MG	DA	3397	1/1	0.92	0.29	60,60,60,60	0
55	MG	AA	1645	1/1	0.92	0.47	50,50,50,50	0
55	MG	DA	3192	1/1	0.92	0.48	62,62,62,62	0
55	MG	BA	3384	1/1	0.92	0.24	73,73,73,73	0
55	MG	DA	3255	1/1	0.92	0.28	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	3014	1/1	0.92	0.56	74,74,74,74	0
55	MG	BA	3048	1/1	0.92	0.54	77,77,77,77	0
55	MG	BA	3512	1/1	0.92	0.27	69,69,69,69	0
55	MG	BA	3520	1/1	0.92	0.46	44,44,44,44	0
55	MG	CA	1610	1/1	0.92	0.27	97,97,97,97	0
55	MG	BA	3372	1/1	0.92	0.27	73,73,73,73	0
55	MG	AA	1699	1/1	0.92	0.26	64,64,64,64	0
55	MG	CA	1701	1/1	0.92	0.42	88,88,88,88	0
55	MG	DA	3063	1/1	0.92	0.53	75,75,75,75	0
55	MG	BA	3085	1/1	0.92	0.17	73,73,73,73	0
55	MG	CA	1782	1/1	0.92	0.38	93,93,93,93	0
55	MG	AA	1805	1/1	0.92	0.35	65,65,65,65	0
55	MG	AA	1788	1/1	0.92	0.52	77,77,77,77	0
55	MG	DA	3516	1/1	0.92	0.33	105,105,105,105	0
55	MG	BA	3602	1/1	0.92	0.25	67,67,67,67	0
55	MG	DA	3414	1/1	0.92	0.31	85,85,85,85	0
55	MG	CA	1694	1/1	0.92	0.47	97,97,97,97	0
55	MG	DA	3082	1/1	0.92	0.38	91,91,91,91	0
55	MG	DA	3229	1/1	0.92	0.50	62,62,62,62	0
55	MG	AA	1825	1/1	0.92	0.24	93,93,93,93	0
55	MG	AA	1654	1/1	0.92	0.44	75,75,75,75	0
55	MG	BA	3288	1/1	0.92	0.46	76,76,76,76	0
55	MG	BA	3549	1/1	0.92	0.34	68,68,68,68	0
55	MG	CA	1776	1/1	0.92	0.50	71,71,71,71	0
55	MG	BA	3545	1/1	0.92	0.38	69,69,69,69	0
55	MG	BA	3419	1/1	0.92	0.53	85,85,85,85	0
55	MG	CA	1602	1/1	0.92	0.28	80,80,80,80	0
55	MG	BA	3426	1/1	0.92	0.49	85,85,85,85	0
55	MG	DA	3416	1/1	0.92	0.49	59,59,59,59	0
55	MG	BA	3338	1/1	0.92	0.21	71,71,71,71	0
55	MG	DA	3510	1/1	0.92	0.32	85,85,85,85	0
55	MG	BA	3477	1/1	0.92	0.46	95,95,95,95	0
55	MG	DA	3392	1/1	0.92	0.42	68,68,68,68	0
55	MG	AA	1650	1/1	0.92	0.49	71,71,71,71	0
55	MG	CA	1678	1/1	0.92	0.23	70,70,70,70	0
55	MG	BA	3159	1/1	0.92	0.51	58,58,58,58	0
55	MG	CA	1788	1/1	0.92	0.33	84,84,84,84	0
55	MG	CA	1605	1/1	0.92	0.38	76,76,76,76	0
55	MG	BA	3615	1/1	0.92	0.41	81,81,81,81	0
55	MG	BA	3351	1/1	0.92	0.96	78,78,78,78	0
55	MG	DA	3185	1/1	0.92	0.35	74,74,74,74	0
55	MG	BA	3347	1/1	0.92	0.43	68,68,68,68	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	0.92	0.58	71,71,71,71	0
55	MG	AA	1748	1/1	0.92	0.42	84,84,84,84	0
55	MG	BA	3174	1/1	0.92	0.81	71,71,71,71	0
55	MG	DA	3248	1/1	0.92	0.48	75,75,75,75	0
55	MG	BA	3333	1/1	0.92	0.47	80,80,80,80	0
55	MG	BA	3299	1/1	0.92	0.49	89,89,89,89	0
55	MG	AA	1661	1/1	0.92	0.34	48,48,48,48	0
55	MG	DA	3324	1/1	0.92	0.20	78,78,78,78	0
55	MG	BA	3208	1/1	0.92	0.10	45,45,45,45	0
55	MG	BA	3315	1/1	0.92	0.34	78,78,78,78	0
55	MG	BA	3279	1/1	0.93	0.09	70,70,70,70	0
55	MG	BA	3156	1/1	0.93	0.29	40,40,40,40	0
55	MG	BA	3389	1/1	0.93	0.23	59,59,59,59	0
55	MG	DA	3325	1/1	0.93	0.54	73,73,73,73	0
55	MG	CA	1613	1/1	0.93	0.28	68,68,68,68	0
55	MG	BA	3499	1/1	0.93	0.39	68,68,68,68	0
55	MG	CA	1620	1/1	0.93	0.46	64,64,64,64	0
55	MG	BB	206	1/1	0.93	0.34	86,86,86,86	0
55	MG	DA	3445	1/1	0.93	0.33	78,78,78,78	0
55	MG	BA	3374	1/1	0.93	0.40	71,71,71,71	0
55	MG	AA	1775	1/1	0.93	0.12	79,79,79,79	0
55	MG	DA	3469	1/1	0.93	0.60	80,80,80,80	0
55	MG	AA	1687	1/1	0.93	0.32	72,72,72,72	0
55	MG	DA	3421	1/1	0.93	0.32	62,62,62,62	0
55	MG	BA	3413	1/1	0.93	0.52	78,78,78,78	0
55	MG	AA	1636	1/1	0.93	0.28	87,87,87,87	0
55	MG	BA	3236	1/1	0.93	0.44	52,52,52,52	0
55	MG	DA	3066	1/1	0.93	0.53	65,65,65,65	0
55	MG	DA	3208	1/1	0.93	0.47	74,74,74,74	0
55	MG	AA	1833	1/1	0.93	0.44	88,88,88,88	0
55	MG	DA	3268	1/1	0.93	0.48	69,69,69,69	0
55	MG	BA	3316	1/1	0.93	0.50	69,69,69,69	0
55	MG	BO	201	1/1	0.93	0.36	62,62,62,62	0
55	MG	DA	3362	1/1	0.93	0.61	53,53,53,53	0
55	MG	BA	3377	1/1	0.93	0.74	62,62,62,62	0
55	MG	DA	3365	1/1	0.93	0.53	58,58,58,58	0
55	MG	AA	1779	1/1	0.93	0.36	72,72,72,72	0
55	MG	DA	3321	1/1	0.93	0.57	66,66,66,66	0
55	MG	BA	3558	1/1	0.93	0.14	63,63,63,63	0
55	MG	BA	3108	1/1	0.93	0.36	86,86,86,86	0
55	MG	BA	3149	1/1	0.93	0.20	80,80,80,80	0
55	MG	DA	3081	1/1	0.93	0.51	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	BB	205	1/1	0.93	0.35	74,74,74,74	0
55	MG	DA	3326	1/1	0.93	0.36	70,70,70,70	0
55	MG	BA	3429	1/1	0.93	0.12	75,75,75,75	0
55	MG	BA	3135	1/1	0.93	0.49	72,72,72,72	0
55	MG	DA	3372	1/1	0.93	0.36	65,65,65,65	0
55	MG	DA	3071	1/1	0.93	0.24	81,81,81,81	0
55	MG	AA	1740	1/1	0.93	0.18	75,75,75,75	0
55	MG	DA	3212	1/1	0.93	0.60	48,48,48,48	0
55	MG	CA	1703	1/1	0.93	0.27	94,94,94,94	0
55	MG	DA	3310	1/1	0.93	0.49	71,71,71,71	0
55	MG	BA	3519	1/1	0.93	0.31	80,80,80,80	0
55	MG	BA	3198	1/1	0.93	0.17	45,45,45,45	0
55	MG	BA	3093	1/1	0.93	0.27	57,57,57,57	0
55	MG	AA	1608	1/1	0.93	0.26	64,64,64,64	0
55	MG	DA	3418	1/1	0.93	0.41	78,78,78,78	0
55	MG	BA	3099	1/1	0.93	0.58	67,67,67,67	0
55	MG	CA	1658	1/1	0.93	0.45	91,91,91,91	0
55	MG	AA	1605	1/1	0.93	0.40	82,82,82,82	0
55	MG	CA	1775	1/1	0.93	0.40	72,72,72,72	0
55	MG	BB	203	1/1	0.93	0.42	65,65,65,65	0
55	MG	BA	3340	1/1	0.93	0.30	77,77,77,77	0
55	MG	DA	3308	1/1	0.93	0.38	97,97,97,97	0
55	MG	BA	3298	1/1	0.93	0.27	65,65,65,65	0
55	MG	DA	3207	1/1	0.93	0.57	66,66,66,66	0
55	MG	BA	3258	1/1	0.93	0.29	45,45,45,45	0
55	MG	BA	3011	1/1	0.93	0.29	42,42,42,42	0
55	MG	CA	1752	1/1	0.93	0.18	70,70,70,70	0
55	MG	DA	3426	1/1	0.93	0.42	58,58,58,58	0
55	MG	BA	3268	1/1	0.93	0.58	67,67,67,67	0
55	MG	DA	3378	1/1	0.93	0.50	63,63,63,63	0
55	MG	BA	3200	1/1	0.93	0.39	62,62,62,62	0
55	MG	DA	3069	1/1	0.93	0.44	60,60,60,60	0
55	MG	DA	3267	1/1	0.93	0.36	64,64,64,64	0
55	MG	BA	3012	1/1	0.93	0.28	45,45,45,45	0
55	MG	CA	1717	1/1	0.93	0.18	106,106,106,106	0
55	MG	B1	201	1/1	0.93	0.30	47,47,47,47	0
55	MG	BA	3616	1/1	0.93	0.38	58,58,58,58	0
55	MG	DA	3172	1/1	0.93	0.10	88,88,88,88	0
55	MG	CA	1806	1/1	0.93	0.48	96,96,96,96	0
55	MG	DA	3124	1/1	0.93	0.57	54,54,54,54	0
55	MG	DA	3224	1/1	0.93	0.47	66,66,66,66	0
55	MG	CA	1680	1/1	0.93	0.55	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	BA	3239	1/1	0.93	0.27	74,74,74,74	0
55	MG	CA	1651	1/1	0.93	0.35	90,90,90,90	0
55	MG	CA	1716	1/1	0.93	0.25	79,79,79,79	0
55	MG	CA	1653	1/1	0.93	0.17	77,77,77,77	0
55	MG	DA	3143	1/1	0.93	0.28	58,58,58,58	0
55	MG	AA	1738	1/1	0.93	0.54	79,79,79,79	0
55	MG	AA	1629	1/1	0.93	0.12	86,86,86,86	0
55	MG	DA	3360	1/1	0.93	0.39	65,65,65,65	0
55	MG	BA	3056	1/1	0.93	0.21	54,54,54,54	0
55	MG	AA	1685	1/1	0.93	0.29	88,88,88,88	0
55	MG	BA	3486	1/1	0.93	0.41	80,80,80,80	0
55	MG	DA	3111	1/1	0.93	0.26	52,52,52,52	0
55	MG	DA	3031	1/1	0.93	0.22	72,72,72,72	0
55	MG	BA	3600	1/1	0.93	0.34	66,66,66,66	0
55	MG	DA	3138	1/1	0.93	0.20	70,70,70,70	0
55	MG	DA	3089	1/1	0.93	0.54	82,82,82,82	0
55	MG	CA	1721	1/1	0.93	0.20	80,80,80,80	0
55	MG	BA	3032	1/1	0.93	0.52	49,49,49,49	0
55	MG	DA	3316	1/1	0.93	0.33	61,61,61,61	0
55	MG	BA	3067	1/1	0.93	0.23	48,48,48,48	0
55	MG	BA	3369	1/1	0.93	0.30	73,73,73,73	0
55	MG	CA	1739	1/1	0.93	0.56	75,75,75,75	0
55	MG	BA	3427	1/1	0.94	0.41	65,65,65,65	0
55	MG	DA	3443	1/1	0.94	0.36	80,80,80,80	0
55	MG	AA	1799	1/1	0.94	0.33	78,78,78,78	0
55	MG	DA	3450	1/1	0.94	0.33	88,88,88,88	0
55	MG	BA	3228	1/1	0.94	0.62	72,72,72,72	0
55	MG	DA	3198	1/1	0.94	0.31	47,47,47,47	0
55	MG	DA	3272	1/1	0.94	0.28	64,64,64,64	0
55	MG	BA	3143	1/1	0.94	0.68	72,72,72,72	0
55	MG	DA	3289	1/1	0.94	0.43	90,90,90,90	0
55	MG	BA	3568	1/1	0.94	0.39	83,83,83,83	0
55	MG	DA	3339	1/1	0.94	0.32	66,66,66,66	0
55	MG	DA	3033	1/1	0.94	0.25	62,62,62,62	0
55	MG	BA	3307	1/1	0.94	0.48	39,39,39,39	0
55	MG	BA	3337	1/1	0.94	0.30	72,72,72,72	0
55	MG	BA	3562	1/1	0.94	0.30	79,79,79,79	0
55	MG	AA	1736	1/1	0.94	0.46	90,90,90,90	0
55	MG	CA	1705	1/1	0.94	0.47	80,80,80,80	0
56	ZN	CQ	101	1/1	0.94	0.14	120,120,120,120	0
55	MG	BA	3025	1/1	0.94	0.36	42,42,42,42	0
55	MG	DA	3148	1/1	0.94	0.48	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	BA	3599	1/1	0.94	0.47	69,69,69,69	0
55	MG	BA	3037	1/1	0.94	0.38	44,44,44,44	0
55	MG	BA	3297	1/1	0.94	0.22	58,58,58,58	0
55	MG	BA	3612	1/1	0.94	0.44	66,66,66,66	0
55	MG	DA	3214	1/1	0.94	0.44	40,40,40,40	0
55	MG	BA	3550	1/1	0.94	0.24	93,93,93,93	0
55	MG	BA	3264	1/1	0.94	0.21	30,30,30,30	0
55	MG	AA	1721	1/1	0.94	0.29	77,77,77,77	0
55	MG	DA	3054	1/1	0.94	0.62	58,58,58,58	0
55	MG	BA	3286	1/1	0.94	0.28	66,66,66,66	0
55	MG	DA	3388	1/1	0.94	0.29	74,74,74,74	0
55	MG	DA	3374	1/1	0.94	0.41	62,62,62,62	0
55	MG	BA	3464	1/1	0.94	0.51	77,77,77,77	0
55	MG	BA	3498	1/1	0.94	0.33	85,85,85,85	0
55	MG	BA	3353	1/1	0.94	0.44	52,52,52,52	0
55	MG	DA	3375	1/1	0.94	0.69	88,88,88,88	0
55	MG	BA	3263	1/1	0.94	0.64	54,54,54,54	0
55	MG	BA	3422	1/1	0.94	0.26	78,78,78,78	0
55	MG	BA	3226	1/1	0.94	0.41	50,50,50,50	0
55	MG	BA	3115	1/1	0.94	0.27	87,87,87,87	0
55	MG	BB	213	1/1	0.94	0.45	66,66,66,66	0
55	MG	DA	3379	1/1	0.94	0.44	85,85,85,85	0
55	MG	DA	3305	1/1	0.94	0.36	77,77,77,77	0
55	MG	DA	3105	1/1	0.94	0.36	45,45,45,45	0
55	MG	AA	1814	1/1	0.94	0.32	83,83,83,83	0
55	MG	BA	3006	1/1	0.94	0.43	38,38,38,38	0
55	MG	BA	3515	1/1	0.94	0.21	72,72,72,72	0
55	MG	CA	1642	1/1	0.94	0.20	91,91,91,91	0
55	MG	BB	211	1/1	0.94	0.29	92,92,92,92	0
55	MG	DA	3423	1/1	0.94	0.89	75,75,75,75	0
55	MG	BA	3197	1/1	0.94	0.53	46,46,46,46	0
55	MG	DA	3083	1/1	0.94	0.49	85,85,85,85	0
55	MG	DA	3453	1/1	0.94	0.24	66,66,66,66	0
55	MG	DA	3323	1/1	0.94	0.14	42,42,42,42	0
55	MG	BA	3346	1/1	0.94	0.33	51,51,51,51	0
55	MG	DA	3035	1/1	0.94	0.26	62,62,62,62	0
55	MG	AA	1666	1/1	0.94	0.52	62,62,62,62	0
55	MG	BA	3308	1/1	0.94	0.32	61,61,61,61	0
55	MG	BA	3287	1/1	0.94	0.39	62,62,62,62	0
55	MG	BA	3312	1/1	0.94	0.48	57,57,57,57	0
55	MG	CA	1743	1/1	0.94	0.49	80,80,80,80	0
55	MG	BA	3242	1/1	0.94	0.44	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	BA	3280	1/1	0.94	0.52	50,50,50,50	0
55	MG	BA	3454	1/1	0.94	0.36	92,92,92,92	0
55	MG	BA	3590	1/1	0.94	0.34	63,63,63,63	0
55	MG	CA	1670	1/1	0.94	0.49	56,56,56,56	0
55	MG	AA	1648	1/1	0.94	0.52	78,78,78,78	0
55	MG	BA	3047	1/1	0.94	0.41	74,74,74,74	0
55	MG	DA	3282	1/1	0.94	0.44	69,69,69,69	0
55	MG	BA	3306	1/1	0.94	0.25	67,67,67,67	0
55	MG	AA	1695	1/1	0.94	0.23	90,90,90,90	0
55	MG	DA	3024	1/1	0.94	0.32	108,108,108,108	0
55	MG	DA	3099	1/1	0.94	0.27	40,40,40,40	0
55	MG	AA	1603	1/1	0.94	0.33	63,63,63,63	0
55	MG	BA	3430	1/1	0.94	0.27	57,57,57,57	0
55	MG	DA	3039	1/1	0.94	0.34	85,85,85,85	0
55	MG	DA	3386	1/1	0.94	0.48	61,61,61,61	0
55	MG	DA	3262	1/1	0.94	0.46	48,48,48,48	0
55	MG	AA	1838	1/1	0.94	0.41	61,61,61,61	0
55	MG	BA	3620	1/1	0.94	0.28	68,68,68,68	0
55	MG	BA	3136	1/1	0.94	0.16	74,74,74,74	0
55	MG	BA	3577	1/1	0.94	0.18	73,73,73,73	0
55	MG	DA	3261	1/1	0.94	0.49	58,58,58,58	0
55	MG	BA	3405	1/1	0.94	0.47	56,56,56,56	0
55	MG	BA	3560	1/1	0.94	0.56	78,78,78,78	0
55	MG	CA	1730	1/1	0.94	0.19	106,106,106,106	0
55	MG	CA	1779	1/1	0.94	0.33	72,72,72,72	0
55	MG	BA	3493	1/1	0.94	0.37	63,63,63,63	0
55	MG	CA	1748	1/1	0.94	0.16	87,87,87,87	0
55	MG	B5	101	1/1	0.94	0.35	45,45,45,45	0
55	MG	DA	3276	1/1	0.94	0.52	68,68,68,68	0
55	MG	AA	1655	1/1	0.94	0.47	88,88,88,88	0
55	MG	BA	3148	1/1	0.94	0.41	32,32,32,32	0
55	MG	AA	1672	1/1	0.94	0.33	87,87,87,87	0
55	MG	AA	1747	1/1	0.94	0.40	88,88,88,88	0
55	MG	BA	3016	1/1	0.94	0.53	39,39,39,39	0
55	MG	DA	3334	1/1	0.94	0.56	68,68,68,68	0
55	MG	CA	1735	1/1	0.94	0.20	89,89,89,89	0
55	MG	AA	1641	1/1	0.94	0.37	57,57,57,57	0
55	MG	DA	3012	1/1	0.94	0.50	66,66,66,66	0
55	MG	DA	3127	1/1	0.94	0.40	74,74,74,74	0
55	MG	BA	3150	1/1	0.94	0.44	36,36,36,36	0
55	MG	BA	3218	1/1	0.94	0.54	48,48,48,48	0
55	MG	BA	3165	1/1	0.94	0.56	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	CA	1724	1/1	0.94	0.51	84,84,84,84	0
55	MG	BA	3386	1/1	0.94	0.50	59,59,59,59	0
55	MG	AA	1676	1/1	0.94	0.38	70,70,70,70	0
55	MG	DA	3270	1/1	0.94	0.28	83,83,83,83	0
55	MG	BA	3450	1/1	0.94	0.18	54,54,54,54	0
55	MG	BA	3224	1/1	0.94	0.11	55,55,55,55	0
55	MG	BA	3440	1/1	0.94	0.44	74,74,74,74	0
55	MG	BA	3076	1/1	0.94	0.33	68,68,68,68	0
55	MG	BA	3141	1/1	0.94	0.48	35,35,35,35	0
55	MG	BA	3529	1/1	0.95	0.38	68,68,68,68	0
55	MG	BA	3044	1/1	0.95	0.33	62,62,62,62	0
55	MG	BA	3491	1/1	0.95	0.53	42,42,42,42	0
55	MG	DA	3170	1/1	0.95	0.44	68,68,68,68	0
55	MG	AA	1642	1/1	0.95	0.68	72,72,72,72	0
55	MG	BA	3125	1/1	0.95	0.53	52,52,52,52	0
55	MG	DA	3228	1/1	0.95	0.47	44,44,44,44	0
55	MG	DA	3013	1/1	0.95	0.53	56,56,56,56	0
55	MG	BA	3508	1/1	0.95	0.41	59,59,59,59	0
55	MG	A1	101	1/1	0.95	0.17	66,66,66,66	0
55	MG	BA	3147	1/1	0.95	0.15	55,55,55,55	0
55	MG	DA	3189	1/1	0.95	0.50	41,41,41,41	0
55	MG	AA	1669	1/1	0.95	0.43	68,68,68,68	0
55	MG	DA	3411	1/1	0.95	0.19	70,70,70,70	0
55	MG	BA	3525	1/1	0.95	0.29	77,77,77,77	0
55	MG	DA	3199	1/1	0.95	0.48	61,61,61,61	0
55	MG	AA	1746	1/1	0.95	0.41	84,84,84,84	0
55	MG	DA	3249	1/1	0.95	0.40	72,72,72,72	0
55	MG	AA	1671	1/1	0.95	0.12	67,67,67,67	0
55	MG	DA	3499	1/1	0.95	0.21	61,61,61,61	0
55	MG	AA	1798	1/1	0.95	0.25	58,58,58,58	0
55	MG	CA	1622	1/1	0.95	0.33	95,95,95,95	0
55	MG	CA	1736	1/1	0.95	0.73	79,79,79,79	0
55	MG	DA	3456	1/1	0.95	0.36	83,83,83,83	0
55	MG	CA	1731	1/1	0.95	0.58	72,72,72,72	0
55	MG	BA	3284	1/1	0.95	0.45	56,56,56,56	0
55	MG	BA	3436	1/1	0.95	0.23	59,59,59,59	0
55	MG	AA	1623	1/1	0.95	0.74	65,65,65,65	0
55	MG	AA	1726	1/1	0.95	0.48	81,81,81,81	0
55	MG	AA	1622	1/1	0.95	0.23	76,76,76,76	0
55	MG	DA	3243	1/1	0.95	0.51	79,79,79,79	0
55	MG	DA	3016	1/1	0.95	0.43	78,78,78,78	0
55	MG	AA	1620	1/1	0.95	0.28	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	AA	1610	1/1	0.95	0.49	51,51,51,51	0
55	MG	BA	3235	1/1	0.95	0.39	54,54,54,54	0
55	MG	AA	1763	1/1	0.95	0.58	53,53,53,53	0
55	MG	BF	301	1/1	0.95	0.07	73,73,73,73	0
55	MG	BA	3528	1/1	0.95	0.44	76,76,76,76	0
55	MG	DA	3190	1/1	0.95	0.57	61,61,61,61	0
55	MG	DA	3046	1/1	0.95	0.34	65,65,65,65	0
55	MG	DA	3205	1/1	0.95	0.54	67,67,67,67	0
55	MG	BA	3050	1/1	0.95	0.48	39,39,39,39	0
55	MG	BA	3373	1/1	0.95	0.44	64,64,64,64	0
55	MG	AA	1658	1/1	0.95	0.65	49,49,49,49	0
55	MG	DA	3452	1/1	0.95	0.21	83,83,83,83	0
55	MG	BA	3352	1/1	0.95	0.35	76,76,76,76	0
55	MG	BA	3107	1/1	0.95	0.43	36,36,36,36	0
55	MG	CA	1621	1/1	0.95	0.36	66,66,66,66	0
55	MG	BA	3082	1/1	0.95	0.36	64,64,64,64	0
55	MG	BA	3003	1/1	0.95	0.44	47,47,47,47	0
55	MG	DA	3258	1/1	0.95	0.32	37,37,37,37	0
55	MG	BA	3170	1/1	0.95	0.48	55,55,55,55	0
55	MG	DA	3022	1/1	0.95	0.55	60,60,60,60	0
55	MG	AA	1818	1/1	0.95	0.60	76,76,76,76	0
55	MG	DA	3216	1/1	0.95	0.30	49,49,49,49	0
55	MG	CA	1793	1/1	0.95	0.34	91,91,91,91	0
55	MG	BA	3043	1/1	0.95	0.25	32,32,32,32	0
55	MG	BA	3237	1/1	0.95	0.49	57,57,57,57	0
55	MG	CA	1744	1/1	0.95	0.27	79,79,79,79	0
55	MG	AA	1827	1/1	0.95	0.28	87,87,87,87	0
55	MG	BA	3522	1/1	0.95	0.48	82,82,82,82	0
55	MG	BA	3040	1/1	0.95	0.36	54,54,54,54	0
55	MG	DA	3275	1/1	0.95	0.36	76,76,76,76	0
55	MG	BA	3275	1/1	0.95	0.21	73,73,73,73	0
55	MG	DA	3250	1/1	0.95	0.39	63,63,63,63	0
55	MG	AA	1796	1/1	0.95	0.14	75,75,75,75	0
55	MG	AA	1667	1/1	0.95	0.33	68,68,68,68	0
55	MG	BA	3180	1/1	0.95	0.40	37,37,37,37	0
55	MG	CA	1728	1/1	0.95	0.66	69,69,69,69	0
55	MG	BA	3049	1/1	0.95	0.40	68,68,68,68	0
55	MG	DA	3345	1/1	0.95	0.39	64,64,64,64	0
55	MG	CA	1617	1/1	0.95	0.24	93,93,93,93	0
55	MG	BA	3153	1/1	0.95	0.44	52,52,52,52	0
55	MG	DA	3317	1/1	0.95	0.22	81,81,81,81	0
55	MG	DA	3167	1/1	0.95	0.40	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	BA	3443	1/1	0.95	0.14	77,77,77,77	0
55	MG	DA	3100	1/1	0.95	0.44	44,44,44,44	0
55	MG	AA	1765	1/1	0.95	0.51	84,84,84,84	0
55	MG	BA	3274	1/1	0.95	0.17	46,46,46,46	0
55	MG	BA	3248	1/1	0.95	0.35	53,53,53,53	0
55	MG	BB	215	1/1	0.95	0.26	82,82,82,82	0
55	MG	AA	1780	1/1	0.95	0.26	86,86,86,86	0
55	MG	AA	1762	1/1	0.95	0.21	80,80,80,80	0
55	MG	AA	1670	1/1	0.95	0.38	63,63,63,63	0
55	MG	DA	3470	1/1	0.95	0.11	80,80,80,80	0
55	MG	DA	3153	1/1	0.95	0.31	70,70,70,70	0
55	MG	AC	104	1/1	0.95	0.47	56,56,56,56	0
55	MG	DA	3122	1/1	0.95	0.49	46,46,46,46	0
55	MG	DA	3036	1/1	0.95	0.21	99,99,99,99	0
55	MG	BA	3576	1/1	0.95	0.41	74,74,74,74	0
55	MG	BA	3177	1/1	0.95	0.51	57,57,57,57	0
55	MG	DA	3176	1/1	0.95	0.55	65,65,65,65	0
55	MG	AC	108	1/1	0.95	0.40	85,85,85,85	0
55	MG	DA	3165	1/1	0.95	0.59	65,65,65,65	0
55	MG	CA	1675	1/1	0.95	0.48	62,62,62,62	0
55	MG	BA	3410	1/1	0.95	0.72	62,62,62,62	0
55	MG	DA	3163	1/1	0.95	0.59	62,62,62,62	0
55	MG	CC	103	1/1	0.95	1.01	72,72,72,72	0
55	MG	BA	3564	1/1	0.95	0.61	84,84,84,84	0
55	MG	DA	3331	1/1	0.95	0.55	50,50,50,50	0
55	MG	CA	1646	1/1	0.95	0.37	76,76,76,76	0
55	MG	BA	3478	1/1	0.95	0.23	63,63,63,63	0
55	MG	AA	1659	1/1	0.95	0.75	69,69,69,69	0
55	MG	DA	3206	1/1	0.95	0.53	65,65,65,65	0
55	MG	BA	3064	1/1	0.95	0.29	49,49,49,49	0
55	MG	BA	3492	1/1	0.95	0.43	77,77,77,77	0
55	MG	DA	3238	1/1	0.95	0.42	60,60,60,60	0
55	MG	AA	1714	1/1	0.95	0.32	107,107,107,107	0
55	MG	BA	3326	1/1	0.95	0.34	52,52,52,52	0
55	MG	BA	3169	1/1	0.95	0.60	63,63,63,63	0
55	MG	DA	3521	1/1	0.95	0.58	69,69,69,69	0
55	MG	DA	3234	1/1	0.96	0.43	52,52,52,52	0
55	MG	CA	1685	1/1	0.96	0.37	93,93,93,93	0
55	MG	BA	3058	1/1	0.96	0.32	62,62,62,62	0
55	MG	BA	3010	1/1	0.96	0.41	46,46,46,46	0
55	MG	DE	303	1/1	0.96	0.35	56,56,56,56	0
55	MG	DA	3241	1/1	0.96	0.47	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	BA	3097	1/1	0.96	0.36	59,59,59,59	0
55	MG	CA	1695	1/1	0.96	0.50	87,87,87,87	0
55	MG	BA	3254	1/1	0.96	0.34	43,43,43,43	0
55	MG	CA	1671	1/1	0.96	0.56	49,49,49,49	0
55	MG	DA	3278	1/1	0.96	0.51	42,42,42,42	0
55	MG	CA	1692	1/1	0.96	0.49	82,82,82,82	0
55	MG	AA	1800	1/1	0.96	0.31	82,82,82,82	0
55	MG	BA	3238	1/1	0.96	0.56	41,41,41,41	0
55	MG	CC	106	1/1	0.96	0.60	96,96,96,96	0
55	MG	BA	3209	1/1	0.96	0.47	39,39,39,39	0
55	MG	BA	3605	1/1	0.96	0.51	47,47,47,47	0
55	MG	CA	1746	1/1	0.96	0.61	57,57,57,57	0
55	MG	DA	3021	1/1	0.96	0.48	51,51,51,51	0
55	MG	BA	3117	1/1	0.96	0.49	60,60,60,60	0
55	MG	BA	3142	1/1	0.96	0.37	51,51,51,51	0
55	MG	DA	3169	1/1	0.96	0.31	69,69,69,69	0
55	MG	BA	3253	1/1	0.96	0.26	51,51,51,51	0
55	MG	AA	1632	1/1	0.96	0.25	67,67,67,67	0
55	MG	CA	1764	1/1	0.96	0.54	72,72,72,72	0
55	MG	CN	201	1/1	0.96	0.15	74,74,74,74	0
55	MG	AA	1646	1/1	0.96	0.41	67,67,67,67	0
55	MG	DA	3232	1/1	0.96	0.42	44,44,44,44	0
55	MG	BA	3184	1/1	0.96	0.23	39,39,39,39	0
55	MG	AA	1686	1/1	0.96	0.36	85,85,85,85	0
55	MG	BA	3008	1/1	0.96	0.49	37,37,37,37	0
55	MG	CA	1690	1/1	0.96	0.36	68,68,68,68	0
55	MG	DA	3311	1/1	0.96	0.41	73,73,73,73	0
55	MG	BA	3406	1/1	0.96	0.51	82,82,82,82	0
55	MG	AN	201	1/1	0.96	0.17	68,68,68,68	0
55	MG	DA	3193	1/1	0.96	0.69	63,63,63,63	0
55	MG	BB	207	1/1	0.96	0.18	83,83,83,83	0
55	MG	BA	3138	1/1	0.96	0.47	46,46,46,46	0
55	MG	DA	3382	1/1	0.96	0.52	78,78,78,78	0
55	MG	CA	1666	1/1	0.96	0.29	71,71,71,71	0
55	MG	CA	1795	1/1	0.96	0.29	76,76,76,76	0
55	MG	DA	3299	1/1	0.96	0.33	38,38,38,38	0
55	MG	BA	3452	1/1	0.96	0.40	41,41,41,41	0
55	MG	DA	3159	1/1	0.96	0.26	37,37,37,37	0
55	MG	DA	3495	1/1	0.96	0.20	63,63,63,63	0
55	MG	DA	3244	1/1	0.96	0.46	71,71,71,71	0
55	MG	AA	1837	1/1	0.96	0.53	73,73,73,73	0
55	MG	DA	3008	1/1	0.96	0.38	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	DA	3109	1/1	0.96	0.23	65,65,65,65	0
55	MG	AA	1741	1/1	0.96	0.31	67,67,67,67	0
55	MG	DA	3001	1/1	0.96	0.46	67,67,67,67	0
55	MG	BA	3380	1/1	0.96	0.17	65,65,65,65	0
55	MG	BA	3221	1/1	0.96	0.37	60,60,60,60	0
55	MG	BU	201	1/1	0.96	0.25	81,81,81,81	0
55	MG	DA	3156	1/1	0.96	0.69	48,48,48,48	0
55	MG	CA	1674	1/1	0.96	0.11	70,70,70,70	0
55	MG	DA	3110	1/1	0.96	0.33	58,58,58,58	0
55	MG	BA	3241	1/1	0.96	0.49	60,60,60,60	0
55	MG	BA	3092	1/1	0.96	0.46	32,32,32,32	0
55	MG	DA	3108	1/1	0.96	0.33	54,54,54,54	0
55	MG	BA	3109	1/1	0.96	0.32	70,70,70,70	0
55	MG	AA	1792	1/1	0.96	0.21	55,55,55,55	0
55	MG	DA	3087	1/1	0.96	0.50	63,63,63,63	0
55	MG	DA	3271	1/1	0.96	0.47	58,58,58,58	0
55	MG	DA	3457	1/1	0.96	0.76	65,65,65,65	0
55	MG	BA	3078	1/1	0.96	0.37	65,65,65,65	0
55	MG	BA	3100	1/1	0.96	0.37	42,42,42,42	0
55	MG	BA	3096	1/1	0.96	0.50	56,56,56,56	0
55	MG	DA	3174	1/1	0.96	0.57	44,44,44,44	0
55	MG	BA	3026	1/1	0.96	0.31	47,47,47,47	0
55	MG	DA	3181	1/1	0.96	0.49	50,50,50,50	0
55	MG	DA	3301	1/1	0.96	0.34	63,63,63,63	0
55	MG	BA	3604	1/1	0.96	0.11	61,61,61,61	0
55	MG	BA	3201	1/1	0.96	0.64	66,66,66,66	0
55	MG	BA	3062	1/1	0.96	0.29	56,56,56,56	0
55	MG	BA	3176	1/1	0.96	0.51	48,48,48,48	0
55	MG	AA	1733	1/1	0.96	0.60	71,71,71,71	0
55	MG	DA	3295	1/1	0.96	0.37	50,50,50,50	0
55	MG	BA	3113	1/1	0.96	0.53	57,57,57,57	0
55	MG	AA	1649	1/1	0.96	0.37	79,79,79,79	0
55	MG	AA	1606	1/1	0.96	0.07	91,91,91,91	0
55	MG	BA	3480	1/1	0.96	0.51	50,50,50,50	0
55	MG	DA	3218	1/1	0.96	0.41	62,62,62,62	0
55	MG	DA	3121	1/1	0.96	0.17	64,64,64,64	0
55	MG	BA	3428	1/1	0.96	0.36	68,68,68,68	0
55	MG	BA	3168	1/1	0.96	0.36	49,49,49,49	0
55	MG	AA	1789	1/1	0.96	0.29	74,74,74,74	0
55	MG	BA	3137	1/1	0.96	0.37	47,47,47,47	0
55	MG	BA	3031	1/1	0.96	0.36	33,33,33,33	0
55	MG	BA	3243	1/1	0.96	0.48	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	AA	1811	1/1	0.96	0.50	67,67,67,67	0
55	MG	DA	3217	1/1	0.96	0.40	55,55,55,55	0
55	MG	CA	1738	1/1	0.96	0.41	63,63,63,63	0
55	MG	DA	3329	1/1	0.96	0.35	44,44,44,44	0
55	MG	BA	3152	1/1	0.96	0.51	40,40,40,40	0
55	MG	CA	1722	1/1	0.96	0.38	75,75,75,75	0
55	MG	BA	3124	1/1	0.96	0.52	45,45,45,45	0
55	MG	DA	3184	1/1	0.96	0.65	61,61,61,61	0
55	MG	BA	3251	1/1	0.96	0.39	68,68,68,68	0
55	MG	BA	3376	1/1	0.97	0.44	73,73,73,73	0
55	MG	BE	303	1/1	0.97	0.40	44,44,44,44	0
55	MG	BA	3095	1/1	0.97	0.47	37,37,37,37	0
55	MG	DA	3161	1/1	0.97	0.44	45,45,45,45	0
55	MG	DA	3149	1/1	0.97	0.62	57,57,57,57	0
55	MG	BA	3102	1/1	0.97	0.28	66,66,66,66	0
55	MG	DA	3132	1/1	0.97	0.31	53,53,53,53	0
55	MG	DA	3265	1/1	0.97	0.41	50,50,50,50	0
55	MG	DA	3246	1/1	0.97	0.43	53,53,53,53	0
55	MG	AA	1601	1/1	0.97	0.36	56,56,56,56	0
55	MG	DA	3257	1/1	0.97	0.33	49,49,49,49	0
55	MG	CA	1603	1/1	0.97	0.35	77,77,77,77	0
55	MG	AA	1750	1/1	0.97	0.54	62,62,62,62	0
55	MG	BA	3504	1/1	0.97	0.33	45,45,45,45	0
55	MG	BA	3555	1/1	0.97	0.23	38,38,38,38	0
55	MG	DA	3126	1/1	0.97	0.26	41,41,41,41	0
55	MG	DA	3160	1/1	0.97	0.40	49,49,49,49	0
55	MG	DA	3256	1/1	0.97	0.44	49,49,49,49	0
55	MG	DA	3288	1/1	0.97	0.37	47,47,47,47	0
55	MG	BA	3456	1/1	0.97	0.50	78,78,78,78	0
55	MG	DA	3155	1/1	0.97	0.46	46,46,46,46	0
55	MG	BA	3192	1/1	0.97	0.33	34,34,34,34	0
55	MG	AC	101	1/1	0.97	0.48	53,53,53,53	0
55	MG	DA	3284	1/1	0.97	0.33	56,56,56,56	0
55	MG	BA	3182	1/1	0.97	0.33	43,43,43,43	0
55	MG	CA	1676	1/1	0.97	0.44	55,55,55,55	0
55	MG	DA	3433	1/1	0.97	0.53	57,57,57,57	0
55	MG	BA	3183	1/1	0.97	0.30	47,47,47,47	0
55	MG	BA	3453	1/1	0.97	0.57	60,60,60,60	0
55	MG	DA	3252	1/1	0.97	0.32	64,64,64,64	0
55	MG	DA	3227	1/1	0.97	0.72	50,50,50,50	0
56	ZN	AG	302	1/1	0.97	0.34	95,95,95,95	0
55	MG	BA	3199	1/1	0.97	0.42	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	BA	3178	1/1	0.97	0.36	36,36,36,36	0
55	MG	DA	3204	1/1	0.97	0.39	51,51,51,51	0
55	MG	BA	3181	1/1	0.97	0.35	39,39,39,39	0
55	MG	DA	3420	1/1	0.97	0.31	67,67,67,67	0
55	MG	BA	3329	1/1	0.97	0.40	65,65,65,65	0
55	MG	DA	3141	1/1	0.97	0.52	38,38,38,38	0
55	MG	DA	3200	1/1	0.97	0.45	44,44,44,44	0
55	MG	BA	3129	1/1	0.97	0.44	52,52,52,52	0
55	MG	BA	3119	1/1	0.97	0.38	62,62,62,62	0
55	MG	BA	3407	1/1	0.97	0.26	59,59,59,59	0
55	MG	BA	3383	1/1	0.97	0.22	71,71,71,71	0
55	MG	BA	3020	1/1	0.97	0.47	41,41,41,41	0
55	MG	DA	3191	1/1	0.97	0.55	46,46,46,46	0
55	MG	BA	3220	1/1	0.97	0.45	44,44,44,44	0
55	MG	BA	3202	1/1	0.97	0.39	51,51,51,51	0
55	MG	DA	3145	1/1	0.97	0.51	60,60,60,60	0
55	MG	DA	3202	1/1	0.97	0.43	47,47,47,47	0
55	MG	BA	3160	1/1	0.97	0.42	42,42,42,42	0
55	MG	BA	3186	1/1	0.97	0.42	36,36,36,36	0
55	MG	BA	3051	1/1	0.97	0.23	74,74,74,74	0
55	MG	DP	201	1/1	0.97	0.35	65,65,65,65	0
55	MG	BA	3557	1/1	0.97	0.47	77,77,77,77	0
55	MG	BA	3077	1/1	0.97	0.45	54,54,54,54	0
55	MG	D3	101	1/1	0.97	0.43	66,66,66,66	0
55	MG	BA	3188	1/1	0.97	0.37	60,60,60,60	0
55	MG	DA	3239	1/1	0.97	0.36	45,45,45,45	0
55	MG	BA	3320	1/1	0.97	0.27	62,62,62,62	0
55	MG	BA	3585	1/1	0.97	0.38	60,60,60,60	0
55	MG	DA	3196	1/1	0.97	0.46	50,50,50,50	0
55	MG	BA	3035	1/1	0.97	0.27	37,37,37,37	0
55	MG	BE	302	1/1	0.97	0.23	56,56,56,56	0
55	MG	BA	3030	1/1	0.97	0.54	44,44,44,44	0
55	MG	BA	3021	1/1	0.97	0.53	41,41,41,41	0
55	MG	BA	3561	1/1	0.97	0.31	74,74,74,74	0
55	MG	BA	3213	1/1	0.97	0.56	49,49,49,49	0
55	MG	DA	3157	1/1	0.97	0.69	47,47,47,47	0
55	MG	BA	3066	1/1	0.97	0.31	62,62,62,62	0
55	MG	BA	3063	1/1	0.97	0.13	43,43,43,43	0
55	MG	DA	3113	1/1	0.97	0.55	43,43,43,43	0
55	MG	BA	3244	1/1	0.97	0.33	58,58,58,58	0
55	MG	DA	3195	1/1	0.97	0.76	70,70,70,70	0
55	MG	DA	3245	1/1	0.97	0.51	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	DA	3221	1/1	0.97	0.70	63,63,63,63	0
55	MG	BA	3022	1/1	0.97	0.45	30,30,30,30	0
55	MG	DA	3162	1/1	0.97	0.38	66,66,66,66	0
55	MG	AA	1657	1/1	0.97	0.45	50,50,50,50	0
55	MG	DA	3286	1/1	0.97	0.14	47,47,47,47	0
55	MG	DA	3210	1/1	0.97	0.42	63,63,63,63	0
55	MG	BA	3028	1/1	0.97	0.41	46,46,46,46	0
55	MG	AA	1784	1/1	0.97	0.47	66,66,66,66	0
55	MG	CC	102	1/1	0.97	0.52	73,73,73,73	0
55	MG	BA	3276	1/1	0.97	0.23	74,74,74,74	0
55	MG	BA	3055	1/1	0.97	0.43	57,57,57,57	0
55	MG	DA	3264	1/1	0.97	0.65	59,59,59,59	0
55	MG	DA	3135	1/1	0.97	0.42	49,49,49,49	0
55	MG	AA	1602	1/1	0.97	0.33	79,79,79,79	0
55	MG	DA	3103	1/1	0.97	0.40	50,50,50,50	0
55	MG	DA	3215	1/1	0.97	0.42	42,42,42,42	0
55	MG	CA	1799	1/1	0.97	0.31	96,96,96,96	0
55	MG	DA	3158	1/1	0.97	0.59	44,44,44,44	0
55	MG	DA	3096	1/1	0.97	0.58	53,53,53,53	0
55	MG	CA	1750	1/1	0.97	0.48	79,79,79,79	0
55	MG	BA	3162	1/1	0.97	0.52	45,45,45,45	0
55	MG	DA	3219	1/1	0.97	0.24	70,70,70,70	0
55	MG	DA	3177	1/1	0.97	0.34	74,74,74,74	0
55	MG	AA	1794	1/1	0.97	0.21	84,84,84,84	0
55	MG	DA	3107	1/1	0.97	0.36	53,53,53,53	0
55	MG	DA	3222	1/1	0.97	0.50	60,60,60,60	0
55	MG	DA	3254	1/1	0.97	0.55	50,50,50,50	0
55	MG	DA	3006	1/1	0.97	0.48	71,71,71,71	0
55	MG	BA	3259	1/1	0.97	0.25	40,40,40,40	0
55	MG	BA	3014	1/1	0.97	0.48	53,53,53,53	0
55	MG	DA	3390	1/1	0.97	0.35	75,75,75,75	0
55	MG	BA	3005	1/1	0.97	0.49	43,43,43,43	0
55	MG	BA	3594	1/1	0.97	0.55	79,79,79,79	0
55	MG	DA	3209	1/1	0.97	0.50	66,66,66,66	0
55	MG	AA	1634	1/1	0.97	0.29	62,62,62,62	0
55	MG	BA	3567	1/1	0.97	0.23	80,80,80,80	0
55	MG	AA	1665	1/1	0.97	0.75	70,70,70,70	0
55	MG	DA	3446	1/1	0.97	0.50	75,75,75,75	0
55	MG	BA	3001	1/1	0.97	0.48	47,47,47,47	0
55	MG	DA	3166	1/1	0.97	0.45	58,58,58,58	0
55	MG	DA	3178	1/1	0.97	0.75	59,59,59,59	0
55	MG	BA	3355	1/1	0.97	0.57	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	DA	3354	1/1	0.97	0.41	73,73,73,73	0
55	MG	BA	3033	1/1	0.97	0.38	38,38,38,38	0
55	MG	BA	3111	1/1	0.97	0.33	59,59,59,59	0
55	MG	DA	3233	1/1	0.97	0.42	52,52,52,52	0
55	MG	BA	3046	1/1	0.97	0.38	39,39,39,39	0
55	MG	DA	3280	1/1	0.97	0.57	46,46,46,46	0
55	MG	BA	3433	1/1	0.97	0.15	70,70,70,70	0
55	MG	BA	3042	1/1	0.98	0.34	41,41,41,41	0
55	MG	DA	3065	1/1	0.98	0.41	74,74,74,74	0
55	MG	CA	1619	1/1	0.98	0.49	61,61,61,61	0
55	MG	DA	3097	1/1	0.98	0.29	52,52,52,52	0
55	MG	CA	1650	1/1	0.98	0.26	102,102,102,102	0
55	MG	BA	3041	1/1	0.98	0.31	46,46,46,46	0
55	MG	BA	3172	1/1	0.98	0.36	34,34,34,34	0
55	MG	BA	3158	1/1	0.98	0.32	41,41,41,41	0
55	MG	BA	3045	1/1	0.98	0.41	45,45,45,45	0
55	MG	DA	3180	1/1	0.98	0.59	52,52,52,52	0
55	MG	BA	3157	1/1	0.98	0.60	45,45,45,45	0
55	MG	BA	3189	1/1	0.98	0.39	49,49,49,49	0
55	MG	AA	1627	1/1	0.98	0.32	53,53,53,53	0
55	MG	AA	1691	1/1	0.98	0.49	50,50,50,50	0
55	MG	DA	3240	1/1	0.98	0.55	42,42,42,42	0
55	MG	DA	3118	1/1	0.98	0.35	71,71,71,71	0
56	ZN	CG	303	1/1	0.98	0.31	118,118,118,118	0
55	MG	BA	3002	1/1	0.98	0.47	43,43,43,43	0
55	MG	BA	3245	1/1	0.98	0.55	49,49,49,49	0
55	MG	DA	3201	1/1	0.98	0.25	47,47,47,47	0
55	MG	DA	3144	1/1	0.98	0.29	60,60,60,60	0
55	MG	DA	3235	1/1	0.98	0.42	48,48,48,48	0
55	MG	BA	3015	1/1	0.98	0.35	38,38,38,38	0
55	MG	BA	3554	1/1	0.98	0.47	45,45,45,45	0
55	MG	AA	1841	1/1	0.98	0.38	59,59,59,59	0
55	MG	BA	3139	1/1	0.98	0.39	35,35,35,35	0
55	MG	BA	3390	1/1	0.98	0.31	60,60,60,60	0
55	MG	BA	3013	1/1	0.98	0.43	34,34,34,34	0
55	MG	CA	1754	1/1	0.98	0.32	86,86,86,86	0
55	MG	BA	3207	1/1	0.98	0.57	41,41,41,41	0
55	MG	BA	3017	1/1	0.98	0.46	25,25,25,25	0
55	MG	BA	3007	1/1	0.98	0.54	53,53,53,53	0
55	MG	BA	3610	1/1	0.98	0.43	61,61,61,61	0
55	MG	BA	3004	1/1	0.98	0.46	35,35,35,35	0
55	MG	CA	1710	1/1	0.98	0.29	106,106,106,106	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	BA	3538	1/1	0.98	0.55	66,66,66,66	0
55	MG	BA	3212	1/1	0.98	0.61	43,43,43,43	0
55	MG	BA	3068	1/1	0.98	0.34	75,75,75,75	0
56	ZN	AQ	102	1/1	0.98	0.09	122,122,122,122	0
55	MG	AA	1707	1/1	0.98	0.58	50,50,50,50	0
55	MG	DA	3104	1/1	0.98	0.40	43,43,43,43	0
55	MG	DA	3101	1/1	0.98	0.33	43,43,43,43	0
55	MG	DA	3171	1/1	0.98	0.34	63,63,63,63	0
55	MG	BA	3190	1/1	0.98	0.33	63,63,63,63	0
55	MG	AA	1842	1/1	0.98	0.46	59,59,59,59	0
55	MG	AA	1783	1/1	0.98	0.60	67,67,67,67	0
55	MG	DA	3102	1/1	0.98	0.37	51,51,51,51	0
55	MG	AA	1619	1/1	0.98	0.40	63,63,63,63	0
55	MG	BA	3229	1/1	0.98	0.12	50,50,50,50	0
55	MG	BA	3009	1/1	0.98	0.33	36,36,36,36	0
55	MG	BA	3036	1/1	0.98	0.54	44,44,44,44	0
55	MG	BA	3382	1/1	0.98	0.39	43,43,43,43	0
55	MG	DA	3079	1/1	0.98	0.38	54,54,54,54	0
55	MG	BA	3269	1/1	0.98	0.45	61,61,61,61	0
55	MG	BA	3079	1/1	0.98	0.41	55,55,55,55	0
55	MG	DA	3106	1/1	0.98	0.41	48,48,48,48	0
55	MG	B0	201	1/1	0.98	0.32	51,51,51,51	0
55	MG	DA	3052	1/1	0.98	0.45	71,71,71,71	0
55	MG	AA	1660	1/1	0.98	0.62	53,53,53,53	0
55	MG	BA	3196	1/1	0.98	0.32	33,33,33,33	0
55	MG	BA	3024	1/1	0.98	0.38	27,27,27,27	0
55	MG	DA	3211	1/1	0.98	0.49	42,42,42,42	0
55	MG	DA	3223	1/1	0.98	0.47	52,52,52,52	0
55	MG	DA	3095	1/1	0.98	0.44	49,49,49,49	0
55	MG	DA	3116	1/1	0.98	0.40	74,74,74,74	0
55	MG	D5	2001	1/1	0.98	0.41	46,46,46,46	0
55	MG	BA	3039	1/1	0.98	0.30	42,42,42,42	0
55	MG	BA	3126	1/1	0.98	0.42	46,46,46,46	0
55	MG	BA	3163	1/1	0.98	0.58	50,50,50,50	0
55	MG	BA	3123	1/1	0.98	0.21	51,51,51,51	0
55	MG	BA	3261	1/1	0.98	0.62	52,52,52,52	0
55	MG	BA	3128	1/1	0.98	0.50	46,46,46,46	0
55	MG	DA	3194	1/1	0.98	0.43	73,73,73,73	0
55	MG	DA	3147	1/1	0.98	0.38	53,53,53,53	0
55	MG	BA	3091	1/1	0.98	0.52	35,35,35,35	0
55	MG	BA	3294	1/1	0.98	0.35	72,72,72,72	0
55	MG	DA	3472	1/1	0.98	0.69	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	DA	3133	1/1	0.98	0.38	42,42,42,42	0
55	MG	BA	3155	1/1	0.98	0.18	45,45,45,45	0
55	MG	AG	301	1/1	0.98	0.57	81,81,81,81	0
55	MG	BA	3255	1/1	0.98	0.38	46,46,46,46	0
55	MG	BA	3230	1/1	0.98	0.59	56,56,56,56	0
55	MG	BA	3283	1/1	0.98	0.38	49,49,49,49	0
55	MG	DA	3296	1/1	0.99	0.66	51,51,51,51	0
55	MG	AA	1604	1/1	0.99	0.33	67,67,67,67	0
55	MG	BA	3023	1/1	0.99	0.36	45,45,45,45	0
55	MG	BA	3131	1/1	0.99	0.32	59,59,59,59	0
55	MG	BA	3018	1/1	0.99	0.35	54,54,54,54	0
55	MG	BA	3216	1/1	0.99	0.32	33,33,33,33	0
55	MG	BA	3608	1/1	0.99	0.37	39,39,39,39	0
55	MG	BA	3074	1/1	0.99	0.47	49,49,49,49	0
55	MG	CA	1792	1/1	0.99	0.62	70,70,70,70	0
55	MG	AA	1609	1/1	0.99	0.41	78,78,78,78	0
55	MG	BA	3029	1/1	0.99	0.42	35,35,35,35	0
55	MG	DA	3142	1/1	0.99	0.52	40,40,40,40	0
55	MG	BA	3233	1/1	0.99	0.41	48,48,48,48	0
55	MG	DA	3213	1/1	0.99	0.48	41,41,41,41	0
55	MG	BA	3262	1/1	0.99	0.57	33,33,33,33	0
55	MG	DA	3115	1/1	0.99	0.52	49,49,49,49	0
55	MG	CA	1726	1/1	0.99	0.62	75,75,75,75	0
55	MG	DA	3474	1/1	0.99	0.60	83,83,83,83	0
55	MG	DA	3203	1/1	0.99	0.27	48,48,48,48	0
55	MG	CA	1706	1/1	0.99	0.42	87,87,87,87	0
55	MG	DA	3114	1/1	0.99	0.56	54,54,54,54	0
55	MG	DA	3463	1/1	0.99	0.20	73,73,73,73	0
55	MG	DE	301	1/1	0.99	0.38	41,41,41,41	0
55	MG	BA	3019	1/1	0.99	0.44	66,66,66,66	0
55	MG	DA	3260	1/1	0.99	0.62	41,41,41,41	0
55	MG	DA	3182	1/1	0.99	0.81	44,44,44,44	0
55	MG	BA	3173	1/1	0.99	0.59	52,52,52,52	0
55	MG	BA	3171	1/1	0.99	0.54	61,61,61,61	0
55	MG	BA	3027	1/1	0.99	0.54	36,36,36,36	0

6.5 Other polymers

There are no such residues in this entry.