



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 16, 2020 – 01:33 pm BST

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](mailto: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.

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

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

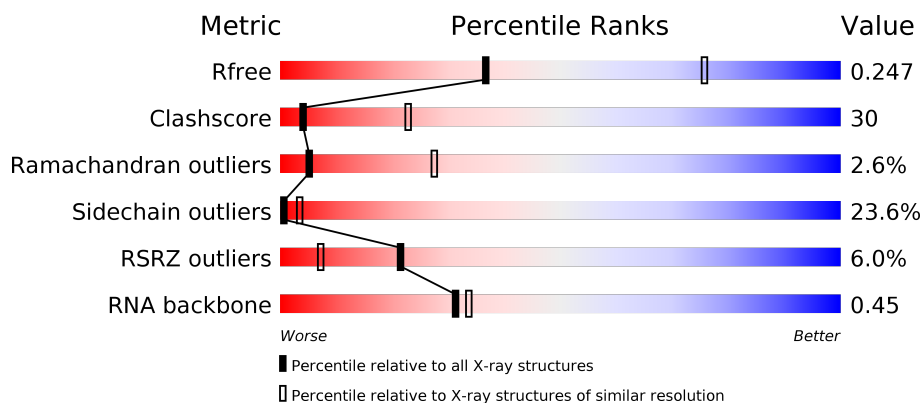
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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))
$R_{free}$	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)
RNA backbone	3102	1173 (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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AA	1506	<div> <div>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>
2	CE	256	<div> <div>10%</div> <div>34%</div> <div>41%</div> <div>16%</div> <div>7%</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	




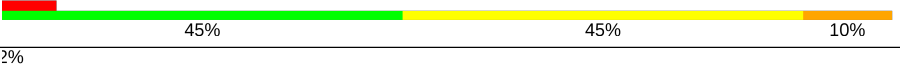
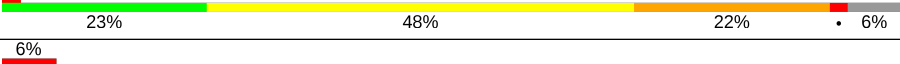
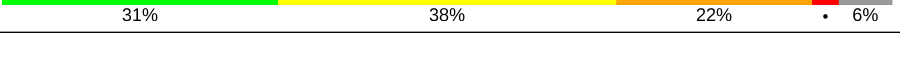
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Mol	Chain	Length	Quality of chain
39	DR	146	
40	B1	118	
40	D1	118	
41	B2	101	
41	D2	101	
42	BS	113	
42	DS	113	
43	BT	96	
43	DT	96	
44	BU	110	
44	DU	110	
45	BV	206	
45	DV	206	
46	B3	85	
46	D3	85	
47	BZ	98	
47	DZ	98	
48	BW	72	
48	DW	72	
49	BX	60	
49	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	C	N	O	P	0	0	0
			62707	27911	11722	20163	2911			
25	DA	2907	Total	C	N	O	P	0	0	0
			62607	27866	11712	20123	2906			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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	C	N	O	P	0	0	0
			2617	1166	486	844	121			
26	DB	122	Total	C	N	O	P	0	0	0
			2617	1166	486	844	121			

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

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

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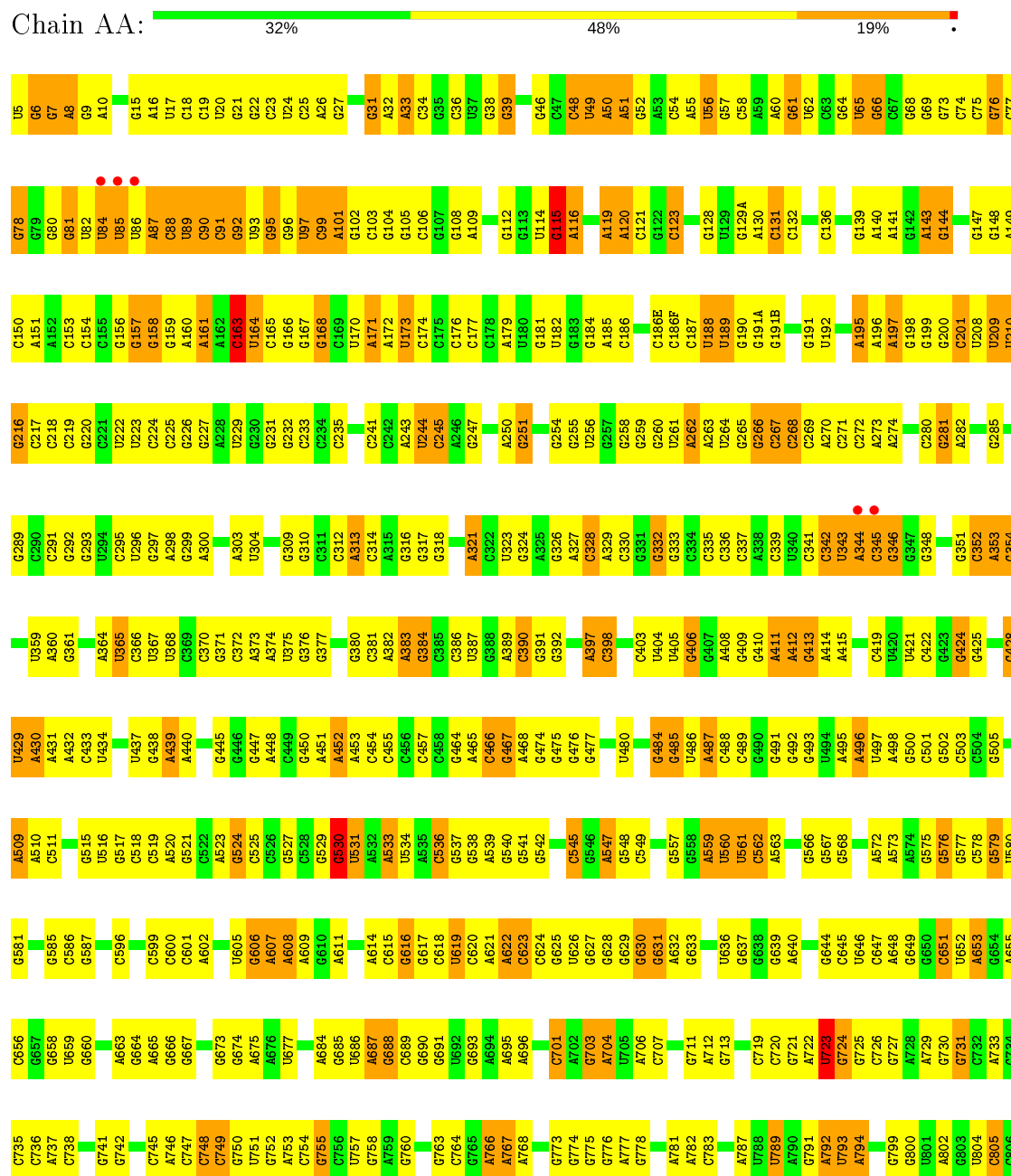
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	CQ	1	Total 1	Zn 1	0	0
56	CG	1	Total 1	Zn 1	0	0

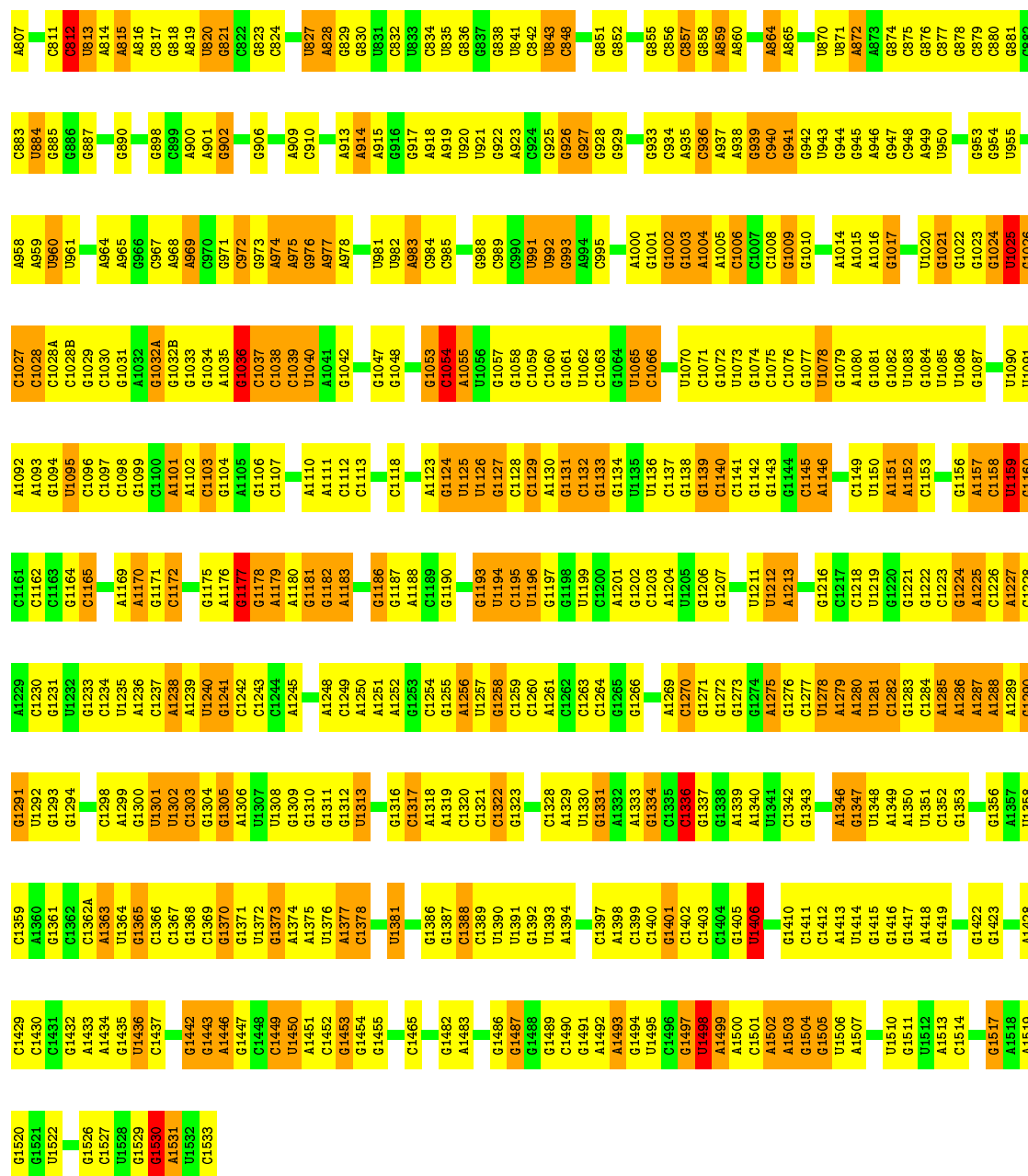
### 3 Residue-property plots

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

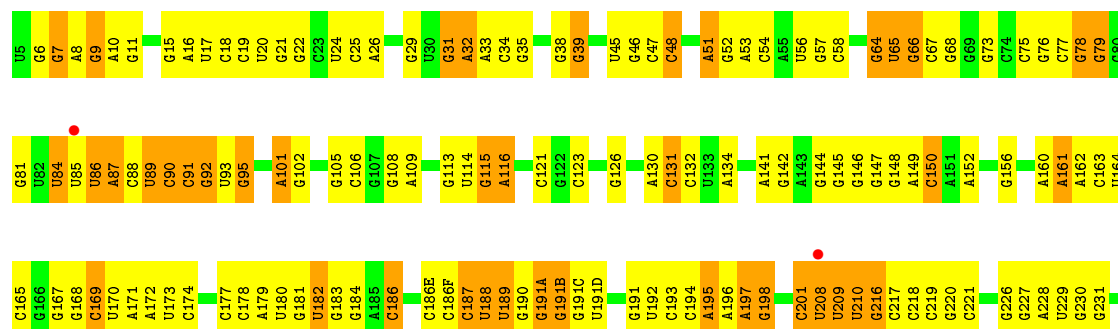




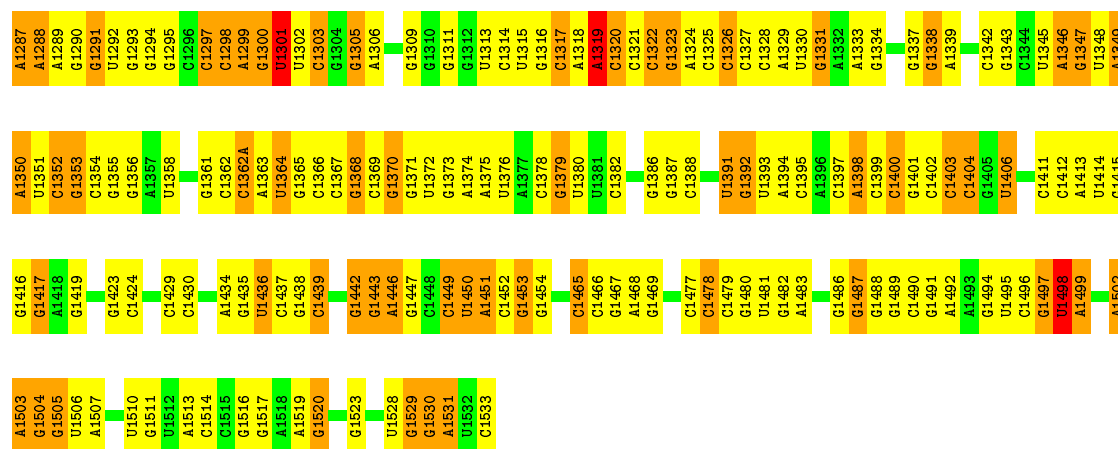


# • Molecule 1: 16S ribosomal RNA

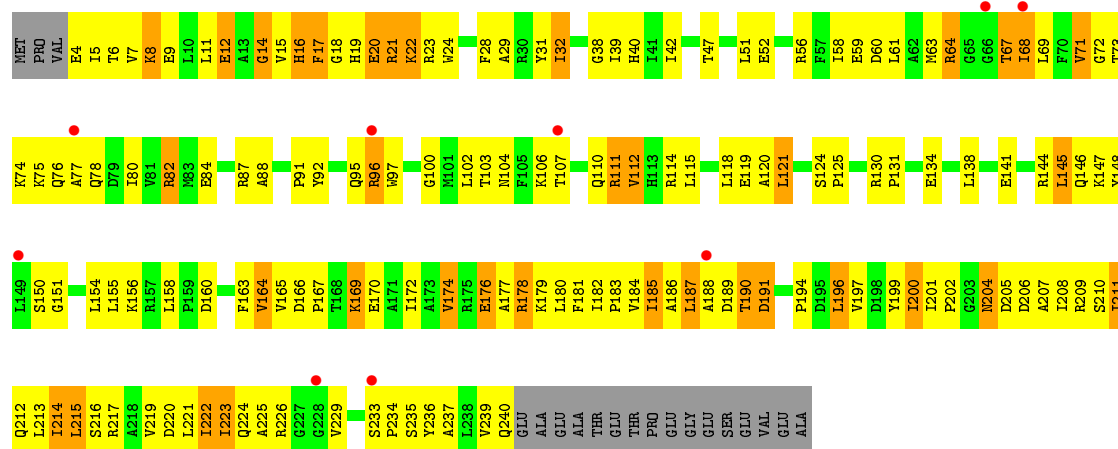
Chain CA:  30%  47%  22%



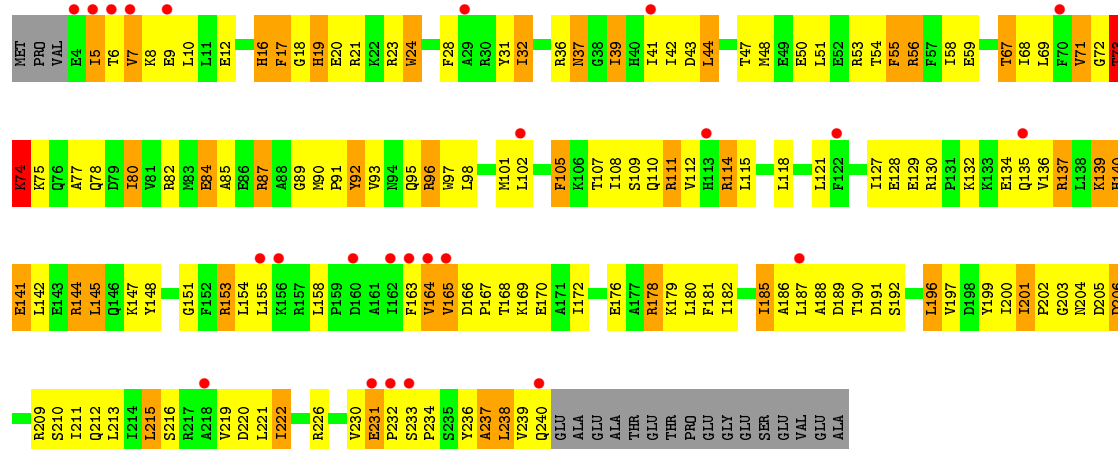
C1223	C1224	C1160	C1161	C1162	C1163	C1164	C1165	C1166	C1100	G1034	A978	G917	U833	G755	G682	C612	G541	G467	C390	A313	C235
G1225	A1101	C980	G1036	G1037	G1038	G1039	G1040	G1041	C1107	A1035	C979	A918	U834	C756	G683	C613	G542	A468	G391	C314	C240
C1226	A1102	G981	G1037	G1038	G1039	G1040	G1041	G1042	C1108	G1036	C980	A919	U835	G757	G684	G616	G543	G474	G392	A315	C241
A1227	G1103	G982	G1038	G1039	G1040	G1041	G1042	G1043	C1109	U836	G983	U920	U836	G758	G685	G617	G544	G475	G393	G316	C242
C1228	C1104	A983	G1039	G1040	G1041	G1042	G1043	G1044	C1110	G1037	G984	G922	U837	G759	G686	G618	G545	G476	G394	A321	A243
	A1105	A984	U1040	U1041	U1042	U1043	U1044	U1045	C1111	G1038	G985	A923	U838	G760	G687	U619	G546	G477	G395	C395	U244
G1231	C1106	C985	A1041	A1042	A1043	A1044	A1045	A1046	C1112	U839	G986	G926	U841	G761	G688	C620	G547	A478	G396	G326	C245
U1232	C1107	G986	G1042	G1043	G1044	G1045	G1046	G1047	C1113	U840	G987	G927	U842	G762	G689	C621	G548	A481	A397	G327	A246
G1233	G1108	G987	G1043	G1044	G1045	G1046	G1047	G1048		U841	G988	G928	U843	G763	G690	A622	G549	A482	C398	A328	G247
C1234	C1109	G988	A1044	A1045	A1046	A1047	A1048	A1049		U842	G989	G929	U844	G764	G691	C624	U551	U404	A329	A329	
U1235	A1110	G989	G1045	G1046	G1047	G1048	G1049	G1050		U843	G990	G930	U845	G765	G692	G625	U552	U405	G332	A250	A250
G1174	A1111	C990	G1046	G1047	G1048	G1049	G1050	G1051		U844	G991	G931	U846	G766	G693	G626	U553	G406	G333	U252	U252
G1175	C1112	U991	G1047	G1048	G1049	G1050	G1051	G1052		U845	G992	G932	U847	G767	G694	G627	U554	G407	G334	U253	U253
A1176	C1113	G993	G1048	G1049	G1050	G1051	G1052	G1053		U846	G993	G933	U848	G768	G695	G628	U555	A408	C339	G339	G254
A1239	A1177	G994	G1049	G1050	G1051	G1052	G1053	G1054		U847	G994	G934	U849	G769	G696	G629	U556	G409	G340	U340	G255
U1240	G1178	C995	A1050	A1051	A1052	A1053	A1054	A1055		U848	G995	A935	U850	G770	G697	G630	U557	G410	G341	U341	U256
C1242	G1179	A996	G1051	G1052	G1053	G1054	G1055	G1056		U849	G996	A936	U851	G771	G698	G631	U558	G411	G342	U342	G257
C1243	A1180	U997	G1052	G1053	G1054	G1055	G1056	G1057		U850	G997	A937	U852	G772	G699	G632	U559	G412	U343	U343	G258
C1244	G1181	G998	G1053	G1054	G1055	G1056	G1057	G1058		U851	G998	A938	U853	G773	G700	G633	U560	G413	U344	G345	G260
	G1182	U999	G1054	G1055	G1056	G1057	G1058	G1059		U852	G999	A939	U854	G774	G701	G634	U561	G414	G346	G346	G261
U1247	A1183	G1000	G1055	G1056	G1057	G1058	G1059	G1060		U853	G1000	G941	U855	G775	G702	G635	U562	G415	C339	U340	G256
A1248	G1184	A1000	G1056	G1057	G1058	G1059	G1060	G1061		U854	A1000	G942	U856	G776	G703	G636	U563	G416	G347	G347	A262
C1249	G1185	G1001	G1057	G1058	G1059	G1060	G1061	G1062		U855	G1001	G943	U857	G777	G704	G637	U564	G417	G348	G348	G262
A1250	G1186	G1002	G1058	G1059	G1060	G1061	G1062	G1063		U856	G1002	U943	U858	G778	G705	G638	U565	G418	G349	G349	G263
A1251	G1187	G1003	G1059	G1060	G1061	G1062	G1063	G1064		U857	G1003	U944	U859	G779	G706	G639	U566	G419	G350	G350	G264
A1252	A1188	A1004	G1060	G1061	G1062	G1063	G1064	G1065		U858	A1004	G945	U860	G780	G707	G640	U567	G420	G351	G351	G265
G1253	G1189	G1005	G1061	G1062	G1063	G1064	G1065	G1066		U859	G1005	G946	U861	G781	G708	G641	U568	G421	G352	G352	G266
C1254	A1190	A1006	G1062	G1063	G1064	G1065	G1066	G1067		U860	A1006	G947	U862	G782	G709	G642	U569	G422	G353	G353	G267
G1255	G1191	C1006	G1063	G1064	G1065	G1066	G1067	G1068		U861	C1006	G948	U863	G783	G710	G643	U570	G423	G354	G354	G268
C1256	C1192	C1007	G1064	G1065	G1066	G1067	G1068	G1069		U862	C1007	G949	U864	G784	G711	G644	U571	G424	G355	G355	G269
A1257	G1193	A1008	G1065	G1066	G1067	G1068	G1069	G1070		U863	A1008	U949	U865	G785	G712	G645	U572	G425	G356	G356	G270
U1257	C1194	G1009	G1066	G1067	G1068	G1069	G1070	G1071		U864	G1009	U950	U866	G786	G713	G646	U573	G426	G357	G357	G271
C1258	U1195	G1010	G1067	G1068	G1069	G1070	G1071	G1072		U865	G1010	U951	U867	G787	G714	G647	U574	G427	G358	G358	G272
C1259	G1196	G1011	G1068	G1069	G1070	G1071	G1072	G1073		U866	G1011	U952	U868	G788	G715	G648	U575	G428	G359	G359	A274
G1197	C1197	G1012	G1069	G1070	G1071	G1072	G1073	G1074		U867	G1012	U953	U869	G789	G716	G649	U576	G429	G360	G360	G275
U1199	G1198	G1013	G1070	G1071	G1072	G1073	G1074	G1075		U868	G1013	U954	U870	G790	G717	G650	U577	G430	G361	G361	A279
C1262	U1199	A1014	G1071	G1072	G1073	G1074	G1075	G1076		U869	A1014	U955	U871	G791	G718	G651	U578	G431	G362	G362	C280
C1263	C1200	A1015	G1072	G1073	G1074	G1075	G1076	G1077		U870	A1015	U956	U872	G792	G719	G652	U579	G432	G363	G363	C281
	A1201	A1016	G1073	G1074	G1075	G1076	G1077	G1078		U871	A1016	U957	U873	G793	G720	G653	U580	G433	G364	G364	A282
G1266	C1201	G1017	G1074	G1075	G1076	G1077	G1078	G1079		U872	G1017	U958	U874	G794	G721	G654	U581	G434	G365	G365	C283
C1267	G1202	G1018	G1075	G1076	G1077	G1078	G1079	G1080		U873	G1018	U959	U875	G795	G722	G655	U582	G435	G366	G366	U287
A1268	C1203	G1019	G1076	G1077	G1078	G1079	G1080	G1081		U874	G1019	U960	U876	G796	G723	G656	U583	G436	G367	G367	A288
U1205	A1204	U1020	G1077	G1078	G1079	G1080	G1081	G1082		U875	U1020	U961	U877	G797	G724	G657	U584	G437	G368	G368	G289
G1206	G1207	G1021	G1078	G1079	G1080	G1081	G1082	G1083		U876	G1021	U962	U878	G798	G725	G658	U585	G438	G369	G369	
G1207	C1208	G1022	G1079	G1080	G1081	G1082	G1083	G1084		U877	G1022	U963	U879	G799	G726	G659	U586	G439	G370	G370	G292
G1272	C1209	G1023	G1080	G1081	G1082	G1083	G1084	G1085		U878	G1023	U964	U880	G800	G727	G660	U587	G440	G371	G371	G293
G1273	G1274	U1024	G1081	G1082	G1083	G1084	G1085	G1086		U879	U1024	U965	U881	G801	G728	G661	U588	G441	G372	G372	U294
A1275	A1276	G1025	G1082	G1083	G1084	G1085	G1086	G1087		U880	G1025	U966	U882	G802	G729	G662	U589	G442	G373	G373	C295
G1276	G1277	G1026	G1083	G1084	G1085	G1086	G1087	G1088		U881	G1026	U967	U883	G803	G730	G663	U590	G443	G374	G374	
U1278	U1279	G1027	G1084	G1085	G1086	G1087	G1088	G1089		U882	G1027	U968	U884	G804	G731	G664	U591	G444	G375	G375	
A1280	A1281	G1028	G1085	G1086	G1087	G1088	G1089	G1090		U883	G1028	U969	U885	G805	G732	G665	U592	G445	G376	G376	
U1281	C1282	C1028A	G1086	G1087	G1088	G1089	G1090	G1091		U884	C1028A	U970	U886	G806	G733	G666	U593	G446	G377	G377	
U1219	G1220	G1028B	G1087	G1088	G1089	G1090	G1091	G1092		U885	G1028B	U971	U887	G807	G734	G667	U594	G447	G378	G378	A298
G1221	G1222	G1029	G1088	G1089	G1090	G1091	G1092	G1093		U886	G1029	U972	U888	G808	G735	G668	U595	G448	G379	G379	G299
A1285	A1286	G1030	G1089	G1090	G1091	G1092	G1093	G1094		U887	G1030	U973	U889	G809	G736	G669	U596	G449	G380	G380	A300
		G1031	G1090	G1091	G1092	G1093	G1094	G1095		U888	G1031	U974	U890	G810	G737	G670	U597	G450	G381	G381	G301
		A1032	G1091	G1092	G1093	G1094	G1095	G1096		U889	A1032	U975	U891	G811	G738	G671	U598	G451	G382	G382	G302
		G1032A	G1092	G1093	G1094	G1095	G1096	G1097		U890	G1032A	U976	U892	G812	G739	G672	U599	G452	G383	G383	
		G1032B	G1093	G1094	G1095	G1096	G1097	G1098		U891	G1032B	U977	U893	G813	G740	G673	U600	G453	G384	G384	G309
		G1033	G1094	G1095	G1096	G1097	G1098	G1099		U892	G1033	U978	U894	G814	G741	G674	U601	G454	G385	G385	
			G1095	G1096	G1097	G1098	G1099	G1100		U893		U979	U895	G815	G742	G675	U602	G455	G386	G386	
			G1096	G1097	G1098	G1099	G1100	G1101		U894		U980	U896	G816	G743	G676	U603	G456	G387	G387	
			G1097	G1098	G1099	G1100	G1101	G1102		U895		U981	U897	G817	G744	G677	U604	G457	G388	G388	
			G1098	G1099	G1100	G1101	G1102	G1103		U896		U982	U898	G818	G745	G678	U605	G458	G389	G389	
			G1099	G1100	G1101	G1102	G1103	G1104		U897		U983	U899	G819	G746	G679	U606	G459	G390	G390	
			G1100	G1101	G1102	G1103	G1104	G1105		U898		U984	U900	G							



### • Molecule 2: 30S RIBOSOMAL PROTEIN S2

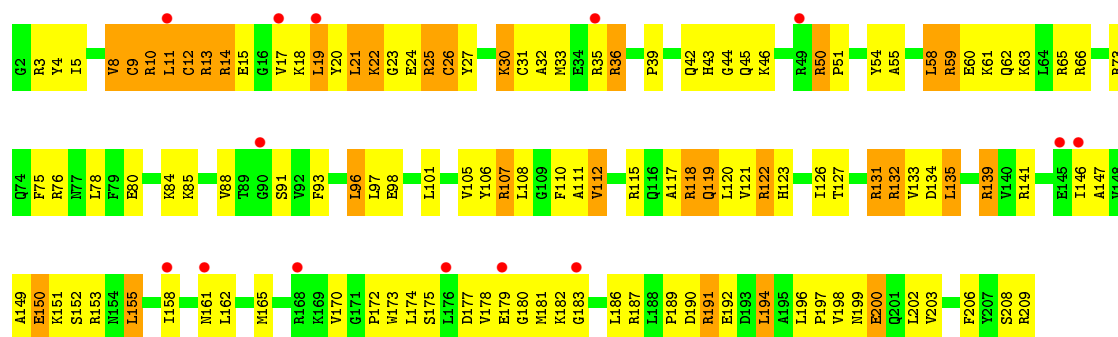


### • Molecule 2: 30S RIBOSOMAL PROTEIN S2

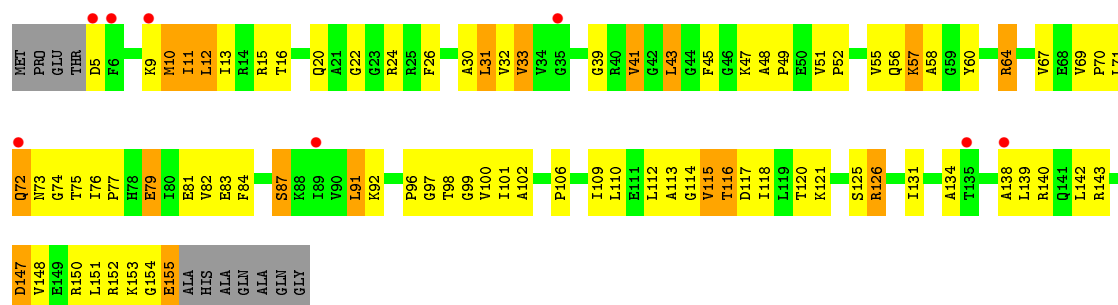
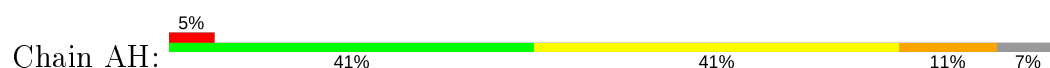


### • Molecule 3: 30S RIBOSOMAL PROTEIN S3

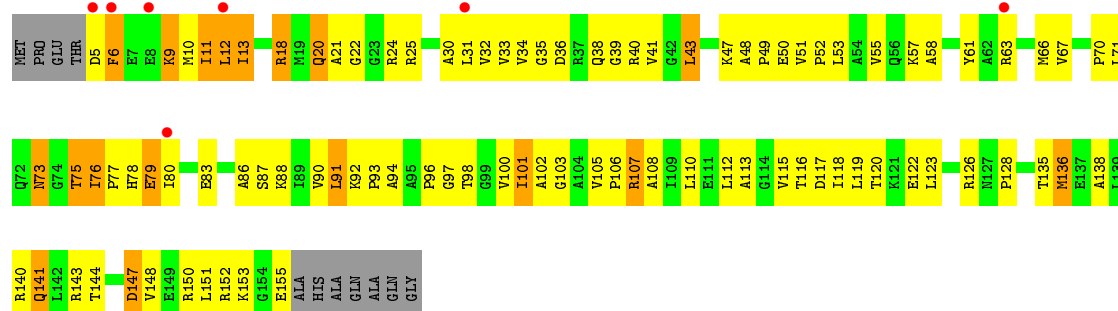




• Molecule 5: 30S RIBOSOMAL PROTEIN S5



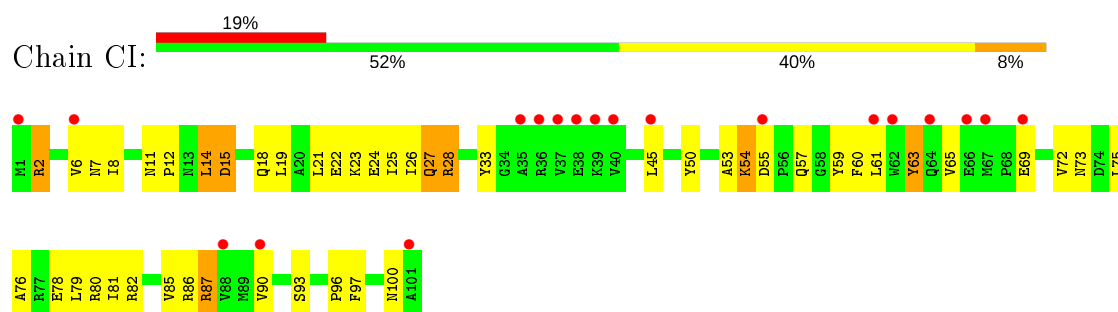
• Molecule 5: 30S RIBOSOMAL PROTEIN S5



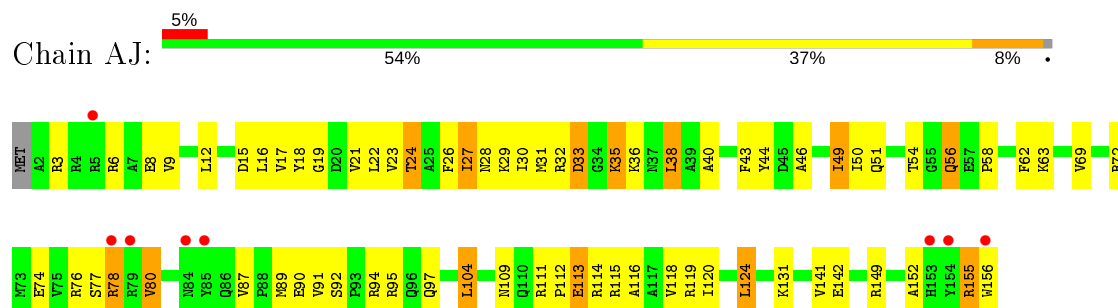
• Molecule 6: 30S RIBOSOMAL PROTEIN S6



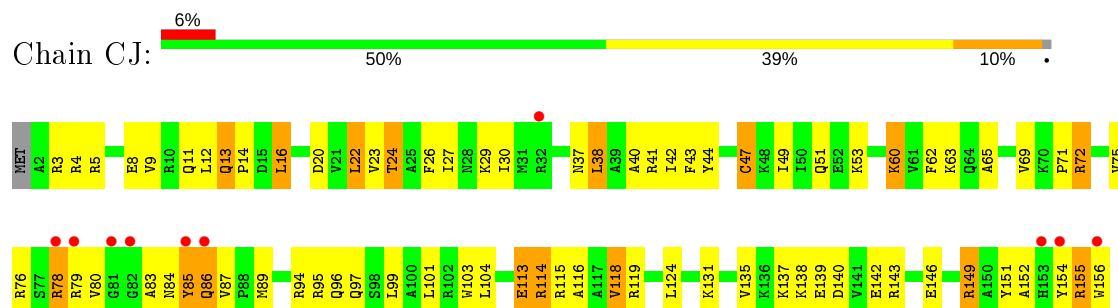
• Molecule 6: 30S RIBOSOMAL PROTEIN S6



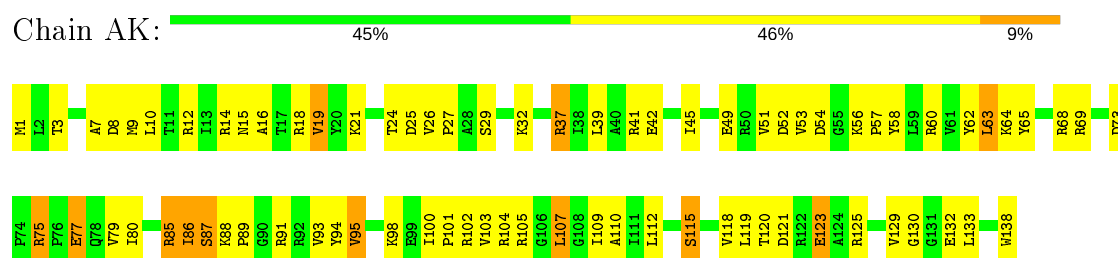
• Molecule 7: 30S RIBOSOMAL PROTEIN S7



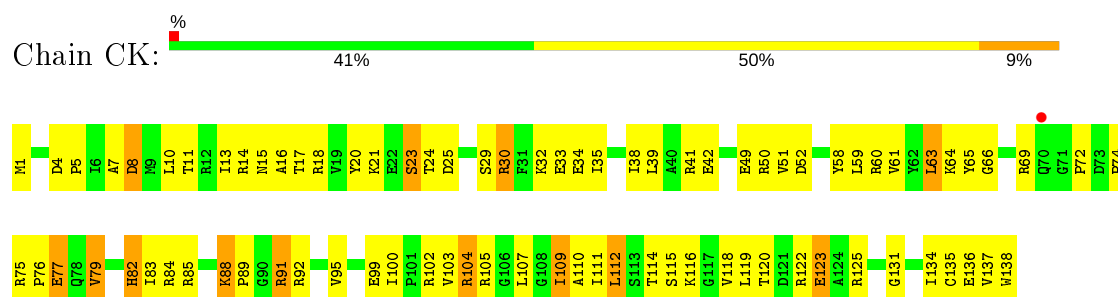
• Molecule 7: 30S RIBOSOMAL PROTEIN S7



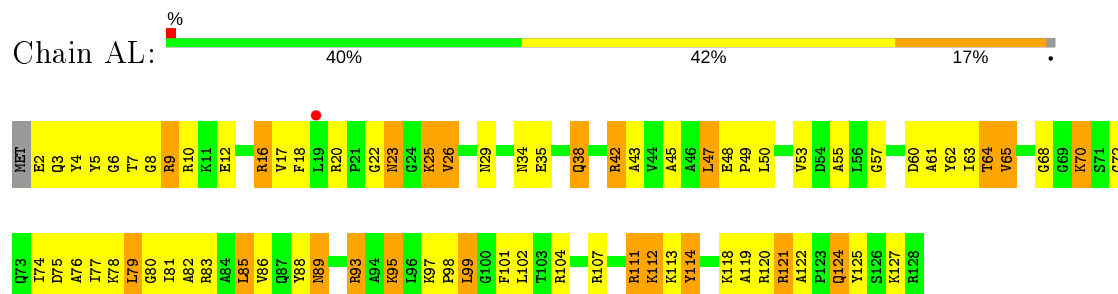
• Molecule 8: 30S RIBOSOMAL PROTEIN S8



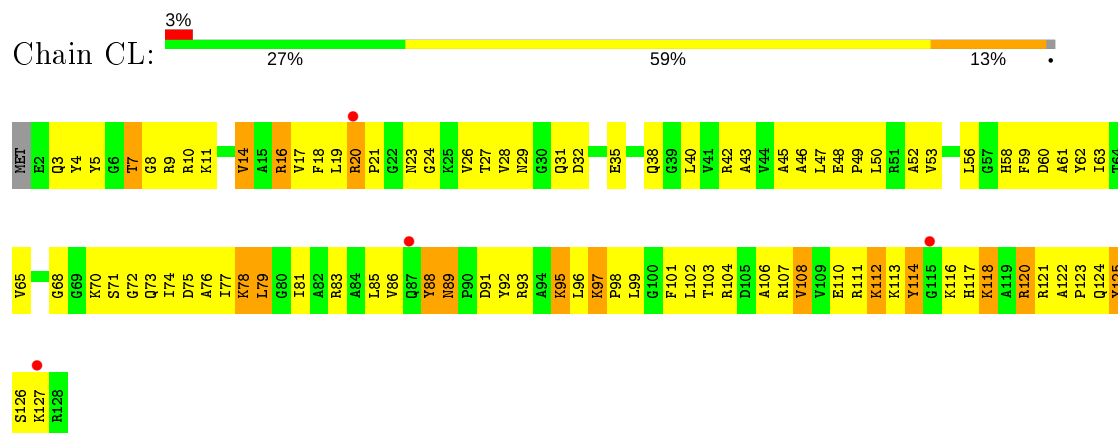
• Molecule 8: 30S RIBOSOMAL PROTEIN S8



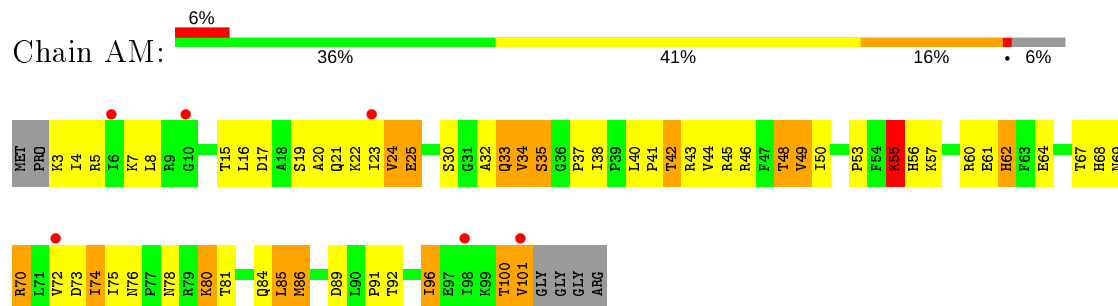
- Molecule 9: 30S RIBOSOMAL PROTEIN S9



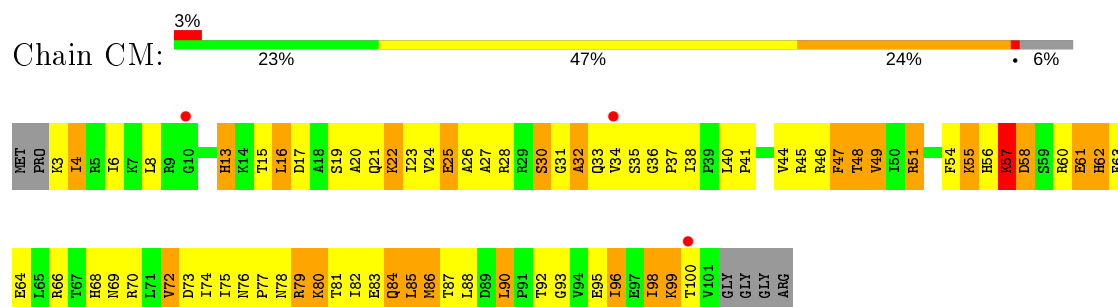
- Molecule 9: 30S RIBOSOMAL PROTEIN S9



- Molecule 10: 30S RIBOSOMAL PROTEIN S10

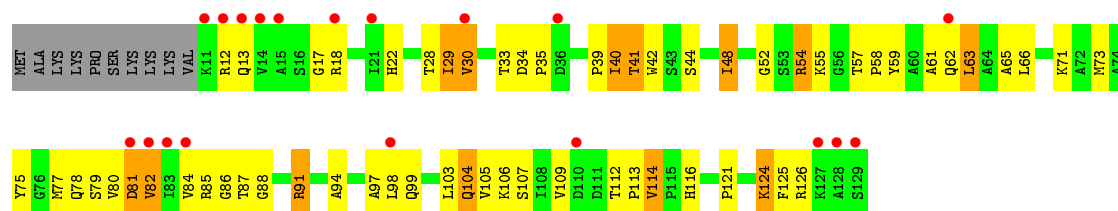


- Molecule 10: 30S RIBOSOMAL PROTEIN S10

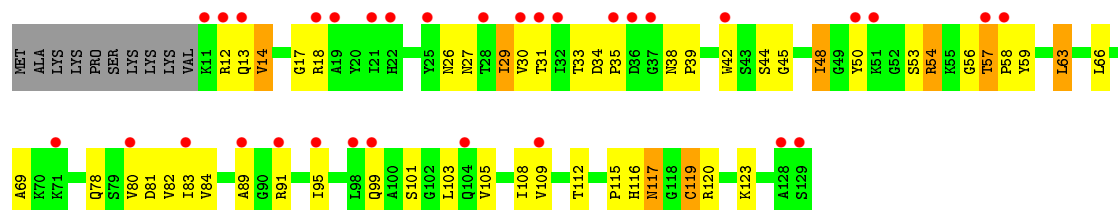


- Molecule 11: 30S RIBOSOMAL PROTEIN S11

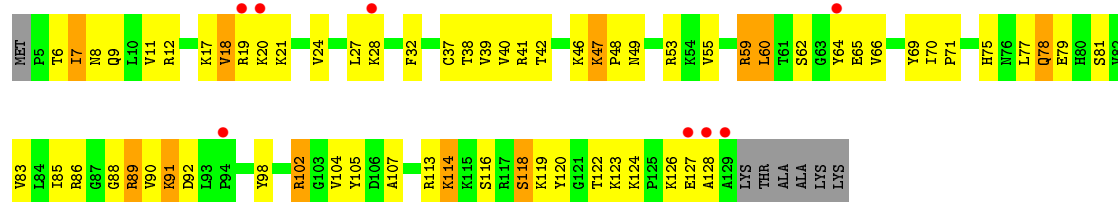




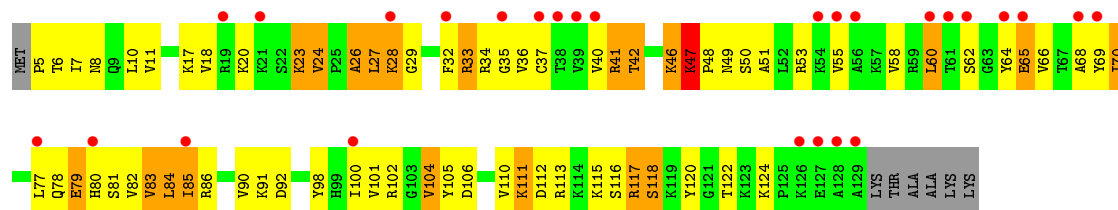
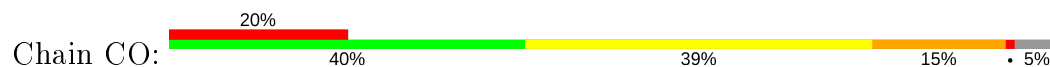
• Molecule 11: 30S RIBOSOMAL PROTEIN S11



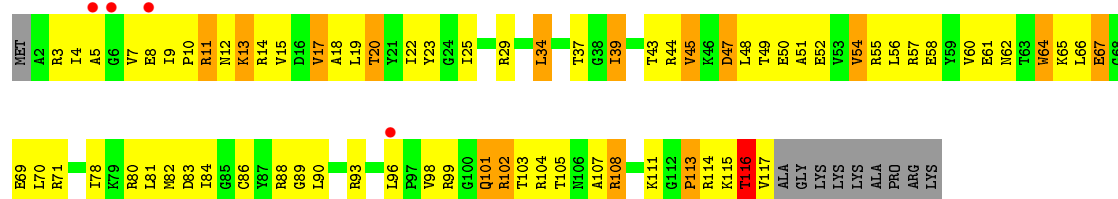
• Molecule 12: 30S RIBOSOMAL PROTEIN S12



• Molecule 12: 30S RIBOSOMAL PROTEIN S12

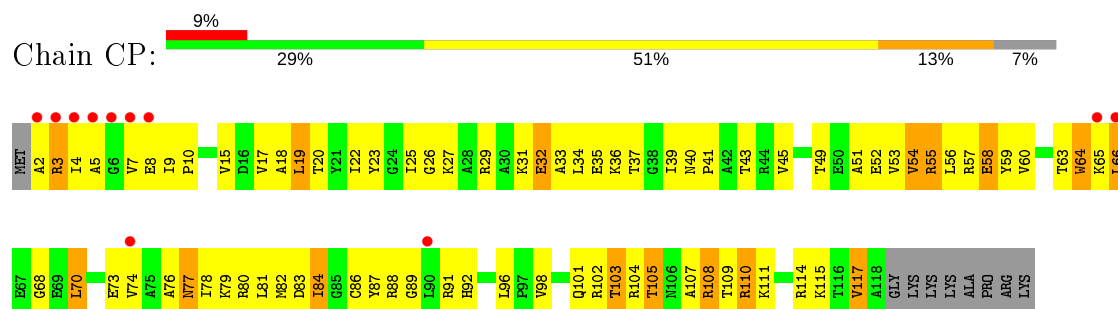


• Molecule 13: 30S RIBOSOMAL PROTEIN S13

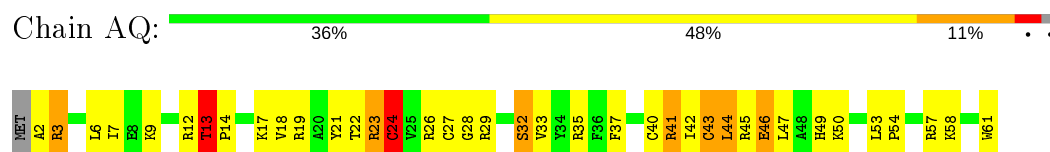




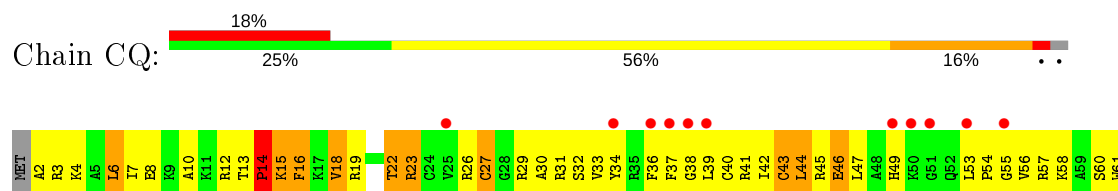
- Molecule 13: 30S RIBOSOMAL PROTEIN S13



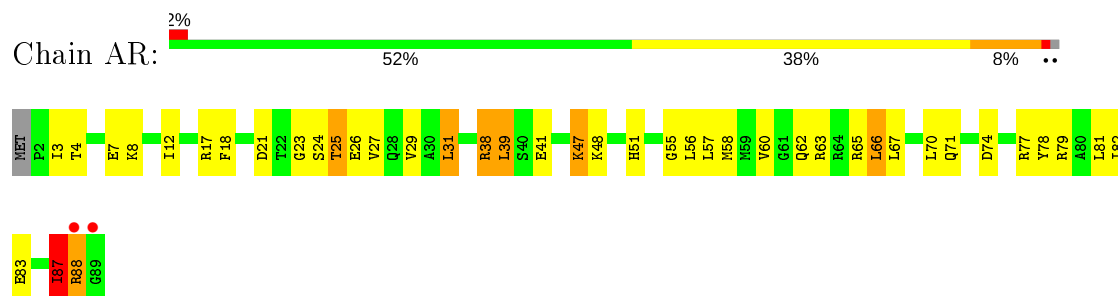
- Molecule 14: 30S RIBOSOMAL PROTEIN S14



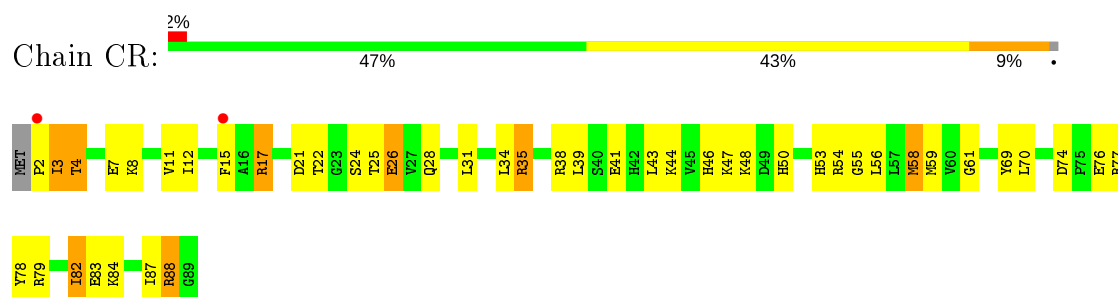
- Molecule 14: 30S RIBOSOMAL PROTEIN S14



- Molecule 15: 30S RIBOSOMAL PROTEIN S15



- Molecule 15: 30S RIBOSOMAL PROTEIN S15



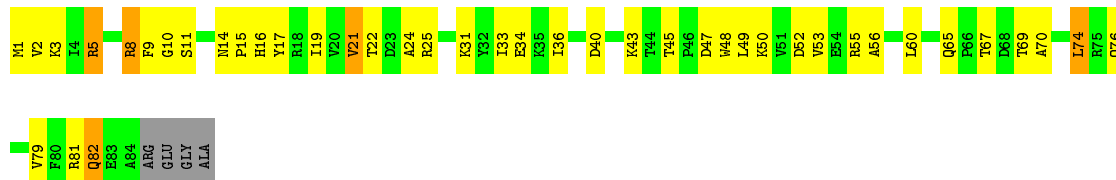
- Molecule 16: 30S RIBOSOMAL PROTEIN S16





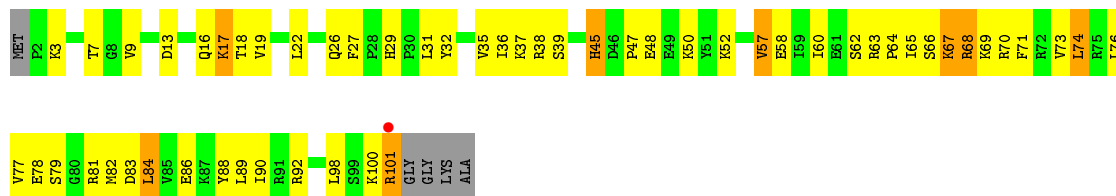
• Molecule 16: 30S RIBOSOMAL PROTEIN S16

Chain CS: 48% 42% 6% 5%



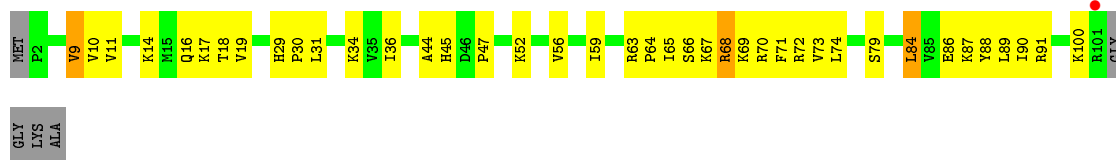
• Molecule 17: 30S RIBOSOMAL PROTEIN S17

Chain AT: 43% 45% 8% 5%



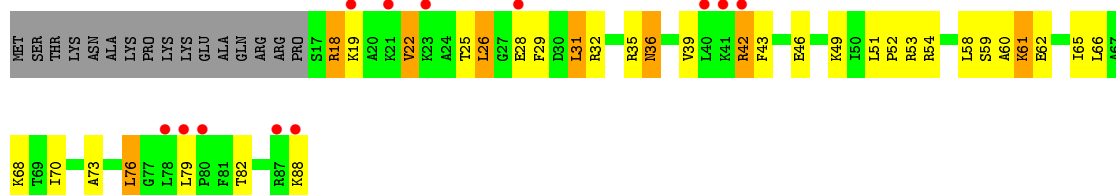
• Molecule 17: 30S RIBOSOMAL PROTEIN S17

Chain CT: 57% 35% 5%



• Molecule 18: 30S RIBOSOMAL PROTEIN S18

Chain AU: 14% 43% 30% 9% 18%



• Molecule 18: 30S RIBOSOMAL PROTEIN S18

Chain CU: 34% 36% 11% 18%

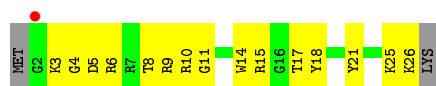


Chain AX: 




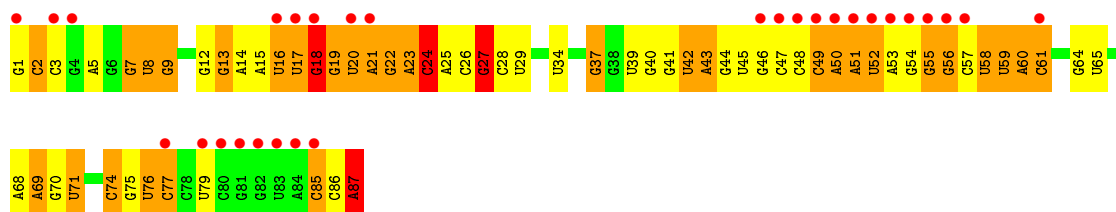
• Molecule 21: 30S RIBOSOMAL PROTEIN THX

Chain CX: 



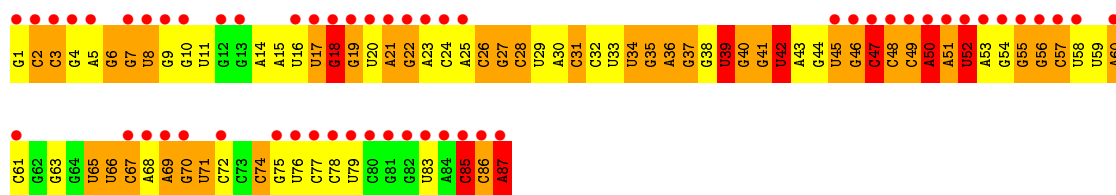
• Molecule 22: TRNA-LEU

Chain AB: 




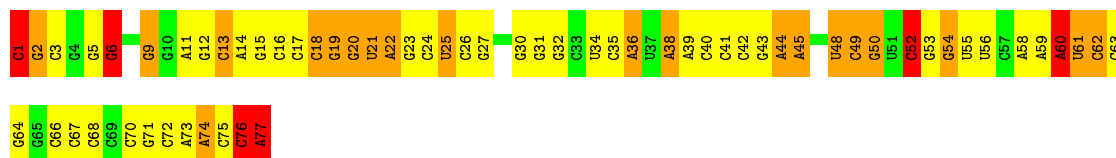
• Molecule 22: TRNA-LEU

Chain CB: 




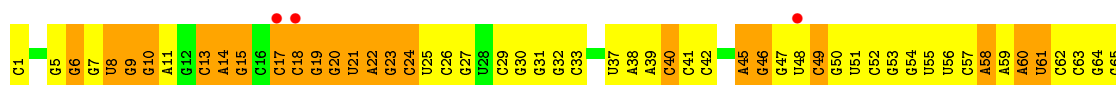
• Molecule 23: TRNA-FMET

Chain AC: 



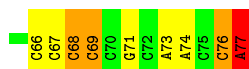
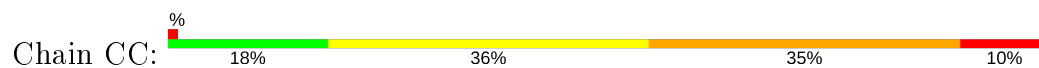
• Molecule 23: TRNA-FMET

Chain AD: 

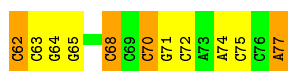
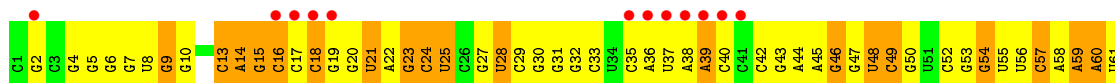
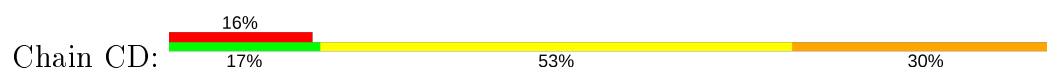




• Molecule 23: TRNA-FMET



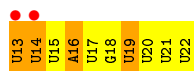
• Molecule 23: TRNA-FMET



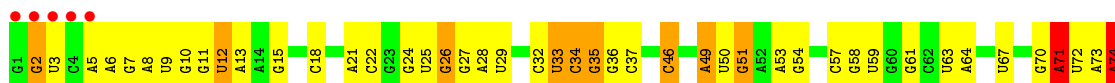
• Molecule 24: MRNA



• Molecule 24: MRNA

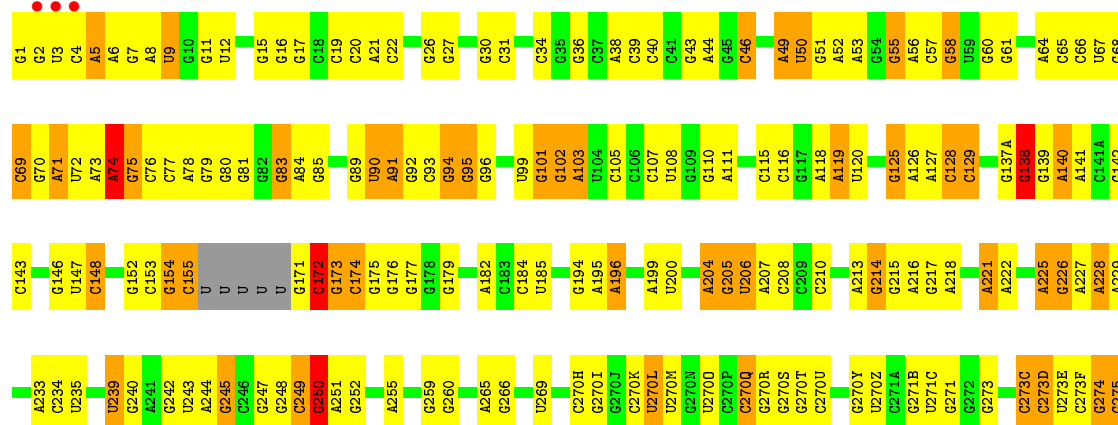


• Molecule 25: RNA (2912-MER)



C1092	G1025	U958	G883	U811	C854G	G599	U525	A363A	A454	C363B	A289	G247	U165
G1093	U1026	A959	C884	C812	G654H	G600	A526	G363B	C455	G363C	C297	G248	G171
U1094	A1027	A960	C885	C813	C654I	C601	C527	G363C	C456	G363C	C297	G249	C172
A1095	A1028	C961	C886	C814	A654J	G602	A528	G363D	A457	G363D	G298	G250	G173
A1096	U1096	G962	A887	C815	C654K	A603	A529	U863E	G458	U863E	A299	A251	
U1097	U1033	G963	C888	C816	G654L	G604	G530	A363F	U459	A363F	A300	G252	
A1098	G1037	C964	C889	C817	C654M	C605	C531	C364	A460	C364	G301		G177
G1099	U1038	G968	A890	G818	G654N	U606	A532	C365		C365	G302		
G1039	G1039		G892	A819	G654O	U607	U534	C366		C366	U303		
			C893	A820	G654P	A608	U534	G370	U464	G370	G304	G259	A181
			C894	A821	C654Q	A609	C535	G372	A466	A371	U305	G260	C184
A1102	G1042	A973	U895	U822	C654R	G609A	A536	U373	G467	G372	G307	G261	U185
A1103	C1043	G974	C896	G823	C654S	C610	C537	U373	G468	U373			
C1104	C974A	C897	A896	G824	A654T	C611	G539	G382	G469	G382	G308	C264	
U1105	A1044	G975	C897	A824	A654U	G612	G540	U383	A470	U383	A310	A265	G188
A1045	A1045		C898	C825	G654V	G612	C541	G384	A471	U384	A311	G266	
A1046	U1047	G978	A899	U826	U654W	U613		C385	A472	C385			G194
A1047	G1047	G979	A900	U827	A655	U614	C546	G386	U475	G386	A314	U269	A195
A1048	A1048	A980	A901	U828	G656	G615	A547	C389	G476	C389	A315	A270B	A196
A1049	A1050	A981	C902	A829	U857	A616	A548	G390	A477	G390	G316		
C1050			C903	G830	C671	G617	G549	G391	A478	G391	G317		A198
U1113	A983	A984	C904	G831	G660	C618A	G550	G392	A479	G391	G318	U270F	U200
G1114	C1053	A1054	U905	C834	U667	G619	U554	C392	A480	G392	G319	C270G	C201
	G1055	C986	G907	A835		G620	G556	C393	G481	C393	A320	C270H	
G1117	G1056	G987	C908	G836		A621	U557	U395	A482	U395	A322	G270I	C207
C1118	A1057	A988	A909	C837	C672	G622	G558	C404	A483	C404	G323	G270J	C208
C1119	U1058	G989	A910	C838	G673		G559	U405	C484	U405	A324	C270K	C209
	G1059	A990	A911	U839	G674	A627	C560	C404	C485	C404	G325	U270L	C210
G1122	U1060	C991	C992	C840	A675	G628	G561	U405		U405	G326	U270M	A213
C991	U1061	C992	A917	U847	A676	G629	U562	C409	G488	C409	G329	U270N	G214
G1123	C993	G993	A918	G848	C683	G630	G563	G410	G489	G410	G330	U270O	G215
A1126	G1063	C994	G919	U779	C683	A631	C564	G411	A490	G411	A330	C270P	A216
A1127	C1064	A995	C925	U779	G684	A632	C565	A492	G492	G412	A331	C270Q	G217
A1128	U1065	C996	U851	G850	A685	A633	U566	G493	G493	C413	A332	G270R	G218
A1129	U1066	G997	A926	U851	G686	C634		G494		C414	A332	G270S	A218
U1067	A1067	C998		G852		C635				C415	A332		
U1130	G1068	U999	U930	G853	C673	G636	A571	G495		C416	A333		A221
G1131	A1069	G999	G931	G854	A637	A637	A572	G495		A415	C334	G270X	A222
C1135	A1070	A1000	G932	C954	A705	A644	G573	G498	G498	C426	C335	G270Y	A223
G1136	G1071	A1001	G932	G855	A706	C644	C580	U504	U499	C426	G341	U270Z	A224
A1137	C1002	G1002	A933	C956	C692	C645	C581	A505	G500	A428	G342	C271A	G225
G1137	G1003	G1003	C957	C957	G640	U639	A575	G506	G500	G439	G343		A225
G1073	A1073	C1004	U938	U858	U694	C640	U576	G507	A501	A423	G338	G271B	G226
G1139	G1074	C1005	G939	G859	U694		G577	G508	A502	G423	U339	U271C	G226
C1075	C1006	C1006	G939	U860	A705	A644	C580	A503	A503	C426	U339	G271	A227
C1076	U1076	C1007	A941	C791	A706	C645	C581	U504	A503	A428	G342		A227
U1142	A1077	U1142	G942	A863	G712	A646	C581	G506	G506	G439	G343	G272	A229
U1078	U1078	A1010	U943	G864	G713	G647	G582	G507	A507	G439	G344	G273	U230
A1142A	C1079	G1011	G944	C865	G713	G648	G583	G508	A507	G440	G344	G275	C231
A1143	U1081	U1012	A945	C866	U714	U714	A586	G509	C509	U441	G352	A276	G332
	U1082	C1013	G946	C867	G715	G651	C587	C510	C510	G442	G353	C277	A233
C1147	U1083	U1014	G947	U868	A716	G652	G651	G511	G511	A443	G354	A278	C234
A1148	U1084	G1015		G869	G717	G653	C589	G512	G512	C444	G355	C279	U235
G1149	A1083		G850		A802	A654	A590	G512		C445	G356	C280	C236
C1150	A1085	G1018	C951	G873	U724	A654	C591	A515	A515	G446	A357	G281	C237
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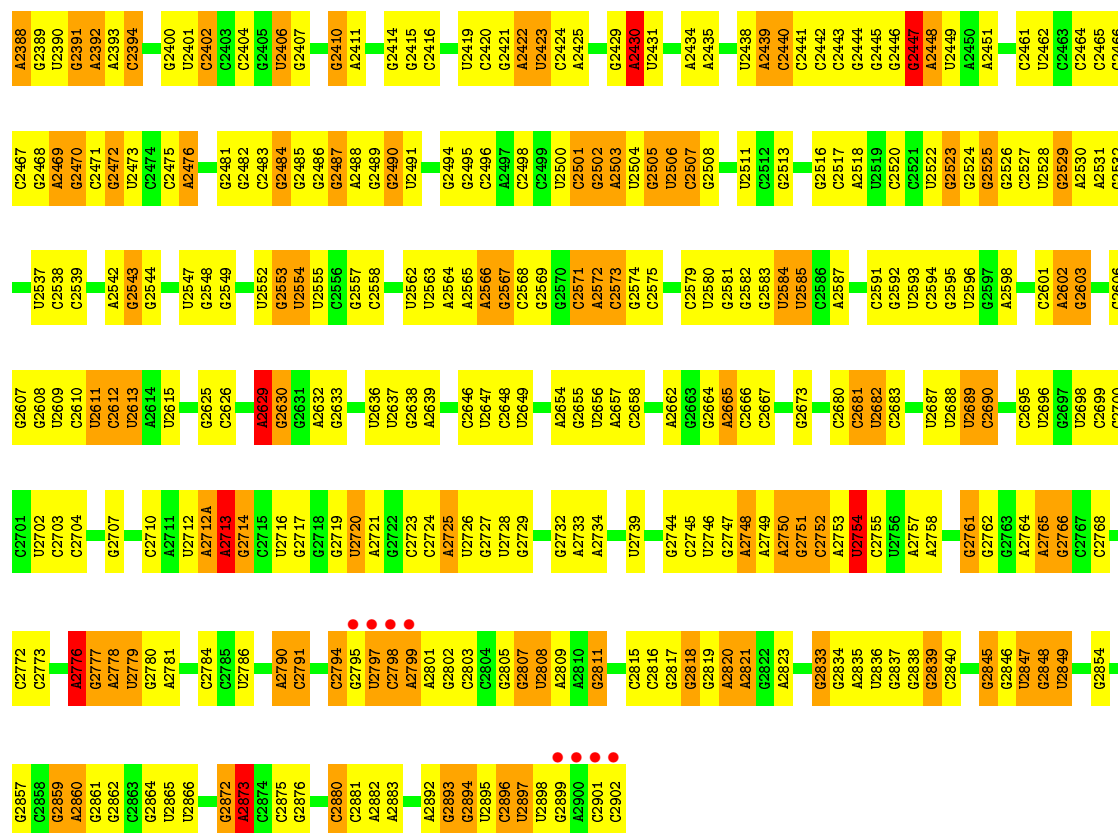
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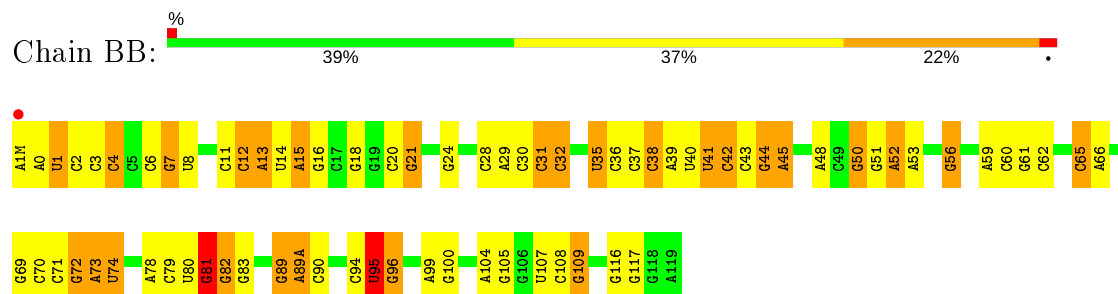


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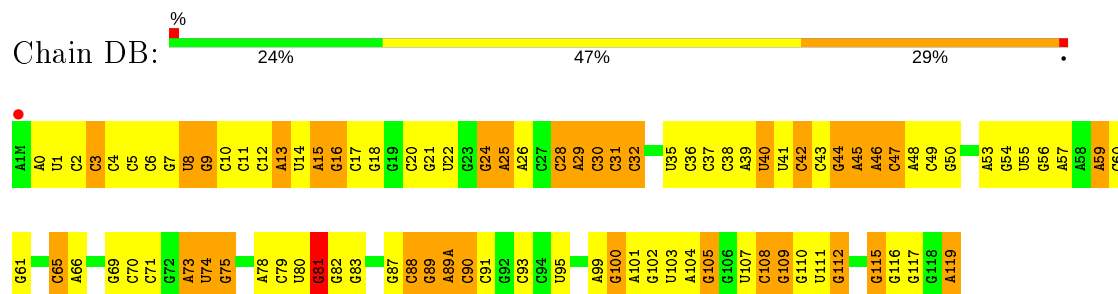
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• Molecule 26: 5S RIBOSOMAL RNA

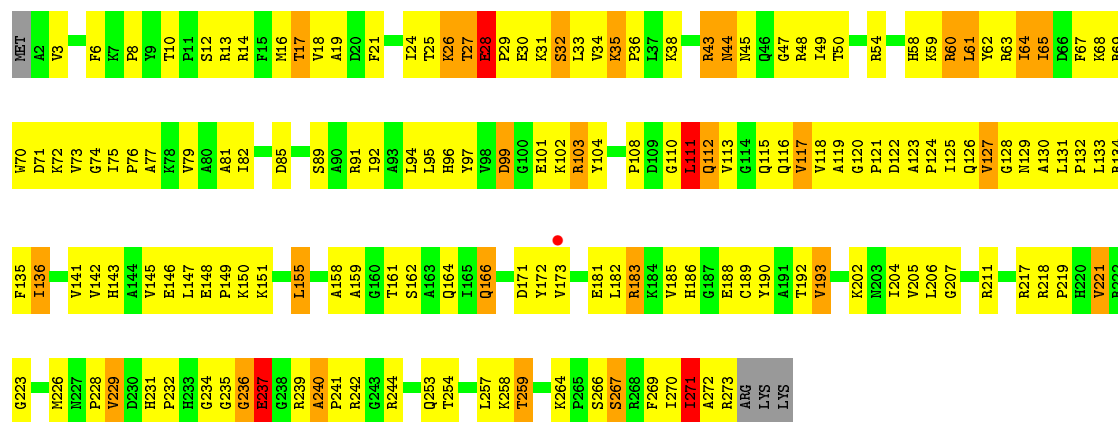


• Molecule 26: 5S RIBOSOMAL RNA

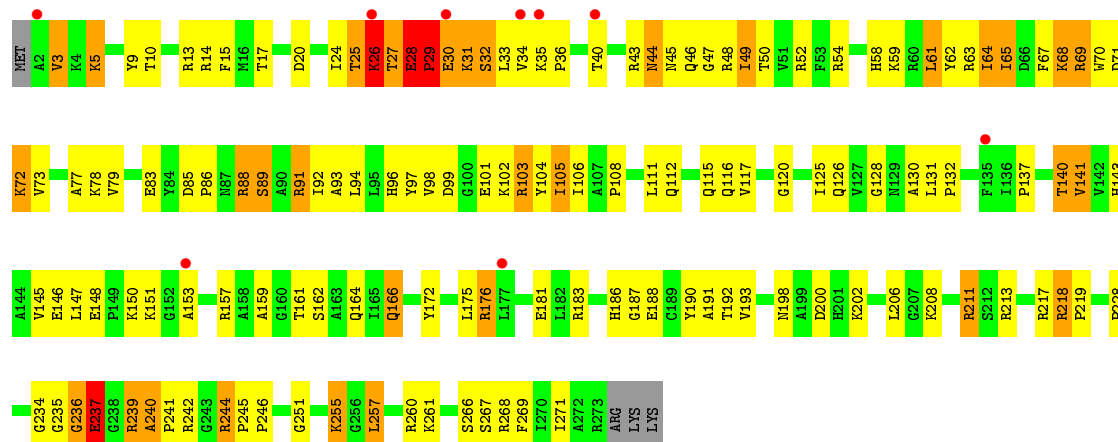


• Molecule 27: 50S ribosomal protein L2

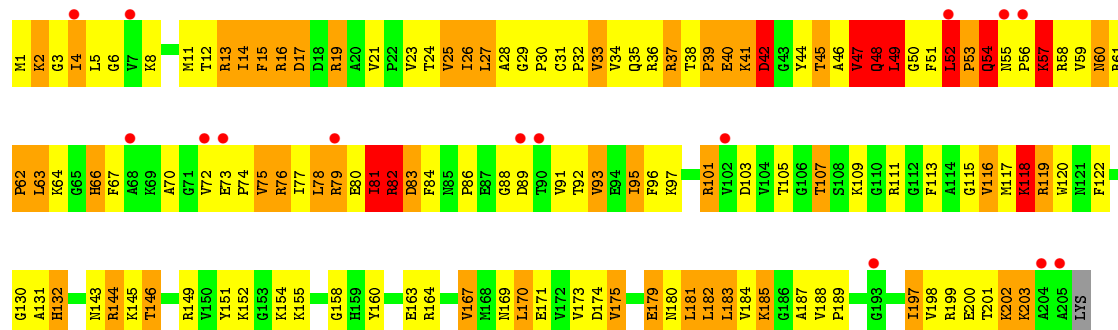




• Molecule 27: 50S ribosomal protein L2

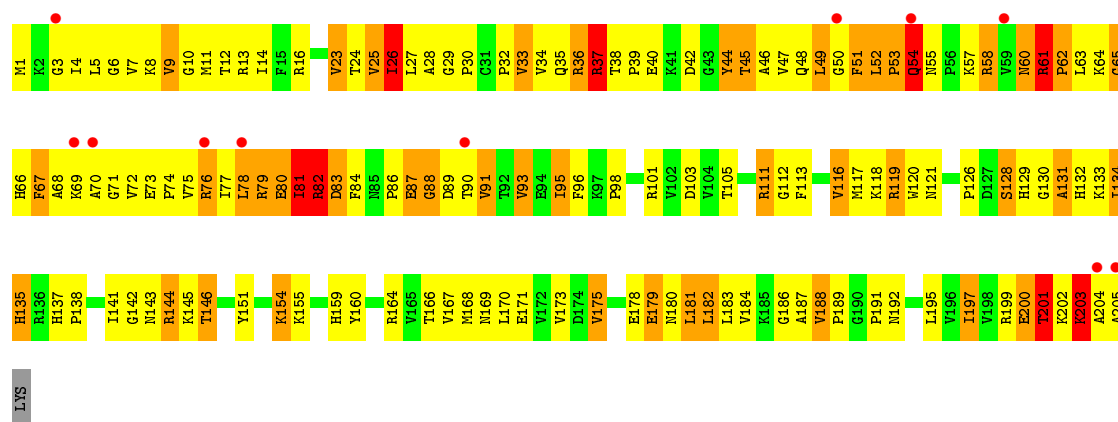


• Molecule 28: 50S ribosomal protein L3

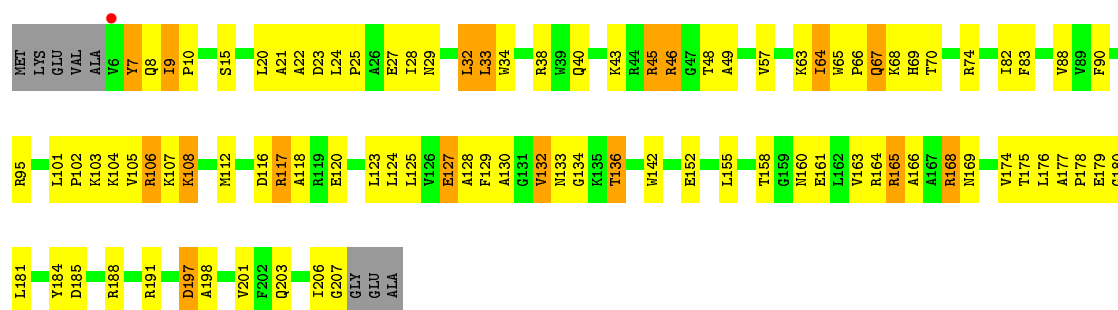


• Molecule 28: 50S ribosomal protein L3

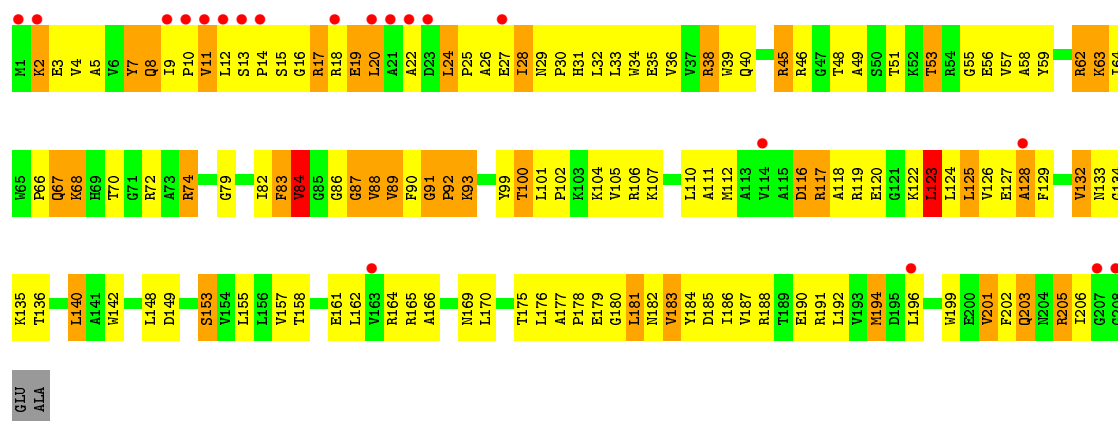




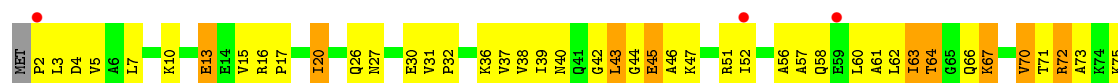
• Molecule 29: 50S ribosomal protein L4

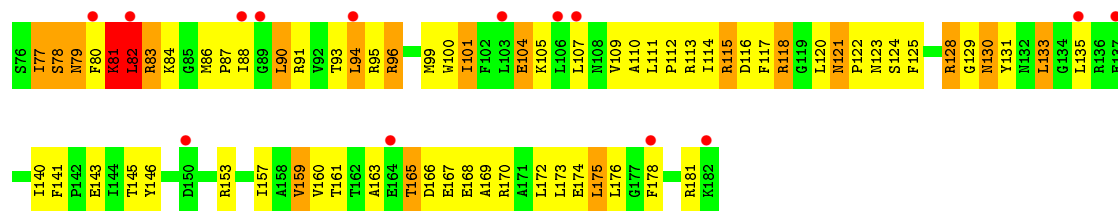


• Molecule 29: 50S ribosomal protein L4

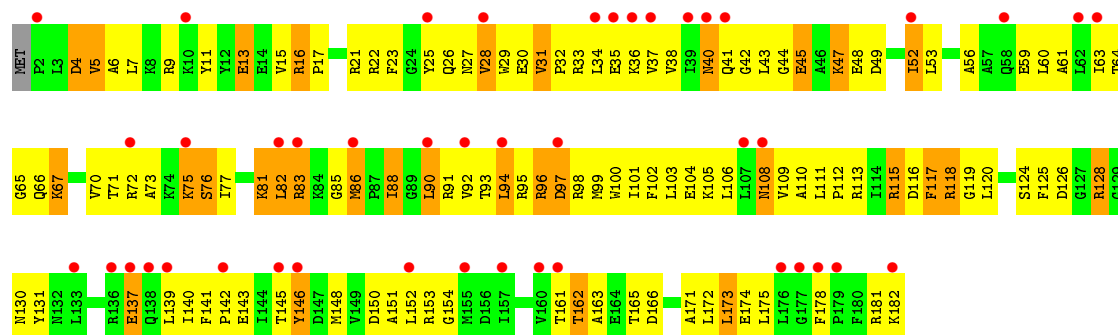


• Molecule 30: 50S ribosomal protein L5

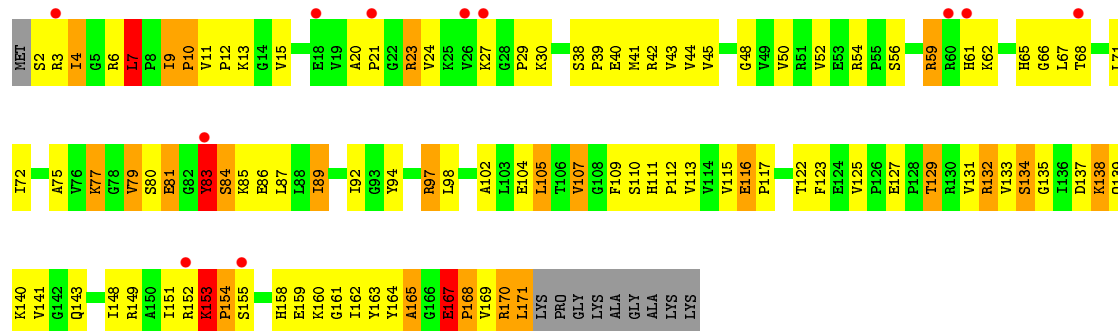




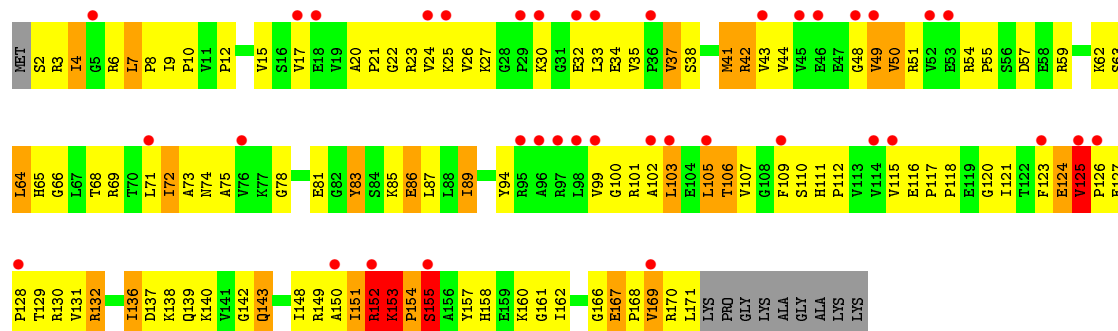
• Molecule 30: 50S ribosomal protein L5



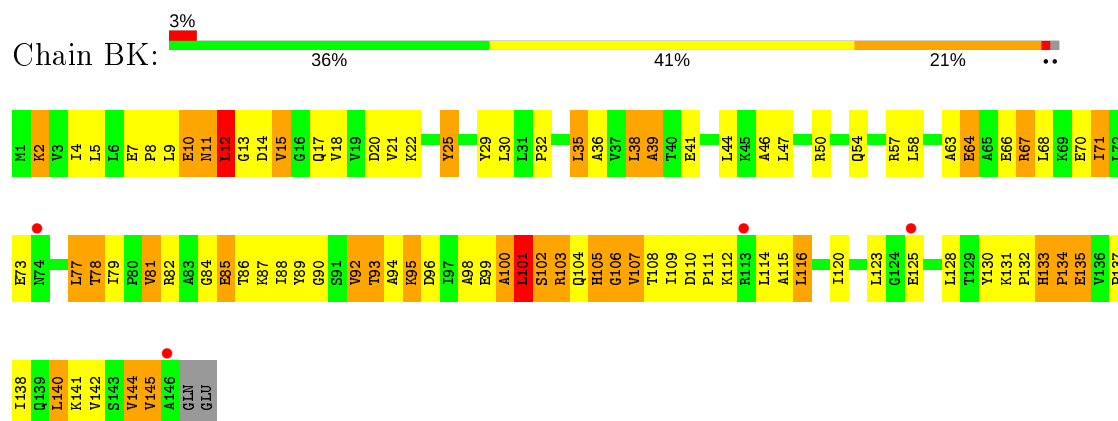
• Molecule 31: 50S ribosomal protein L6



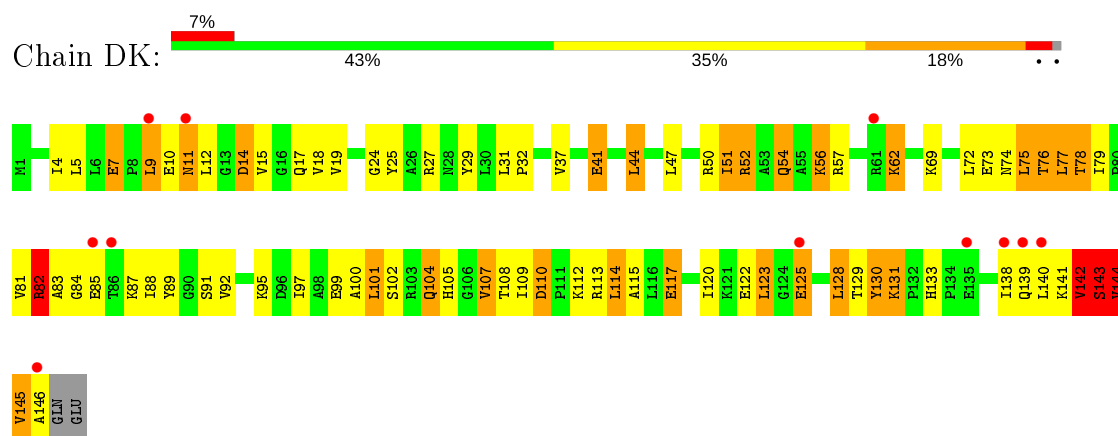
• Molecule 31: 50S ribosomal protein L6



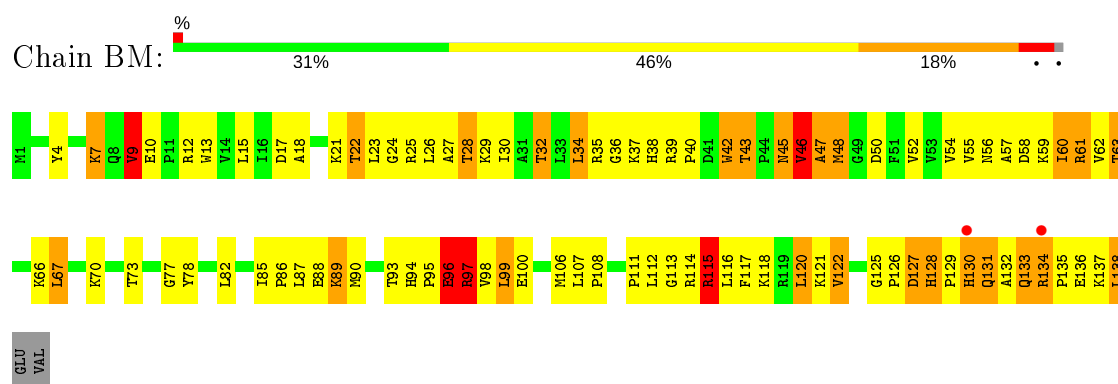
- Molecule 32: 50S ribosomal protein L9



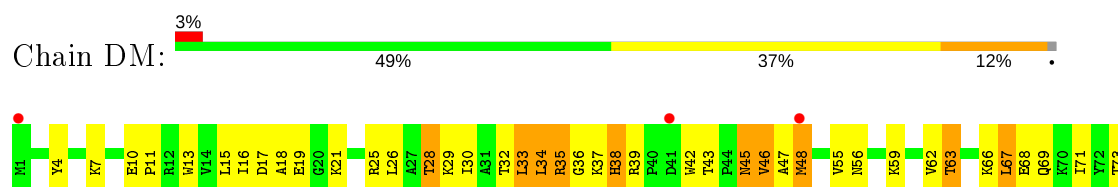
- Molecule 32: 50S ribosomal protein L9



- Molecule 33: 50S ribosomal protein L13



- Molecule 33: 50S ribosomal protein L13





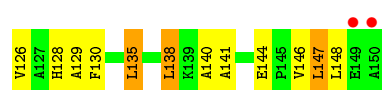
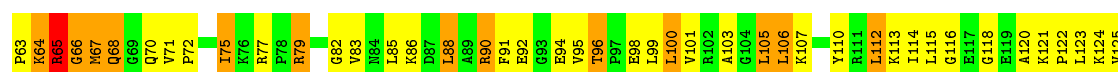
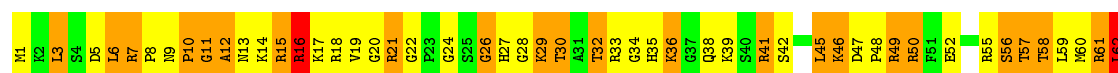
- Molecule 34: 50S ribosomal protein L14



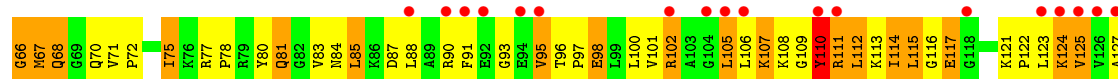
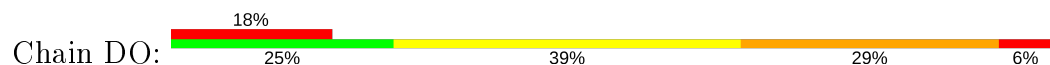
- Molecule 34: 50S ribosomal protein L14



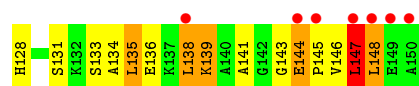
- Molecule 35: 50S ribosomal protein L15



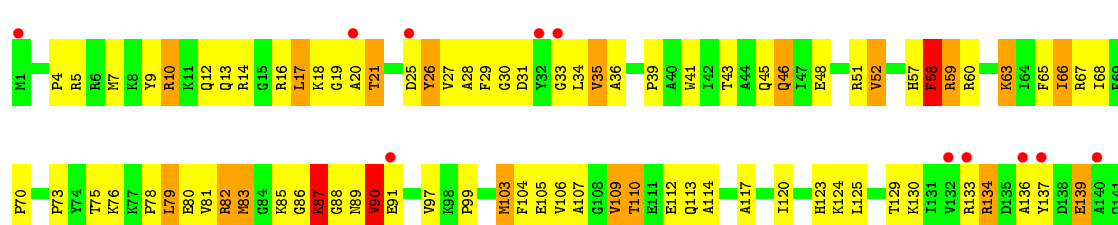
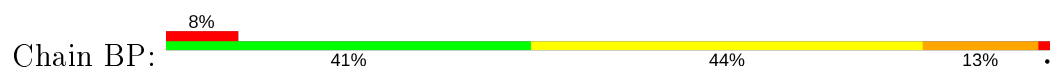
- Molecule 35: 50S ribosomal protein L15



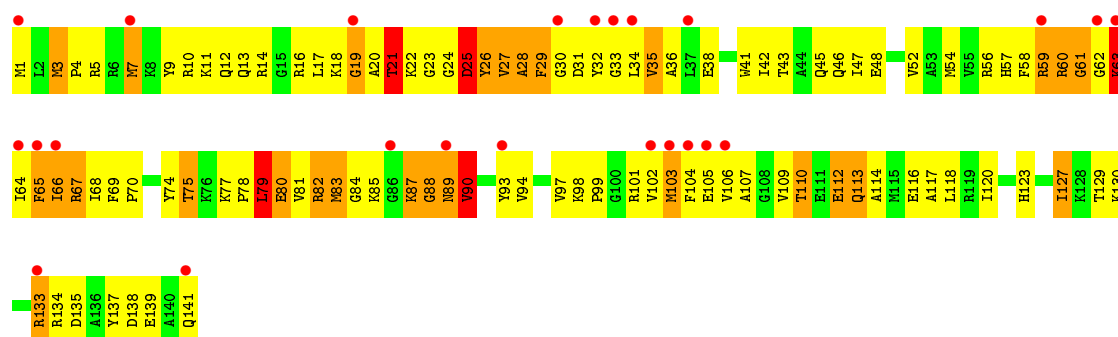




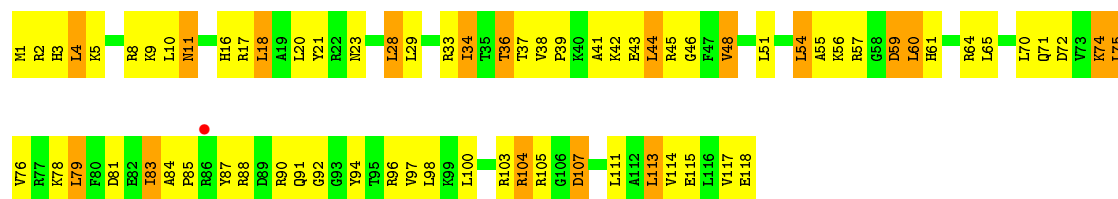
- Molecule 36: 50S ribosomal protein L16



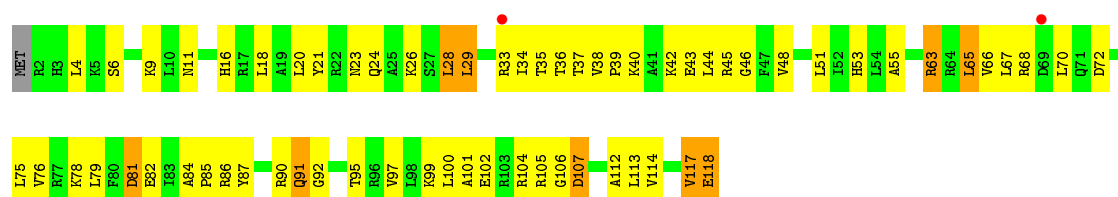
- Molecule 36: 50S ribosomal protein L16



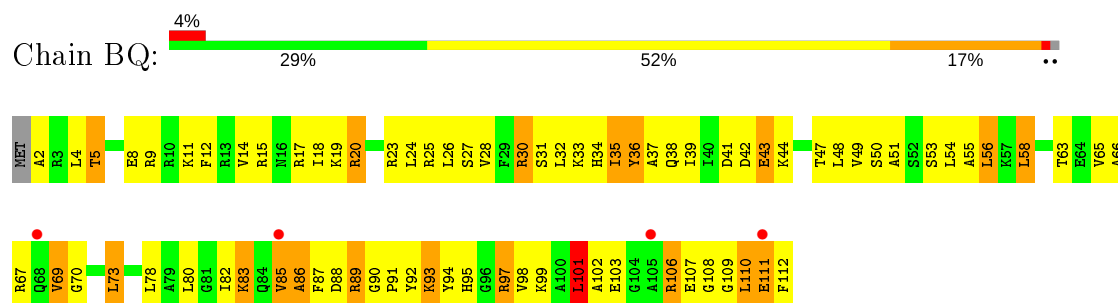
- Molecule 37: 50S ribosomal protein L17



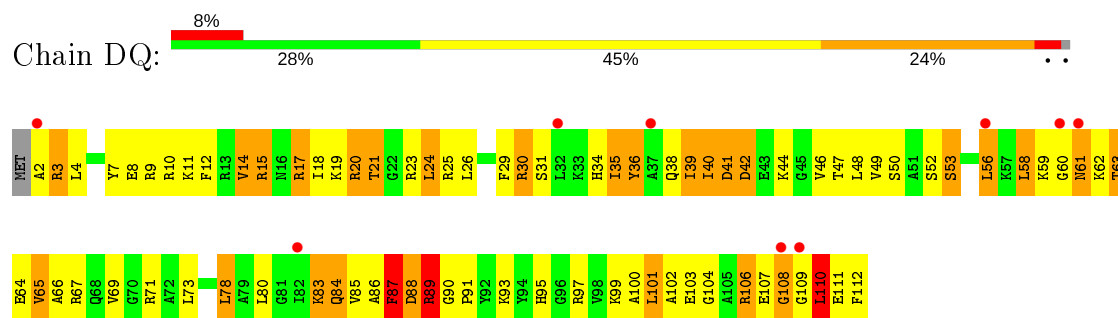
- Molecule 37: 50S ribosomal protein L17



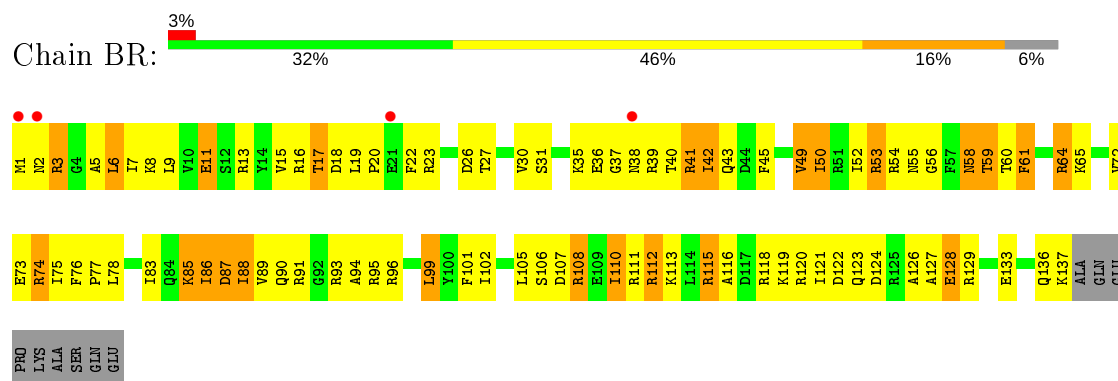
- Molecule 38: 50S ribosomal protein L18



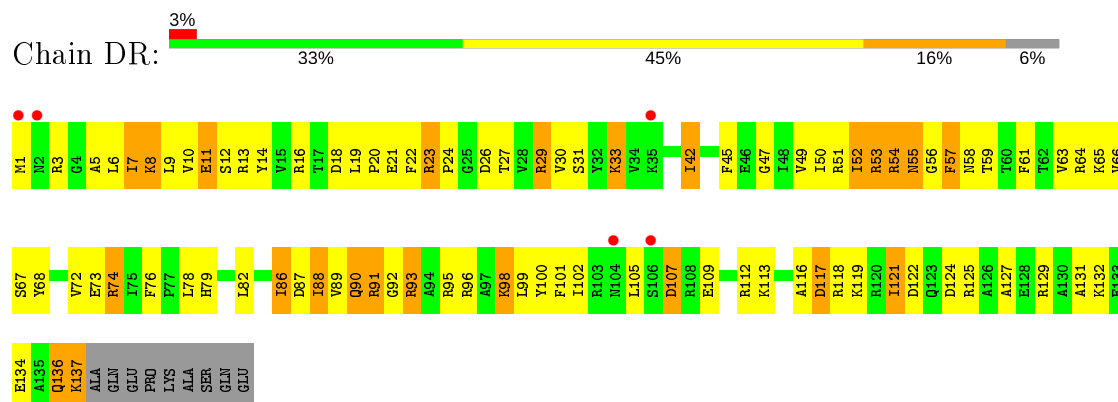
- Molecule 38: 50S ribosomal protein L18



- Molecule 39: 50S ribosomal protein L19



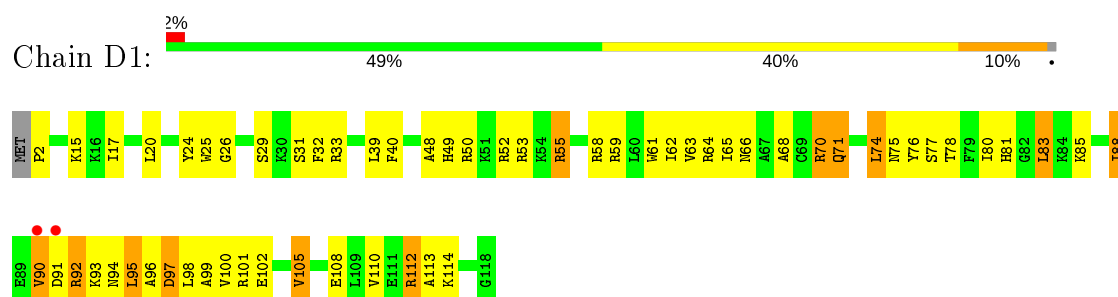
- Molecule 39: 50S ribosomal protein L19



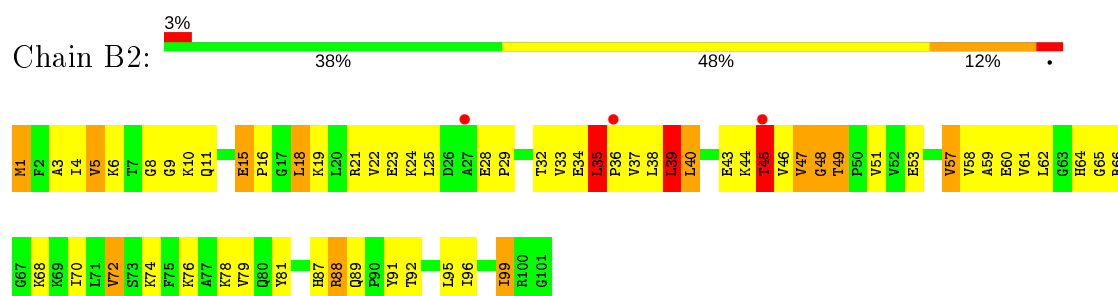
- Molecule 40: 50S ribosomal protein L20

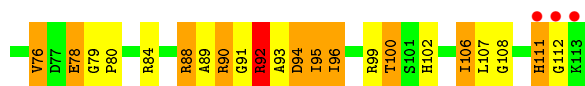


• Molecule 40: 50S ribosomal protein L20



• Molecule 41: 50S ribosomal protein L21

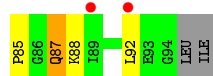




- Molecule 42: 50S ribosomal protein L22



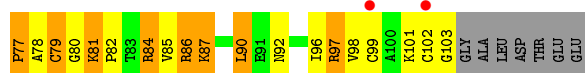
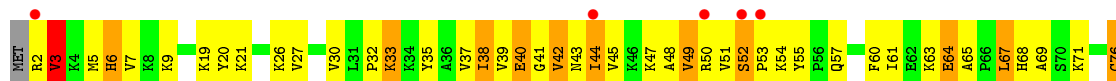
- Molecule 43: 50S ribosomal protein L23



- Molecule 43: 50S ribosomal protein L23

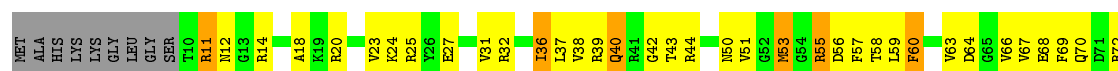


- Molecule 44: 50S ribosomal protein L24



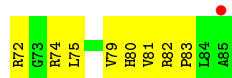
- Molecule 44: 50S ribosomal protein L24



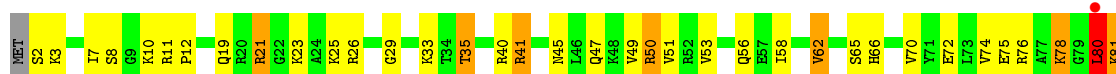




- Molecule 46: 50S ribosomal protein L27



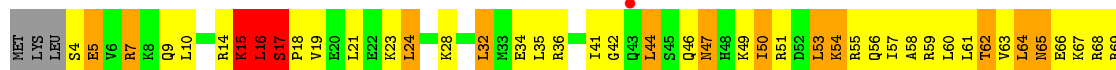
- Molecule 47: 50S ribosomal protein L28



- Molecule 47: 50S ribosomal protein L28

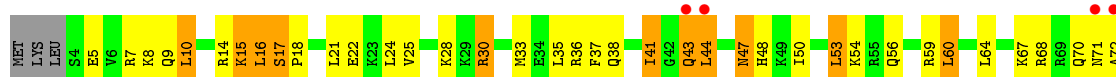


- Molecule 48: 50S ribosomal protein L29

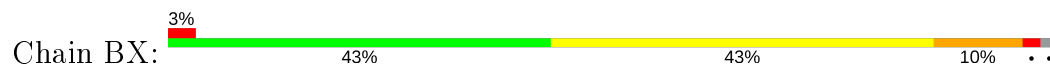


- Molecule 48: 50S ribosomal protein L29

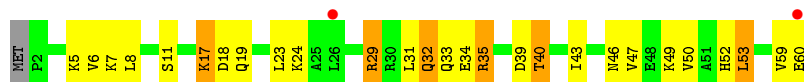




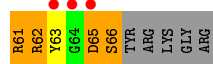
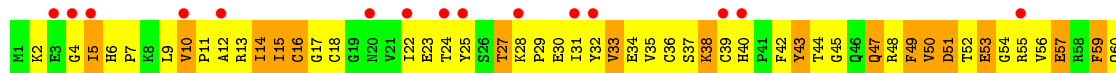
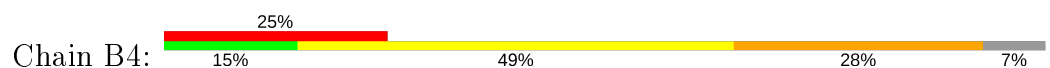
- Molecule 49: 50S ribosomal protein L30



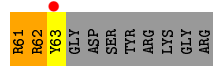
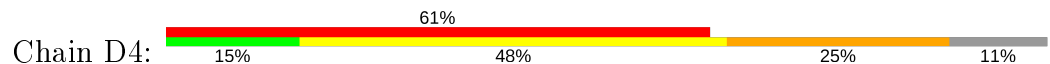
- Molecule 49: 50S ribosomal protein L30



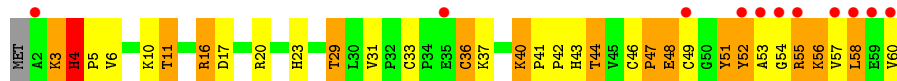
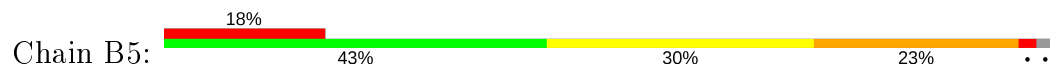
- Molecule 50: 50S ribosomal protein L31



- Molecule 50: 50S ribosomal protein L31

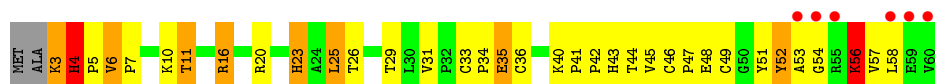


- Molecule 51: 50S ribosomal protein L32

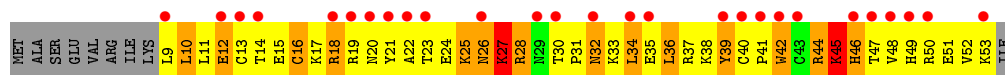


- Molecule 51: 50S ribosomal protein L32

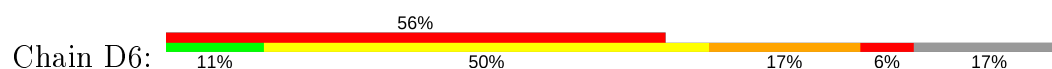




- Molecule 52: 50S ribosomal protein L33



- Molecule 52: 50S ribosomal protein L33



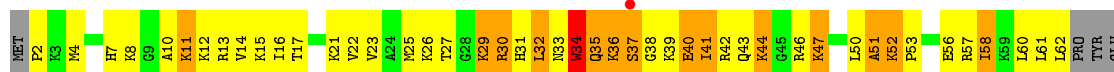
- Molecule 53: 50S ribosomal protein L34



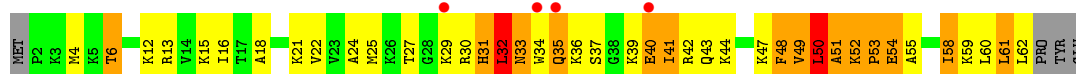
- Molecule 53: 50S ribosomal protein L34



- 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, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 <sup>2</sup> )	77.4	Xtriage
Anisotropy	0.190	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 67.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	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 <sup>2</sup> )	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.*

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	AA	0.44	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%)	9	39
3	AF	203/239 (85%)	179 (88%)	24 (12%)	0	100	100
3	CF	204/239 (85%)	179 (88%)	23 (11%)	2 (1%)	15	53
4	AG	206/208 (99%)	179 (87%)	24 (12%)	3 (2%)	10	42
4	CG	206/208 (99%)	179 (87%)	25 (12%)	2 (1%)	15	53
5	AH	149/162 (92%)	137 (92%)	10 (7%)	2 (1%)	12	45
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%)	22	60
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	16
11	AN	117/129 (91%)	102 (87%)	14 (12%)	1 (1%)	17	55
11	CN	117/129 (91%)	104 (89%)	13 (11%)	0	100	100
12	AO	123/132 (93%)	105 (85%)	16 (13%)	2 (2%)	9	40
12	CO	123/132 (93%)	105 (85%)	15 (12%)	3 (2%)	6	29
13	AP	114/126 (90%)	89 (78%)	23 (20%)	2 (2%)	8	37
13	CP	115/126 (91%)	96 (84%)	17 (15%)	2 (2%)	9	39
14	AQ	58/61 (95%)	49 (84%)	9 (16%)	0	100	100
14	CQ	58/61 (95%)	49 (84%)	8 (14%)	1 (2%)	9	39
15	AR	86/89 (97%)	74 (86%)	11 (13%)	1 (1%)	13	48
15	CR	86/89 (97%)	76 (88%)	10 (12%)	0	100	100
16	AS	82/88 (93%)	71 (87%)	8 (10%)	3 (4%)	3	19
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%)	11	43
18	CU	70/88 (80%)	61 (87%)	9 (13%)	0	100	100
19	AV	76/93 (82%)	68 (90%)	6 (8%)	2 (3%)	5	27
19	CV	76/93 (82%)	60 (79%)	12 (16%)	4 (5%)	2	11
20	AW	97/106 (92%)	84 (87%)	13 (13%)	0	100	100
20	CW	97/106 (92%)	80 (82%)	16 (16%)	1 (1%)	15	53
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%)	8	36
27	DD	270/276 (98%)	248 (92%)	15 (6%)	7 (3%)	5	27
28	BE	203/206 (98%)	149 (73%)	30 (15%)	24 (12%)	0	1
28	DE	203/206 (98%)	144 (71%)	41 (20%)	18 (9%)	1	3
29	BF	200/210 (95%)	179 (90%)	21 (10%)	0	100	100
29	DF	206/210 (98%)	168 (82%)	30 (15%)	8 (4%)	3	17
30	BG	179/182 (98%)	154 (86%)	20 (11%)	5 (3%)	5	25
30	DG	179/182 (98%)	150 (84%)	28 (16%)	1 (1%)	25	64

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	BH	168/180 (93%)	133 (79%)	28 (17%)	7 (4%)	3	16
31	DH	168/180 (93%)	125 (74%)	35 (21%)	8 (5%)	2	13
32	BK	144/148 (97%)	102 (71%)	32 (22%)	10 (7%)	1	6
32	DK	144/148 (97%)	113 (78%)	28 (19%)	3 (2%)	7	33
33	BM	136/140 (97%)	113 (83%)	16 (12%)	7 (5%)	2	12
33	DM	136/140 (97%)	119 (88%)	15 (11%)	2 (2%)	10	42
34	BN	120/122 (98%)	111 (92%)	9 (8%)	0	100	100
34	DN	120/122 (98%)	113 (94%)	6 (5%)	1 (1%)	19	57
35	BO	148/150 (99%)	107 (72%)	27 (18%)	14 (10%)	0	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%)	6	31
36	DP	139/141 (99%)	93 (67%)	30 (22%)	16 (12%)	0	2
37	B0	116/118 (98%)	101 (87%)	13 (11%)	2 (2%)	9	39
37	D0	115/118 (98%)	109 (95%)	6 (5%)	0	100	100
38	BQ	109/112 (97%)	86 (79%)	20 (18%)	3 (3%)	5	25
38	DQ	109/112 (97%)	87 (80%)	19 (17%)	3 (3%)	5	25
39	BR	135/146 (92%)	114 (84%)	21 (16%)	0	100	100
39	DR	135/146 (92%)	119 (88%)	14 (10%)	2 (2%)	10	42
40	B1	115/118 (98%)	103 (90%)	11 (10%)	1 (1%)	17	55
40	D1	115/118 (98%)	101 (88%)	14 (12%)	0	100	100
41	B2	99/101 (98%)	92 (93%)	5 (5%)	2 (2%)	7	34
41	D2	99/101 (98%)	78 (79%)	14 (14%)	7 (7%)	1	5
42	BS	111/113 (98%)	97 (87%)	10 (9%)	4 (4%)	3	19
42	DS	111/113 (98%)	103 (93%)	8 (7%)	0	100	100
43	BT	90/96 (94%)	84 (93%)	4 (4%)	2 (2%)	6	31
43	DT	90/96 (94%)	78 (87%)	10 (11%)	2 (2%)	6	31
44	BU	100/110 (91%)	80 (80%)	15 (15%)	5 (5%)	2	12
44	DU	100/110 (91%)	70 (70%)	24 (24%)	6 (6%)	1	9
45	BV	173/206 (84%)	129 (75%)	37 (21%)	7 (4%)	3	17
45	DV	177/206 (86%)	132 (75%)	35 (20%)	10 (6%)	2	10
46	B3	74/85 (87%)	67 (90%)	5 (7%)	2 (3%)	5	26

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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	22
47	DZ	95/98 (97%)	84 (88%)	10 (10%)	1 (1%)	14	50
48	BW	64/72 (89%)	58 (91%)	4 (6%)	2 (3%)	4	23
48	DW	67/72 (93%)	60 (90%)	6 (9%)	1 (2%)	10	42
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	23
50	D4	61/71 (86%)	32 (52%)	28 (46%)	1 (2%)	9	40
51	B5	57/60 (95%)	49 (86%)	7 (12%)	1 (2%)	8	37
51	D5	56/60 (93%)	48 (86%)	7 (12%)	1 (2%)	8	37
52	B6	43/54 (80%)	27 (63%)	14 (33%)	2 (5%)	2	14
52	D6	43/54 (80%)	29 (67%)	10 (23%)	4 (9%)	0	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	1
All	All	11335/12052 (94%)	9588 (85%)	1457 (13%)	290 (3%)	5	27

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%)	0	3
2	CE	205/220 (93%)	159 (78%)	46 (22%)	1	4
3	AF	159/188 (85%)	120 (76%)	39 (24%)	0	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	4
5	AH	116/123 (94%)	88 (76%)	28 (24%)	0	3
5	CH	116/123 (94%)	89 (77%)	27 (23%)	1	4
6	AI	90/90 (100%)	76 (84%)	14 (16%)	2	13
6	CI	90/90 (100%)	74 (82%)	16 (18%)	2	9
7	AJ	126/127 (99%)	104 (82%)	22 (18%)	2	10
7	CJ	126/127 (99%)	89 (71%)	37 (29%)	0	1
8	AK	119/119 (100%)	100 (84%)	19 (16%)	2	12
8	CK	119/119 (100%)	94 (79%)	25 (21%)	1	5
9	AL	98/99 (99%)	70 (71%)	28 (29%)	0	2
9	CL	98/99 (99%)	69 (70%)	29 (30%)	0	1
10	AM	89/92 (97%)	66 (74%)	23 (26%)	0	2
10	CM	89/92 (97%)	60 (67%)	29 (33%)	0	1
11	AN	90/99 (91%)	74 (82%)	16 (18%)	2	9
11	CN	90/99 (91%)	73 (81%)	17 (19%)	1	8
12	AO	104/109 (95%)	88 (85%)	16 (15%)	2	13
12	CO	104/109 (95%)	80 (77%)	24 (23%)	1	4
13	AP	94/101 (93%)	71 (76%)	23 (24%)	0	3
13	CP	94/101 (93%)	75 (80%)	19 (20%)	1	6
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%)	3	16
15	CR	79/80 (99%)	66 (84%)	13 (16%)	2	11
16	AS	72/74 (97%)	53 (74%)	19 (26%)	0	2
16	CS	72/74 (97%)	62 (86%)	10 (14%)	3	16
17	AT	95/97 (98%)	82 (86%)	13 (14%)	3	17
17	CT	95/97 (98%)	89 (94%)	6 (6%)	18	51

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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%)	0	3
19	AV	67/80 (84%)	47 (70%)	20 (30%)	0	1
19	CV	67/80 (84%)	53 (79%)	14 (21%)	1	5
20	AW	76/82 (93%)	60 (79%)	16 (21%)	1	5
20	CW	76/82 (93%)	55 (72%)	21 (28%)	0	2
21	AX	20/22 (91%)	17 (85%)	3 (15%)	3	14
21	CX	20/22 (91%)	20 (100%)	0	100	100
27	BD	214/218 (98%)	172 (80%)	42 (20%)	1	7
27	DD	214/218 (98%)	162 (76%)	52 (24%)	0	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	2
30	BG	155/156 (99%)	115 (74%)	40 (26%)	0	2
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	9
34	BN	100/100 (100%)	83 (83%)	17 (17%)	2	10
34	DN	100/100 (100%)	78 (78%)	22 (22%)	1	4
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%)	0	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	1
40	B1	93/94 (99%)	76 (82%)	17 (18%)	1	9
40	D1	93/94 (99%)	80 (86%)	13 (14%)	3	16
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	3
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	5
46	B3	61/67 (91%)	54 (88%)	7 (12%)	5	24
46	D3	62/67 (92%)	47 (76%)	15 (24%)	0	3
47	BZ	82/83 (99%)	64 (78%)	18 (22%)	1	4
47	DZ	82/83 (99%)	64 (78%)	18 (22%)	1	4
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	7
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	1
53	B7	42/42 (100%)	34 (81%)	8 (19%)	1	8
53	D7	42/42 (100%)	32 (76%)	10 (24%)	0	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	7
All	All	9579/9996 (96%)	7317 (76%)	2262 (24%)	1	3

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	AA	1506/1506 (100%)	-0.57	5 (0%) 94 84	50, 98, 179, 234	0
1	CA	1506/1506 (100%)	-0.56	4 (0%) 94 84	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%) 17 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%) 18 5	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 69	94, 116, 128, 136	0
9	AL	127/128 (99%)	-0.31	1 (0%) 86 65	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 1	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 <sup>2</sup> )	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 1	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 15	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 1	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 54	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 65	66, 91, 110, 169	0
26	DB	122/122 (100%)	-0.47	1 (0%) 86 65	84, 120, 141, 189	0
27	BD	272/276 (98%)	0.09	1 (0%) 92 79	35, 57, 79, 96	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	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%) 25 9	52, 88, 137, 159	0
29	BF	202/210 (96%)	-0.13	1 (0%) 91 75	38, 70, 108, 123	0
29	DF	208/210 (99%)	0.59	20 (9%) 8 2	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%) 18 5	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 65	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 65	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 3	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 40	54, 69, 104, 148	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	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%) 25 9	64, 80, 104, 121	0
44	BU	102/110 (92%)	0.37	7 (6%) 16 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 14	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 7	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 14	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 5	65, 79, 94, 123	0
All	All	21104/21634 (97%)	0.11	1258 (5%) 21 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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
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( $\text{\AA}^2$ )	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( $\text{\AA}^2$ )	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( $\text{\AA}^2$ )	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( $\text{\AA}^2$ )	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( $\text{\AA}^2$ )	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( $\text{\AA}^2$ )	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( $\text{\AA}^2$ )	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( $\text{\AA}^2$ )	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( $\text{\AA}^2$ )	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( $\text{\AA}^2$ )	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( $\text{\AA}^2$ )	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( $\text{\AA}^2$ )	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( $\text{\AA}^2$ )	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( $\text{\AA}^2$ )	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( $\text{\AA}^2$ )	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( $\text{\AA}^2$ )	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( $\text{\AA}^2$ )	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( $\text{\AA}^2$ )	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( $\text{\AA}^2$ )	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( $\text{\AA}^2$ )	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( $\text{\AA}^2$ )	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( $\text{\AA}^2$ )	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( $\text{\AA}^2$ )	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( $\text{\AA}^2$ )	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( $\text{\AA}^2$ )	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( $\text{\AA}^2$ )	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( $\text{\AA}^2$ )	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( $\text{\AA}^2$ )	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( $\text{\AA}^2$ )	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( $\text{\AA}^2$ )	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( $\text{\AA}^2$ )	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( $\text{\AA}^2$ )	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( $\text{\AA}^2$ )	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( $\text{\AA}^2$ )	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( $\text{\AA}^2$ )	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( $\text{\AA}^2$ )	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( $\text{\AA}^2$ )	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( $\text{\AA}^2$ )	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( $\text{\AA}^2$ )	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( $\text{\AA}^2$ )	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.