wwPDB X-ray Structure Validation Summary Report ⓘ

May 21, 2020 – 04:14 am BST

PDB ID	:	4V8D
Title	:	Structure analysis of ribosomal decoding (cognate tRNA-tyr complex).
Authors	:	Jenner, L.; Demeshkina, N.; Yusupov, M.; Yusupova, G.
Deposited on	:	2011-12-07
Resolution	:	3.00 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

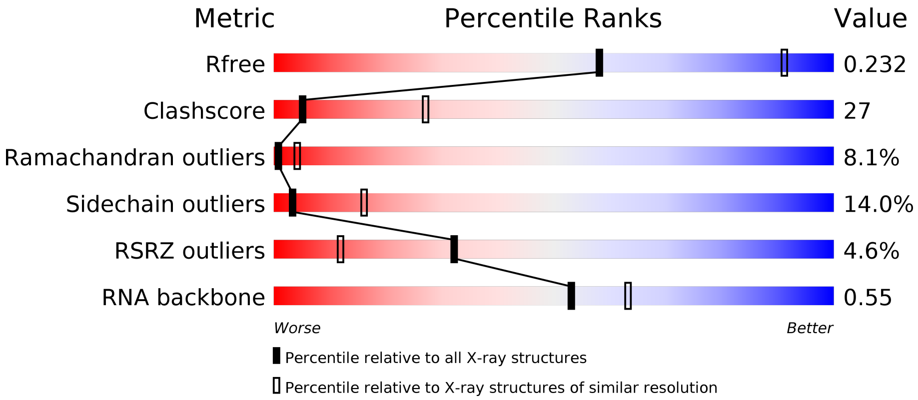
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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

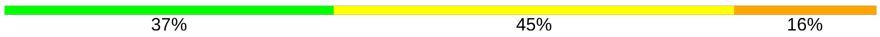
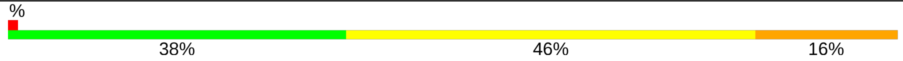
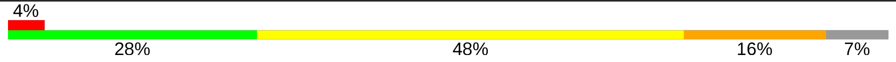
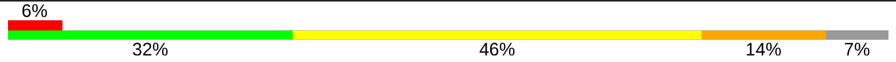
The reported resolution of this entry is 3.00 Å.

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 >=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 <=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	
1	CA	1506	
2	AE	256	
2	CE	256	

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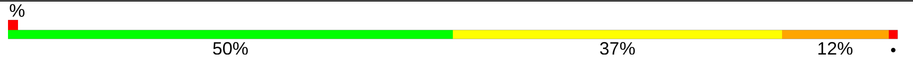
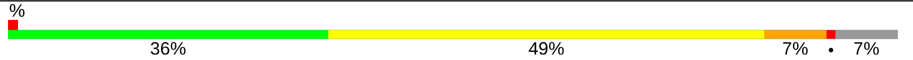
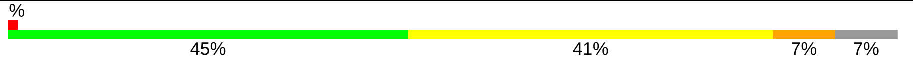
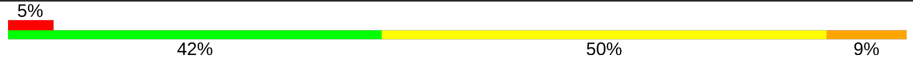
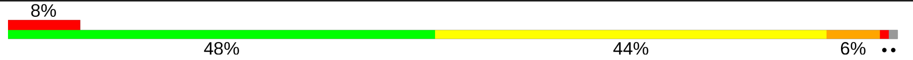
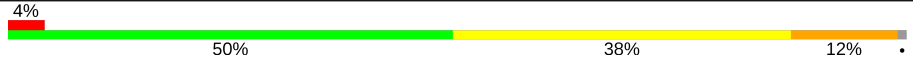
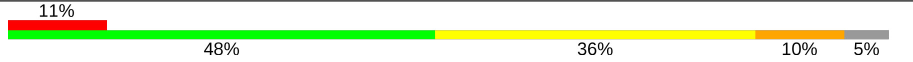
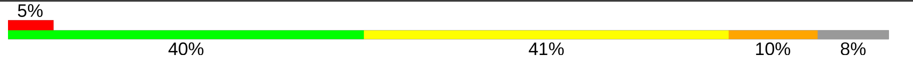
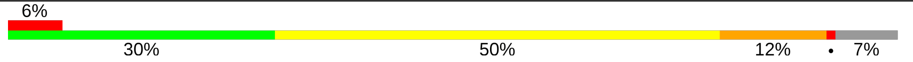
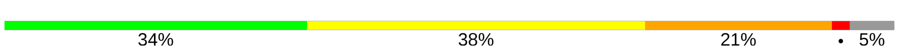
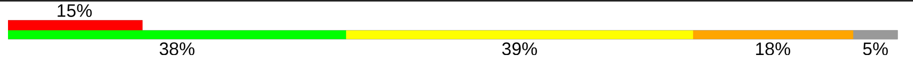
Mol	Chain	Length	Quality of chain
3	AF	239	
3	CF	239	
4	AG	208	
4	CG	208	
5	AH	162	
5	CH	162	
6	AI	101	
6	CI	101	
7	AJ	156	
7	CJ	156	
8	AK	138	
8	CK	138	
9	AL	128	
9	CL	128	
10	AM	105	
10	CM	105	
11	AN	129	
11	CN	129	
12	AO	132	
12	CO	132	
13	AP	126	
13	CP	126	
14	AQ	61	
14	CQ	61	
15	AR	89	

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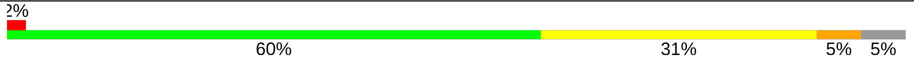
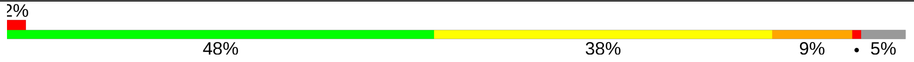
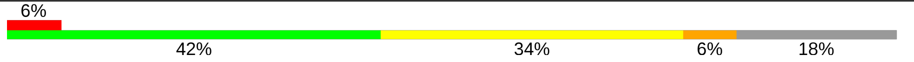
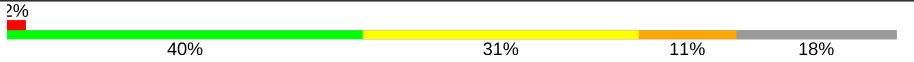
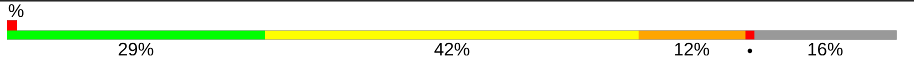
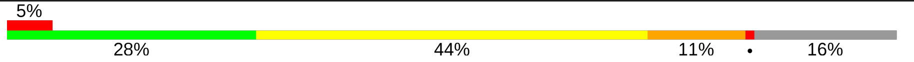
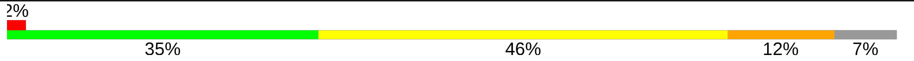
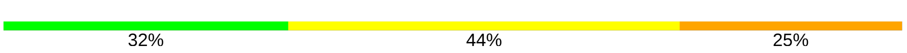
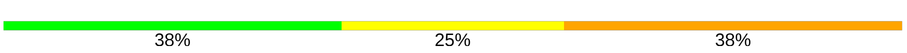
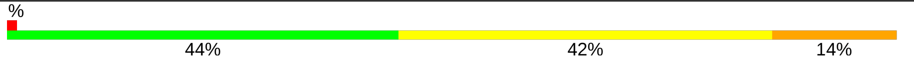
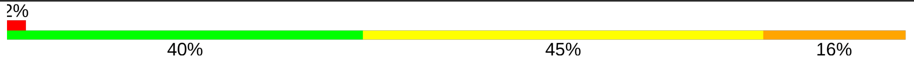
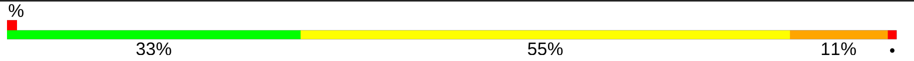
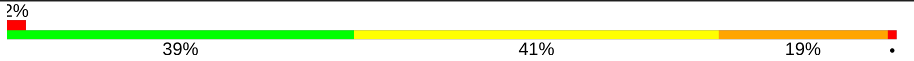
Mol	Chain	Length	Quality of chain
15	CR	89	
16	AS	88	
16	CS	88	
17	AT	105	
17	CT	105	
18	AU	88	
18	CU	88	
19	AV	93	
19	CV	93	
20	AW	106	
20	CW	106	
21	AX	27	
21	CX	27	
22	AB	85	
22	AD	85	
22	CB	85	
22	CD	85	
23	AC	77	
23	CC	77	
24	A1	16	
24	C1	16	
25	BA	2912	
25	DA	2912	
26	BB	122	
26	DB	122	

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Mol	Chain	Length	Quality of chain
27	BD	276	46% 42% 9% • •
27	DD	276	48% 41% 8% • •
28	BE	206	2% 43% 37% 18% •
28	DE	206	4% 30% 49% 19% •
29	BF	210	% 49% 40% 7% •
29	DF	210	10% 38% 42% 18% • •
30	BG	182	19% 35% 53% 12% •
30	DG	182	4% 41% 47% 11% • •
31	BH	180	2% 33% 40% 18% • 6%
31	DH	180	31% 38% 42% 13% • 6%
32	BK	148	5% 31% 46% 20% • •
32	DK	148	% 39% 47% 13% •
33	BM	140	% 46% 39% 13% • •
33	DM	140	% 36% 45% 16% • •
34	BN	122	57% 37% 7%
34	DN	122	52% 38% 10% •
35	BO	150	5% 35% 37% 24% •
35	DO	150	15% 29% 38% 23% 9%
36	BP	141	4% 38% 43% 17% •
36	DP	141	10% 25% 54% 18% •
37	B0	118	40% 46% 13% •
37	D0	118	% 39% 49% 10% • •
38	BQ	112	9% 38% 48% 13% •
38	DQ	112	5% 39% 46% 13% • •
39	BR	146	3% 34% 45% 15% • 6%

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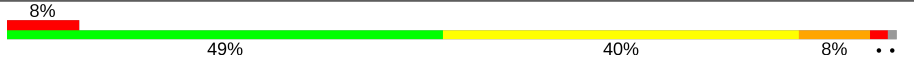
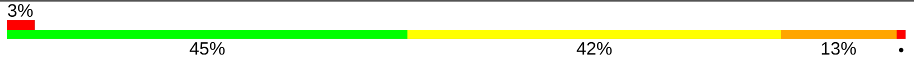
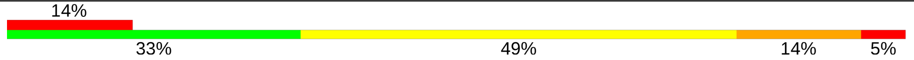
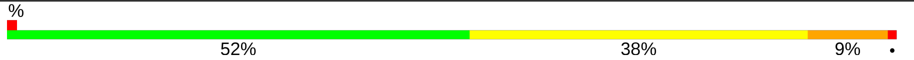
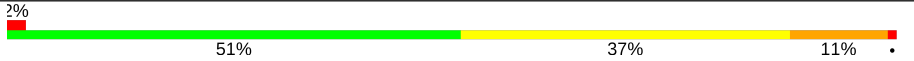
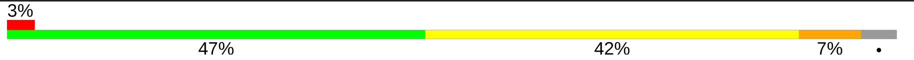
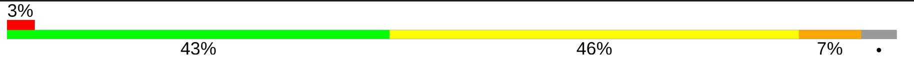
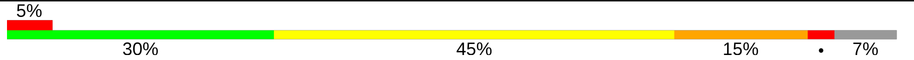
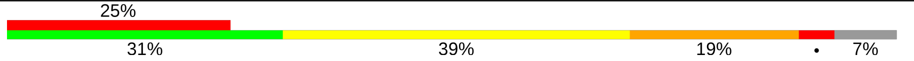
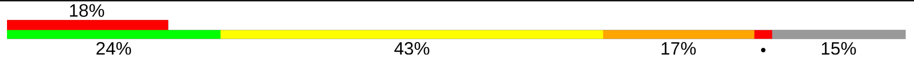
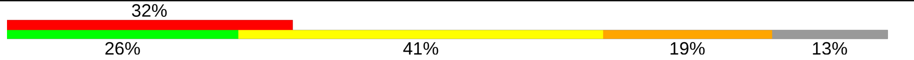
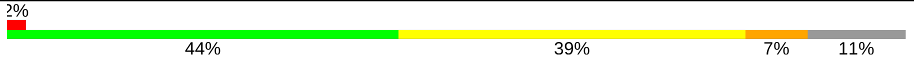
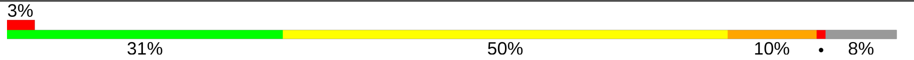
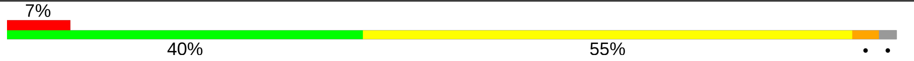
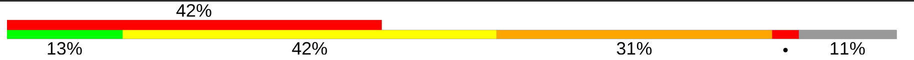
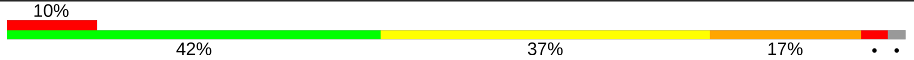
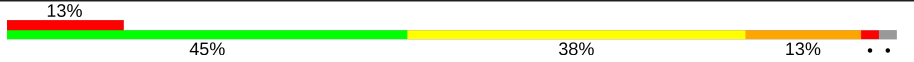
Mol	Chain	Length	Quality of chain
39	DR	146	
40	B1	118	
40	D1	118	
41	B2	101	
41	D2	101	
42	BS	113	
42	DS	113	
43	BT	96	
43	DT	96	
44	BU	110	
44	DU	110	
45	BV	206	
45	DV	206	
46	B3	85	
46	D3	85	
47	BZ	98	
47	DZ	98	
48	BW	72	
48	DW	72	
49	BX	60	
49	DX	60	
50	B4	71	
50	D4	71	
51	B5	60	
51	D5	60	

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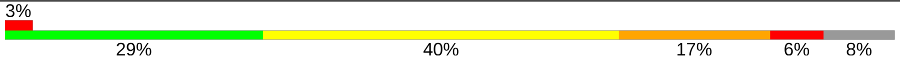
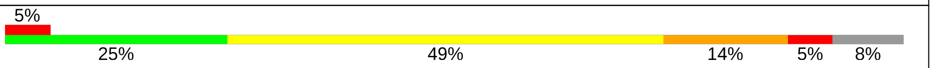
Mol	Chain	Length	Quality of chain
52	B6	54	
52	D6	54	
53	B7	49	
53	D7	49	
54	B8	65	
54	D8	65	

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	1613	-	-	-	X
55	MG	AA	1643	-	-	-	X
55	MG	AA	1666	-	-	-	X
55	MG	AA	1683	-	-	-	X
55	MG	AA	1726	-	-	-	X
55	MG	AA	1728	-	-	-	X
55	MG	AA	1736	-	-	-	X
55	MG	AA	1750	-	-	-	X
55	MG	AA	1758	-	-	-	X
55	MG	AA	1768	-	-	-	X
55	MG	AA	1772	-	-	-	X
55	MG	AA	1775	-	-	-	X
55	MG	AA	1785	-	-	-	X
55	MG	AA	1791	-	-	-	X
55	MG	AA	1800	-	-	-	X
55	MG	AA	1804	-	-	-	X
55	MG	AA	1805	-	-	-	X
55	MG	AA	1806	-	-	-	X
55	MG	AA	1809	-	-	-	X
55	MG	AA	1815	-	-	-	X
55	MG	AA	1818	-	-	-	X
55	MG	AC	107	-	-	-	X
55	MG	BA	3041	-	-	-	X
55	MG	BA	3069	-	-	-	X
55	MG	BA	3078	-	-	-	X
55	MG	BA	3100	-	-	-	X
55	MG	BA	3122	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	BA	3137	-	-	-	X
55	MG	BA	3155	-	-	-	X
55	MG	BA	3171	-	-	-	X
55	MG	BA	3189	-	-	-	X
55	MG	BA	3192	-	-	-	X
55	MG	BA	3195	-	-	-	X
55	MG	BA	3209	-	-	-	X
55	MG	BA	3222	-	-	-	X
55	MG	BA	3245	-	-	-	X
55	MG	BA	3263	-	-	-	X
55	MG	BA	3266	-	-	-	X
55	MG	BA	3274	-	-	-	X
55	MG	BA	3300	-	-	-	X
55	MG	BA	3309	-	-	-	X
55	MG	BA	3323	-	-	-	X
55	MG	BA	3324	-	-	-	X
55	MG	BA	3333	-	-	-	X
55	MG	BA	3344	-	-	-	X
55	MG	BA	3353	-	-	-	X
55	MG	BA	3372	-	-	-	X
55	MG	BA	3373	-	-	-	X
55	MG	BA	3380	-	-	-	X
55	MG	BA	3382	-	-	-	X
55	MG	BA	3386	-	-	-	X
55	MG	BA	3391	-	-	-	X
55	MG	BA	3396	-	-	-	X
55	MG	BA	3406	-	-	-	X
55	MG	BA	3413	-	-	-	X
55	MG	BA	3421	-	-	-	X
55	MG	BA	3422	-	-	-	X
55	MG	BA	3426	-	-	-	X
55	MG	BA	3429	-	-	-	X
55	MG	BA	3433	-	-	-	X
55	MG	BA	3438	-	-	-	X
55	MG	BA	3440	-	-	-	X
55	MG	BA	3446	-	-	-	X
55	MG	BA	3451	-	-	-	X
55	MG	BA	3455	-	-	-	X
55	MG	BA	3456	-	-	-	X
55	MG	BA	3463	-	-	-	X
55	MG	BA	3472	-	-	-	X
55	MG	BA	3477	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	BA	3479	-	-	-	X
55	MG	BA	3487	-	-	-	X
55	MG	BA	3503	-	-	-	X
55	MG	BA	3504	-	-	-	X
55	MG	BA	3509	-	-	-	X
55	MG	BA	3510	-	-	-	X
55	MG	BA	3537	-	-	-	X
55	MG	BA	3540	-	-	-	X
55	MG	BA	3546	-	-	-	X
55	MG	BA	3550	-	-	-	X
55	MG	BB	203	-	-	-	X
55	MG	BB	208	-	-	-	X
55	MG	CA	1673	-	-	-	X
55	MG	CA	1678	-	-	-	X
55	MG	CA	1701	-	-	-	X
55	MG	CA	1722	-	-	-	X
55	MG	CA	1736	-	-	-	X
55	MG	CA	1740	-	-	-	X
55	MG	CA	1742	-	-	-	X
55	MG	CA	1759	-	-	-	X
55	MG	CA	1761	-	-	-	X
55	MG	CA	1762	-	-	-	X
55	MG	CA	1768	-	-	-	X
55	MG	CA	1773	-	-	-	X
55	MG	CA	1790	-	-	-	X
55	MG	CA	1804	-	-	-	X
55	MG	CA	1808	-	-	-	X
55	MG	CA	1812	-	-	-	X
55	MG	CA	1817	-	-	-	X
55	MG	CA	1819	-	-	-	X
55	MG	CB	103	-	-	-	X
55	MG	CK	201	-	-	-	X
55	MG	CR	101	-	-	-	X
55	MG	DA	3054	-	-	-	X
55	MG	DA	3085	-	-	-	X
55	MG	DA	3099	-	-	-	X
55	MG	DA	3100	-	-	-	X
55	MG	DA	3120	-	-	-	X
55	MG	DA	3172	-	-	-	X
55	MG	DA	3176	-	-	-	X
55	MG	DA	3207	-	-	-	X
55	MG	DA	3221	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	DA	3225	-	-	-	X
55	MG	DA	3227	-	-	-	X
55	MG	DA	3228	-	-	-	X
55	MG	DA	3238	-	-	-	X
55	MG	DA	3262	-	-	-	X
55	MG	DA	3279	-	-	-	X
55	MG	DA	3291	-	-	-	X
55	MG	DA	3330	-	-	-	X
55	MG	DA	3336	-	-	-	X
55	MG	DA	3342	-	-	-	X
55	MG	DA	3358	-	-	-	X
55	MG	DA	3365	-	-	-	X
55	MG	DA	3372	-	-	-	X
55	MG	DA	3382	-	-	-	X
55	MG	DA	3399	-	-	-	X
55	MG	DA	3409	-	-	-	X
55	MG	DA	3423	-	-	-	X
55	MG	DA	3425	-	-	-	X
55	MG	DA	3446	-	-	-	X
55	MG	DB	210	-	-	-	X

2 Entry composition

There are 56 unique types of molecules in this entry. The entry contains 299676 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	1502	Total 32284	C 14370	N 5982	O 10431	P 1501	0	0	0
1	CA	1502	Total 32287	C 14370	N 5982	O 10433	P 1502	0	0	0

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

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

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

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

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

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

- 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 1155 729 218 204 4	0	0	0
5	CH	151	Total C N O S 1155 729 218 204 4	0	0	0

- 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 843 531 155 154 3	0	0	0
6	CI	101	Total C N O S 843 531 155 154 3	0	0	0

- 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 1257 781 252 218 6	0	0	0
7	CJ	155	Total C N O S 1257 781 252 218 6	0	0	0

- 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 1116 705 215 193 3	0	0	0
8	CK	138	Total C N O S 1116 705 215 193 3	0	0	0

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

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

- 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 801 504 157 139 1	0	0	0

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

- 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 885 549 168 165 3	0	0	0
11	CN	119	Total C N O S 885 549 168 165 3	0	0	0

- 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 975 614 196 164 1	0	0	0
12	CO	125	Total C N O S 975 614 196 164 1	0	0	0

- 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 928 574 191 161 2	0	0	0
13	CP	117	Total C N O S 933 577 192 162 2	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
14	AQ	58	Total C N O S 476 303 99 70 4	0	0	0
14	CQ	58	Total C N O S 476 303 99 70 4	0	0	0

- 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 734 459 147 126 2	0	0	0
15	CR	88	Total C N O S 734 459 147 126 2	0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
22	AB	85	Total 1814	C 813	N 323	O 592	P 85	S 1	0	0	0
22	AD	85	Total 1814	C 813	N 323	O 592	P 85	S 1	0	0	0
22	CB	85	Total 1814	C 813	N 323	O 592	P 85	S 1	0	0	0
22	CD	85	Total 1814	C 813	N 323	O 592	P 85	S 1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AC	77	Total 1643	C 732	N 298	O 536	P 77	0	0	0
23	CC	77	Total 1643	C 732	N 298	O 536	P 77	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AC	18	C	U	CONFLICT	GB AP012306.1
CC	18	C	U	CONFLICT	GB AP012306.1

- Molecule 24 is a RNA chain called MRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	A1	16	Total 346	C 156	N 69	O 105	P 16	0	0	0
24	C1	16	Total 346	C 156	N 69	O 105	P 16	0	0	0

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

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

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BA	161	U	-	INSERTION	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	166	U	-	INSERTION	GB AP008226.1
DA	654A	A	G	CONFLICT	GB AP008226.1
DA	654E	C	G	CONFLICT	GB AP008226.1
DA	654P	G	C	CONFLICT	GB AP008226.1
DA	654T	A	C	CONFLICT	GB AP008226.1
DA	1058	U	G	CONFLICT	GB AP008226.1
DA	1080	A	C	CONFLICT	GB AP008226.1

- Molecule 26 is a RNA chain called 5S RIBOSOMAL RNA.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- 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 933 588 171 170 4	0	0	0
34	DN	122	Total C N O S 933 588 171 170 4	0	0	0

- 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 1145 712 232 198 3	0	0	0
35	DO	150	Total C N O S 1145 712 232 198 3	0	0	0

- 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 1122 715 212 188 7	0	0	0
36	DP	141	Total C N O S 1122 715 212 188 7	0	0	0

- 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 968 604 203 160 1	0	0	0
37	D0	117	Total C N O 960 599 202 159	0	0	0

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

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

- 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 785	C 505	N 150	O 125	S 5	0	0	0
44	DU	102	Total 785	C 505	N 150	O 125	S 5	0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	B7	45	Total 391	C 240	N 97	O 52	S 2	0	0	0
53	D7	45	Total 391	C 240	N 97	O 52	S 2	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	B8	60	Total 480	C 306	N 98	O 74	S 2	0	0	0
54	D8	60	Total 480	C 306	N 98	O 74	S 2	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
55	BA	568	Total Mg 568 568	2	0
55	CA	219	Total Mg 219 219	0	0
55	AB	4	Total Mg 4 4	0	0
55	BE	3	Total Mg 3 3	0	0
55	B1	2	Total Mg 2 2	0	0
55	AN	1	Total Mg 1 1	0	0
55	CR	1	Total Mg 1 1	0	0
55	AS	1	Total Mg 1 1	0	0
55	B5	1	Total Mg 1 1	0	0
55	BB	18	Total Mg 18 18	0	0
55	DO	1	Total Mg 1 1	0	0
55	D8	1	Total Mg 1 1	0	0
55	D3	1	Total Mg 1 1	0	0
55	BF	3	Total Mg 3 3	0	0
55	B2	1	Total Mg 1 1	0	0
55	AA	220	Total Mg 220 220	1	0
55	D7	1	Total Mg 1 1	0	0
55	AR	1	Total Mg 1 1	0	0
55	B6	1	Total Mg 1 1	0	0
55	CG	2	Total Mg 2 2	0	0
55	A1	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	AD	3	Total 3	Mg 3	0	0
55	DD	3	Total 3	Mg 3	0	0
55	D0	1	Total 1	Mg 1	0	0
55	CC	9	Total 9	Mg 9	0	0
55	DE	1	Total 1	Mg 1	0	0
55	B3	3	Total 3	Mg 3	0	0
55	DA	488	Total 488	Mg 488	0	0
55	D5	2	Total 2	Mg 2	0	0
55	B7	1	Total 1	Mg 1	0	0
55	AG	2	Total 2	Mg 2	0	0
55	BO	2	Total 2	Mg 2	0	0
55	D1	1	Total 1	Mg 1	0	0
55	CB	4	Total 4	Mg 4	0	0
55	AC	8	Total 8	Mg 8	0	0
55	CD	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	BW	1	Total 1	Mg 1	0	0
55	CK	1	Total 1	Mg 1	0	0
55	DB	20	Total 20	Mg 20	0	0

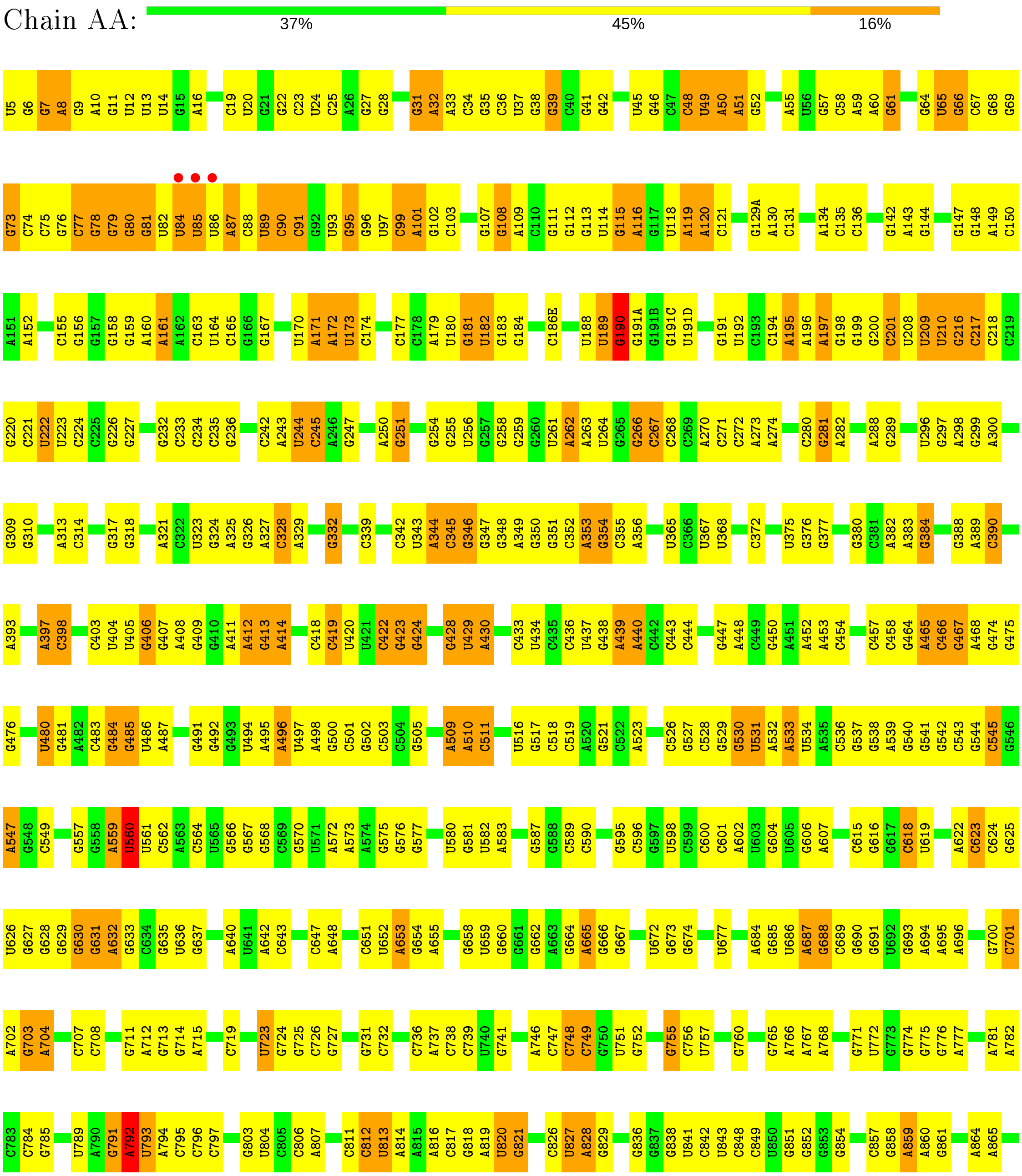
- Molecule 56 is ZINC ION (three-letter code: ZN) (formula: Zn).

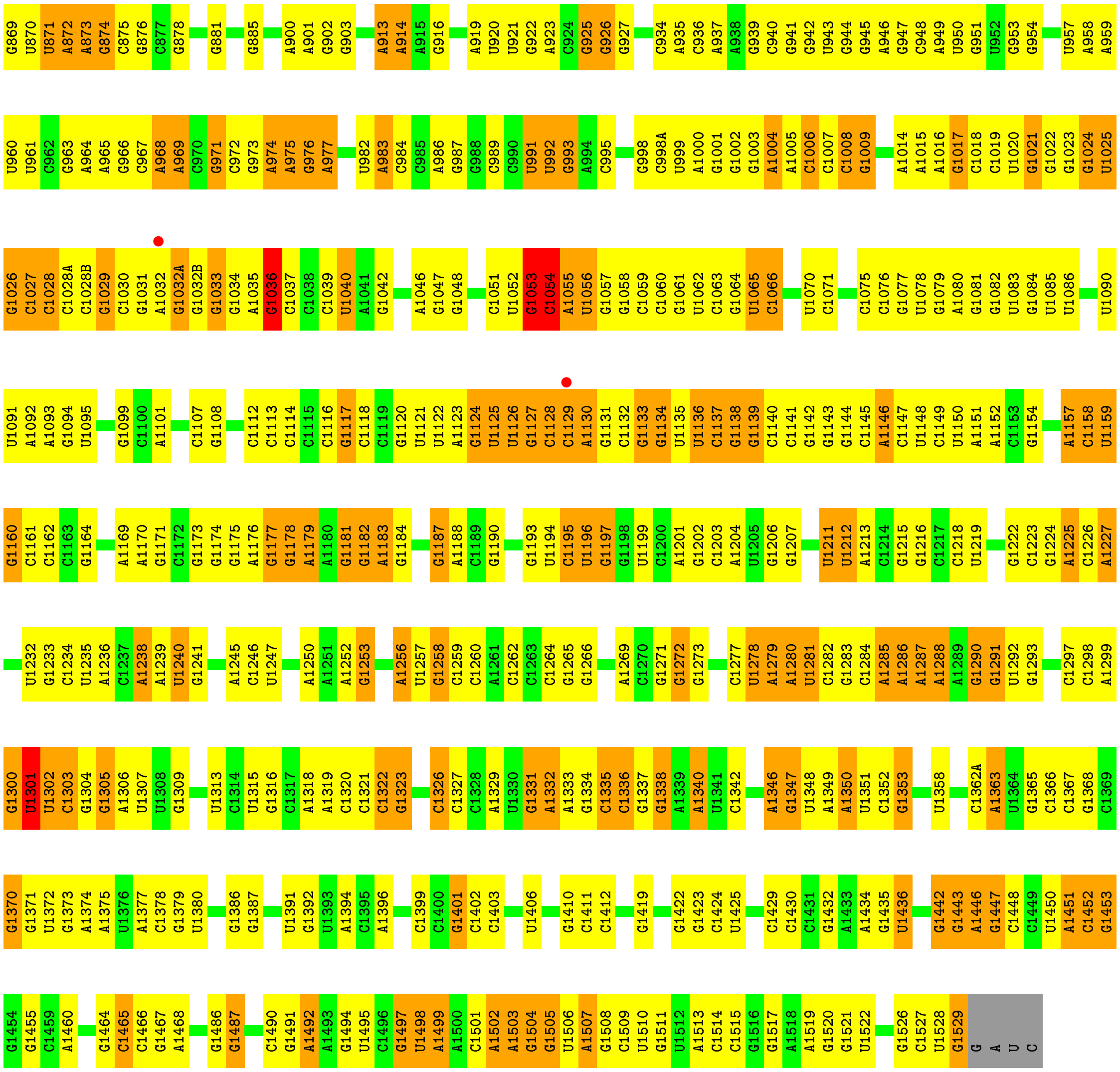
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	AG	1	Total Zn 1 1	0	0
56	AQ	1	Total Zn 1 1	0	0
56	CQ	1	Total Zn 1 1	0	0
56	CG	1	Total Zn 1 1	0	0

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.

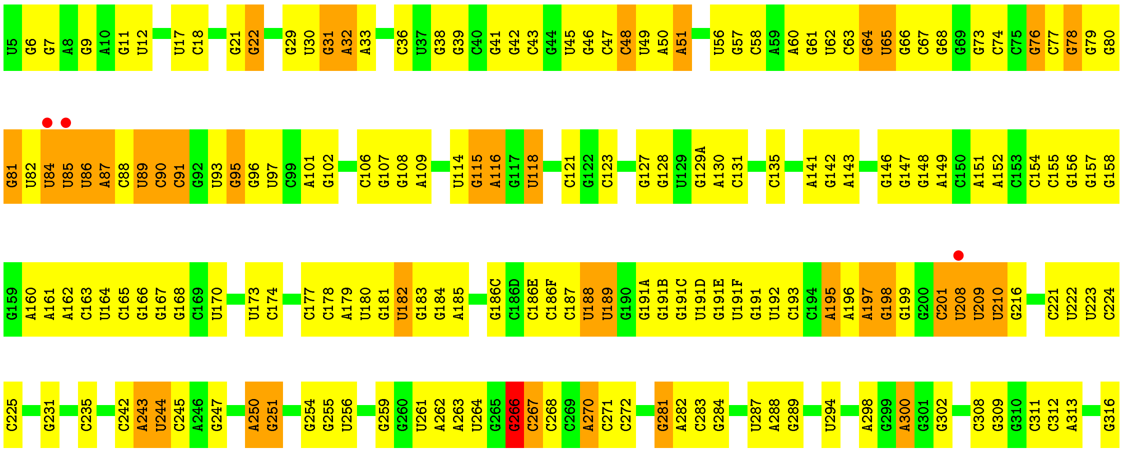
- Molecule 1: 16S ribosomal RNA

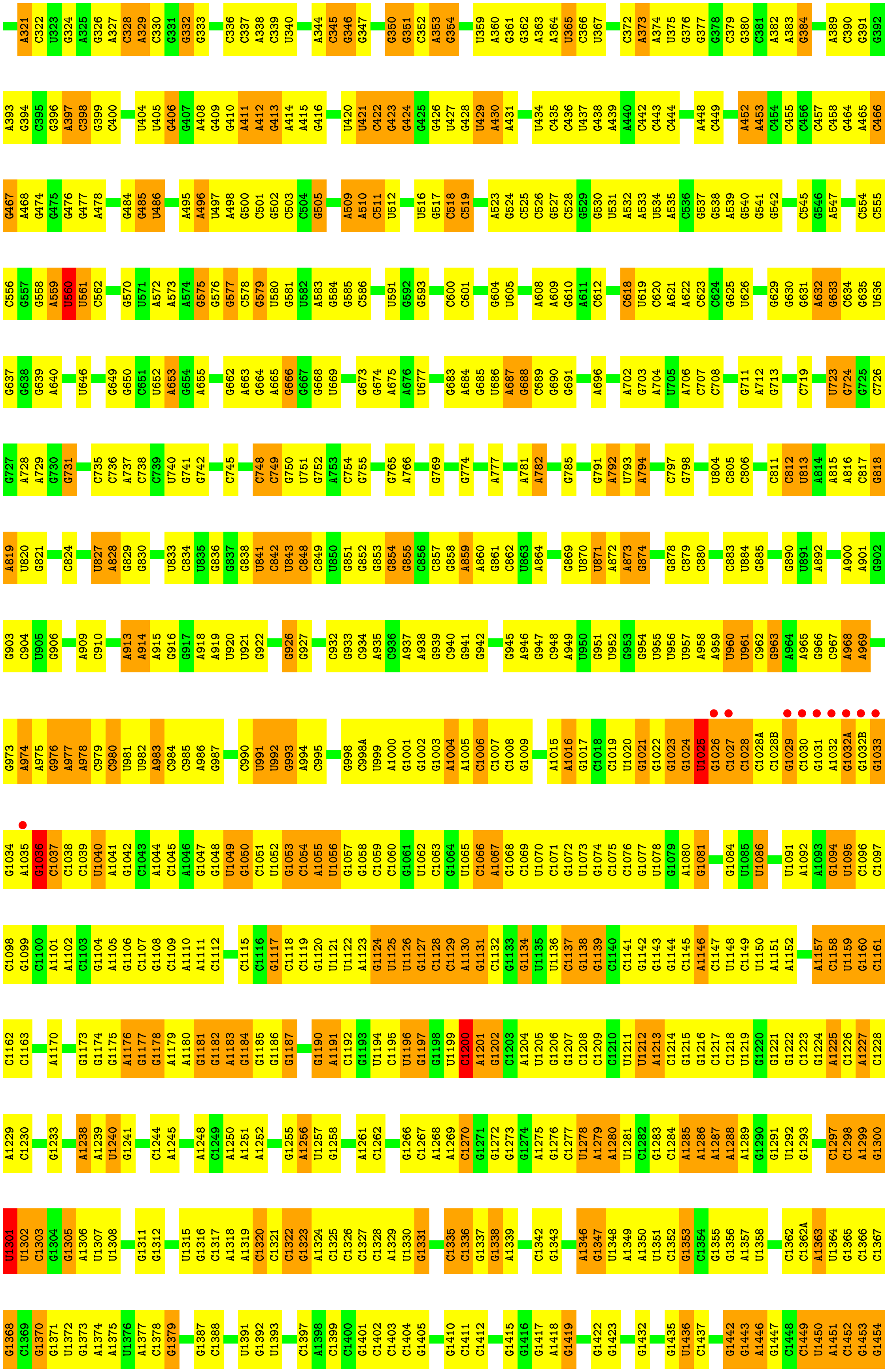




• Molecule 1: 16S ribosomal RNA

Chain CA:

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A393 G394 C395 G396 A397 C398 G399 C400 U404 U405 G406 G407 A408 G409 G410 A411 A412 G413 A414 A415 G416 U420 U421 C422 G423 G424 G425 G426 U427 G428 U429 A430 A431 U434 C435 C436 U437 G438 A439 A440 C442 C443 C444 A448 C449 A452 A453 C454 C455 C456 C457 C458 G464 A465 C466
G467 A468 G474 G475 G476 G477 A478 G484 G485 U486 A495 A496 U497 A498 G500 C501 G502 C503 C504 G505 A509 A510 C511 U512 U516 G517 C518 C519 A523 G524 C525 C526 G527 C528 G529 G530 U531 A532 A533 U534 A535 C536 G537 G538 A539 G540 G541 G542 C545 G546 A547 C554 C555
C556 G557 G558 A559 U560 U561 C562 G570 U571 A572 A573 A574 G575 G576 G577 C578 G579 U580 G581 U582 A583 G584 G585 C586 U591 G592 G593 C600 C601 G604 U605 A608 A609 G610 A611 C612 C618 U619 C620 A621 A622 C623 C624 G625 U626 G629 G630 G631 A632 G633 C634 G635 U636
G637 G638 G639 A640 U646 G649 G650 C651 U652 A653 G654 A655 G662 A663 G664 A665 G666 G667 G668 U669 G673 G674 A675 A676 U677 G683 A684 G685 U686 A687 G688 C689 G690 G691 A696 A702 G703 A704 U705 A706 C707 C708 G711 A712 G713 C719 U723 G724 G725 G726
G727 A728 A729 G730 G731 C735 C736 A737 C738 C739 U740 G741 G742 C745 C748 C749 G750 U751 G752 A753 C754 G755 G765 A766 G769 G774 A777 A781 A782 G785 G791 A792 U793 A794 C797 G798 U804 C805 C806 C811 C812 U813 A814 A815 A816 C817 G818
A819 U820 G821 C824 U827 A828 G829 G830 U833 C834 U835 G836 G837 G838 U841 C842 U843 C848 C849 U850 G851 G852 G853 G854 G855 C856 C857 G858 A859 A860 G861 C862 G863 A864 G869 U870 U871 A872 A873 G874 G878 C879 C880 C883 U884 G885 G890 U891 A892 A900 A901 G902
G903 C904 U905 G906 A909 C910 A913 A914 A915 G916 G917 A918 A919 U920 U921 G922 G926 G927 C932 G933 C934 A935 C936 A937 A938 G939 C940 G941 G942 G945 A946 G947 C948 A949 U950 G951 U952 G953 G954 U955 U956 U957 A958 A959 U960 U961 C962 G963 A964 A965 G966 C967 A968 A969
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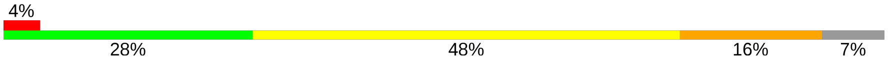
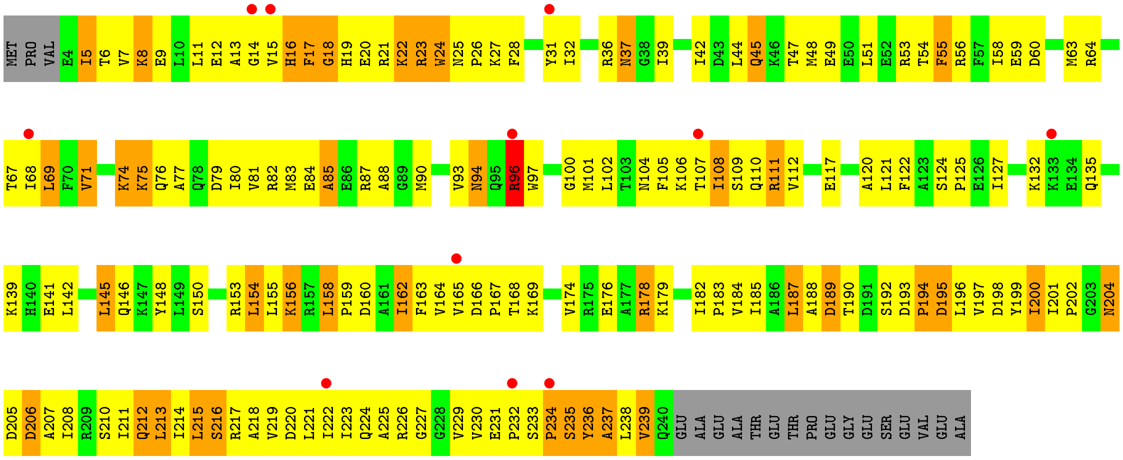
C1098 G1099 C1100 A1101 A1102 C1103 G1104 A1105 G1106 C1107 G1108 C1109 A1110 A1111 C1112 C1115 C1116 G1117 C1118 C1119 G1120 U1121 U1122 A1123 G1124 U1125 U1126 G1127 C1128 C1129 A1130 G1131 C1132 G1133 G1134 U1135 U1136 C1137 G1138 G1139 C1140 C1141 G1142 G1143 G1144 C1145 A1146 C1147 U1148 C1149 U1150 A1151 A1152 A1157 C1158 U1159 G1160 C1161
C1162 C1163 A1170 G1173 G1174 G1175 A1176 G1177 G1178 A1179 A1180 G1181 G1182 A1183 G1184 G1185 G1186 G1187 G1190 A1191 C1192 G1193 U1194 C1195 U1196 G1197 G1198 U1199 C1200 A1201 G1202 C1203 A1204 U1205 G1206 G1207 C1208 C1209 C1210 U1211 U1212 A1213 C1214 G1215 G1216 C1217 C1218 U1219 G1220 G1221 G1222 C1223 G1224 A1225 C1226 A1227 C1228
A1229 C1230 G1233 A1238 A1239 U1240 G1241 C1244 A1245 A1248 C1249 A1250 A1251 A1252 G1255 A1256 U1257 G1258 A1261 C1262 G1266 C1267 A1268 A1269 C1270 G1271 G1272 G1273 G1274 A1275 G1276 C1277 U1278 A1279 A1280 U1281 C1282 G1283 C1284 A1285 A1286 A1287 A1288 A1289 G1290 G1291 U1292 G1293 C1297 C1298 A1299 G1300
U1301 U1302 C1303 G1304 G1305 A1306 U1307 U1308 G1311 G1312 U1315 G1316 C1317 A1318 A1319 C1320 C1321 C1322 G1323 A1324 C1325 C1326 C1327 C1328 A1329 U1330 G1331 C1335 C1336 G1337 G1338 A1339 C1342 G1343 A1346 G1347 U1348 A1349 A1350 U1351 C1352 G1353 C1354 G1355 G1356 A1357 U1358 C1362 C1362A A1363 U1364 G1365 C1366 C1367
G1368 C1369 G1370 G1371 U1372 G1373 A1374 A1375 U1376 A1377 C1378 G1379 G1387 C1388 U1391 G1392 U1393 C1397 A1398 C1399 C1400 G1401 C1402 C1403 C1404 G1405 G1410 C1411 C1412 G1415 G1416 G1417 A1418 G1419 G1422 G1423 G1432 G1435 U1436 C1437 G1442 G1443 A1446 G1447 C1448 C1449 U1450 A1451 G1452 G1453 G1454

- Molecule 2: 30S RIBOSOMAL PROTEIN S2

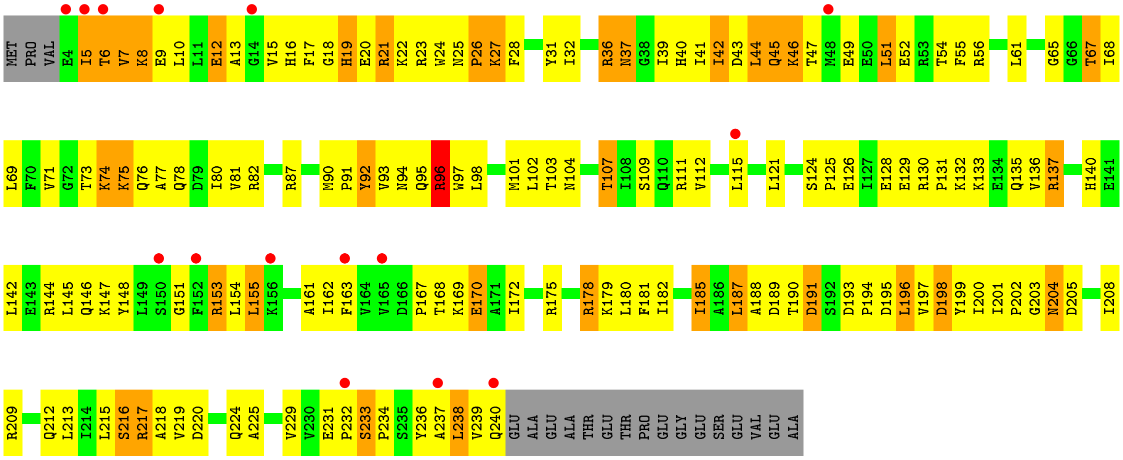
Chain AE:





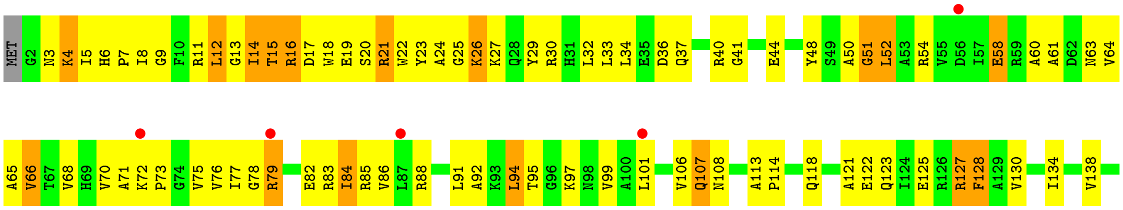
- Molecule 2: 30S RIBOSOMAL PROTEIN S2

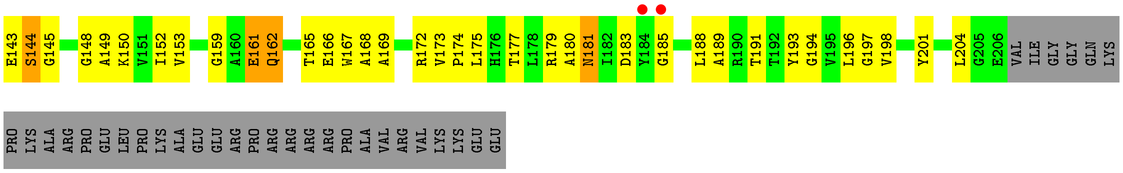
Chain CE:



- Molecule 3: 30S RIBOSOMAL PROTEIN S3

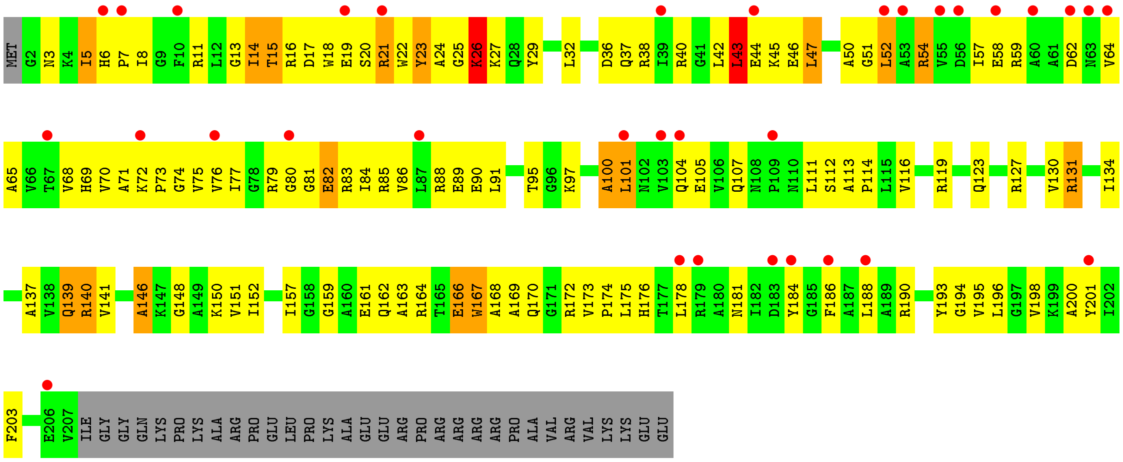
Chain AF:





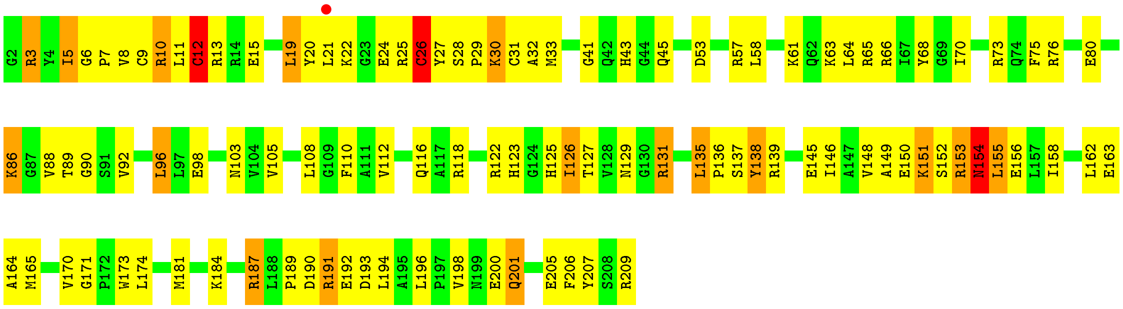
• Molecule 3: 30S RIBOSOMAL PROTEIN S3

Chain CF:



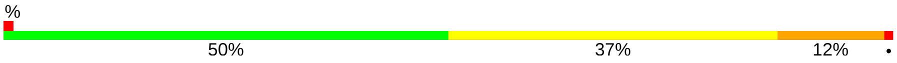
• Molecule 4: 30S RIBOSOMAL PROTEIN S4

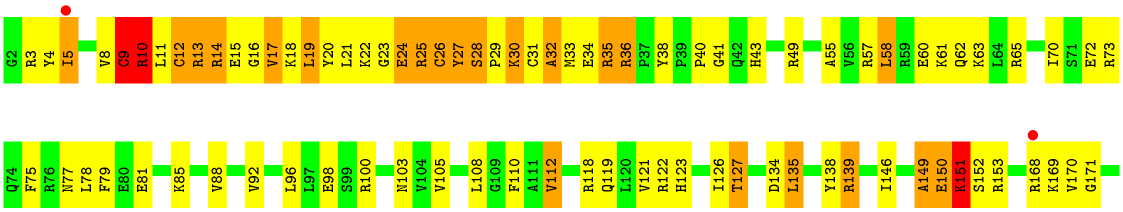
Chain AG:

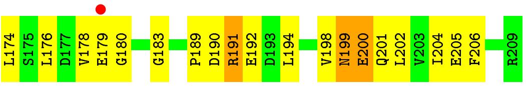


• Molecule 4: 30S RIBOSOMAL PROTEIN S4

Chain CG:

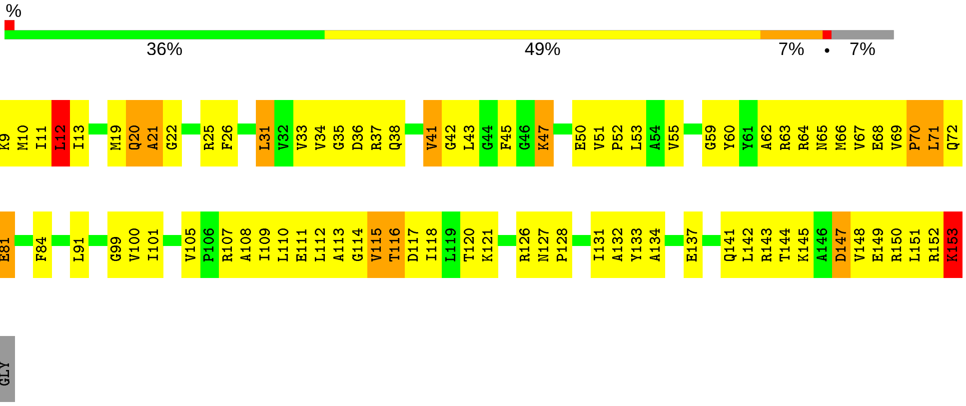






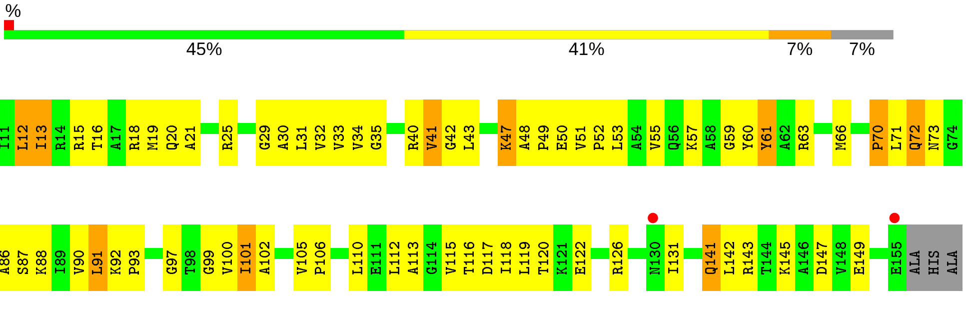
- Molecule 5: 30S RIBOSOMAL PROTEIN S5

Chain AH:



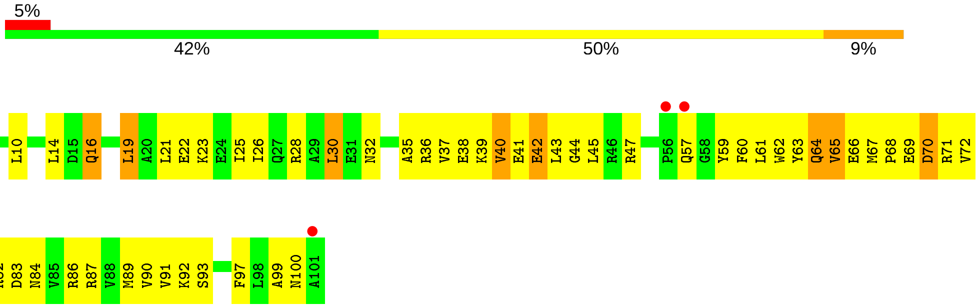
- Molecule 5: 30S RIBOSOMAL PROTEIN S5

Chain CH:



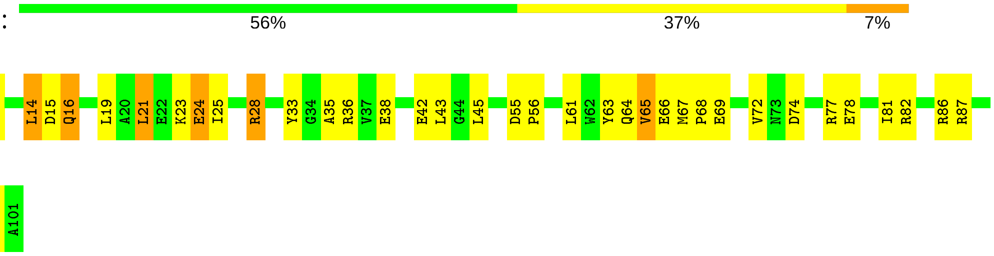
- Molecule 6: 30S RIBOSOMAL PROTEIN S6

Chain AI:

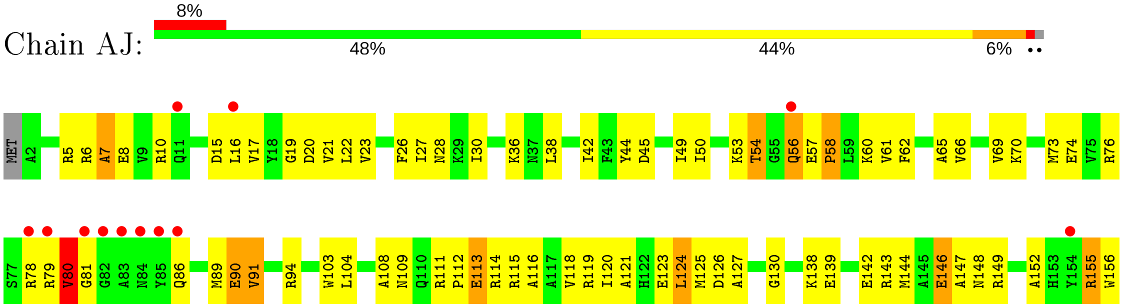


- Molecule 6: 30S RIBOSOMAL PROTEIN S6

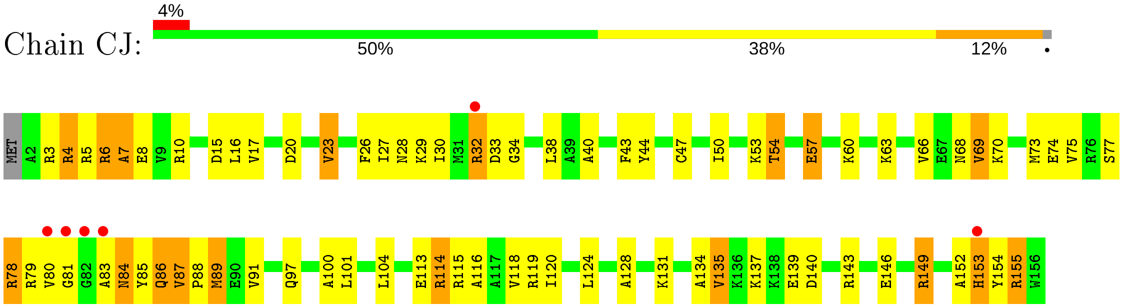
Chain CI:



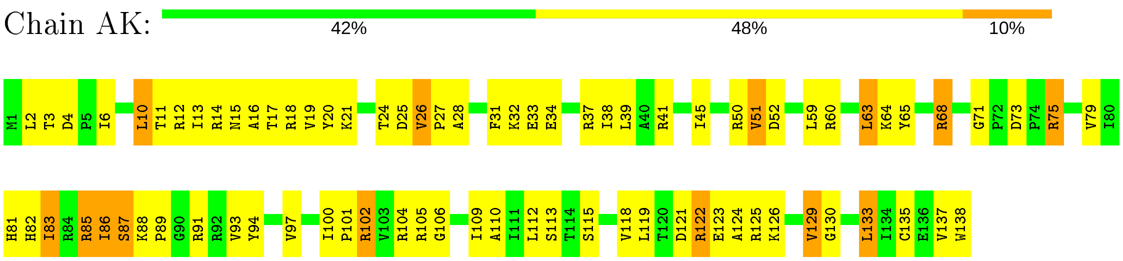
- Molecule 7: 30S RIBOSOMAL PROTEIN S7



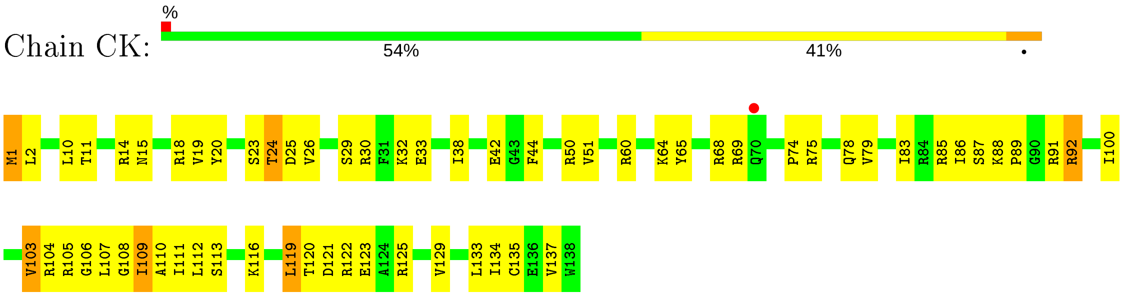
- Molecule 7: 30S RIBOSOMAL PROTEIN S7



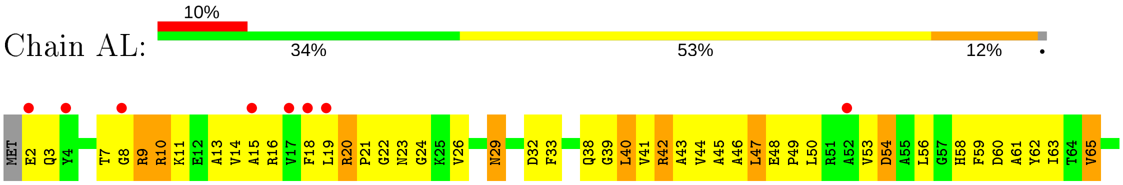
- Molecule 8: 30S RIBOSOMAL PROTEIN S8

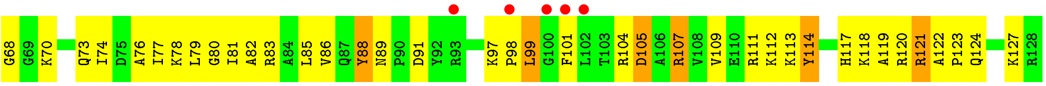


- Molecule 8: 30S RIBOSOMAL PROTEIN S8



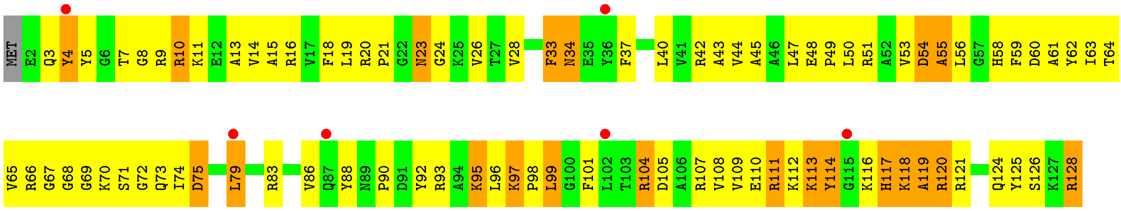
- Molecule 9: 30S RIBOSOMAL PROTEIN S9





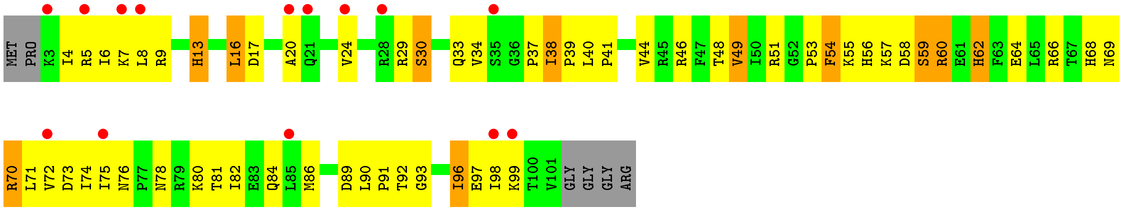
- Molecule 9: 30S RIBOSOMAL PROTEIN S9

Chain CL:



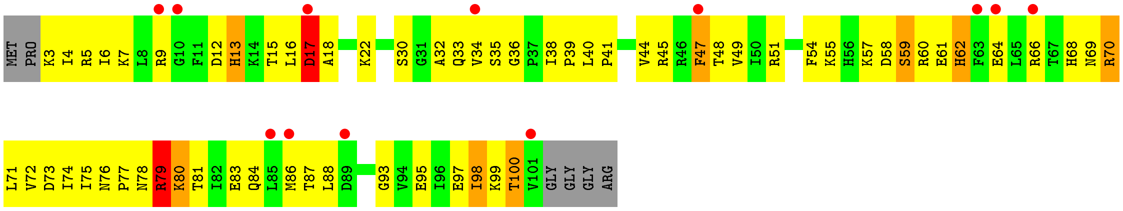
- Molecule 10: 30S RIBOSOMAL PROTEIN S10

Chain AM:



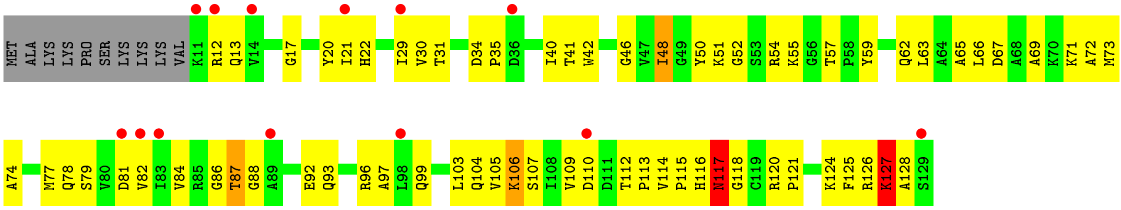
- Molecule 10: 30S RIBOSOMAL PROTEIN S10

Chain CM:



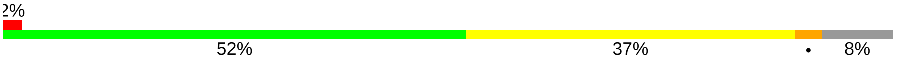
- Molecule 11: 30S RIBOSOMAL PROTEIN S11

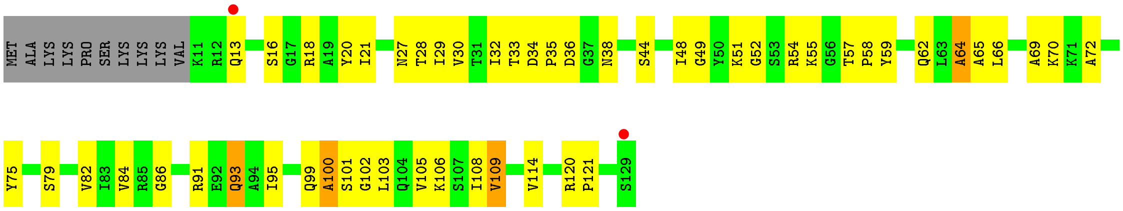
Chain AN:



- Molecule 11: 30S RIBOSOMAL PROTEIN S11

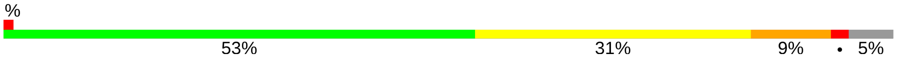
Chain CN:

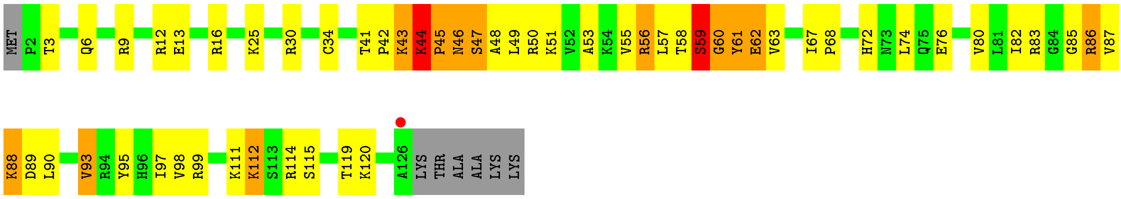




- Molecule 12: 30S RIBOSOMAL PROTEIN S12

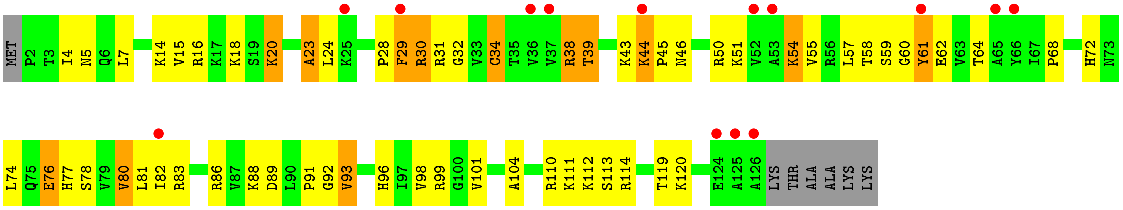
Chain AO:





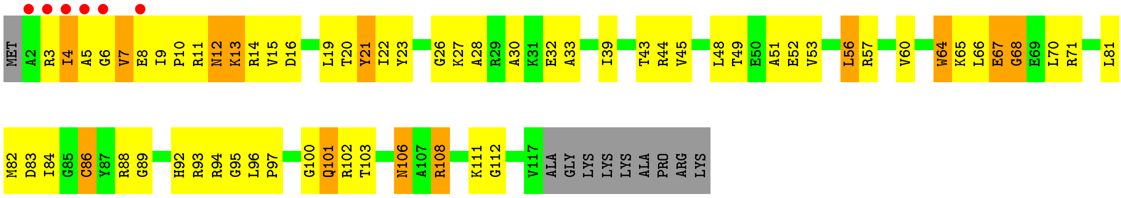
- Molecule 12: 30S RIBOSOMAL PROTEIN S12

Chain CO:



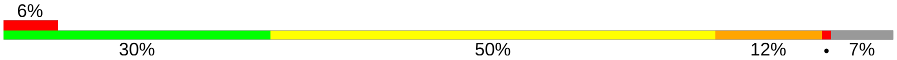
- Molecule 13: 30S RIBOSOMAL PROTEIN S13

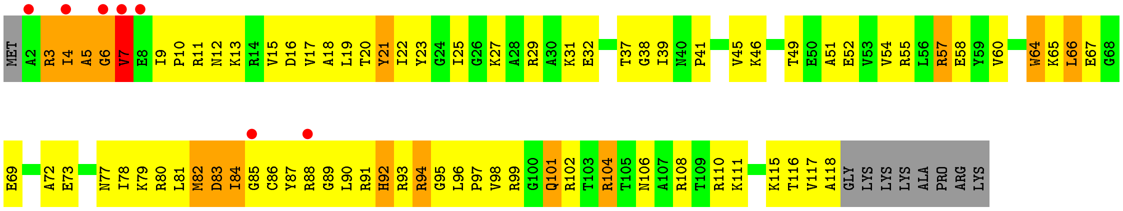
Chain AP:



- Molecule 13: 30S RIBOSOMAL PROTEIN S13

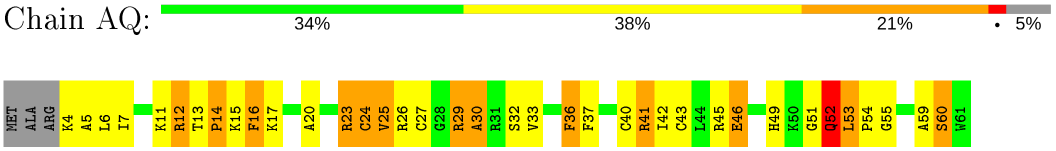
Chain CP:





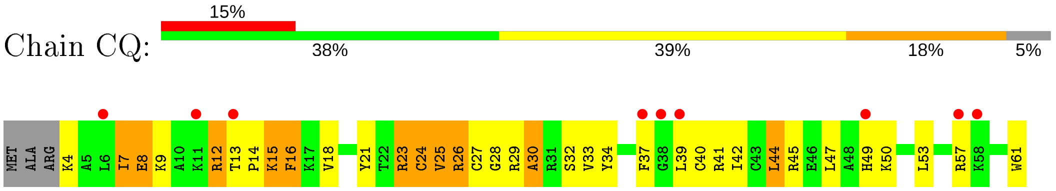
- Molecule 14: 30S RIBOSOMAL PROTEIN S14

Chain AQ:



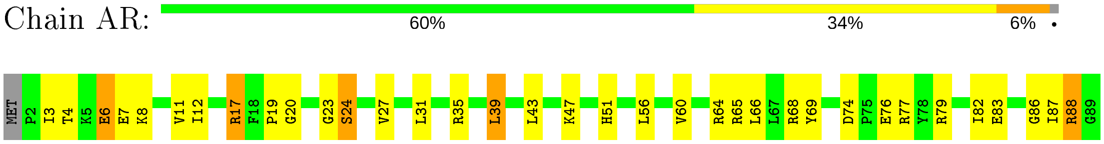
- Molecule 14: 30S RIBOSOMAL PROTEIN S14

Chain CQ:



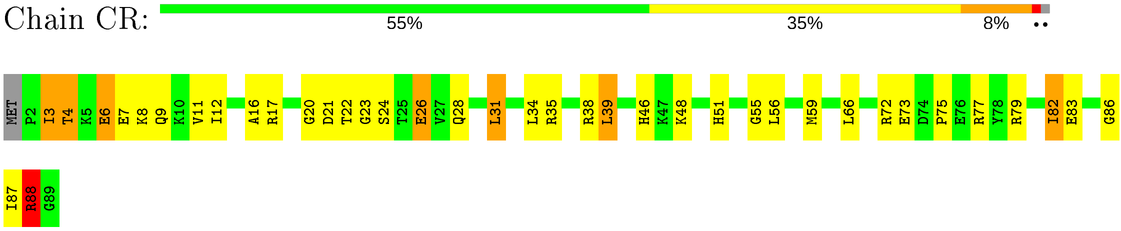
- Molecule 15: 30S RIBOSOMAL PROTEIN S15

Chain AR:



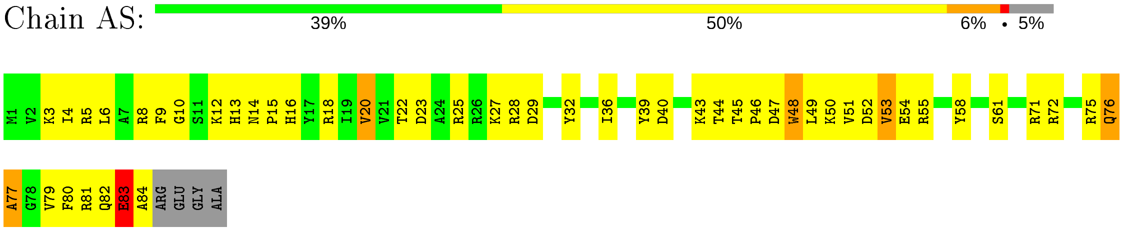
- Molecule 15: 30S RIBOSOMAL PROTEIN S15

Chain CR:



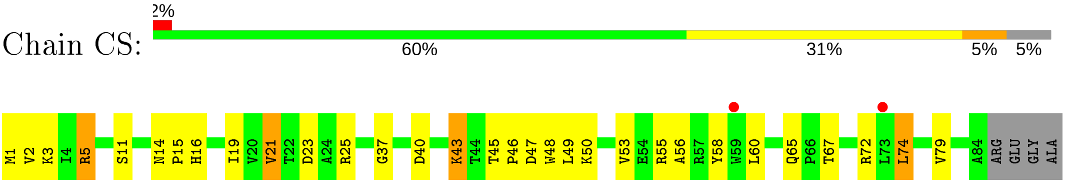
- Molecule 16: 30S RIBOSOMAL PROTEIN S16

Chain AS:



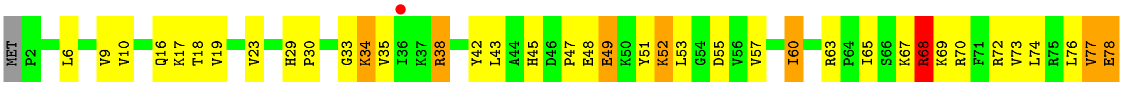
- Molecule 16: 30S RIBOSOMAL PROTEIN S16

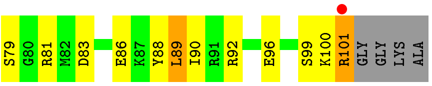
Chain CS:



- Molecule 17: 30S RIBOSOMAL PROTEIN S17

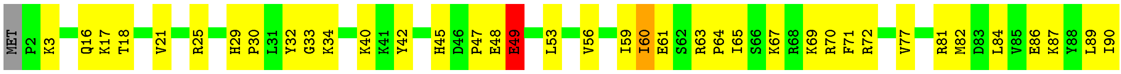
Chain AT:

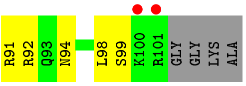




- Molecule 17: 30S RIBOSOMAL PROTEIN S17

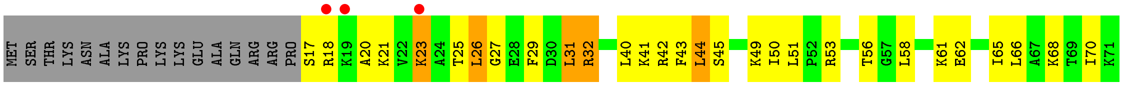
Chain CT:

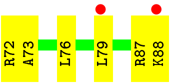




- Molecule 18: 30S RIBOSOMAL PROTEIN S18

Chain AU:





- Molecule 18: 30S RIBOSOMAL PROTEIN S18

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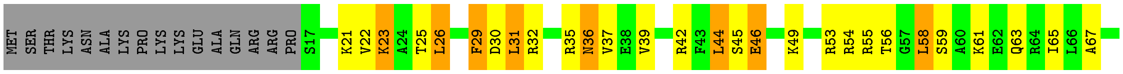

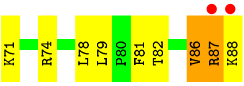

- Molecule 19: 30S RIBOSOMAL PROTEIN S19

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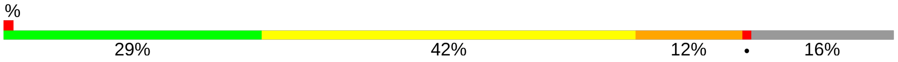

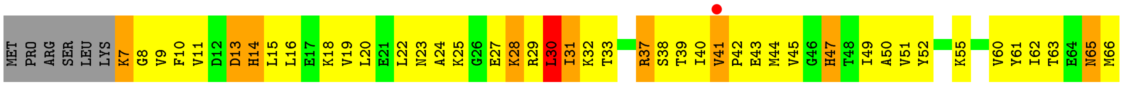

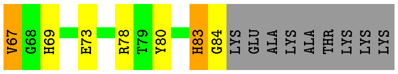

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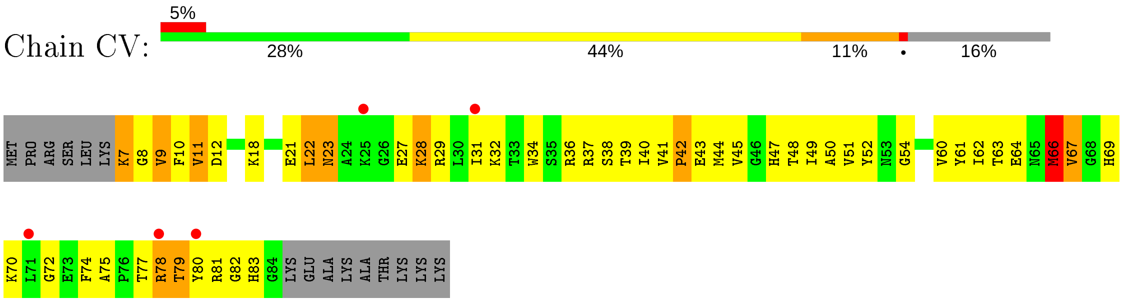

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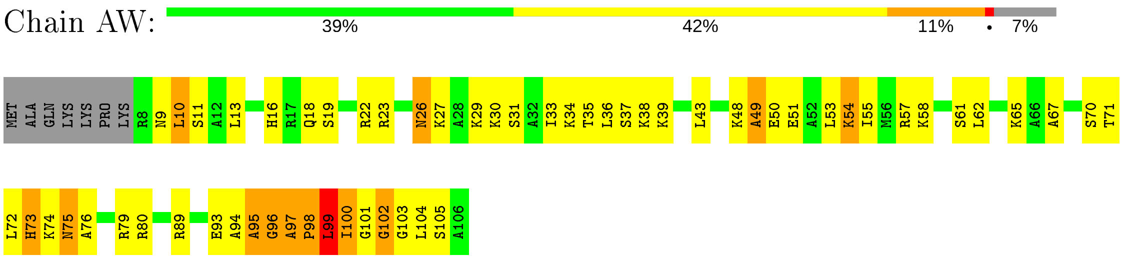
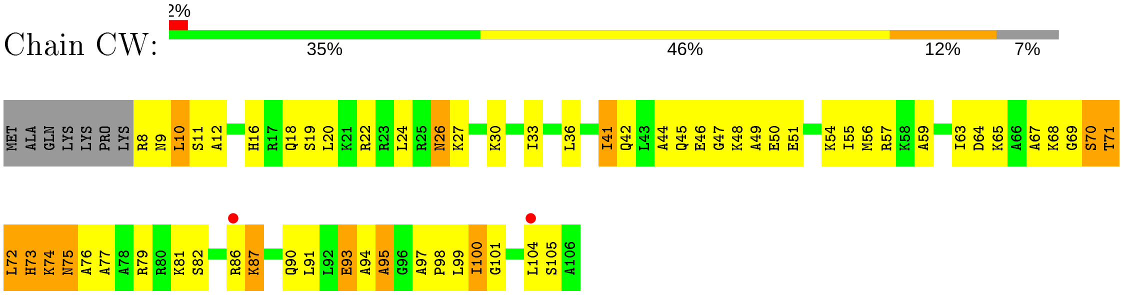
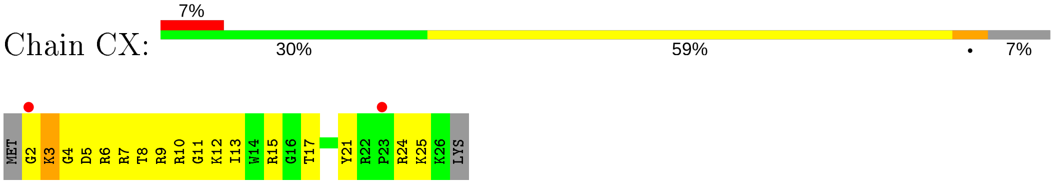


- Molecule 20: 30S RIBOSOMAL PROTEIN S20

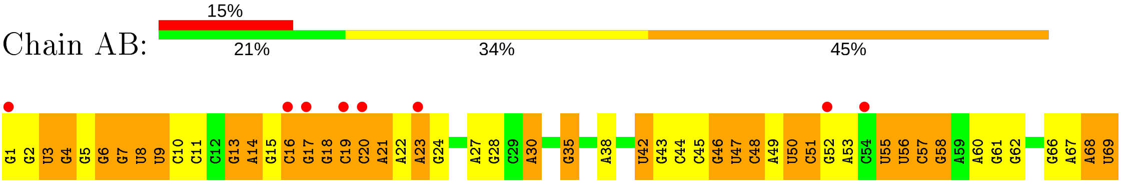


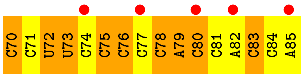
- Molecule 21: 30S RIBOSOMAL PROTEIN THX

- Molecule 21: 30S RIBOSOMAL PROTEIN THX



- Molecule 22: TRNA-TYR





- Molecule 22: TRNA-TYR

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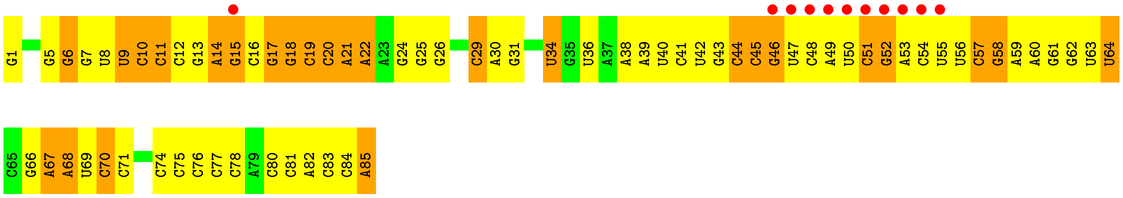

- Molecule 22: TRNA-TYR

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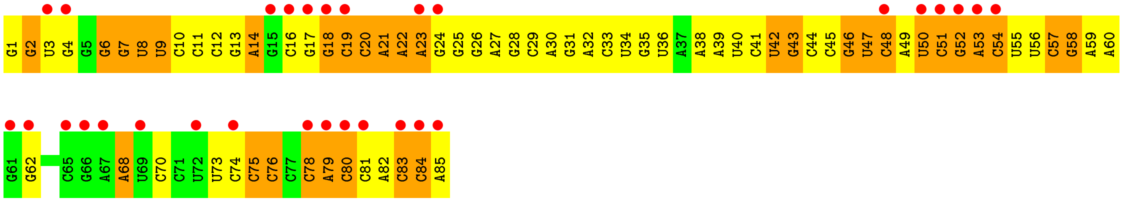

- Molecule 22: TRNA-TYR

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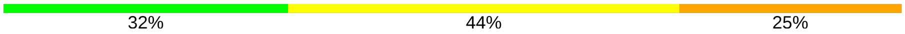

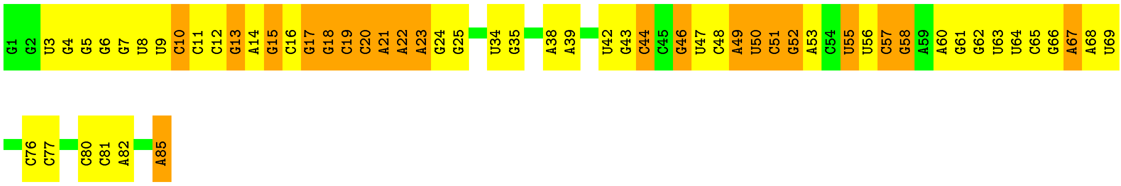

- Molecule 23: TRNA-FMET

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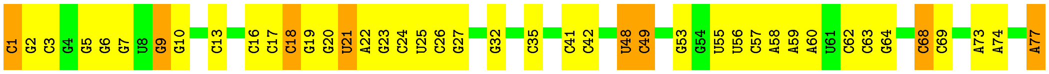

- Molecule 23: TRNA-FMET

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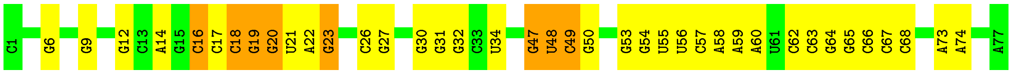

- Molecule 24: MRNA

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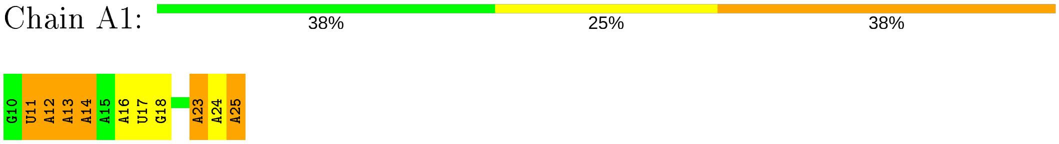
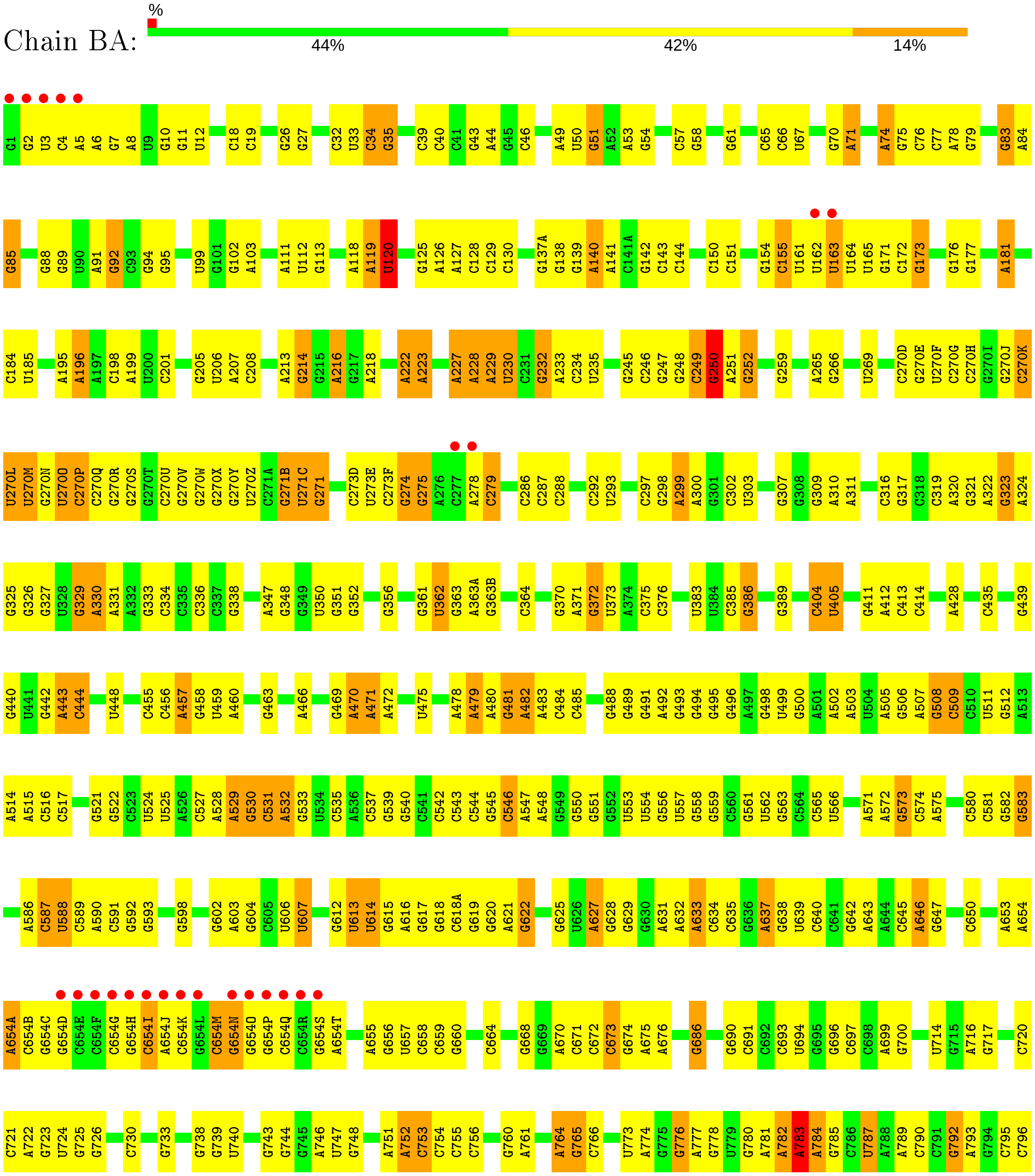


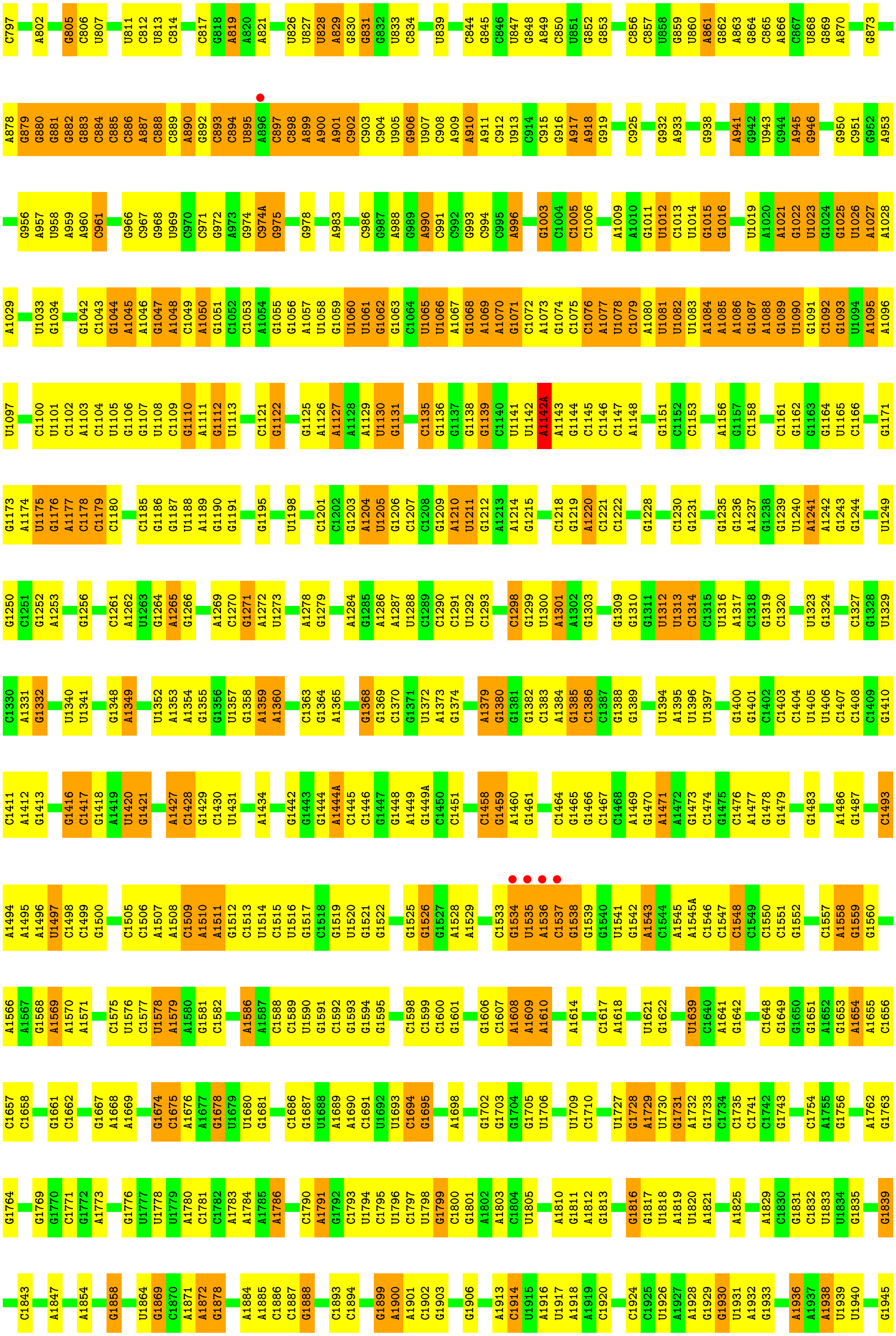
- Molecule 24: MRNA

Chain C1:

- Molecule 25: RNA (2912-MER)

Chain BA:

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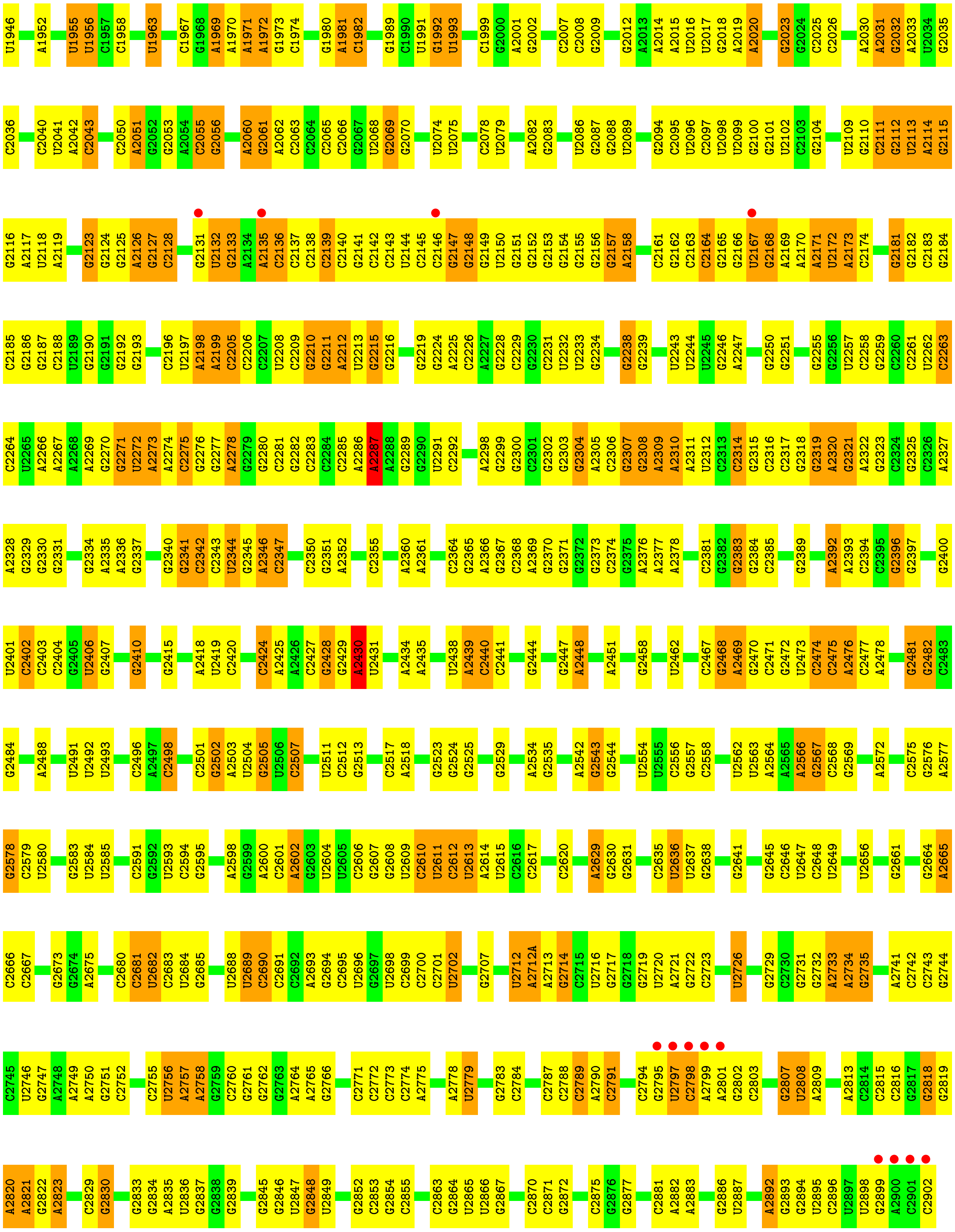
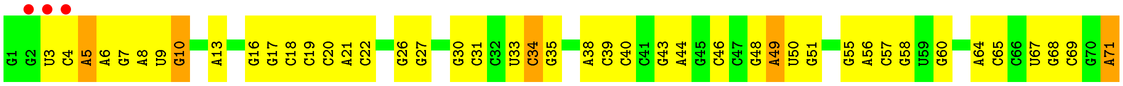
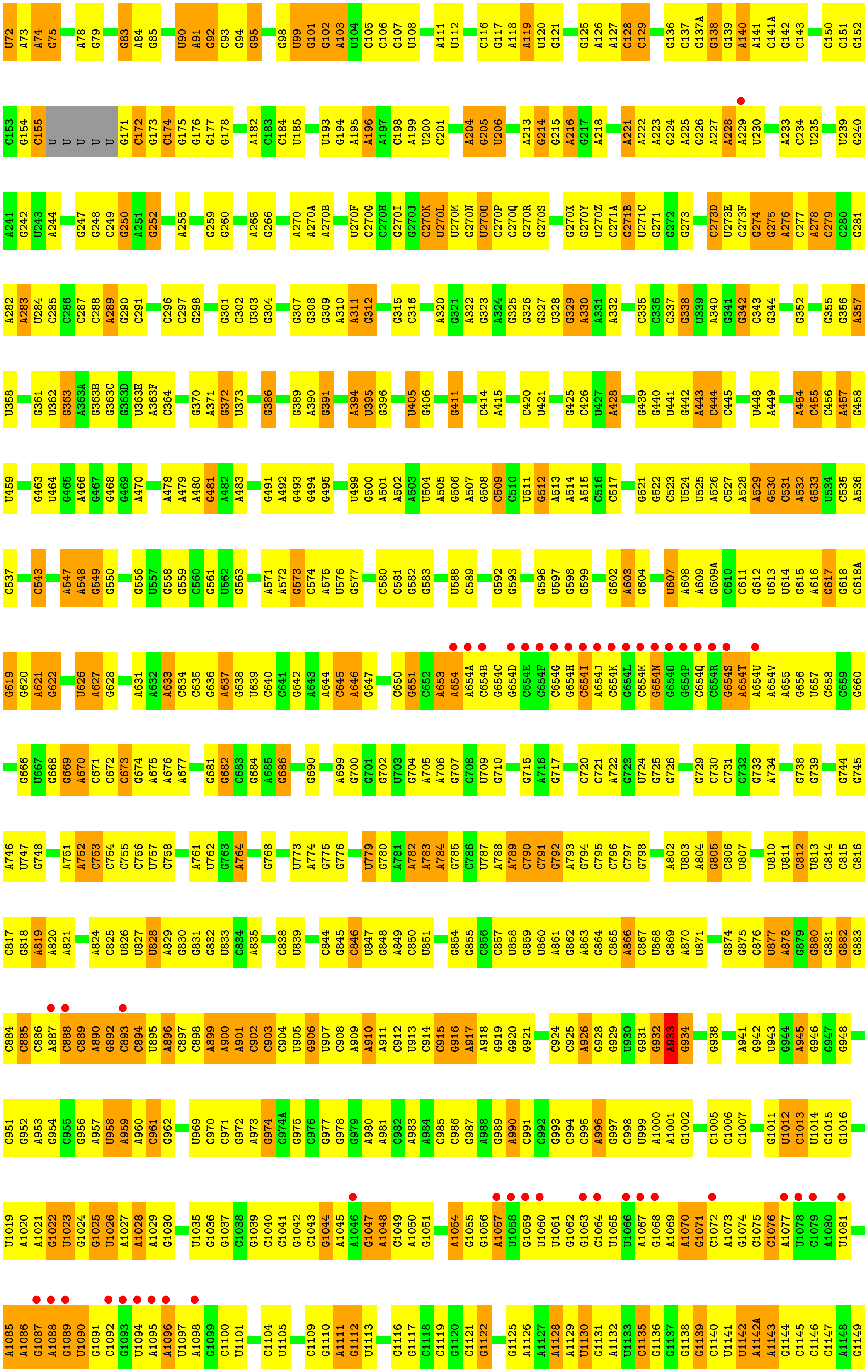


- Molecule 25: RNA (2912-MER)

Chain DA:

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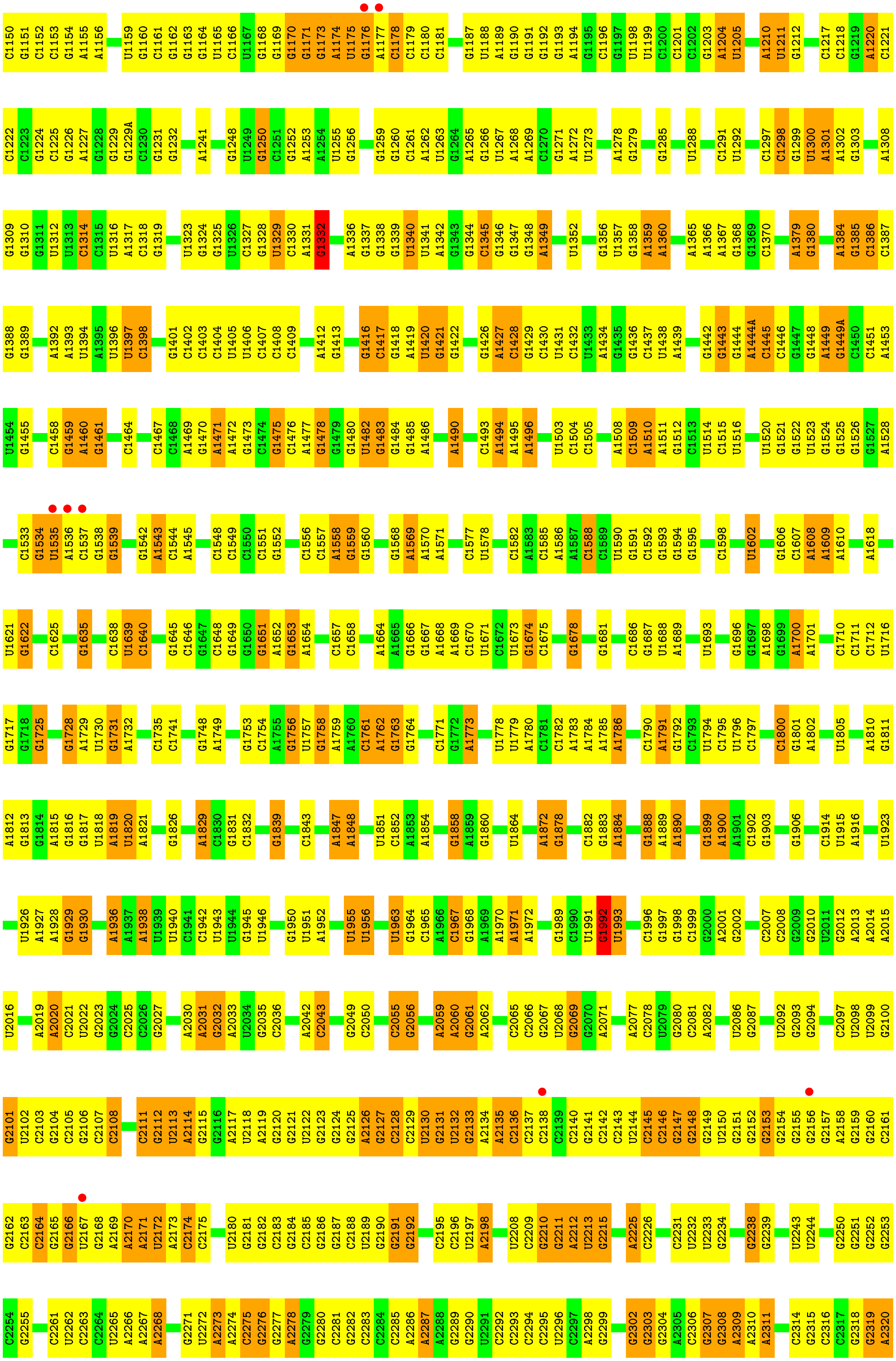
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G1717 G1718 G1725 G1728 A1729 U1730 G1731 A1732 C1735 C1741 G1748 A1749 G1753 C1754 A1755 G1756 U1757 G1758 A1759 A1760 C1761 A1762 G1763 G1764 C1771 G1772 A1773 U1778 U1779 A1780 C1781 C1782 A1783 A1784 A1785 A1786 C1790 A1791 G1792 C1793 U1794 C1795 U1796 C1797 C1800 G1801 A1802 U1805 A1810 G1811
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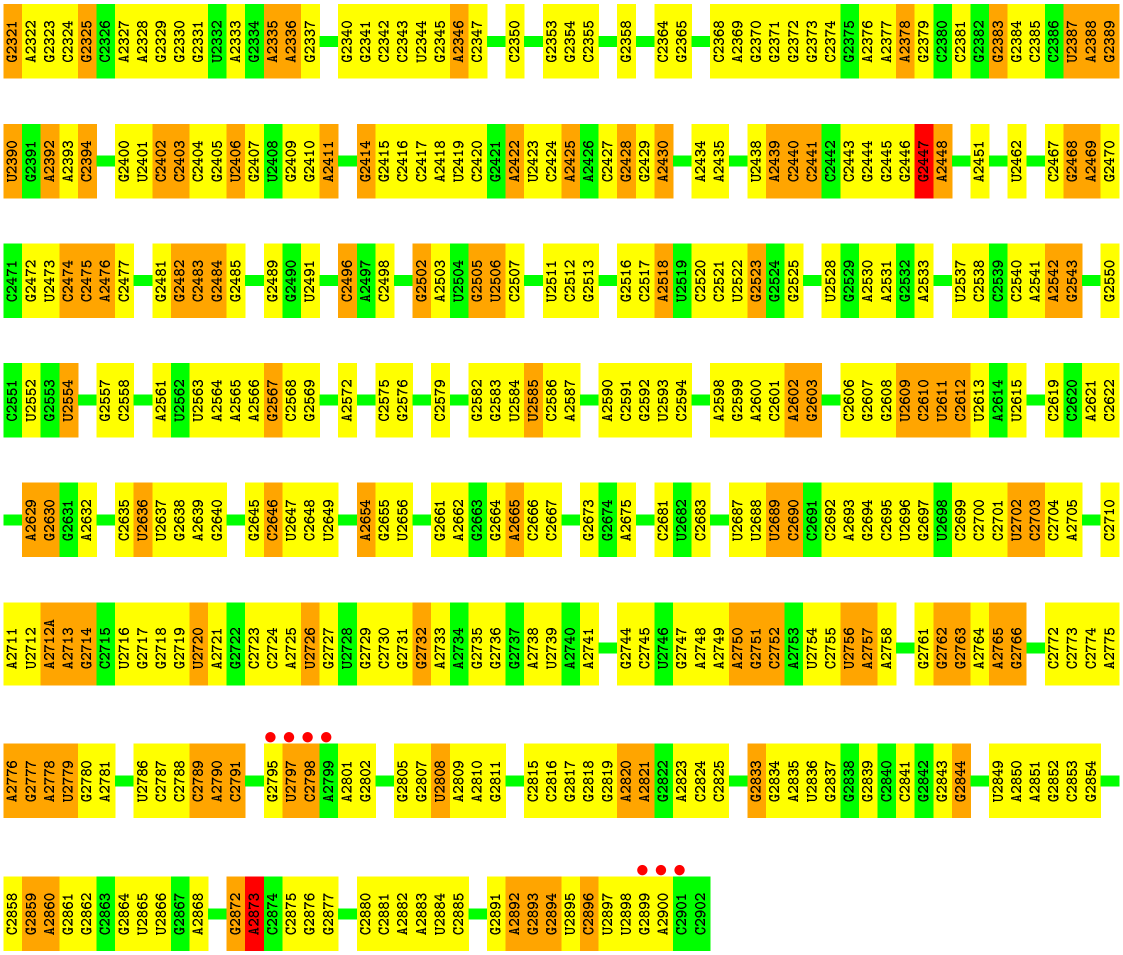
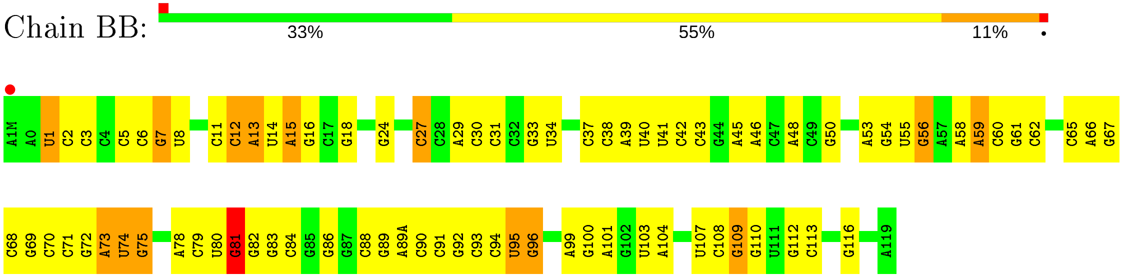
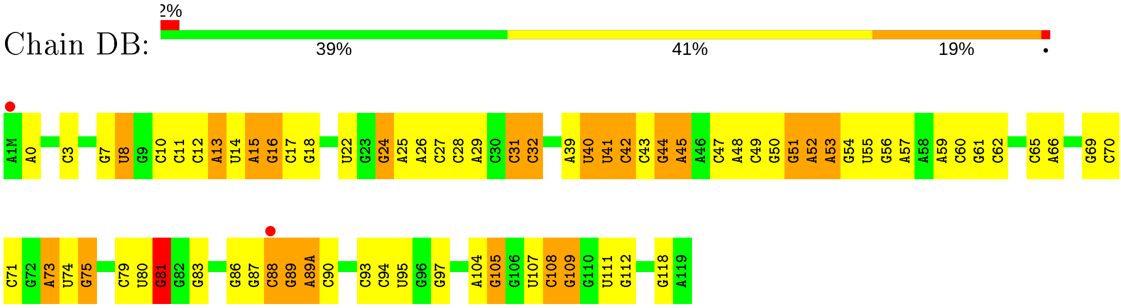
C2254 G2255 C2261 U2262 C2263 C2264 U2265 A2266 A2267 A2268 G2271 U2272 A2273 A2274 C2275 G2276 G2277 A2278 G2279 G2280 C2281 G2282 C2283 C2284 C2285 A2286 A2287 A2288 G2289 G2290 U2291 C2292 C2293 C2294 C2295 U2296 C2297 A2298 G2299 G2302 G2303 G2304 A2305 C2306 G2307 G2308 A2309 A2310 A2311 C2314 G2315 C2316 C2317 G2318 G2319 A2320



- Molecule 26: 5S RIBOSOMAL RNA

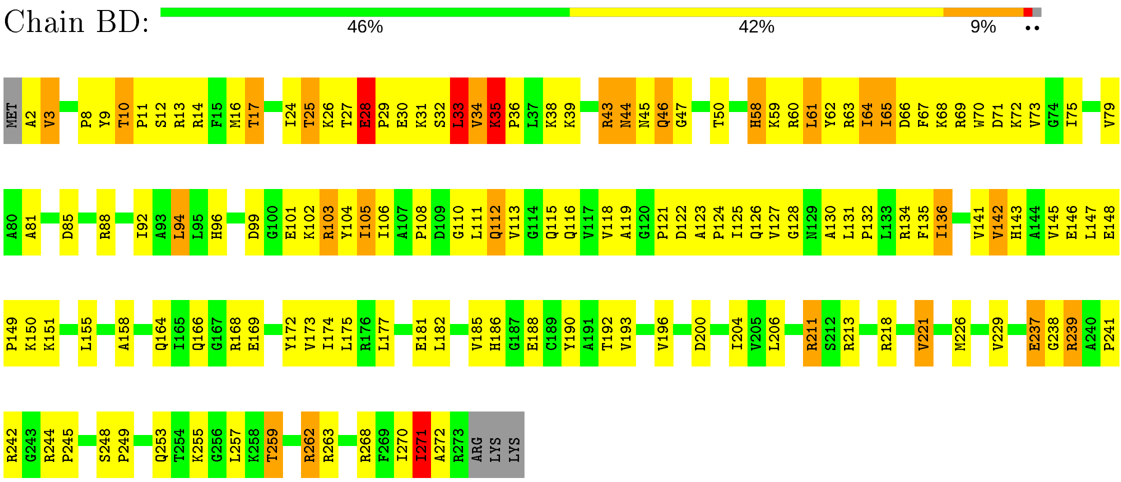


- Molecule 26: 5S RIBOSOMAL RNA



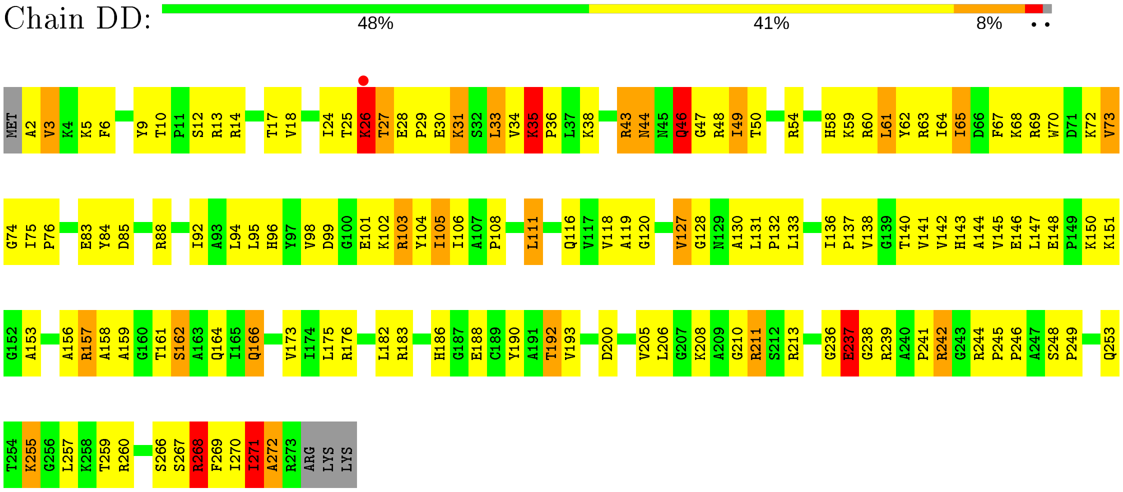
- Molecule 27: 50S ribosomal protein L2

Chain BD:



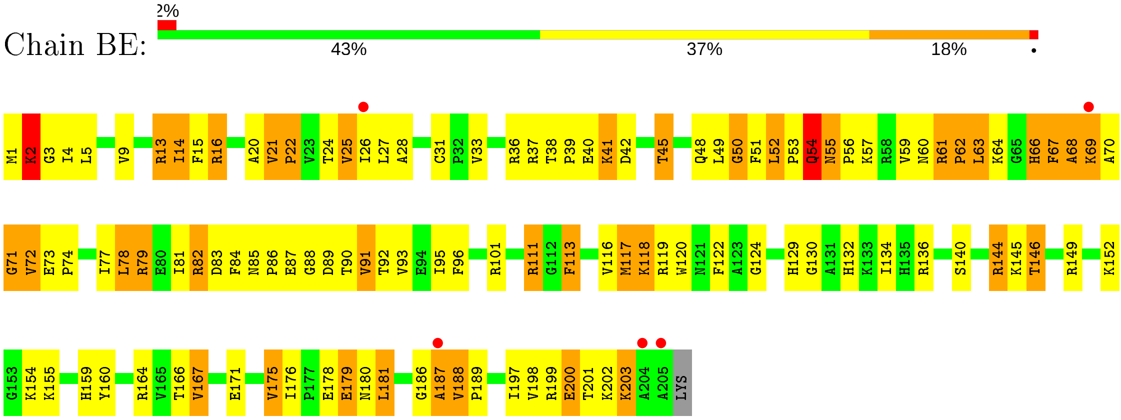
- Molecule 27: 50S ribosomal protein L2

Chain DD:



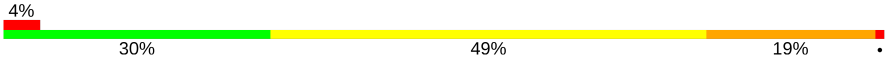
- Molecule 28: 50S ribosomal protein L3

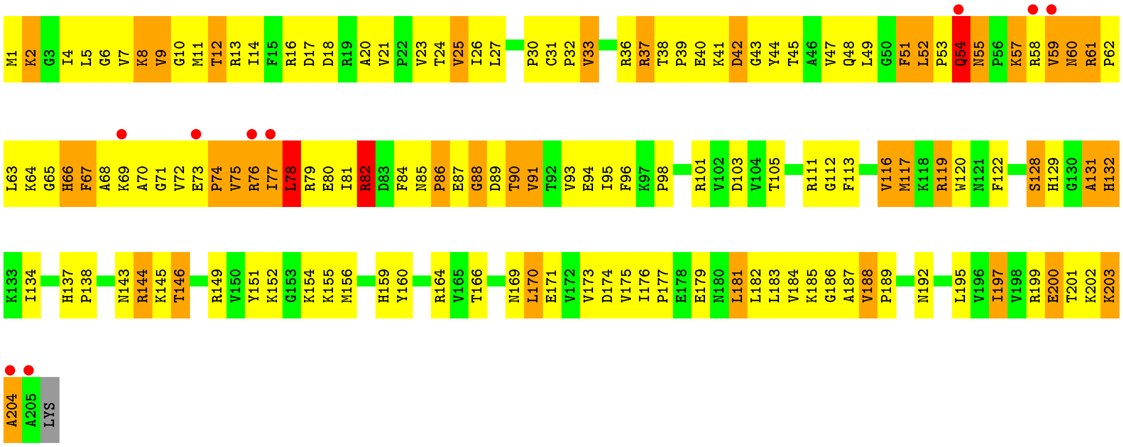
Chain BE:



- Molecule 28: 50S ribosomal protein L3

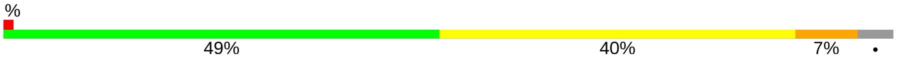
Chain DE:

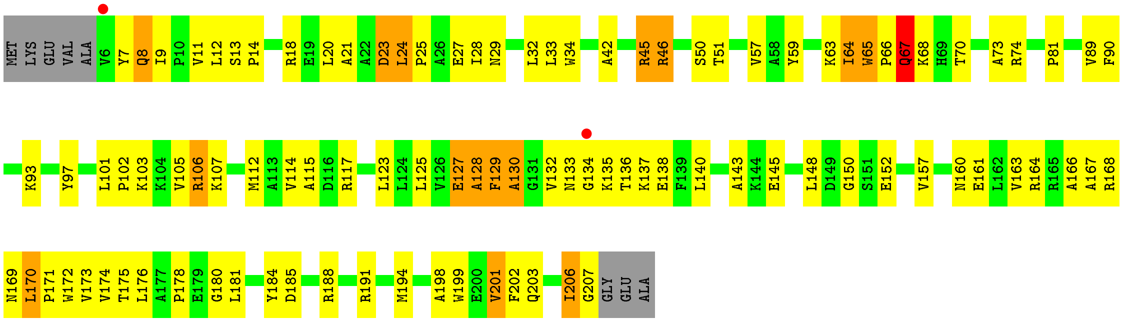




- Molecule 29: 50S ribosomal protein L4

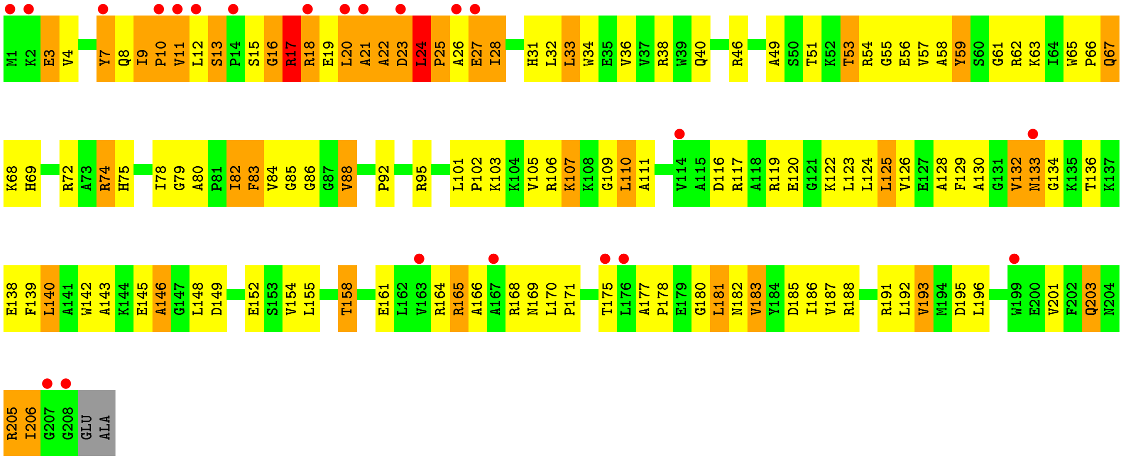
Chain BF:





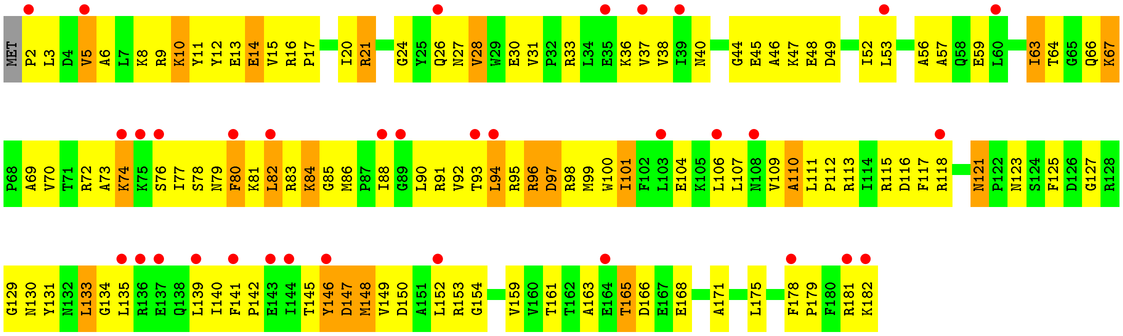
- Molecule 29: 50S ribosomal protein L4

Chain DF:



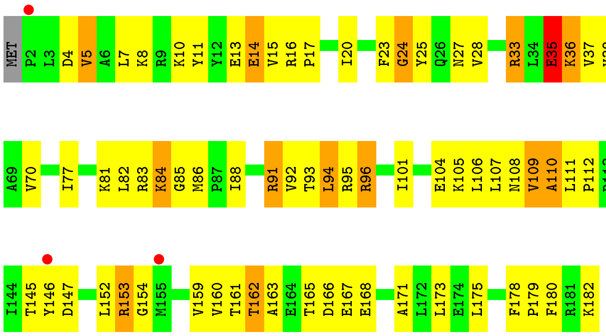
- Molecule 30: 50S ribosomal protein L5

Chain BG:



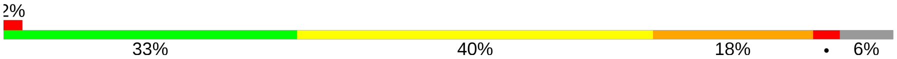
- Molecule 30: 50S ribosomal protein L5

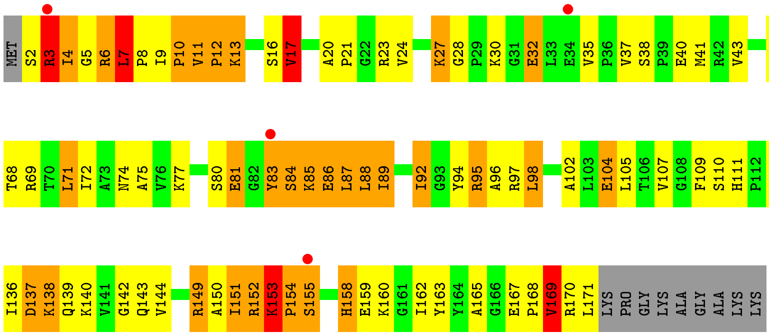
Chain DG:



- Molecule 31: 50S ribosomal protein L6

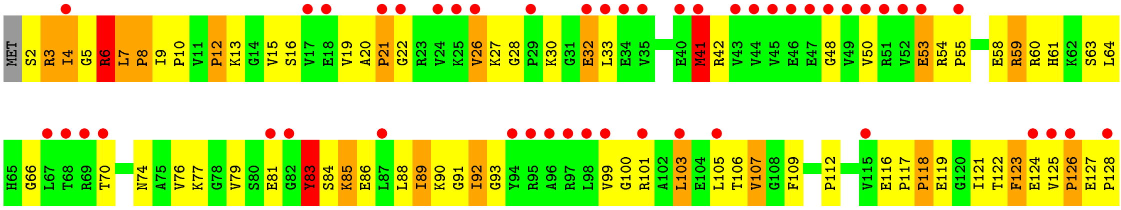
Chain BH:

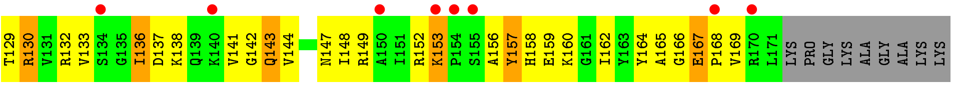




- Molecule 31: 50S ribosomal protein L6

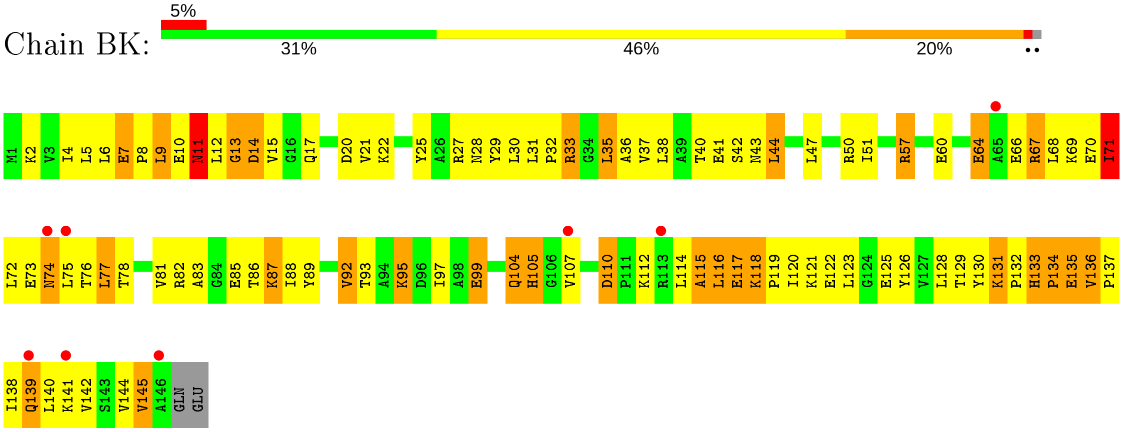
Chain DH:





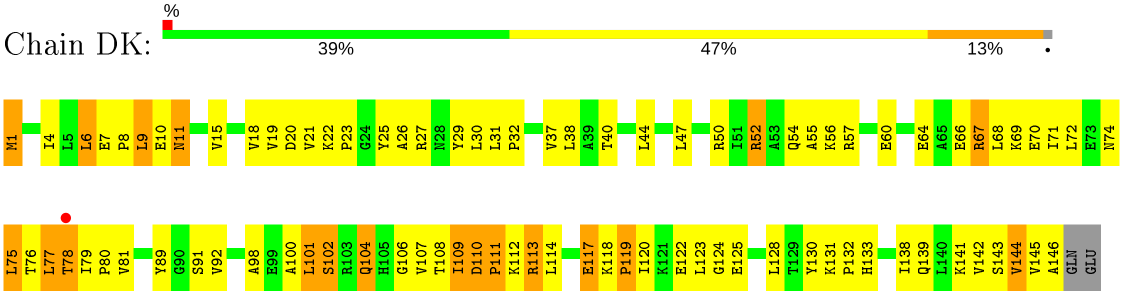
- Molecule 32: 50S ribosomal protein L9

Chain BK:



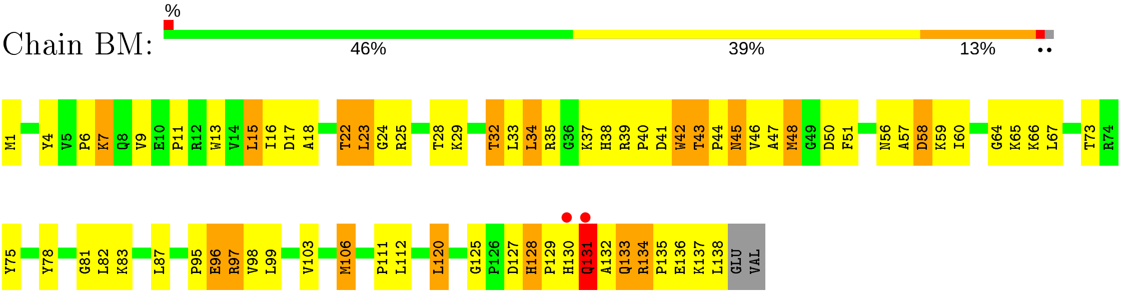
- Molecule 32: 50S ribosomal protein L9

Chain DK:



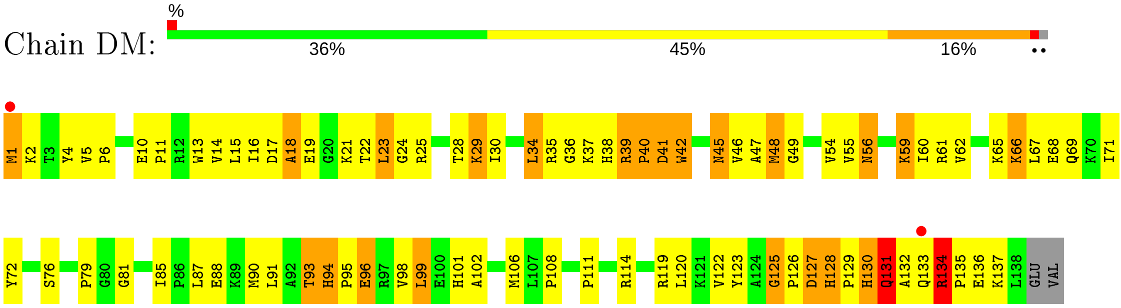
- Molecule 33: 50S ribosomal protein L13

Chain BM:

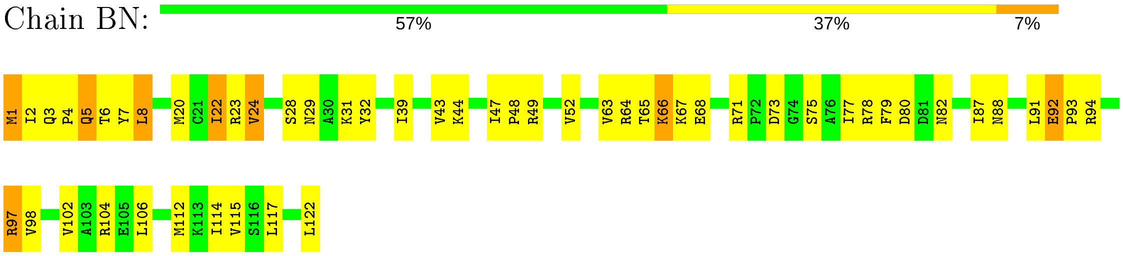


- Molecule 33: 50S ribosomal protein L13

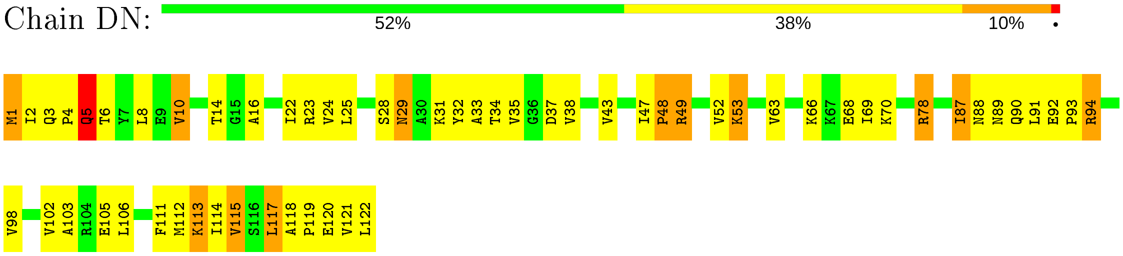
Chain DM:



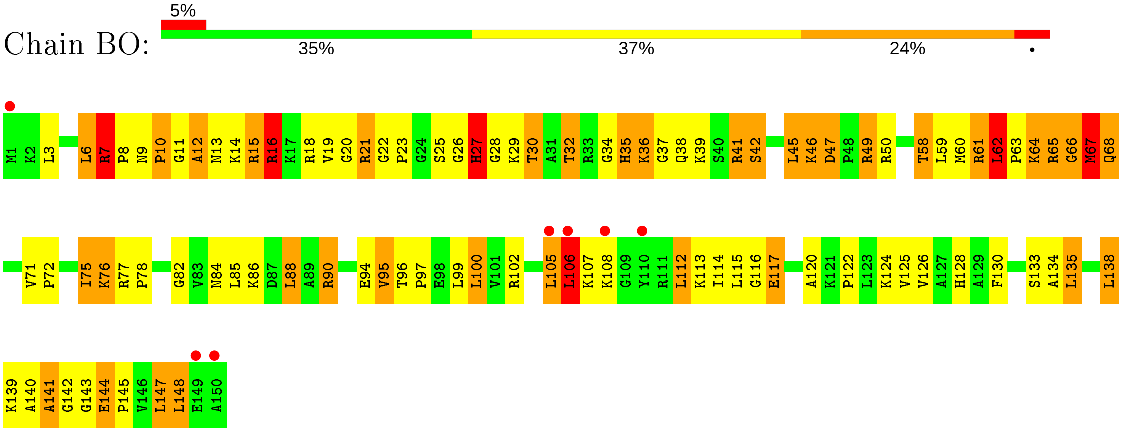
- Molecule 34: 50S ribosomal protein L14



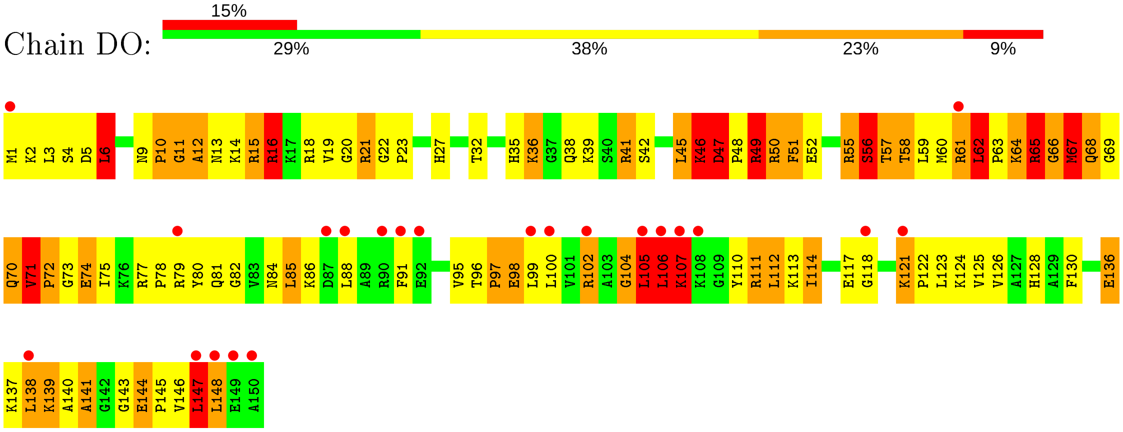
- Molecule 34: 50S ribosomal protein L14



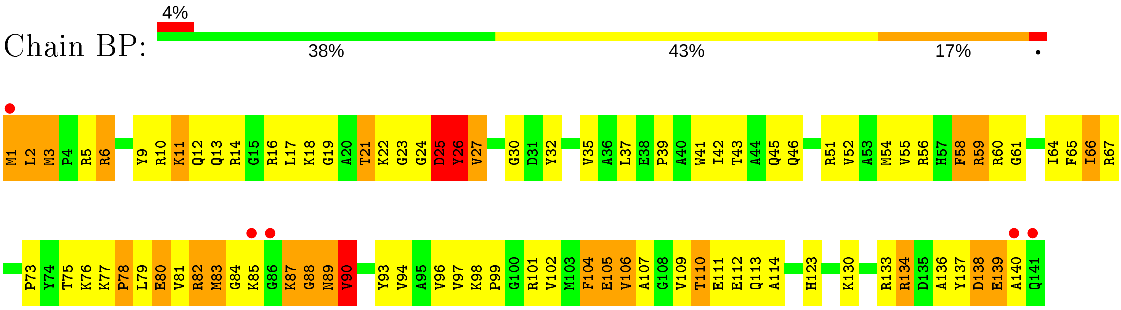
- Molecule 35: 50S ribosomal protein L15



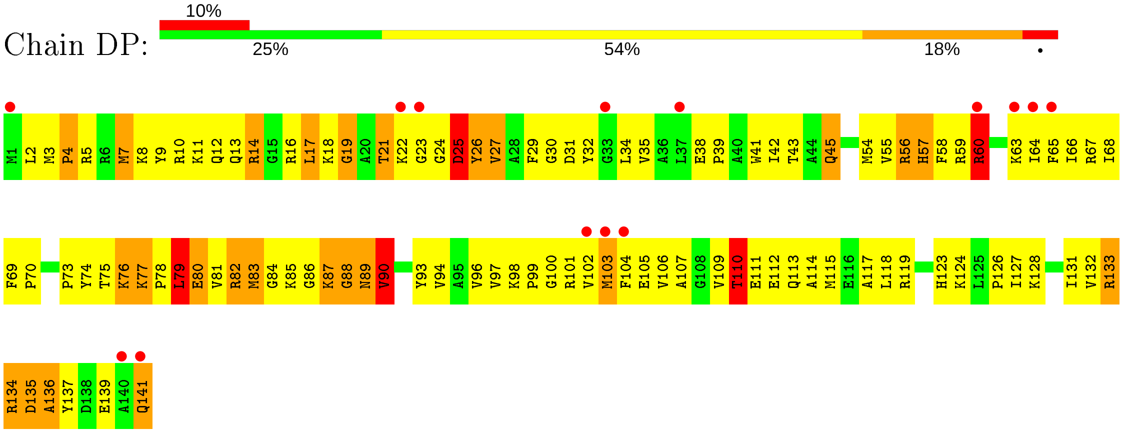
- Molecule 35: 50S ribosomal protein L15



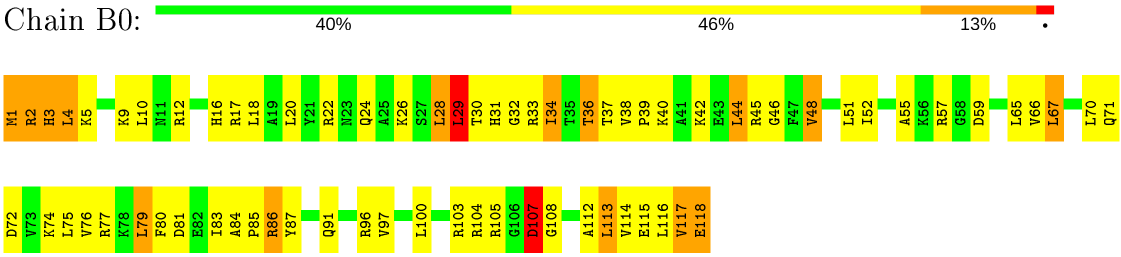
- Molecule 36: 50S ribosomal protein L16



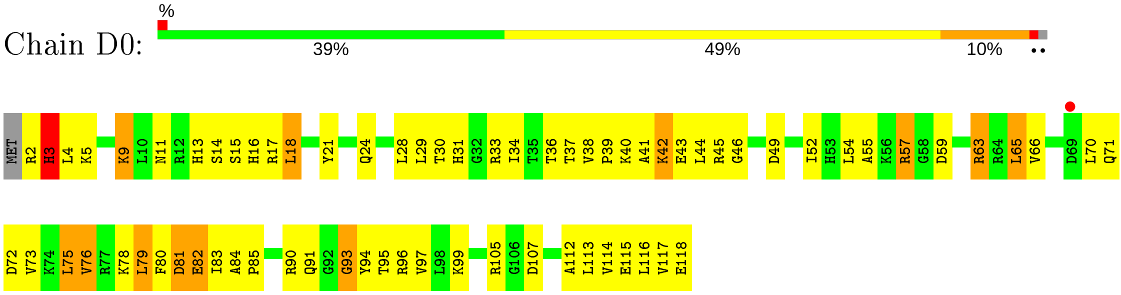
- Molecule 36: 50S ribosomal protein L16



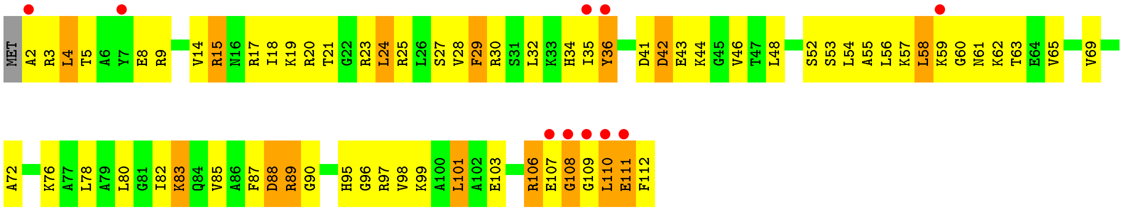
- Molecule 37: 50S ribosomal protein L17



- Molecule 37: 50S ribosomal protein L17

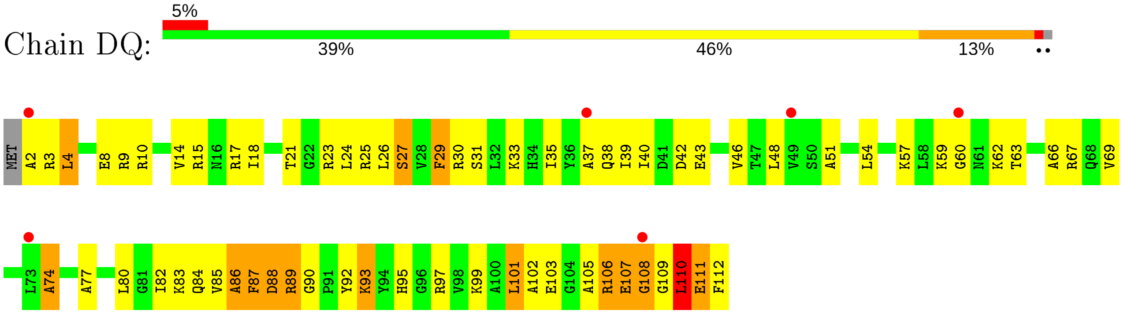


- Molecule 38: 50S ribosomal protein L18



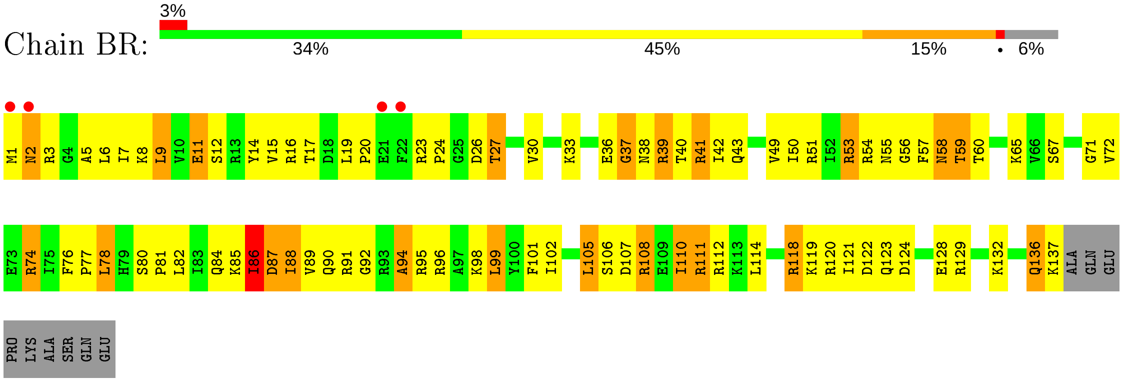
- Molecule 38: 50S ribosomal protein L18

Chain DQ:



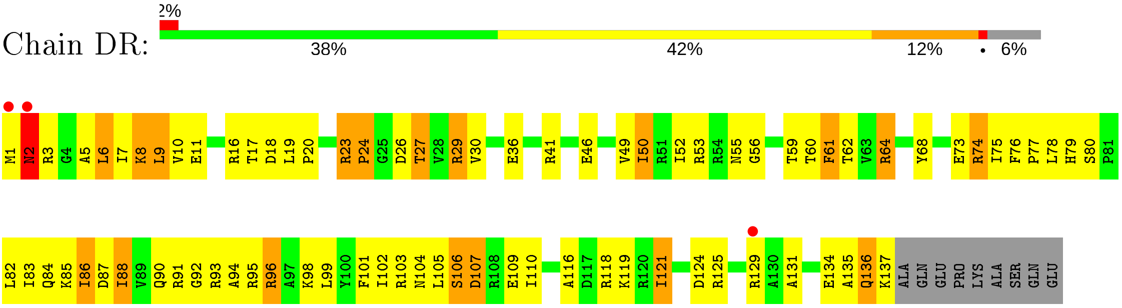
- Molecule 39: 50S ribosomal protein L19

Chain BR:



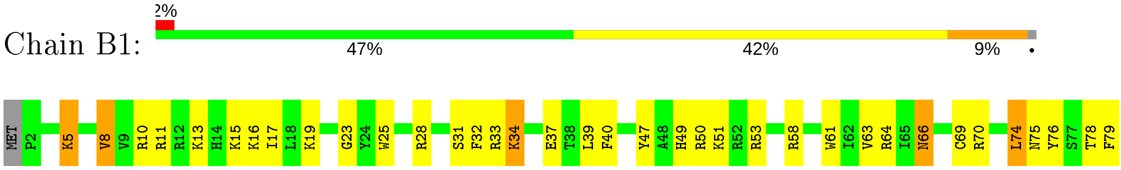
- Molecule 39: 50S ribosomal protein L19

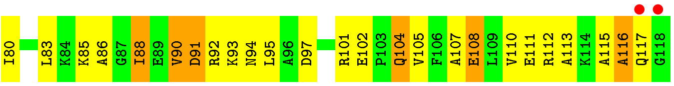
Chain DR:



- Molecule 40: 50S ribosomal protein L20

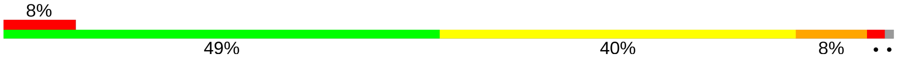
Chain B1:

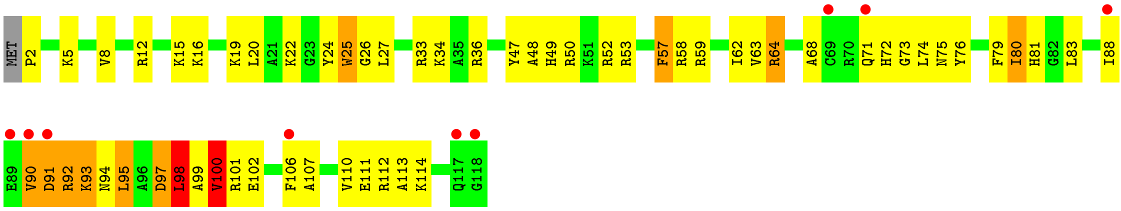




- Molecule 40: 50S ribosomal protein L20

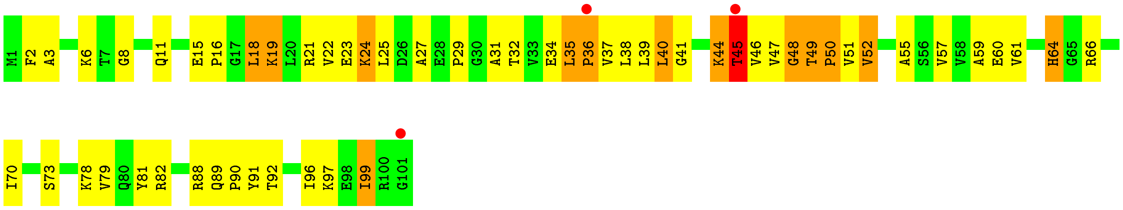
Chain D1:





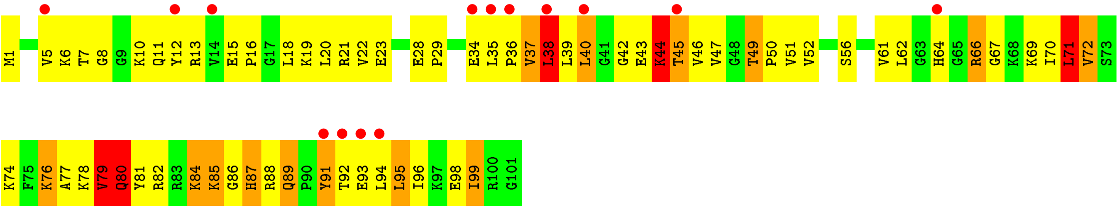
- Molecule 41: 50S ribosomal protein L21

Chain B2:



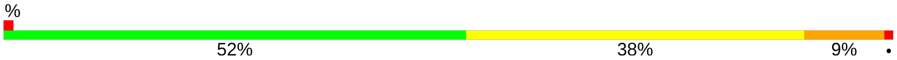
- Molecule 41: 50S ribosomal protein L21

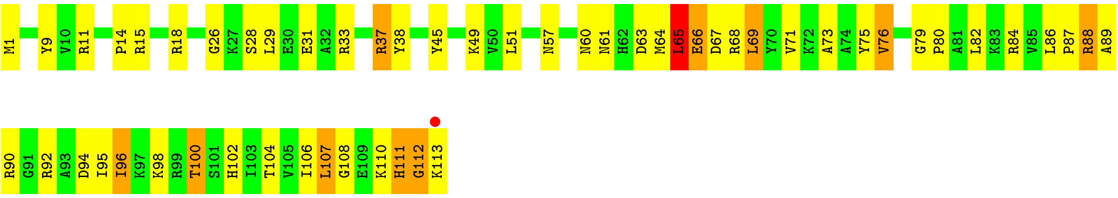
Chain D2:



- Molecule 42: 50S ribosomal protein L22

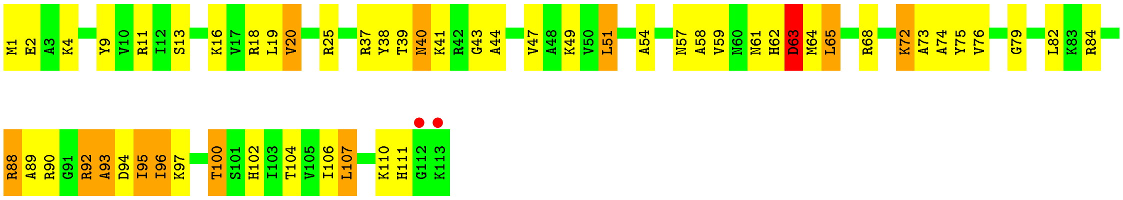
Chain BS:





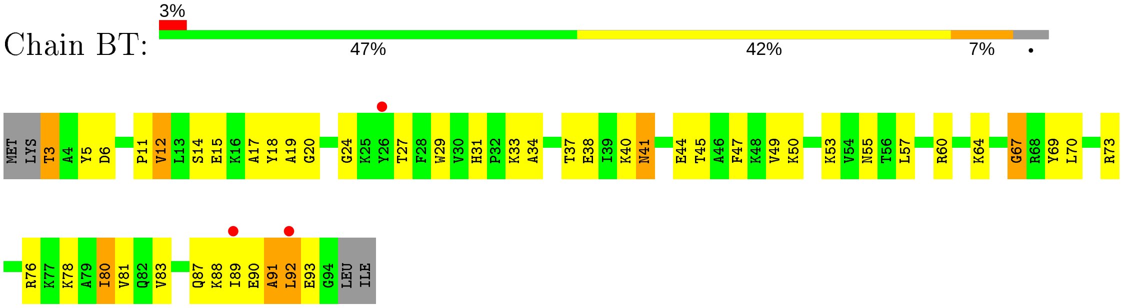
- Molecule 42: 50S ribosomal protein L22

Chain DS:



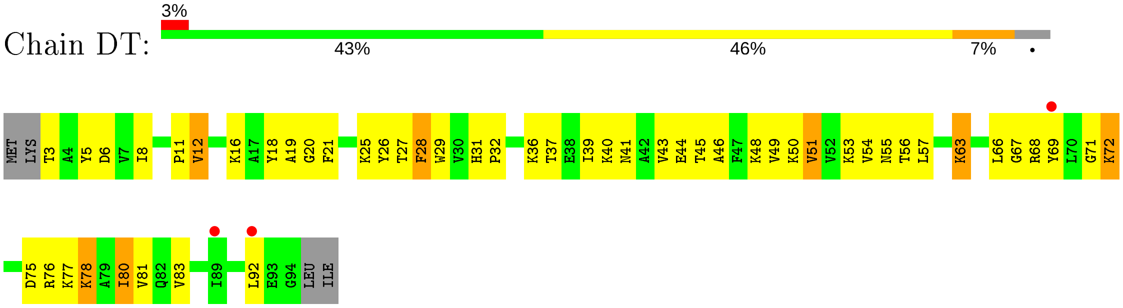
- Molecule 43: 50S ribosomal protein L23

Chain BT:



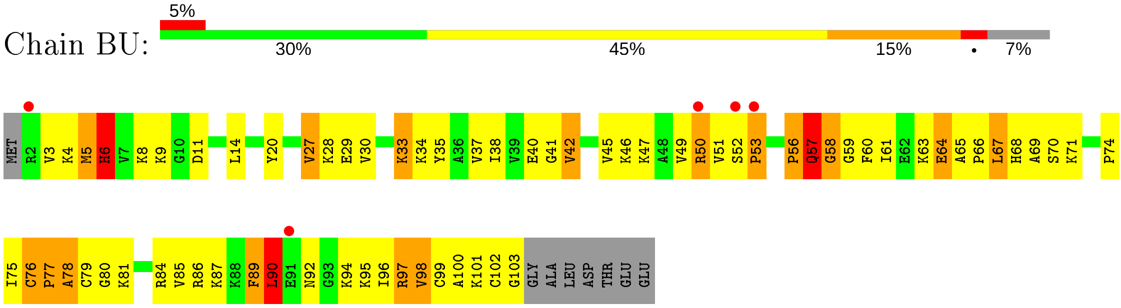
- Molecule 43: 50S ribosomal protein L23

Chain DT:



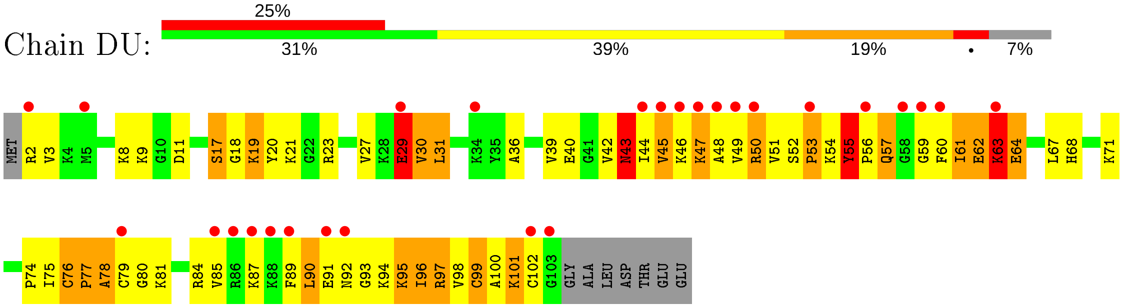
- Molecule 44: 50S ribosomal protein L24

Chain BU:

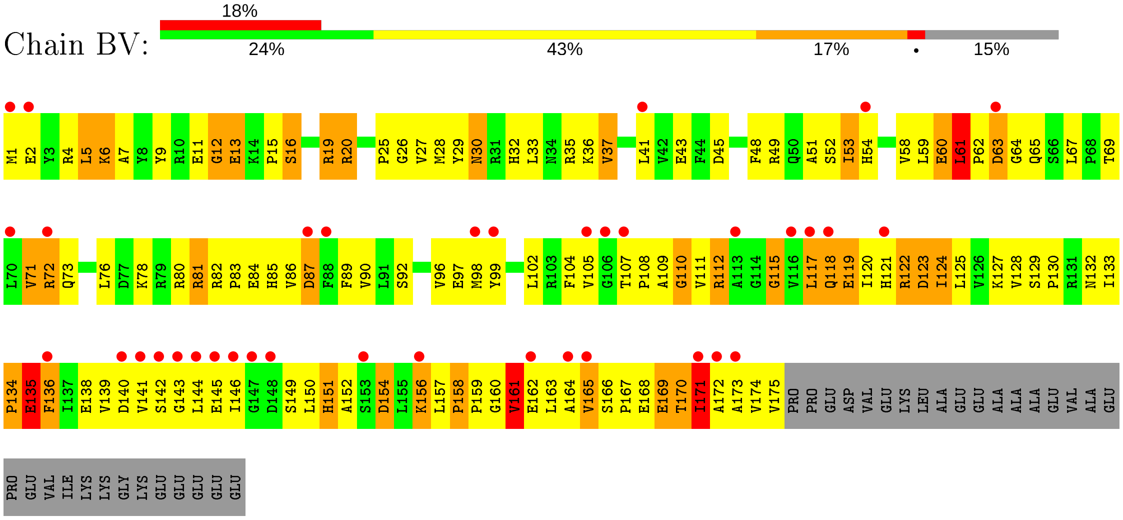


- Molecule 44: 50S ribosomal protein L24

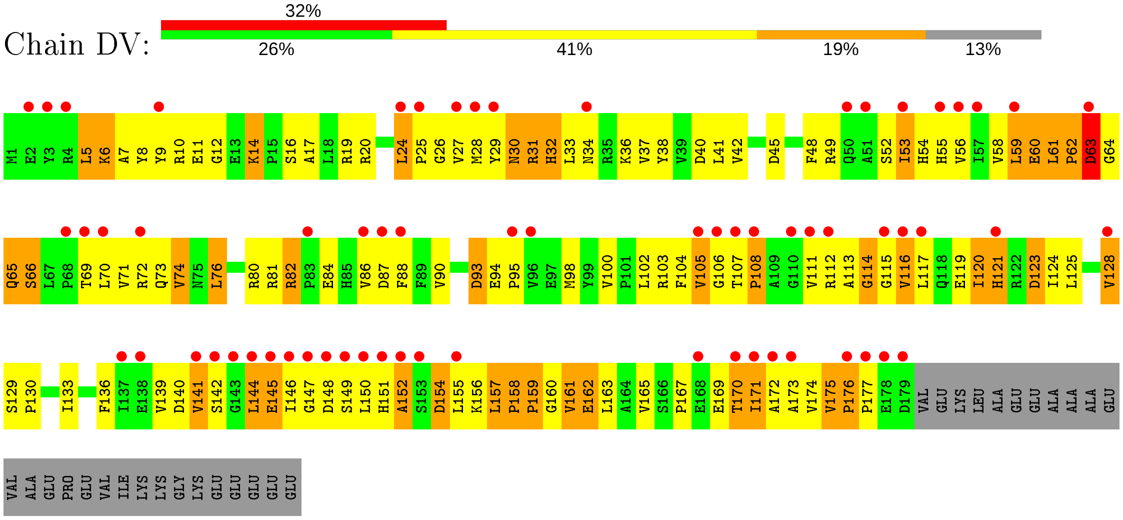
Chain DU:



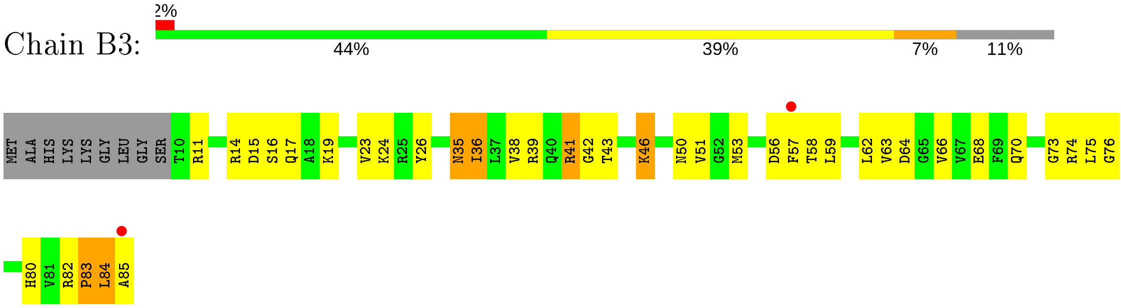
- Molecule 45: 50S ribosomal protein L25



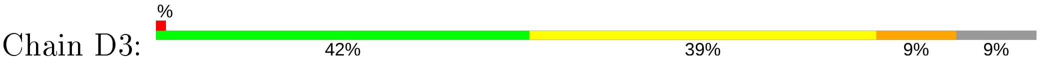
- Molecule 45: 50S ribosomal protein L25

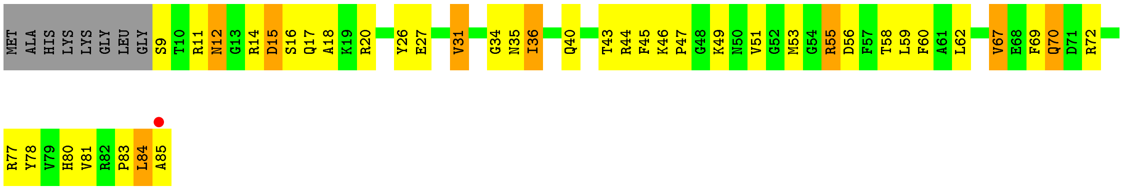


- Molecule 46: 50S ribosomal protein L27



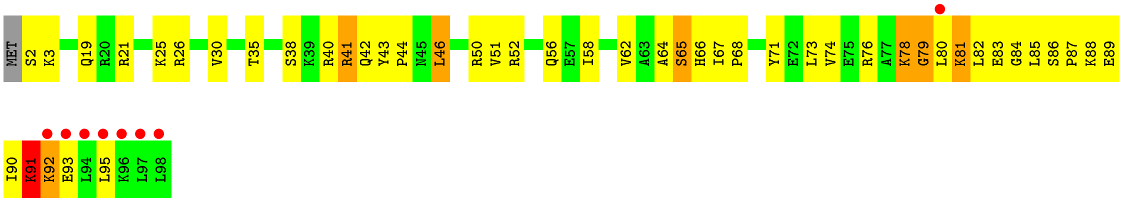
- Molecule 46: 50S ribosomal protein L27





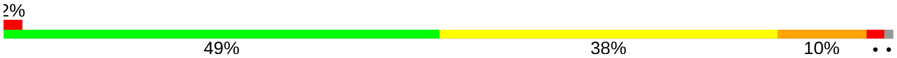
- Molecule 47: 50S ribosomal protein L28

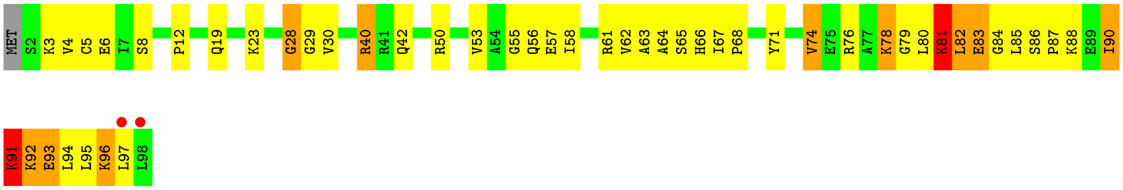
Chain BZ:



- Molecule 47: 50S ribosomal protein L28

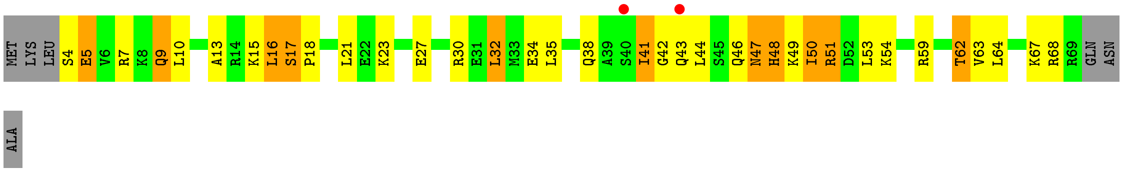
Chain DZ:





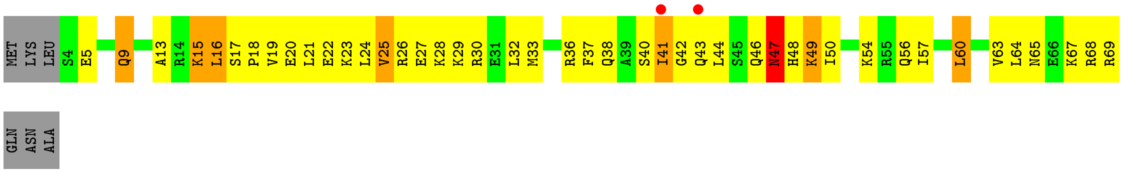
- Molecule 48: 50S ribosomal protein L29

Chain BW:



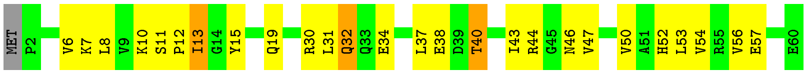
- Molecule 48: 50S ribosomal protein L29

Chain DW:



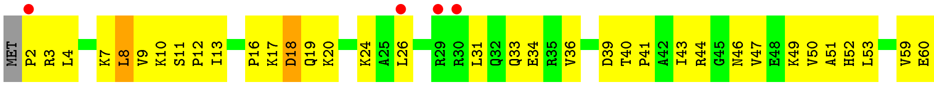
- Molecule 49: 50S ribosomal protein L30

Chain BX:



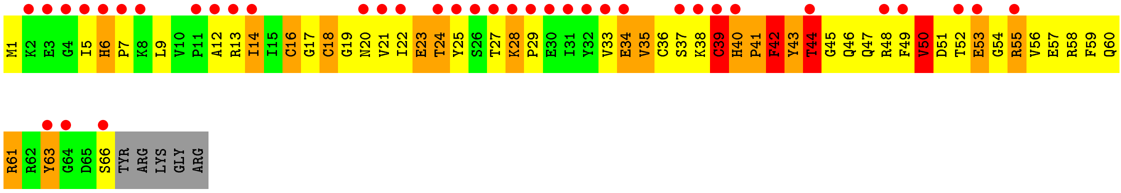
- Molecule 49: 50S ribosomal protein L30

Chain DX:



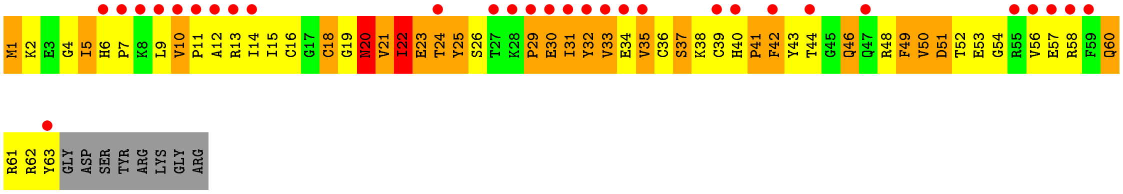
- Molecule 50: 50S ribosomal protein L31

Chain B4:



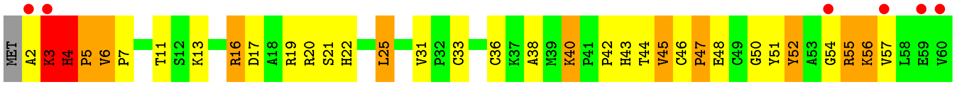
- Molecule 50: 50S ribosomal protein L31

Chain D4:



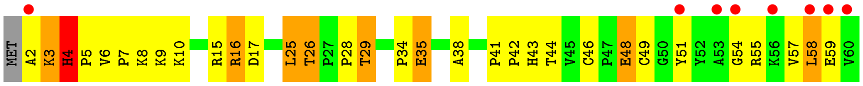
- Molecule 51: 50S ribosomal protein L32

Chain B5:



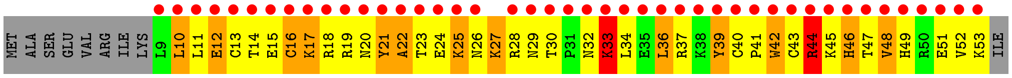
- Molecule 51: 50S ribosomal protein L32

Chain D5:



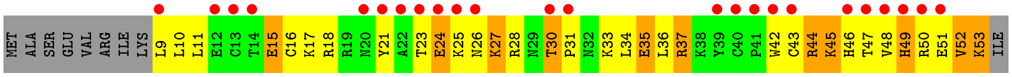
- Molecule 52: 50S ribosomal protein L33

Chain B6:



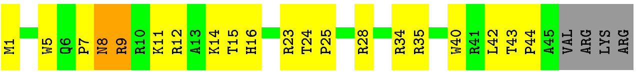
- Molecule 52: 50S ribosomal protein L33

Chain D6:



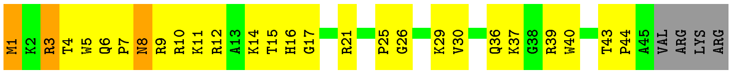
- Molecule 53: 50S ribosomal protein L34

Chain B7:



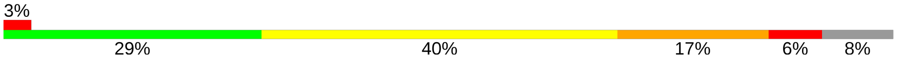
- Molecule 53: 50S ribosomal protein L34

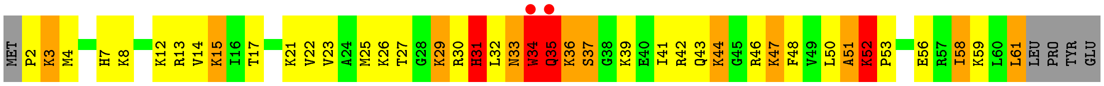
Chain D7:



- Molecule 54: 50S ribosomal protein L35

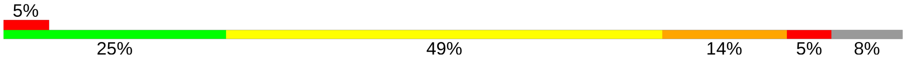
Chain B8:

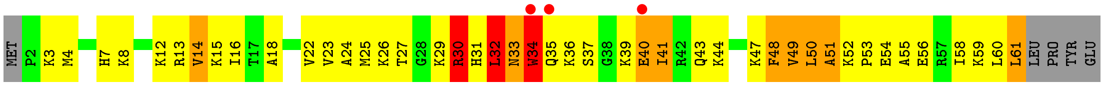




- Molecule 54: 50S ribosomal protein L35

Chain D8:





4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	210.67Å 451.75Å 625.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	154.06 – 3.00 257.02 – 3.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (154.06-3.00) 93.5 (257.02-3.00)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.20 (at 3.01Å)	Xtriage
Refinement program	PHENIX dev_810	Depositor
R, R_{free}	0.203 , 0.235 0.204 , 0.232	Depositor DCC
R_{free} test set	2000 reflections (0.17%)	wwPDB-VP
Wilson B-factor (Å^2)	78.2	Xtriage
Anisotropy	0.228	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 82.8	EDS
L-test for twinning[2]	$< \|L\| >= 0.47$, $< L^2 >= 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	299676	wwPDB-VP
Average B, all atoms (Å^2)	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.47% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: MIA, 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	0.28	0/36139	0.67	20/56406 (0.0%)
1	CA	0.28	0/36142	0.66	20/56410 (0.0%)
2	AE	0.22	0/1959	0.42	0/2642
2	CE	0.22	0/1959	0.42	0/2642
3	AF	0.22	0/1629	0.42	0/2195
3	CF	0.21	0/1636	0.40	0/2205
4	AG	0.29	1/1733 (0.1%)	0.44	0/2318
4	CG	0.27	0/1733	0.47	0/2318
5	AH	0.24	0/1171	0.44	0/1576
5	CH	0.24	0/1171	0.44	0/1576
6	AI	0.24	0/856	0.42	0/1154
6	CI	0.24	0/856	0.42	0/1154
7	AJ	0.22	0/1276	0.40	0/1709
7	CJ	0.22	0/1276	0.38	0/1709
8	AK	0.23	0/1136	0.44	0/1527
8	CK	0.22	0/1136	0.42	0/1527
9	AL	0.23	0/1029	0.41	0/1379
9	CL	0.22	0/1029	0.42	0/1379
10	AM	0.22	0/814	0.42	0/1095
10	CM	0.21	0/814	0.43	0/1095
11	AN	0.24	0/900	0.44	0/1213
11	CN	0.24	0/900	0.43	0/1213
12	AO	0.26	0/991	0.49	0/1327
12	CO	0.25	0/991	0.49	0/1327
13	AP	0.22	0/938	0.45	0/1258
13	CP	0.20	0/943	0.41	0/1265
14	AQ	0.27	0/485	0.47	0/643
14	CQ	0.23	0/485	0.43	0/643
15	AR	0.24	0/745	0.43	0/992
15	CR	0.23	0/745	0.39	0/992
16	AS	0.22	0/721	0.44	0/970
16	CS	0.23	0/721	0.42	0/970

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	AT	0.23	0/847	0.43	0/1131
17	CT	0.24	0/847	0.42	0/1131
18	AU	0.25	0/596	0.45	0/790
18	CU	0.24	0/596	0.44	0/790
19	AV	0.23	0/638	0.45	0/860
19	CV	0.22	0/638	0.43	0/860
20	AW	0.22	0/765	0.42	0/1007
20	CW	0.23	0/765	0.45	0/1007
21	AX	0.22	0/221	0.41	0/288
21	CX	0.21	0/221	0.40	0/288
22	AB	0.28	0/1992	0.60	0/3099
22	AD	0.21	0/1992	0.50	0/3099
22	CB	0.26	0/1992	0.57	0/3099
22	CD	0.20	0/1992	0.49	0/3099
23	AC	0.25	0/1835	0.59	1/2859 (0.0%)
23	CC	0.24	0/1835	0.57	0/2859
24	A1	0.33	0/389	0.64	0/604
24	C1	0.38	0/389	0.65	0/604
25	BA	0.37	0/70233	0.75	52/109643 (0.0%)
25	DA	0.33	1/70122 (0.0%)	0.70	54/109469 (0.0%)
26	BB	0.33	0/2928	0.80	11/4568 (0.2%)
26	DB	0.29	0/2928	0.74	4/4568 (0.1%)
27	BD	0.32	0/2165	0.58	1/2919 (0.0%)
27	DD	0.29	0/2165	0.52	0/2919
28	BE	0.29	0/1601	0.55	0/2160
28	DE	0.27	0/1601	0.52	0/2160
29	BF	0.28	0/1620	0.50	0/2194
29	DF	0.26	0/1662	0.52	0/2249
30	BG	0.24	0/1499	0.43	0/2016
30	DG	0.21	0/1499	0.42	0/2016
31	BH	0.25	0/1332	0.50	0/1802
31	DH	0.21	0/1332	0.44	0/1802
32	BK	0.24	0/1151	0.49	0/1558
32	DK	0.23	0/1151	0.51	0/1558
33	BM	0.26	0/1131	0.49	0/1525
33	DM	0.23	0/1131	0.44	0/1525
34	BN	0.27	0/943	0.46	0/1269
34	DN	0.26	0/943	0.46	0/1269
35	BO	0.28	0/1162	0.58	0/1544
35	DO	0.24	0/1162	0.45	0/1544
36	BP	0.27	0/1143	0.46	0/1527
36	DP	0.24	0/1143	0.41	0/1527
37	B0	0.26	0/982	0.48	0/1312

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
37	D0	0.25	0/974	0.45	0/1302
38	BQ	0.26	0/892	0.50	0/1187
38	DQ	0.23	0/892	0.46	0/1187
39	BR	0.28	0/1155	0.49	0/1542
39	DR	0.25	0/1155	0.44	0/1542
40	B1	0.28	0/982	0.49	0/1306
40	D1	0.24	0/982	0.44	0/1306
41	B2	0.26	0/790	0.48	0/1057
41	D2	0.27	0/790	0.51	0/1057
42	BS	0.27	0/911	0.47	0/1220
42	DS	0.26	0/911	0.44	0/1220
43	BT	0.31	0/739	0.49	0/993
43	DT	0.28	0/739	0.46	0/993
44	BU	0.29	0/798	0.52	0/1064
44	DU	0.26	0/798	0.48	0/1064
45	BV	0.23	0/1427	0.48	1/1935 (0.1%)
45	DV	0.22	0/1460	0.43	0/1982
46	B3	0.28	0/615	0.46	0/819
46	D3	0.26	0/621	0.44	0/827
47	BZ	0.27	0/770	0.50	0/1022
47	DZ	0.26	0/770	0.50	0/1022
48	BW	0.28	0/560	0.52	0/741
48	DW	0.25	0/560	0.45	0/741
49	BX	0.25	0/474	0.42	0/635
49	DX	0.22	0/474	0.41	0/635
50	B4	0.22	0/545	0.49	0/733
50	D4	0.23	0/527	0.51	0/709
51	B5	0.25	0/473	0.51	0/639
51	D5	0.24	0/473	0.54	0/639
52	B6	0.26	0/396	0.46	0/529
52	D6	0.23	0/396	0.51	0/529
53	B7	0.31	0/399	0.44	0/526
53	D7	0.26	0/399	0.44	0/526
54	B8	0.33	0/486	0.55	0/638
54	D8	0.33	0/486	0.67	0/638
All	All	0.30	2/324157 (0.0%)	0.65	164/485451 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
31	BH	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	DA	2873	A	N7-C5	-5.99	1.35	1.39
4	AG	12	CYS	CB-SG	5.09	1.90	1.82

The worst 5 of 164 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	DA	2311	A	N1-C2-N3	12.09	135.35	129.30
25	DA	2311	A	N1-C6-N6	10.02	124.61	118.60
25	BA	673	C	C2-N3-C4	-10.01	114.89	119.90
26	BB	95	U	C5-C4-O4	9.25	131.45	125.90
25	DA	673	C	C2-N3-C4	-9.13	115.33	119.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
31	BH	153	LYS	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32284	0	16296	1132	1
1	CA	32287	0	16295	1151	1
2	AE	1924	0	1975	160	0
2	CE	1924	0	1975	155	0
3	AF	1605	0	1668	115	0
3	CF	1612	0	1677	117	0
4	AG	1703	0	1763	116	0
4	CG	1703	0	1763	116	0
5	AH	1155	0	1213	75	0
5	CH	1155	0	1213	63	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	AI	843	0	857	52	0
6	CI	843	0	857	41	0
7	AJ	1257	0	1296	66	0
7	CJ	1257	0	1296	73	0
8	AK	1116	0	1177	76	0
8	CK	1116	0	1177	48	0
9	AL	1010	0	1037	80	0
9	CL	1010	0	1037	112	0
10	AM	801	0	849	76	0
10	CM	801	0	849	83	0
11	AN	885	0	904	58	0
11	CN	885	0	904	38	0
12	AO	975	0	1062	96	0
12	CO	975	0	1062	66	0
13	AP	928	0	987	76	0
13	CP	933	0	992	81	0
14	AQ	476	0	511	42	0
14	CQ	476	0	511	39	0
15	AR	734	0	771	33	0
15	CR	734	0	771	32	0
16	AS	705	0	725	57	0
16	CS	705	0	725	23	0
17	AT	834	0	904	43	0
17	CT	834	0	904	39	0
18	AU	591	0	662	27	0
18	CU	591	0	662	37	0
19	AV	624	0	636	52	0
19	CV	624	0	636	67	0
20	AW	763	0	861	63	0
20	CW	763	0	861	58	0
21	AX	217	0	234	18	0
21	CX	217	0	234	20	0
22	AB	1814	0	932	112	0
22	AD	1814	0	932	110	0
22	CB	1814	0	932	111	0
22	CD	1814	0	932	99	0
23	AC	1643	0	837	41	0
23	CC	1643	0	837	38	0
24	A1	346	0	174	19	0
24	C1	346	0	174	17	0
25	BA	62707	0	31614	1935	0
25	DA	62607	0	31565	2087	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	BB	2617	0	1328	89	0
26	DB	2617	0	1328	108	0
27	BD	2115	0	2195	197	0
27	DD	2115	0	2195	189	0
28	BE	1568	0	1634	146	0
28	DE	1568	0	1634	183	0
29	BF	1585	0	1632	111	0
29	DF	1627	0	1680	162	0
30	BG	1474	0	1535	129	0
30	DG	1474	0	1535	101	0
31	BH	1307	0	1382	147	0
31	DH	1307	0	1382	101	1
32	BK	1136	0	1223	102	0
32	DK	1136	0	1223	79	0
33	BM	1104	0	1180	75	0
33	DM	1104	0	1180	82	0
34	BN	933	0	996	51	0
34	DN	933	0	996	55	0
35	BO	1145	0	1228	176	0
35	DO	1145	0	1228	299	0
36	BP	1122	0	1179	140	0
36	DP	1122	0	1179	166	0
37	B0	968	0	1033	75	0
37	D0	960	0	1021	66	0
38	BQ	882	0	943	84	0
38	DQ	882	0	943	79	0
39	BR	1141	0	1202	98	0
39	DR	1141	0	1202	94	0
40	B1	964	0	1022	74	0
40	D1	964	0	1022	84	0
41	B2	779	0	852	72	0
41	D2	779	0	852	114	0
42	BS	900	0	964	41	0
42	DS	900	0	964	52	0
43	BT	725	0	778	48	0
43	DT	725	0	778	50	0
44	BU	785	0	878	99	0
44	DU	785	0	878	91	0
45	BV	1397	0	1430	138	0
45	DV	1428	0	1454	125	0
46	B3	607	0	628	41	0
46	D3	613	0	633	45	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
47	BZ	763	0	848	50	0
47	DZ	763	0	848	48	0
48	BW	558	0	610	38	0
48	DW	558	0	610	43	0
49	BX	469	0	518	21	0
49	DX	469	0	518	24	0
50	B4	533	0	522	128	0
50	D4	515	0	510	71	0
51	B5	459	0	480	92	0
51	D5	459	0	476	39	0
52	B6	389	0	404	80	0
52	D6	389	0	404	51	0
53	B7	391	0	432	17	0
53	D7	391	0	432	25	0
54	B8	480	0	549	116	0
54	D8	480	0	549	81	0
55	A1	1	0	0	0	0
55	AA	220	0	0	0	0
55	AB	4	0	0	0	0
55	AC	8	0	0	0	0
55	AD	3	0	0	0	0
55	AG	2	0	0	0	0
55	AN	1	0	0	0	0
55	AR	1	0	0	0	0
55	AS	1	0	0	0	0
55	B0	1	0	0	0	0
55	B1	2	0	0	0	0
55	B2	1	0	0	0	0
55	B3	3	0	0	0	0
55	B5	1	0	0	0	0
55	B6	1	0	0	0	0
55	B7	1	0	0	0	0
55	BA	568	0	0	0	0
55	BB	18	0	0	0	0
55	BD	1	0	0	0	0
55	BE	3	0	0	0	0
55	BF	3	0	0	0	0
55	BO	2	0	0	0	0
55	BW	1	0	0	0	0
55	CA	219	0	0	0	0
55	CB	4	0	0	0	0
55	CC	9	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	CD	1	0	0	0	0
55	CG	2	0	0	0	0
55	CK	1	0	0	0	0
55	CR	1	0	0	0	0
55	D0	1	0	0	0	0
55	D1	1	0	0	0	0
55	D3	1	0	0	0	0
55	D5	2	0	0	0	0
55	D7	1	0	0	0	0
55	D8	1	0	0	0	0
55	DA	488	0	0	0	0
55	DB	20	0	0	0	0
55	DD	3	0	0	0	0
55	DE	1	0	0	0	0
55	DO	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	299676	0	200977	13379	2

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 27.

The worst 5 of 13379 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)
35:DO:46:LYS:HD3	35:DO:51:PHE:CD1	1.38	1.55
54:B8:34:TRP:CB	54:B8:35:GLN:HB2	1.34	1.55
50:B4:37:SER:HB3	50:B4:42:PHE:CD1	1.40	1.52
35:DO:71:VAL:HG13	35:DO:72:PRO:CD	1.44	1.47
35:BO:19:VAL:HG23	35:BO:27:HIS:CB	1.45	1.46

All (2) 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]	1.97	0.23
1:CA:86:U:O2'	25:DA:276:A:OP2[3_545]	2.19	0.01

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%)	170 (72%)	44 (19%)	21 (9%)	1	3
2	CE	235/256 (92%)	161 (68%)	48 (20%)	26 (11%)	0	2
3	AF	203/239 (85%)	157 (77%)	36 (18%)	10 (5%)	2	13
3	CF	204/239 (85%)	151 (74%)	40 (20%)	13 (6%)	1	7
4	AG	206/208 (99%)	169 (82%)	29 (14%)	8 (4%)	3	17
4	CG	206/208 (99%)	167 (81%)	24 (12%)	15 (7%)	1	5
5	AH	149/162 (92%)	128 (86%)	16 (11%)	5 (3%)	3	20
5	CH	149/162 (92%)	129 (87%)	18 (12%)	2 (1%)	12	45
6	AI	99/101 (98%)	88 (89%)	8 (8%)	3 (3%)	4	24
6	CI	99/101 (98%)	92 (93%)	7 (7%)	0	100	100
7	AJ	153/156 (98%)	127 (83%)	21 (14%)	5 (3%)	4	21
7	CJ	153/156 (98%)	131 (86%)	16 (10%)	6 (4%)	3	17
8	AK	136/138 (99%)	113 (83%)	15 (11%)	8 (6%)	1	9
8	CK	136/138 (99%)	116 (85%)	17 (12%)	3 (2%)	6	31
9	AL	125/128 (98%)	90 (72%)	26 (21%)	9 (7%)	1	5
9	CL	125/128 (98%)	86 (69%)	30 (24%)	9 (7%)	1	5
10	AM	97/105 (92%)	77 (79%)	17 (18%)	3 (3%)	4	23
10	CM	97/105 (92%)	79 (81%)	13 (13%)	5 (5%)	2	12
11	AN	117/129 (91%)	101 (86%)	11 (9%)	5 (4%)	2	15
11	CN	117/129 (91%)	97 (83%)	16 (14%)	4 (3%)	3	20
12	AO	123/132 (93%)	104 (85%)	7 (6%)	12 (10%)	0	2
12	CO	123/132 (93%)	96 (78%)	21 (17%)	6 (5%)	2	13
13	AP	114/126 (90%)	76 (67%)	26 (23%)	12 (10%)	0	2
13	CP	115/126 (91%)	83 (72%)	18 (16%)	14 (12%)	0	1
14	AQ	56/61 (92%)	37 (66%)	7 (12%)	12 (21%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	CQ	56/61 (92%)	39 (70%)	9 (16%)	8 (14%)	0	1
15	AR	86/89 (97%)	68 (79%)	14 (16%)	4 (5%)	2	14
15	CR	86/89 (97%)	82 (95%)	2 (2%)	2 (2%)	6	30
16	AS	82/88 (93%)	64 (78%)	13 (16%)	5 (6%)	1	8
16	CS	82/88 (93%)	72 (88%)	10 (12%)	0	100	100
17	AT	98/105 (93%)	83 (85%)	9 (9%)	6 (6%)	1	8
17	CT	98/105 (93%)	85 (87%)	10 (10%)	3 (3%)	4	23
18	AU	70/88 (80%)	53 (76%)	13 (19%)	4 (6%)	1	10
18	CU	70/88 (80%)	60 (86%)	7 (10%)	3 (4%)	2	15
19	AV	76/93 (82%)	56 (74%)	12 (16%)	8 (10%)	0	2
19	CV	76/93 (82%)	53 (70%)	16 (21%)	7 (9%)	1	3
20	AW	97/106 (92%)	75 (77%)	14 (14%)	8 (8%)	1	4
20	CW	97/106 (92%)	72 (74%)	16 (16%)	9 (9%)	0	3
21	AX	23/27 (85%)	19 (83%)	2 (9%)	2 (9%)	1	3
21	CX	23/27 (85%)	18 (78%)	2 (9%)	3 (13%)	0	1
27	BD	270/276 (98%)	227 (84%)	30 (11%)	13 (5%)	2	13
27	DD	270/276 (98%)	226 (84%)	32 (12%)	12 (4%)	2	15
28	BE	203/206 (98%)	146 (72%)	34 (17%)	23 (11%)	0	2
28	DE	203/206 (98%)	134 (66%)	40 (20%)	29 (14%)	0	1
29	BF	200/210 (95%)	177 (88%)	14 (7%)	9 (4%)	2	14
29	DF	206/210 (98%)	153 (74%)	30 (15%)	23 (11%)	0	2
30	BG	179/182 (98%)	139 (78%)	27 (15%)	13 (7%)	1	5
30	DG	179/182 (98%)	140 (78%)	28 (16%)	11 (6%)	1	8
31	BH	168/180 (93%)	113 (67%)	20 (12%)	35 (21%)	0	0
31	DH	168/180 (93%)	108 (64%)	36 (21%)	24 (14%)	0	1
32	BK	144/148 (97%)	90 (62%)	39 (27%)	15 (10%)	0	2
32	DK	144/148 (97%)	98 (68%)	36 (25%)	10 (7%)	1	6
33	BM	136/140 (97%)	107 (79%)	21 (15%)	8 (6%)	1	9
33	DM	136/140 (97%)	106 (78%)	16 (12%)	14 (10%)	0	2
34	BN	120/122 (98%)	114 (95%)	4 (3%)	2 (2%)	9	39
34	DN	120/122 (98%)	106 (88%)	10 (8%)	4 (3%)	4	21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	BO	148/150 (99%)	99 (67%)	29 (20%)	20 (14%)	0	1
35	DO	148/150 (99%)	92 (62%)	25 (17%)	31 (21%)	0	0
36	BP	139/141 (99%)	102 (73%)	19 (14%)	18 (13%)	0	1
36	DP	139/141 (99%)	92 (66%)	31 (22%)	16 (12%)	0	2
37	B0	116/118 (98%)	97 (84%)	11 (10%)	8 (7%)	1	6
37	D0	115/118 (98%)	95 (83%)	15 (13%)	5 (4%)	2	15
38	BQ	109/112 (97%)	85 (78%)	17 (16%)	7 (6%)	1	7
38	DQ	109/112 (97%)	73 (67%)	26 (24%)	10 (9%)	1	3
39	BR	135/146 (92%)	105 (78%)	21 (16%)	9 (7%)	1	6
39	DR	135/146 (92%)	108 (80%)	18 (13%)	9 (7%)	1	6
40	B1	115/118 (98%)	102 (89%)	8 (7%)	5 (4%)	2	15
40	D1	115/118 (98%)	91 (79%)	18 (16%)	6 (5%)	2	12
41	B2	99/101 (98%)	81 (82%)	12 (12%)	6 (6%)	1	8
41	D2	99/101 (98%)	68 (69%)	17 (17%)	14 (14%)	0	1
42	BS	111/113 (98%)	92 (83%)	13 (12%)	6 (5%)	2	11
42	DS	111/113 (98%)	92 (83%)	15 (14%)	4 (4%)	3	19
43	BT	90/96 (94%)	81 (90%)	5 (6%)	4 (4%)	2	15
43	DT	90/96 (94%)	72 (80%)	13 (14%)	5 (6%)	2	10
44	BU	100/110 (91%)	65 (65%)	21 (21%)	14 (14%)	0	1
44	DU	100/110 (91%)	62 (62%)	19 (19%)	19 (19%)	0	0
45	BV	173/206 (84%)	112 (65%)	32 (18%)	29 (17%)	0	0
45	DV	177/206 (86%)	109 (62%)	39 (22%)	29 (16%)	0	1
46	B3	74/85 (87%)	65 (88%)	6 (8%)	3 (4%)	3	16
46	D3	75/85 (88%)	64 (85%)	8 (11%)	3 (4%)	3	17
47	BZ	95/98 (97%)	79 (83%)	12 (13%)	4 (4%)	3	16
47	DZ	95/98 (97%)	76 (80%)	11 (12%)	8 (8%)	1	4
48	BW	64/72 (89%)	53 (83%)	6 (9%)	5 (8%)	1	4
48	DW	64/72 (89%)	54 (84%)	6 (9%)	4 (6%)	1	7
49	BX	57/60 (95%)	51 (90%)	5 (9%)	1 (2%)	8	37
49	DX	57/60 (95%)	49 (86%)	5 (9%)	3 (5%)	2	11
50	B4	64/71 (90%)	36 (56%)	12 (19%)	16 (25%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
50	D4	61/71 (86%)	22 (36%)	22 (36%)	17 (28%)	0	0
51	B5	57/60 (95%)	44 (77%)	6 (10%)	7 (12%)	0	1
51	D5	57/60 (95%)	46 (81%)	8 (14%)	3 (5%)	2	11
52	B6	43/54 (80%)	24 (56%)	12 (28%)	7 (16%)	0	1
52	D6	43/54 (80%)	26 (60%)	8 (19%)	9 (21%)	0	0
53	B7	43/49 (88%)	42 (98%)	1 (2%)	0	100	100
53	D7	43/49 (88%)	42 (98%)	1 (2%)	0	100	100
54	B8	58/65 (89%)	42 (72%)	8 (14%)	8 (14%)	0	1
54	D8	58/65 (89%)	37 (64%)	13 (22%)	8 (14%)	0	1
All	All	11319/12052 (94%)	8735 (77%)	1671 (15%)	913 (8%)	1	4

5 of 913 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AE	195	ASP
2	AE	236	TYR
2	AE	237	ALA
3	AF	4	LYS
3	AF	12	LEU

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%)	165 (80%)	40 (20%)	1	7
2	CE	205/220 (93%)	180 (88%)	25 (12%)	5	21
3	AF	159/188 (85%)	141 (89%)	18 (11%)	6	24
3	CF	160/188 (85%)	143 (89%)	17 (11%)	6	26
4	AG	180/180 (100%)	160 (89%)	20 (11%)	6	25
4	CG	180/180 (100%)	160 (89%)	20 (11%)	6	25
5	AH	116/123 (94%)	97 (84%)	19 (16%)	2	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	CH	116/123 (94%)	102 (88%)	14 (12%)	5	21
6	AI	90/90 (100%)	80 (89%)	10 (11%)	6	25
6	CI	90/90 (100%)	81 (90%)	9 (10%)	7	29
7	AJ	126/127 (99%)	106 (84%)	20 (16%)	2	12
7	CJ	126/127 (99%)	105 (83%)	21 (17%)	2	11
8	AK	119/119 (100%)	106 (89%)	13 (11%)	6	25
8	CK	119/119 (100%)	111 (93%)	8 (7%)	16	49
9	AL	98/99 (99%)	86 (88%)	12 (12%)	5	21
9	CL	98/99 (99%)	81 (83%)	17 (17%)	2	10
10	AM	89/92 (97%)	79 (89%)	10 (11%)	6	24
10	CM	89/92 (97%)	78 (88%)	11 (12%)	4	20
11	AN	90/99 (91%)	79 (88%)	11 (12%)	5	21
11	CN	90/99 (91%)	85 (94%)	5 (6%)	21	56
12	AO	104/109 (95%)	95 (91%)	9 (9%)	10	37
12	CO	104/109 (95%)	94 (90%)	10 (10%)	8	32
13	AP	94/101 (93%)	87 (93%)	7 (7%)	13	44
13	CP	94/101 (93%)	83 (88%)	11 (12%)	5	22
14	AQ	48/50 (96%)	42 (88%)	6 (12%)	4	20
14	CQ	48/50 (96%)	44 (92%)	4 (8%)	11	39
15	AR	79/80 (99%)	73 (92%)	6 (8%)	13	43
15	CR	79/80 (99%)	67 (85%)	12 (15%)	3	14
16	AS	72/74 (97%)	68 (94%)	4 (6%)	21	56
16	CS	72/74 (97%)	64 (89%)	8 (11%)	6	25
17	AT	95/97 (98%)	85 (90%)	10 (10%)	7	27
17	CT	95/97 (98%)	92 (97%)	3 (3%)	39	74
18	AU	63/77 (82%)	57 (90%)	6 (10%)	8	32
18	CU	63/77 (82%)	51 (81%)	12 (19%)	1	8
19	AV	67/80 (84%)	55 (82%)	12 (18%)	2	9
19	CV	67/80 (84%)	58 (87%)	9 (13%)	4	17
20	AW	76/82 (93%)	68 (90%)	8 (10%)	7	27
20	CW	76/82 (93%)	66 (87%)	10 (13%)	4	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	AX	20/22 (91%)	20 (100%)	0	100	100
21	CX	20/22 (91%)	20 (100%)	0	100	100
27	BD	214/218 (98%)	178 (83%)	36 (17%)	2	11
27	DD	214/218 (98%)	181 (85%)	33 (15%)	2	13
28	BE	165/166 (99%)	135 (82%)	30 (18%)	1	9
28	DE	165/166 (99%)	139 (84%)	26 (16%)	2	12
29	BF	161/166 (97%)	141 (88%)	20 (12%)	4	20
29	DF	165/166 (99%)	140 (85%)	25 (15%)	3	14
30	BG	155/156 (99%)	135 (87%)	20 (13%)	4	19
30	DG	155/156 (99%)	139 (90%)	16 (10%)	7	28
31	BH	142/148 (96%)	122 (86%)	20 (14%)	3	16
31	DH	142/148 (96%)	124 (87%)	18 (13%)	4	19
32	BK	122/124 (98%)	101 (83%)	21 (17%)	2	10
32	DK	122/124 (98%)	106 (87%)	16 (13%)	4	18
33	BM	117/119 (98%)	98 (84%)	19 (16%)	2	12
33	DM	117/119 (98%)	97 (83%)	20 (17%)	2	10
34	BN	100/100 (100%)	92 (92%)	8 (8%)	12	40
34	DN	100/100 (100%)	87 (87%)	13 (13%)	4	19
35	BO	116/116 (100%)	84 (72%)	32 (28%)	0	2
35	DO	116/116 (100%)	80 (69%)	36 (31%)	0	1
36	BP	111/111 (100%)	94 (85%)	17 (15%)	2	13
36	DP	111/111 (100%)	89 (80%)	22 (20%)	1	7
37	B0	101/101 (100%)	85 (84%)	16 (16%)	2	12
37	D0	100/101 (99%)	82 (82%)	18 (18%)	1	9
38	BQ	87/88 (99%)	73 (84%)	14 (16%)	2	12
38	DQ	87/88 (99%)	79 (91%)	8 (9%)	9	34
39	BR	120/127 (94%)	99 (82%)	21 (18%)	2	10
39	DR	120/127 (94%)	102 (85%)	18 (15%)	3	14
40	B1	93/94 (99%)	85 (91%)	8 (9%)	10	37
40	D1	93/94 (99%)	82 (88%)	11 (12%)	5	22
41	B2	82/82 (100%)	70 (85%)	12 (15%)	3	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
41	D2	82/82 (100%)	69 (84%)	13 (16%)	2	12
42	BS	92/92 (100%)	79 (86%)	13 (14%)	3	16
42	DS	92/92 (100%)	76 (83%)	16 (17%)	2	10
43	BT	74/78 (95%)	65 (88%)	9 (12%)	5	21
43	DT	74/78 (95%)	63 (85%)	11 (15%)	3	14
44	BU	85/91 (93%)	72 (85%)	13 (15%)	2	13
44	DU	85/91 (93%)	67 (79%)	18 (21%)	1	5
45	BV	154/179 (86%)	126 (82%)	28 (18%)	1	9
45	DV	158/179 (88%)	138 (87%)	20 (13%)	4	19
46	B3	61/67 (91%)	57 (93%)	4 (7%)	16	49
46	D3	62/67 (92%)	55 (89%)	7 (11%)	6	24
47	BZ	82/83 (99%)	69 (84%)	13 (16%)	2	12
47	DZ	82/83 (99%)	68 (83%)	14 (17%)	2	10
48	BW	62/67 (92%)	51 (82%)	11 (18%)	2	9
48	DW	62/67 (92%)	51 (82%)	11 (18%)	2	9
49	BX	51/52 (98%)	46 (90%)	5 (10%)	8	30
49	DX	51/52 (98%)	48 (94%)	3 (6%)	19	54
50	B4	59/63 (94%)	49 (83%)	10 (17%)	2	11
50	D4	57/63 (90%)	46 (81%)	11 (19%)	1	8
51	B5	51/52 (98%)	42 (82%)	9 (18%)	2	10
51	D5	51/52 (98%)	41 (80%)	10 (20%)	1	7
52	B6	44/52 (85%)	34 (77%)	10 (23%)	1	4
52	D6	44/52 (85%)	40 (91%)	4 (9%)	9	34
53	B7	38/42 (90%)	33 (87%)	5 (13%)	4	18
53	D7	38/42 (90%)	33 (87%)	5 (13%)	4	18
54	B8	50/55 (91%)	37 (74%)	13 (26%)	0	2
54	D8	50/55 (91%)	41 (82%)	9 (18%)	1	9
All	All	9565/9996 (96%)	8229 (86%)	1336 (14%)	3	16

5 of 1336 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
47	BZ	26	ARG

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Mol	Chain	Res	Type
5	CH	75	THR
44	DU	64	GLU
48	BW	50	ILE
2	CE	5	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 282 such sidechains are listed below:

Mol	Chain	Res	Type
47	BZ	56	GLN
5	CH	141	GLN
45	DV	75	ASN
49	BX	19	GLN
54	B8	31	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1501/1506 (99%)	295 (19%)	43 (2%)
1	CA	1501/1506 (99%)	296 (19%)	49 (3%)
22	AB	83/85 (97%)	38 (45%)	8 (9%)
22	AD	83/85 (97%)	26 (31%)	5 (6%)
22	CB	83/85 (97%)	38 (45%)	9 (10%)
22	CD	83/85 (97%)	25 (30%)	4 (4%)
23	AC	76/77 (98%)	11 (14%)	1 (1%)
23	CC	76/77 (98%)	13 (17%)	3 (3%)
24	A1	15/16 (93%)	6 (40%)	2 (13%)
24	C1	15/16 (93%)	6 (40%)	3 (20%)
25	BA	2911/2912 (99%)	542 (18%)	51 (1%)
25	DA	2905/2912 (99%)	569 (19%)	53 (1%)
26	BB	121/122 (99%)	17 (14%)	0
26	DB	121/122 (99%)	27 (22%)	1 (0%)
All	All	9574/9606 (99%)	1909 (19%)	232 (2%)

5 of 1909 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	7	G
1	AA	8	A
1	AA	9	G
1	AA	13	U

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Mol	Chain	Res	Type
1	AA	32	A

5 of 232 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	BA	2566	A
1	CA	509	A
25	DA	2211	G
25	BA	2689	U
1	CA	201	C

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
22	MIA	CB	38	22	24,31,32	1.96	2 (8%)	26,44,47	2.38	9 (34%)
22	MIA	AB	38	22	24,31,32	1.83	2 (8%)	26,44,47	2.35	10 (38%)
22	MIA	AD	38	22	24,31,32	1.89	2 (8%)	26,44,47	2.74	10 (38%)
22	MIA	CD	38	22	24,31,32	1.91	2 (8%)	26,44,47	2.79	10 (38%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	MIA	CB	38	22	-	4/11/33/34	0/3/3/3
22	MIA	AB	38	22	-	4/11/33/34	0/3/3/3
22	MIA	AD	38	22	-	8/11/33/34	0/3/3/3
22	MIA	CD	38	22	-	7/11/33/34	0/3/3/3

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	CB	38	MIA	C6-N6	6.56	1.46	1.34
22	CB	38	MIA	C13-C14	6.35	1.50	1.32
22	CD	38	MIA	C6-N6	6.28	1.46	1.34
22	AD	38	MIA	C6-N6	6.19	1.45	1.34
22	CD	38	MIA	C13-C14	6.12	1.49	1.32

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	CD	38	MIA	C11-S10-C2	10.19	109.88	102.27
22	AD	38	MIA	C11-S10-C2	9.70	109.51	102.27
22	CB	38	MIA	C11-S10-C2	7.57	107.92	102.27
22	AB	38	MIA	C11-S10-C2	5.97	106.72	102.27
22	AB	38	MIA	C12-C13-C14	-5.85	115.77	127.14

There are no chirality outliers.

5 of 23 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	CB	38	MIA	N1-C2-S10-C11
22	CB	38	MIA	N3-C2-S10-C11
22	CB	38	MIA	C12-C13-C14-C15
22	CB	38	MIA	C12-C13-C14-C16
22	AB	38	MIA	N1-C2-S10-C11

There are no ring outliers.

4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	CB	38	MIA	3	0
22	AB	38	MIA	1	0
22	AD	38	MIA	3	0
22	CD	38	MIA	4	0

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 1608 ligands modelled in this entry, 1608 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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	AA	1502/1506 (99%)	-0.36	5 (0%)	94	84	54, 99, 183, 246	0
1	CA	1502/1506 (99%)	-0.28	13 (0%)	84	63	59, 100, 182, 245	0
2	AE	237/256 (92%)	0.24	11 (4%)	32	12	98, 139, 177, 190	0
2	CE	237/256 (92%)	0.57	15 (6%)	20	6	106, 152, 189, 209	0
3	AF	205/239 (85%)	0.29	7 (3%)	45	19	88, 113, 149, 158	0
3	CF	206/239 (86%)	1.03	33 (16%)	1	1	101, 135, 165, 180	0
4	AG	208/208 (100%)	-0.32	1 (0%)	91	75	81, 107, 131, 143	0
4	CG	208/208 (100%)	0.24	3 (1%)	75	49	75, 95, 123, 135	0
5	AH	151/162 (93%)	0.01	2 (1%)	77	51	78, 99, 125, 164	0
5	CH	151/162 (93%)	0.19	2 (1%)	77	51	84, 106, 131, 167	0
6	AI	101/101 (100%)	0.44	5 (4%)	28	10	67, 99, 115, 141	0
6	CI	101/101 (100%)	-0.07	0	100	100	76, 96, 115, 153	0
7	AJ	155/156 (99%)	0.40	12 (7%)	13	4	96, 114, 143, 161	0
7	CJ	155/156 (99%)	0.05	6 (3%)	39	15	100, 119, 147, 158	0
8	AK	138/138 (100%)	-0.28	0	100	100	81, 103, 117, 132	0
8	CK	138/138 (100%)	0.02	1 (0%)	87	69	81, 109, 125, 136	0
9	AL	127/128 (99%)	0.51	13 (10%)	6	2	83, 138, 159, 166	0
9	CL	127/128 (99%)	0.09	6 (4%)	31	11	95, 147, 165, 171	0
10	AM	99/105 (94%)	0.77	14 (14%)	2	1	81, 140, 167, 178	0
10	CM	99/105 (94%)	0.83	12 (12%)	4	1	103, 154, 174, 180	0
11	AN	119/129 (92%)	0.77	13 (10%)	5	2	62, 95, 130, 161	0
11	CN	119/129 (92%)	0.21	2 (1%)	70	41	74, 99, 133, 164	0
12	AO	125/132 (94%)	-0.22	1 (0%)	86	65	59, 75, 107, 162	0
12	CO	125/132 (94%)	0.62	14 (11%)	5	1	63, 91, 126, 166	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
13	AP	116/126 (92%)	0.23	6 (5%)	27	10	75, 124, 143, 155	0
13	CP	117/126 (92%)	0.19	7 (5%)	21	7	91, 145, 161, 169	0
14	AQ	58/61 (95%)	-0.15	0	100	100	87, 103, 120, 127	0
14	CQ	58/61 (95%)	1.17	9 (15%)	2	1	108, 125, 150, 154	0
15	AR	88/89 (98%)	-0.14	0	100	100	70, 94, 116, 120	0
15	CR	88/89 (98%)	-0.06	0	100	100	67, 96, 124, 136	0
16	AS	84/88 (95%)	-0.36	0	100	100	87, 109, 134, 174	0
16	CS	84/88 (95%)	0.32	2 (2%)	59	30	76, 91, 118, 157	0
17	AT	100/105 (95%)	-0.35	2 (2%)	65	36	80, 102, 118, 129	0
17	CT	100/105 (95%)	0.03	2 (2%)	65	36	75, 100, 126, 144	0
18	AU	72/88 (81%)	0.56	5 (6%)	16	5	77, 97, 135, 164	0
18	CU	72/88 (81%)	0.17	2 (2%)	53	25	85, 103, 149, 172	0
19	AV	78/93 (83%)	0.12	1 (1%)	77	51	97, 120, 145, 156	0
19	CV	78/93 (83%)	0.55	5 (6%)	19	6	128, 152, 178, 186	0
20	AW	99/106 (93%)	-0.17	0	100	100	97, 121, 148, 153	0
20	CW	99/106 (93%)	0.21	2 (2%)	65	36	86, 106, 141, 153	0
21	AX	25/27 (92%)	0.21	1 (4%)	38	15	97, 107, 121, 153	0
21	CX	25/27 (92%)	0.78	2 (8%)	12	4	101, 129, 150, 171	0
22	AB	84/85 (98%)	0.73	13 (15%)	2	1	76, 148, 167, 178	0
22	AD	84/85 (98%)	0.30	11 (13%)	3	1	70, 147, 206, 218	0
22	CB	84/85 (98%)	1.60	30 (35%)	0	0	92, 155, 171, 179	0
22	CD	84/85 (98%)	-0.64	0	100	100	74, 147, 207, 212	0
23	AC	77/77 (100%)	-0.42	0	100	100	66, 91, 135, 155	0
23	CC	77/77 (100%)	-0.59	0	100	100	79, 104, 143, 165	0
24	A1	16/16 (100%)	-0.21	0	100	100	66, 97, 168, 177	0
24	C1	16/16 (100%)	-0.18	0	100	100	75, 107, 176, 183	0
25	BA	2912/2912 (100%)	-0.04	42 (1%)	75	49	39, 68, 206, 243	0
25	DA	2907/2912 (99%)	-0.18	66 (2%)	60	31	49, 82, 226, 247	0
26	BB	122/122 (100%)	-0.27	1 (0%)	86	65	65, 92, 113, 183	0
26	DB	122/122 (100%)	-0.46	2 (1%)	72	44	78, 110, 139, 198	0
27	BD	272/276 (98%)	0.03	0	100	100	39, 59, 82, 104	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
27	DD	272/276 (98%)	-0.08	1 (0%) 92 79	45, 67, 87, 120	0
28	BE	205/206 (99%)	0.11	5 (2%) 59 30	44, 77, 125, 150	0
28	DE	205/206 (99%)	0.07	9 (4%) 34 13	56, 93, 144, 157	0
29	BF	202/210 (96%)	0.08	2 (0%) 82 59	42, 75, 110, 127	0
29	DF	208/210 (99%)	0.84	22 (10%) 6 2	53, 93, 155, 185	0
30	BG	181/182 (99%)	0.94	34 (18%) 1 0	79, 105, 136, 146	0
30	DG	181/182 (99%)	0.37	8 (4%) 34 13	96, 128, 157, 168	0
31	BH	170/180 (94%)	0.13	4 (2%) 59 30	71, 105, 126, 151	0
31	DH	170/180 (94%)	1.56	56 (32%) 0 0	143, 193, 217, 231	0
32	BK	146/148 (98%)	0.46	8 (5%) 25 9	72, 120, 141, 153	0
32	DK	146/148 (98%)	-0.20	1 (0%) 87 69	73, 120, 147, 151	0
33	BM	138/140 (98%)	0.08	2 (1%) 75 49	58, 79, 115, 136	0
33	DM	138/140 (98%)	0.12	2 (1%) 75 49	72, 104, 137, 147	0
34	BN	122/122 (100%)	-0.07	0 100 100	55, 71, 87, 93	0
34	DN	122/122 (100%)	0.04	0 100 100	66, 85, 103, 110	0
35	BO	150/150 (100%)	0.32	7 (4%) 31 11	45, 82, 109, 167	0
35	DO	150/150 (100%)	0.85	22 (14%) 2 1	45, 93, 136, 174	0
36	BP	141/141 (100%)	0.17	5 (3%) 44 18	55, 77, 105, 140	0
36	DP	141/141 (100%)	0.43	14 (9%) 7 2	58, 100, 130, 154	0
37	B0	118/118 (100%)	0.01	0 100 100	53, 74, 96, 106	0
37	D0	117/118 (99%)	0.03	1 (0%) 84 63	62, 81, 100, 117	0
38	BQ	111/112 (99%)	0.73	10 (9%) 9 3	71, 91, 116, 130	0
38	DQ	111/112 (99%)	0.24	6 (5%) 25 9	73, 109, 135, 157	0
39	BR	137/146 (93%)	0.15	4 (2%) 51 23	66, 85, 135, 167	0
39	DR	137/146 (93%)	0.07	3 (2%) 62 33	73, 94, 154, 184	0
40	B1	117/118 (99%)	0.00	2 (1%) 70 41	50, 70, 98, 140	0
40	D1	117/118 (99%)	0.49	9 (7%) 13 4	60, 99, 137, 155	0
41	B2	101/101 (100%)	0.08	3 (2%) 50 22	46, 91, 116, 128	0
41	D2	101/101 (100%)	0.97	14 (13%) 2 1	63, 122, 139, 150	0
42	BS	113/113 (100%)	-0.04	1 (0%) 84 63	44, 67, 99, 152	0
42	DS	113/113 (100%)	0.16	2 (1%) 68 40	61, 75, 109, 161	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
43	BT	92/96 (95%)	0.35	3 (3%)	46	20	54, 69, 95, 112	0
43	DT	92/96 (95%)	0.22	3 (3%)	46	20	65, 81, 109, 122	0
44	BU	102/110 (92%)	0.48	5 (4%)	29	11	70, 94, 144, 165	0
44	DU	102/110 (92%)	1.47	27 (26%)	0	0	78, 111, 162, 172	0
45	BV	175/206 (84%)	1.29	37 (21%)	1	0	79, 120, 189, 194	0
45	DV	179/206 (86%)	1.88	65 (36%)	0	0	111, 152, 207, 219	0
46	B3	76/85 (89%)	0.16	2 (2%)	56	27	51, 72, 92, 125	0
46	D3	77/85 (90%)	-0.04	1 (1%)	77	51	64, 87, 110, 151	0
47	BZ	97/98 (98%)	0.44	8 (8%)	11	3	48, 71, 115, 155	0
47	DZ	97/98 (98%)	-0.07	2 (2%)	63	34	54, 74, 126, 152	0
48	BW	66/72 (91%)	0.35	2 (3%)	50	22	59, 79, 95, 127	0
48	DW	66/72 (91%)	0.40	2 (3%)	50	22	75, 99, 121, 134	0
49	BX	59/60 (98%)	-0.03	0	100	100	61, 77, 112, 131	0
49	DX	59/60 (98%)	0.58	4 (6%)	17	5	76, 103, 136, 159	0
50	B4	66/71 (92%)	2.42	38 (57%)	0	0	112, 153, 176, 181	0
50	D4	63/71 (88%)	1.98	30 (47%)	0	0	141, 181, 191, 201	0
51	B5	59/60 (98%)	0.38	6 (10%)	6	2	43, 81, 156, 165	0
51	D5	59/60 (98%)	0.82	8 (13%)	3	1	61, 84, 169, 188	0
52	B6	45/54 (83%)	5.94	44 (97%)	0	0	117, 148, 164, 173	0
52	D6	45/54 (83%)	2.59	24 (53%)	0	0	131, 164, 181, 185	0
53	B7	45/49 (91%)	-0.03	0	100	100	38, 48, 68, 85	0
53	D7	45/49 (91%)	0.00	0	100	100	52, 59, 74, 94	0
54	B8	60/65 (92%)	0.35	2 (3%)	46	20	51, 68, 88, 115	0
54	D8	60/65 (92%)	0.34	3 (5%)	28	10	64, 80, 106, 132	0
All	All	21100/21658 (97%)	0.13	975 (4%)	32	12	38, 95, 177, 247	0

The worst 5 of 975 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
25	DA	654(J)	A	19.6
29	DF	1	MET	18.4
25	DA	654(L)	G	15.7
25	BA	654(J)	A	14.8
25	DA	654(K)	C	14.1

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
22	MIA	AD	38	29/30	0.92	0.18	98,122,141,145	0
22	MIA	CB	38	29/30	0.94	0.19	63,95,112,126	0
22	MIA	CD	38	29/30	0.94	0.21	101,121,146,154	0
22	MIA	AB	38	29/30	0.96	0.18	65,78,90,93	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
55	MG	DA	3229	1/1	-0.26	0.38	118,118,118,118	0
55	MG	AA	1758	1/1	-0.20	0.45	165,165,165,165	0
55	MG	DA	3407	1/1	-0.02	0.23	103,103,103,103	0
55	MG	CA	1786	1/1	0.06	0.27	111,111,111,111	0
55	MG	AD	101	1/1	0.09	0.32	154,154,154,154	0
55	MG	BA	3380	1/1	0.12	0.43	98,98,98,98	0
55	MG	CA	1803	1/1	0.19	0.24	103,103,103,103	0
55	MG	AA	1788	1/1	0.26	0.27	98,98,98,98	0
55	MG	DA	3176	1/1	0.30	0.54	105,105,105,105	0
55	MG	D1	201	1/1	0.31	0.26	89,89,89,89	0
55	MG	DA	3397	1/1	0.35	0.19	105,105,105,105	0
55	MG	AA	1643	1/1	0.42	0.53	127,127,127,127	0
55	MG	CA	1816	1/1	0.44	0.31	102,102,102,102	0
55	MG	DA	3330	1/1	0.45	0.65	100,100,100,100	0
55	MG	AA	1666	1/1	0.47	0.43	103,103,103,103	0
55	MG	CA	1806	1/1	0.47	0.27	103,103,103,103	0
55	MG	BA	3503	1/1	0.48	0.46	111,111,111,111	0
55	MG	AA	1735	1/1	0.49	0.20	102,102,102,102	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
55	MG	DA	3417	1/1	0.49	0.34	135,135,135,135	0
55	MG	CA	1697	1/1	0.50	0.16	84,84,84,84	0
55	MG	AA	1689	1/1	0.51	0.32	107,107,107,107	0
55	MG	CA	1733	1/1	0.51	0.37	103,103,103,103	0
55	MG	AA	1783	1/1	0.51	0.36	167,167,167,167	0
55	MG	BA	3436	1/1	0.53	0.18	107,107,107,107	0
55	MG	DA	3189	1/1	0.54	0.18	86,86,86,86	0
55	MG	DA	3462	1/1	0.56	0.23	98,98,98,98	0
55	MG	BA	3331	1/1	0.57	0.30	106,106,106,106	0
55	MG	CA	1644	1/1	0.57	0.17	101,101,101,101	0
55	MG	DA	3344	1/1	0.59	0.26	89,89,89,89	0
55	MG	BA	3079	1/1	0.60	0.27	103,103,103,103	0
55	MG	BA	3462	1/1	0.60	0.21	116,116,116,116	0
55	MG	DA	3410	1/1	0.60	0.31	103,103,103,103	0
55	MG	DA	3199	1/1	0.61	0.16	85,85,85,85	0
55	MG	BA	3314	1/1	0.61	0.23	83,83,83,83	0
55	MG	AA	1781	1/1	0.61	0.37	87,87,87,87	0
55	MG	CA	1804	1/1	0.62	0.40	108,108,108,108	0
55	MG	CA	1683	1/1	0.63	0.30	121,121,121,121	0
55	MG	BA	3544	1/1	0.64	0.33	82,82,82,82	0
55	MG	BA	3413	1/1	0.64	0.44	83,83,83,83	0
55	MG	AA	1618	1/1	0.64	0.22	91,91,91,91	0
55	MG	BA	3546	1/1	0.64	0.47	101,101,101,101	0
55	MG	BA	3382	1/1	0.67	0.53	93,93,93,93	0
55	MG	AA	1715	1/1	0.67	0.37	101,101,101,101	0
55	MG	BA	3463	1/1	0.67	0.80	101,101,101,101	0
55	MG	BA	3358	1/1	0.67	0.34	98,98,98,98	0
55	MG	BA	3224	1/1	0.69	0.32	78,78,78,78	0
55	MG	DA	3125	1/1	0.69	0.40	74,74,74,74	0
55	MG	AA	1686	1/1	0.70	0.18	91,91,91,91	0
55	MG	DO	201	1/1	0.71	0.15	98,98,98,98	0
55	MG	CA	1727	1/1	0.71	0.12	84,84,84,84	0
55	MG	AA	1802	1/1	0.71	0.21	75,75,75,75	0
55	MG	AA	1726	1/1	0.71	0.45	94,94,94,94	0
55	MG	AA	1611	1/1	0.71	0.27	94,94,94,94	0
55	MG	AA	1754	1/1	0.72	0.38	95,95,95,95	0
55	MG	CA	1669	1/1	0.72	0.28	85,85,85,85	0
55	MG	DA	3476	1/1	0.73	0.23	104,104,104,104	0
55	MG	DA	3275	1/1	0.73	0.21	85,85,85,85	0
55	MG	AA	1777	1/1	0.73	0.27	115,115,115,115	0
55	MG	BA	3428	1/1	0.74	0.40	91,91,91,91	0
55	MG	BA	3271	1/1	0.74	0.20	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	BA	3482	1/1	0.74	0.17	82,82,82,82	0
55	MG	DA	3222	1/1	0.74	0.16	75,75,75,75	0
55	MG	DA	3187	1/1	0.75	0.30	101,101,101,101	0
55	MG	CA	1759	1/1	0.75	0.51	99,99,99,99	0
55	MG	DA	3294	1/1	0.76	0.38	91,91,91,91	0
55	MG	CR	101	1/1	0.76	0.68	135,135,135,135	0
55	MG	DA	3343	1/1	0.76	0.34	91,91,91,91	0
55	MG	BA	3349	1/1	0.76	0.34	80,80,80,80	0
55	MG	CA	1722	1/1	0.76	0.61	106,106,106,106	0
55	MG	BA	3438	1/1	0.77	0.51	84,84,84,84	0
55	MG	BA	3425	1/1	0.77	0.24	87,87,87,87	0
55	MG	BA	3430	1/1	0.77	0.27	105,105,105,105	0
55	MG	DA	3246	1/1	0.77	0.28	89,89,89,89	0
55	MG	BB	203	1/1	0.77	0.43	71,71,71,71	0
55	MG	AA	1751	1/1	0.78	0.30	105,105,105,105	0
55	MG	BA	3066	1/1	0.78	0.20	99,99,99,99	0
55	MG	AA	1625	1/1	0.78	0.28	68,68,68,68	0
55	MG	BA	3132	1/1	0.79	0.21	76,76,76,76	0
55	MG	BA	3293	1/1	0.79	0.35	96,96,96,96	0
55	MG	BA	3203	1/1	0.79	0.23	106,106,106,106	0
55	MG	CA	1743	1/1	0.79	0.28	106,106,106,106	0
55	MG	DA	3262	1/1	0.79	0.68	99,99,99,99	0
55	MG	BA	3558	1/1	0.79	0.34	85,85,85,85	0
55	MG	AA	1671	1/1	0.80	0.20	95,95,95,95	0
55	MG	BA	3258	1/1	0.81	0.47	76,76,76,76	0
55	MG	BA	3320	1/1	0.81	0.42	85,85,85,85	0
55	MG	CA	1713	1/1	0.82	0.22	82,82,82,82	0
55	MG	BA	3009	1/1	0.83	0.32	58,58,58,58	0
55	MG	CA	1674	1/1	0.83	0.36	88,88,88,88	0
55	MG	AG	302	1/1	0.83	0.34	109,109,109,109	0
55	MG	BA	3347	1/1	0.83	0.61	79,79,79,79	0
55	MG	DA	3379	1/1	0.83	0.25	87,87,87,87	0
55	MG	CA	1756	1/1	0.83	0.29	83,83,83,83	0
55	MG	AA	1657	1/1	0.83	0.35	76,76,76,76	0
55	MG	AA	1694	1/1	0.83	0.20	142,142,142,142	0
55	MG	AA	1615	1/1	0.83	0.30	90,90,90,90	0
55	MG	AA	1786	1/1	0.84	0.28	89,89,89,89	0
55	MG	BA	3317	1/1	0.84	0.43	70,70,70,70	0
55	MG	DA	3171	1/1	0.84	0.16	73,73,73,73	0
55	MG	DA	3295	1/1	0.84	0.35	76,76,76,76	0
55	MG	BA	3296	1/1	0.84	0.36	60,60,60,60	0
55	MG	BA	3232	1/1	0.85	0.22	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
55	MG	BA	3092	1/1	0.85	0.31	67,67,67,67	0
55	MG	DA	3089	1/1	0.85	0.43	60,60,60,60	0
55	MG	BA	3040	1/1	0.85	0.37	74,74,74,74	0
55	MG	AA	1756	1/1	0.85	0.26	85,85,85,85	0
55	MG	BB	209	1/1	0.86	0.18	96,96,96,96	0
55	MG	DA	3483	1/1	0.86	0.41	82,82,82,82	0
55	MG	BA	3306	1/1	0.86	0.30	84,84,84,84	0
55	MG	CA	1652	1/1	0.86	0.13	94,94,94,94	0
55	MG	DA	3357	1/1	0.87	0.16	87,87,87,87	0
55	MG	BA	3415	1/1	0.87	0.21	65,65,65,65	0
55	MG	DA	3324	1/1	0.87	0.19	91,91,91,91	0
55	MG	DA	3349	1/1	0.87	0.24	78,78,78,78	0
55	MG	DA	3373	1/1	0.87	0.45	88,88,88,88	0
55	MG	BA	3548	1/1	0.87	0.35	95,95,95,95	0
55	MG	DA	3232	1/1	0.87	0.13	56,56,56,56	0
55	MG	DA	3254	1/1	0.87	0.15	80,80,80,80	0
55	MG	BA	3340	1/1	0.88	0.37	69,69,69,69	0
55	MG	DA	3304	1/1	0.88	0.12	77,77,77,77	0
55	MG	CA	1739	1/1	0.88	0.23	80,80,80,80	0
55	MG	AA	1820	1/1	0.88	0.12	82,82,82,82	0
55	MG	AC	104	1/1	0.88	0.38	64,64,64,64	0
55	MG	BA	3031	1/1	0.88	0.39	54,54,54,54	0
55	MG	AA	1725	1/1	0.88	0.31	100,100,100,100	0
55	MG	BO	201	1/1	0.89	0.12	78,78,78,78	0
55	MG	AA	1681	1/1	0.89	0.39	72,72,72,72	0
55	MG	BA	3326	1/1	0.89	0.32	67,67,67,67	0
55	MG	AA	1684	1/1	0.89	0.32	83,83,83,83	0
55	MG	AA	1661	1/1	0.89	0.35	56,56,56,56	0
55	MG	CA	1670	1/1	0.89	0.40	67,67,67,67	0
55	MG	BA	3528	1/1	0.89	0.38	32,32,32,32	0
55	MG	DA	3381	1/1	0.89	0.24	90,90,90,90	0
55	MG	DA	3168	1/1	0.89	0.40	87,87,87,87	0
55	MG	BA	3063	1/1	0.89	0.19	80,80,80,80	0
55	MG	DA	3312	1/1	0.89	0.33	75,75,75,75	0
55	MG	AA	1771	1/1	0.89	0.47	108,108,108,108	0
55	MG	BA	3134	1/1	0.90	0.33	59,59,59,59	0
55	MG	DA	3186	1/1	0.90	0.27	60,60,60,60	0
55	MG	BA	3530	1/1	0.90	0.31	71,71,71,71	0
55	MG	DA	3438	1/1	0.90	0.35	79,79,79,79	0
55	MG	CA	1811	1/1	0.90	0.35	69,69,69,69	0
55	MG	CA	1609	1/1	0.90	0.34	71,71,71,71	0
55	MG	BA	3469	1/1	0.90	0.36	124,124,124,124	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	CA	1715	1/1	0.90	0.30	89,89,89,89	0
55	MG	BA	3524	1/1	0.90	0.34	43,43,43,43	0
55	MG	BA	3454	1/1	0.90	0.54	80,80,80,80	0
55	MG	DA	3073	1/1	0.90	0.30	84,84,84,84	0
55	MG	DA	3301	1/1	0.90	0.31	90,90,90,90	0
55	MG	BA	3564	1/1	0.91	0.24	112,112,112,112	0
55	MG	AC	103	1/1	0.91	0.35	66,66,66,66	0
55	MG	BA	3212	1/1	0.91	0.34	68,68,68,68	0
55	MG	AA	1796	1/1	0.91	0.42	102,102,102,102	0
55	MG	AA	1651	1/1	0.91	0.47	79,79,79,79	0
55	MG	AA	1664	1/1	0.91	0.21	53,53,53,53	0
55	MG	BA	3181	1/1	0.91	0.31	69,69,69,69	0
55	MG	AA	1807	1/1	0.91	0.24	88,88,88,88	0
55	MG	CA	1605	1/1	0.91	0.18	90,90,90,90	0
55	MG	AA	1707	1/1	0.91	0.18	81,81,81,81	0
55	MG	BA	3303	1/1	0.92	0.39	73,73,73,73	0
55	MG	AA	1714	1/1	0.92	0.23	89,89,89,89	0
55	MG	DA	3181	1/1	0.92	0.16	50,50,50,50	0
55	MG	AA	1663	1/1	0.92	0.36	72,72,72,72	0
55	MG	BA	3013	1/1	0.92	0.30	52,52,52,52	0
55	MG	CA	1689	1/1	0.92	0.32	73,73,73,73	0
55	MG	BA	3319	1/1	0.93	0.54	64,64,64,64	0
55	MG	BA	3283	1/1	0.93	0.26	56,56,56,56	0
55	MG	BA	3096	1/1	0.93	0.43	63,63,63,63	0
55	MG	BA	3174	1/1	0.93	0.38	46,46,46,46	0
55	MG	CA	1619	1/1	0.93	0.12	68,68,68,68	0
55	MG	BA	3046	1/1	0.93	0.38	56,56,56,56	0
55	MG	BA	3099	1/1	0.93	0.23	75,75,75,75	0
55	MG	BA	3193	1/1	0.93	0.13	46,46,46,46	0
55	MG	CA	1623	1/1	0.93	0.35	75,75,75,75	0
55	MG	CA	1645	1/1	0.94	0.25	84,84,84,84	0
55	MG	CA	1639	1/1	0.94	0.38	59,59,59,59	0
55	MG	DA	3019	1/1	0.94	0.26	79,79,79,79	0
55	MG	AA	1632	1/1	0.94	0.23	55,55,55,55	0
55	MG	BA	3035	1/1	0.94	0.42	61,61,61,61	0
55	MG	AA	1811	1/1	0.94	0.47	65,65,65,65	0
55	MG	BA	3118	1/1	0.94	0.41	49,49,49,49	0
55	MG	BA	3226	1/1	0.94	0.18	69,69,69,69	0
55	MG	CA	1695	1/1	0.94	0.30	69,69,69,69	0
55	MG	CA	1643	1/1	0.94	0.37	80,80,80,80	0
55	MG	BA	3515	1/1	0.94	0.20	81,81,81,81	0
55	MG	BA	3020	1/1	0.95	0.30	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	DA	3198	1/1	0.95	0.35	48,48,48,48	0
55	MG	AA	1622	1/1	0.95	0.22	87,87,87,87	0
55	MG	AA	1619	1/1	0.95	0.38	58,58,58,58	0
55	MG	CA	1663	1/1	0.95	0.45	80,80,80,80	0
55	MG	DA	3174	1/1	0.95	0.38	63,63,63,63	0
55	MG	AA	1634	1/1	0.95	0.34	67,67,67,67	0
55	MG	BA	3187	1/1	0.95	0.51	73,73,73,73	0
55	MG	AC	101	1/1	0.95	0.30	55,55,55,55	0
55	MG	BA	3476	1/1	0.95	0.41	47,47,47,47	0
55	MG	DE	301	1/1	0.95	0.28	59,59,59,59	0
55	MG	BA	3190	1/1	0.95	0.36	86,86,86,86	0
55	MG	BA	3030	1/1	0.96	0.35	41,41,41,41	0
55	MG	CA	1603	1/1	0.96	0.30	60,60,60,60	0
55	MG	BA	3539	1/1	0.96	0.25	35,35,35,35	0
55	MG	DA	3023	1/1	0.96	0.10	47,47,47,47	0
55	MG	BA	3025	1/1	0.96	0.46	46,46,46,46	0
55	MG	AA	1720	1/1	0.96	0.35	83,83,83,83	0
55	MG	DA	3093	1/1	0.96	0.32	52,52,52,52	0
55	MG	CA	1676	1/1	0.96	0.36	76,76,76,76	0
55	MG	BA	3549	1/1	0.96	0.46	55,55,55,55	0
55	MG	CA	1706	1/1	0.97	0.43	79,79,79,79	0
55	MG	DA	3463	1/1	0.97	0.22	84,84,84,84	0
55	MG	BA	3140	1/1	0.97	0.28	67,67,67,67	0
55	MG	BA	3160	1/1	0.97	0.31	44,44,44,44	0
55	MG	DA	3157	1/1	0.97	0.28	51,51,51,51	0
55	MG	BA	3169	1/1	0.97	0.37	45,45,45,45	0
55	MG	BA	3230	1/1	0.97	0.43	48,48,48,48	0
55	MG	BA	3068	1/1	0.98	0.41	56,56,56,56	0
55	MG	BA	3059	1/1	0.98	0.32	63,63,63,63	0
55	MG	BA	3016	1/1	0.98	0.36	48,48,48,48	0
55	MG	BA	3101	1/1	0.98	0.33	66,66,66,66	0
55	MG	BA	3555	1/1	0.98	0.25	47,47,47,47	0
55	MG	DA	3161	1/1	0.98	0.25	55,55,55,55	0
55	MG	DA	3124	1/1	0.98	0.29	47,47,47,47	0
55	MG	AA	1658	1/1	0.99	0.35	56,56,56,56	0
55	MG	BA	3291	1/1	-	-	56,56,56,56	1
55	MG	BA	3456	1/1	-0.34	0.48	168,168,168,168	0
55	MG	CB	104	1/1	-0.32	0.35	147,147,147,147	0
55	MG	BA	3420	1/1	-0.24	0.26	114,114,114,114	0
55	MG	CA	1808	1/1	-0.23	0.55	153,153,153,153	0
55	MG	CA	1673	1/1	-0.10	0.65	136,136,136,136	0
55	MG	BA	3189	1/1	-0.07	0.67	108,108,108,108	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
55	MG	AA	1809	1/1	-0.06	0.49	204,204,204,204	0
55	MG	CA	1768	1/1	-0.04	0.43	138,138,138,138	0
55	MG	DA	3279	1/1	-0.02	0.53	135,135,135,135	0
55	MG	AA	1764	1/1	-0.01	0.33	146,146,146,146	0
55	MG	BA	3393	1/1	-0.01	0.34	118,118,118,118	0
55	MG	DA	3398	1/1	-0.00	0.34	101,101,101,101	0
55	MG	AA	1613	1/1	0.04	0.48	116,116,116,116	0
55	MG	BA	3397	1/1	0.05	0.34	131,131,131,131	0
55	MG	DA	3366	1/1	0.05	0.35	105,105,105,105	0
55	MG	DA	3372	1/1	0.05	0.69	125,125,125,125	0
55	MG	AA	1779	1/1	0.05	0.26	119,119,119,119	0
55	MG	CA	1702	1/1	0.06	0.29	106,106,106,106	0
55	MG	BA	3202	1/1	0.08	0.33	97,97,97,97	0
55	MG	DA	3391	1/1	0.12	0.35	102,102,102,102	0
55	MG	BA	3195	1/1	0.13	0.64	97,97,97,97	0
55	MG	DA	3227	1/1	0.13	2.16	118,118,118,118	0
55	MG	DA	3336	1/1	0.15	0.60	115,115,115,115	0
55	MG	BA	3446	1/1	0.15	0.41	121,121,121,121	0
55	MG	DB	215	1/1	0.16	0.30	129,129,129,129	0
55	MG	DA	3291	1/1	0.17	0.48	149,149,149,149	0
55	MG	CA	1773	1/1	0.19	0.61	139,139,139,139	0
55	MG	DD	303	1/1	0.20	0.16	69,69,69,69	0
55	MG	AC	107	1/1	0.20	0.43	124,124,124,124	0
55	MG	BA	3386	1/1	0.23	0.42	115,115,115,115	0
55	MG	CA	1630	1/1	0.23	0.18	149,149,149,149	0
55	MG	BA	3429	1/1	0.24	0.55	146,146,146,146	0
55	MG	DA	3188	1/1	0.25	0.26	113,113,113,113	0
55	MG	CA	1761	1/1	0.25	0.55	143,143,143,143	0
55	MG	DA	3393	1/1	0.25	0.20	116,116,116,116	0
55	MG	AA	1648	1/1	0.25	0.36	115,115,115,115	0
55	MG	AA	1810	1/1	0.26	0.28	148,148,148,148	0
55	MG	BA	3422	1/1	0.26	0.70	110,110,110,110	0
55	MG	CA	1747	1/1	0.26	0.34	109,109,109,109	0
55	MG	AA	1724	1/1	0.27	0.20	78,78,78,78	0
55	MG	AA	1785	1/1	0.27	2.25	125,125,125,125	0
55	MG	BA	3451	1/1	0.28	0.50	101,101,101,101	0
55	MG	DA	3351	1/1	0.28	0.22	151,151,151,151	0
55	MG	BA	3078	1/1	0.28	0.52	101,101,101,101	0
55	MG	DA	3035	1/1	0.28	0.32	124,124,124,124	0
55	MG	CA	1781	1/1	0.30	0.21	172,172,172,172	0
55	MG	CA	1740	1/1	0.30	0.56	122,122,122,122	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	CA	1610	1/1	0.31	0.24	118,118,118,118	0
55	MG	BA	3163	1/1	0.32	0.34	86,86,86,86	0
55	MG	DA	3100	1/1	0.33	0.44	116,116,116,116	0
55	MG	AA	1703	1/1	0.33	0.31	106,106,106,106	0
55	MG	DA	3076	1/1	0.33	0.33	107,107,107,107	0
55	MG	BA	3439	1/1	0.34	0.38	115,115,115,115	0
55	MG	DB	210	1/1	0.34	0.80	128,128,128,128	0
55	MG	CA	1793	1/1	0.34	0.23	110,110,110,110	0
55	MG	BA	3343	1/1	0.35	0.32	114,114,114,114	0
55	MG	DA	3050	1/1	0.35	0.27	90,90,90,90	0
55	MG	A1	101	1/1	0.35	0.20	102,102,102,102	0
55	MG	BA	3125	1/1	0.36	0.32	107,107,107,107	0
55	MG	BA	3178	1/1	0.36	0.38	96,96,96,96	0
55	MG	CA	1792	1/1	0.38	0.18	104,104,104,104	0
55	MG	AA	1815	1/1	0.39	0.41	114,114,114,114	0
55	MG	CA	1716	1/1	0.39	0.31	103,103,103,103	0
55	MG	AA	1730	1/1	0.39	0.29	113,113,113,113	0
55	MG	BA	3550	1/1	0.40	1.22	131,131,131,131	0
55	MG	BA	3373	1/1	0.40	0.48	92,92,92,92	0
55	MG	CA	1680	1/1	0.40	0.20	99,99,99,99	0
55	MG	BA	3406	1/1	0.41	1.35	182,182,182,182	0
55	MG	DA	3469	1/1	0.42	0.31	109,109,109,109	0
55	MG	DA	3263	1/1	0.42	0.29	96,96,96,96	0
55	MG	CA	1737	1/1	0.43	0.23	122,122,122,122	0
55	MG	CA	1675	1/1	0.43	0.39	111,111,111,111	0
55	MG	BA	3448	1/1	0.44	0.24	104,104,104,104	0
55	MG	DA	3172	1/1	0.44	0.42	122,122,122,122	0
55	MG	CA	1809	1/1	0.44	0.35	93,93,93,93	0
55	MG	AA	1804	1/1	0.45	0.43	113,113,113,113	0
55	MG	CA	1621	1/1	0.45	0.19	97,97,97,97	0
55	MG	CA	1753	1/1	0.45	0.24	103,103,103,103	0
55	MG	DA	3192	1/1	0.45	0.17	90,90,90,90	0
55	MG	CA	1763	1/1	0.46	0.16	100,100,100,100	0
55	MG	DA	3167	1/1	0.46	0.17	95,95,95,95	0
55	MG	DB	209	1/1	0.46	0.33	130,130,130,130	0
55	MG	AB	102	1/1	0.46	0.29	96,96,96,96	0
55	MG	CA	1745	1/1	0.46	0.29	159,159,159,159	0
55	MG	AA	1814	1/1	0.47	0.34	107,107,107,107	0
55	MG	CA	1742	1/1	0.47	0.92	108,108,108,108	0
55	MG	DA	3238	1/1	0.48	0.41	105,105,105,105	0
55	MG	CA	1729	1/1	0.48	0.38	102,102,102,102	0
55	MG	DA	3402	1/1	0.49	0.20	124,124,124,124	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
55	MG	CC	103	1/1	0.49	0.23	114,114,114,114	0
55	MG	DA	3036	1/1	0.49	0.20	100,100,100,100	0
55	MG	AA	1757	1/1	0.49	0.40	101,101,101,101	0
55	MG	BA	3338	1/1	0.50	0.28	91,91,91,91	0
55	MG	BA	3122	1/1	0.50	0.53	106,106,106,106	0
55	MG	CB	102	1/1	0.50	0.19	102,102,102,102	0
55	MG	AC	105	1/1	0.50	0.36	102,102,102,102	0
55	MG	B6	101	1/1	0.51	0.32	102,102,102,102	0
55	MG	DA	3039	1/1	0.51	0.23	101,101,101,101	0
55	MG	BA	3082	1/1	0.51	0.36	100,100,100,100	0
55	MG	AD	102	1/1	0.52	0.23	125,125,125,125	0
55	MG	DA	3218	1/1	0.52	0.27	86,86,86,86	0
55	MG	CA	1813	1/1	0.52	0.24	108,108,108,108	0
55	MG	AD	103	1/1	0.52	0.23	89,89,89,89	0
55	MG	DA	3194	1/1	0.52	0.33	104,104,104,104	0
55	MG	CA	1805	1/1	0.52	0.18	102,102,102,102	0
55	MG	BA	3378	1/1	0.52	0.26	140,140,140,140	0
55	MG	DA	3359	1/1	0.53	0.14	111,111,111,111	0
55	MG	AA	1819	1/1	0.53	0.32	126,126,126,126	0
55	MG	CA	1710	1/1	0.53	0.17	118,118,118,118	0
55	MG	DA	3024	1/1	0.53	0.35	104,104,104,104	0
55	MG	CA	1672	1/1	0.53	0.17	119,119,119,119	0
55	MG	BA	3192	1/1	0.53	0.47	92,92,92,92	0
55	MG	AA	1706	1/1	0.54	0.21	91,91,91,91	0
55	MG	CA	1701	1/1	0.54	1.26	108,108,108,108	0
55	MG	BA	3467	1/1	0.55	0.25	69,69,69,69	0
55	MG	DB	211	1/1	0.55	0.22	111,111,111,111	0
55	MG	CA	1817	1/1	0.55	0.44	106,106,106,106	0
55	MG	BA	3453	1/1	0.55	0.21	75,75,75,75	0
55	MG	DA	3221	1/1	0.56	1.32	154,154,154,154	0
55	MG	BA	3268	1/1	0.56	0.25	90,90,90,90	0
55	MG	BA	3401	1/1	0.56	0.29	86,86,86,86	0
55	MG	CC	105	1/1	0.56	0.13	94,94,94,94	0
55	MG	AA	1743	1/1	0.56	0.25	107,107,107,107	0
55	MG	BA	3062	1/1	0.56	0.36	79,79,79,79	0
55	MG	BA	3037	1/1	0.57	0.35	105,105,105,105	0
55	MG	BA	3041	1/1	0.57	0.48	80,80,80,80	0
55	MG	BA	3281	1/1	0.57	0.28	78,78,78,78	0
55	MG	CA	1764	1/1	0.57	0.22	117,117,117,117	0
55	MG	BA	3335	1/1	0.57	0.34	102,102,102,102	0
55	MG	DA	3342	1/1	0.57	0.93	122,122,122,122	0
55	MG	DA	3439	1/1	0.58	0.36	107,107,107,107	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	DA	3443	1/1	0.58	0.26	94,94,94,94	0
55	MG	BA	3479	1/1	0.58	0.55	146,146,146,146	0
55	MG	BA	3396	1/1	0.58	0.55	87,87,87,87	0
55	MG	AA	1738	1/1	0.58	0.26	91,91,91,91	0
55	MG	DB	206	1/1	0.58	0.31	89,89,89,89	0
55	MG	DB	212	1/1	0.58	0.33	120,120,120,120	0
55	MG	BA	3509	1/1	0.58	0.46	97,97,97,97	0
55	MG	DA	3383	1/1	0.58	0.20	107,107,107,107	0
55	MG	BA	3557	1/1	0.58	0.33	94,94,94,94	0
55	MG	BA	3452	1/1	0.58	0.35	103,103,103,103	0
55	MG	BA	3472	1/1	0.58	0.63	133,133,133,133	0
55	MG	DA	3308	1/1	0.59	0.30	99,99,99,99	0
55	MG	BD	301	1/1	0.59	0.21	80,80,80,80	0
55	MG	DA	3444	1/1	0.59	0.23	109,109,109,109	0
55	MG	BA	3566	1/1	0.60	0.33	83,83,83,83	0
55	MG	BA	3537	1/1	0.60	0.47	73,73,73,73	0
55	MG	BA	3483	1/1	0.60	0.35	120,120,120,120	0
55	MG	DA	3426	1/1	0.60	0.32	103,103,103,103	0
55	MG	AA	1741	1/1	0.60	0.22	98,98,98,98	0
55	MG	BA	3543	1/1	0.60	0.39	101,101,101,101	0
55	MG	BA	3137	1/1	0.60	0.44	88,88,88,88	0
55	MG	BA	3433	1/1	0.60	0.42	99,99,99,99	0
55	MG	DA	3321	1/1	0.60	0.16	112,112,112,112	0
55	MG	AA	1696	1/1	0.60	0.39	112,112,112,112	0
55	MG	DA	3446	1/1	0.60	0.43	166,166,166,166	0
55	MG	AA	1765	1/1	0.60	0.28	149,149,149,149	0
55	MG	CA	1796	1/1	0.60	0.18	146,146,146,146	0
55	MG	DA	3486	1/1	0.61	0.20	101,101,101,101	0
55	MG	DA	3479	1/1	0.61	0.17	97,97,97,97	0
55	MG	DB	208	1/1	0.61	0.30	99,99,99,99	0
55	MG	AA	1818	1/1	0.61	0.47	124,124,124,124	0
55	MG	CA	1700	1/1	0.61	0.33	96,96,96,96	0
55	MG	DA	3328	1/1	0.61	0.27	84,84,84,84	0
55	MG	DA	3353	1/1	0.61	0.24	102,102,102,102	0
55	MG	DA	3163	1/1	0.61	0.37	75,75,75,75	0
55	MG	DA	3206	1/1	0.61	0.29	109,109,109,109	0
55	MG	DA	3261	1/1	0.61	0.22	78,78,78,78	0
55	MG	AA	1784	1/1	0.61	0.22	112,112,112,112	0
55	MG	AR	101	1/1	0.62	0.19	114,114,114,114	0
55	MG	BA	3565	1/1	0.62	0.38	105,105,105,105	0
55	MG	DA	3281	1/1	0.62	0.23	90,90,90,90	0
55	MG	BA	3353	1/1	0.62	0.45	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\AA^2$)	Q<0.9
55	MG	DA	3290	1/1	0.62	0.17	99,99,99,99	0
55	MG	AA	1637	1/1	0.62	0.23	112,112,112,112	0
55	MG	DA	3382	1/1	0.62	0.48	121,121,121,121	0
55	MG	DA	3421	1/1	0.62	0.32	84,84,84,84	0
55	MG	BA	3262	1/1	0.62	0.40	87,87,87,87	0
55	MG	AA	1697	1/1	0.62	0.29	101,101,101,101	0
55	MG	CA	1696	1/1	0.62	0.20	104,104,104,104	0
55	MG	BA	3445	1/1	0.63	0.27	82,82,82,82	0
55	MG	CA	1819	1/1	0.63	0.45	134,134,134,134	0
55	MG	DA	3484	1/1	0.63	0.23	84,84,84,84	0
55	MG	DA	3299	1/1	0.63	0.19	84,84,84,84	0
55	MG	BA	3440	1/1	0.63	0.56	96,96,96,96	0
55	MG	AC	102	1/1	0.63	0.37	106,106,106,106	0
55	MG	BA	3404	1/1	0.63	0.35	100,100,100,100	0
55	MG	DA	3054	1/1	0.63	0.42	108,108,108,108	0
55	MG	B3	102	1/1	0.63	0.35	107,107,107,107	0
55	MG	CA	1687	1/1	0.64	0.29	99,99,99,99	0
55	MG	AA	1755	1/1	0.64	0.30	88,88,88,88	0
55	MG	AA	1791	1/1	0.64	0.47	90,90,90,90	0
55	MG	BA	3274	1/1	0.64	0.47	108,108,108,108	0
55	MG	BA	3155	1/1	0.64	0.98	114,114,114,114	0
55	MG	BB	201	1/1	0.64	0.29	97,97,97,97	0
55	MG	AA	1708	1/1	0.64	0.14	77,77,77,77	0
55	MG	BA	3399	1/1	0.64	0.32	99,99,99,99	0
55	MG	AA	1801	1/1	0.64	0.19	130,130,130,130	0
55	MG	CA	1671	1/1	0.64	0.22	100,100,100,100	0
55	MG	BA	3411	1/1	0.64	0.30	102,102,102,102	0
55	MG	DA	3079	1/1	0.64	0.25	103,103,103,103	0
55	MG	DA	3414	1/1	0.64	0.30	111,111,111,111	0
55	MG	BA	3484	1/1	0.64	0.36	87,87,87,87	0
55	MG	CA	1778	1/1	0.64	0.24	133,133,133,133	0
55	MG	AA	1763	1/1	0.65	0.21	92,92,92,92	0
55	MG	AA	1729	1/1	0.65	0.29	84,84,84,84	0
55	MG	DA	3423	1/1	0.65	0.88	118,118,118,118	0
55	MG	AA	1631	1/1	0.65	0.24	84,84,84,84	0
55	MG	CA	1767	1/1	0.65	0.19	87,87,87,87	0
55	MG	AA	1736	1/1	0.65	0.56	108,108,108,108	0
55	MG	CA	1815	1/1	0.65	0.19	95,95,95,95	0
55	MG	DA	3409	1/1	0.65	0.51	124,124,124,124	0
55	MG	D5	102	1/1	0.65	0.24	104,104,104,104	0
55	MG	DA	3459	1/1	0.65	0.28	76,76,76,76	0
55	MG	DA	3370	1/1	0.65	0.32	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	CA	1810	1/1	0.65	0.27	101,101,101,101	0
55	MG	AA	1626	1/1	0.65	0.32	91,91,91,91	0
55	MG	CA	1757	1/1	0.66	0.28	95,95,95,95	0
55	MG	BA	3051	1/1	0.66	0.31	103,103,103,103	0
55	MG	DB	204	1/1	0.66	0.37	94,94,94,94	0
55	MG	BA	3301	1/1	0.66	0.26	84,84,84,84	0
55	MG	BA	3510	1/1	0.66	0.48	108,108,108,108	0
55	MG	BA	3444	1/1	0.66	0.21	87,87,87,87	0
55	MG	BB	208	1/1	0.66	0.42	117,117,117,117	0
55	MG	DA	3390	1/1	0.66	0.21	92,92,92,92	0
55	MG	DB	217	1/1	0.66	0.29	97,97,97,97	0
55	MG	DA	3451	1/1	0.66	0.23	92,92,92,92	0
55	MG	DA	3092	1/1	0.66	0.17	87,87,87,87	0
55	MG	DA	3228	1/1	0.66	0.54	103,103,103,103	0
55	MG	BA	3475	1/1	0.67	0.32	212,212,212,212	0
55	MG	AA	1727	1/1	0.67	0.22	95,95,95,95	0
55	MG	BA	3568	1/1	0.67	0.20	106,106,106,106	0
55	MG	BA	3058	1/1	0.67	0.30	88,88,88,88	0
55	MG	BA	3376	1/1	0.67	0.27	83,83,83,83	0
55	MG	AA	1688	1/1	0.67	0.15	93,93,93,93	0
55	MG	BA	3209	1/1	0.67	0.48	78,78,78,78	0
55	MG	BA	3290	1/1	0.67	0.24	75,75,75,75	0
55	MG	CA	1682	1/1	0.67	0.13	100,100,100,100	0
55	MG	BA	3333	1/1	0.67	0.52	80,80,80,80	0
55	MG	BA	3316	1/1	0.67	0.39	87,87,87,87	0
55	MG	AA	1762	1/1	0.67	0.18	121,121,121,121	0
55	MG	CA	1709	1/1	0.67	0.34	110,110,110,110	0
55	MG	BB	204	1/1	0.67	0.32	91,91,91,91	0
55	MG	CA	1748	1/1	0.67	0.31	76,76,76,76	0
55	MG	CA	1749	1/1	0.67	0.25	117,117,117,117	0
55	MG	BA	3412	1/1	0.67	0.39	89,89,89,89	0
55	MG	BA	3288	1/1	0.67	0.26	75,75,75,75	0
55	MG	CA	1707	1/1	0.68	0.31	109,109,109,109	0
55	MG	DA	3389	1/1	0.68	0.28	97,97,97,97	0
55	MG	CA	1667	1/1	0.68	0.21	98,98,98,98	0
55	MG	DA	3296	1/1	0.68	0.16	93,93,93,93	0
55	MG	BA	3243	1/1	0.68	0.26	79,79,79,79	0
55	MG	AA	1713	1/1	0.68	0.35	98,98,98,98	0
55	MG	CA	1693	1/1	0.68	0.26	103,103,103,103	0
55	MG	BA	3455	1/1	0.69	0.78	89,89,89,89	0
55	MG	BA	3176	1/1	0.69	0.27	78,78,78,78	0
55	MG	DB	216	1/1	0.69	0.16	100,100,100,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
55	MG	AA	1750	1/1	0.69	0.45	134,134,134,134	0
55	MG	BA	3289	1/1	0.69	0.34	95,95,95,95	0
55	MG	CA	1788	1/1	0.69	0.24	132,132,132,132	0
55	MG	BA	3334	1/1	0.69	0.28	67,67,67,67	0
55	MG	CA	1776	1/1	0.69	0.31	118,118,118,118	0
55	MG	B3	103	1/1	0.69	0.32	83,83,83,83	0
55	MG	DA	3121	1/1	0.69	0.20	104,104,104,104	0
55	MG	DA	3425	1/1	0.69	0.42	88,88,88,88	0
55	MG	BA	3266	1/1	0.69	0.41	71,71,71,71	0
55	MG	DA	3159	1/1	0.70	0.32	68,68,68,68	0
55	MG	DA	3319	1/1	0.70	0.21	95,95,95,95	0
55	MG	BA	3344	1/1	0.70	0.68	84,84,84,84	0
55	MG	CA	1790	1/1	0.70	0.51	142,142,142,142	0
55	MG	DA	3350	1/1	0.70	0.33	120,120,120,120	0
55	MG	B1	202	1/1	0.70	0.33	86,86,86,86	0
55	MG	CA	1708	1/1	0.70	0.18	124,124,124,124	0
55	MG	AA	1773	1/1	0.70	0.35	130,130,130,130	0
55	MG	DA	3448	1/1	0.70	0.19	129,129,129,129	0
55	MG	CC	104	1/1	0.70	0.21	98,98,98,98	0
55	MG	DA	3250	1/1	0.70	0.24	62,62,62,62	0
55	MG	DA	3300	1/1	0.70	0.34	75,75,75,75	0
55	MG	AA	1702	1/1	0.71	0.36	89,89,89,89	0
55	MG	DA	3219	1/1	0.71	0.26	128,128,128,128	0
55	MG	AA	1687	1/1	0.71	0.26	108,108,108,108	0
55	MG	CA	1704	1/1	0.71	0.37	88,88,88,88	0
55	MG	B2	201	1/1	0.71	0.36	91,91,91,91	0
55	MG	DA	3413	1/1	0.71	0.37	86,86,86,86	0
55	MG	BA	3426	1/1	0.71	0.47	86,86,86,86	0
55	MG	BA	3501	1/1	0.71	0.35	86,86,86,86	0
55	MG	BA	3372	1/1	0.71	0.46	76,76,76,76	0
55	MG	DA	3406	1/1	0.71	0.35	129,129,129,129	0
55	MG	CA	1692	1/1	0.71	0.10	157,157,157,157	0
55	MG	CC	106	1/1	0.71	0.35	94,94,94,94	0
55	MG	DA	3368	1/1	0.72	0.20	97,97,97,97	0
55	MG	CB	101	1/1	0.72	0.18	106,106,106,106	0
55	MG	DA	3179	1/1	0.72	0.33	88,88,88,88	0
55	MG	BA	3513	1/1	0.72	0.29	92,92,92,92	0
55	MG	BA	3279	1/1	0.72	0.40	75,75,75,75	0
55	MG	DA	3386	1/1	0.72	0.23	130,130,130,130	0
55	MG	DA	3399	1/1	0.72	0.58	117,117,117,117	0
55	MG	D8	101	1/1	0.72	0.16	88,88,88,88	0
55	MG	DA	3445	1/1	0.72	0.15	118,118,118,118	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	BB	217	1/1	0.72	0.31	104,104,104,104	0
55	MG	DA	3334	1/1	0.72	0.31	87,87,87,87	0
55	MG	BA	3128	1/1	0.72	0.23	71,71,71,71	0
55	MG	CK	201	1/1	0.72	1.47	124,124,124,124	0
55	MG	CA	1658	1/1	0.72	0.33	90,90,90,90	0
55	MG	AA	1806	1/1	0.72	0.40	85,85,85,85	0
55	MG	DA	3310	1/1	0.72	0.29	105,105,105,105	0
55	MG	CA	1780	1/1	0.72	0.21	88,88,88,88	0
55	MG	CA	1799	1/1	0.72	0.18	81,81,81,81	0
55	MG	DA	3346	1/1	0.72	0.23	102,102,102,102	0
55	MG	CA	1762	1/1	0.72	0.44	108,108,108,108	0
55	MG	CA	1797	1/1	0.72	0.36	85,85,85,85	0
55	MG	AA	1799	1/1	0.73	0.21	101,101,101,101	0
55	MG	DA	3252	1/1	0.73	0.17	99,99,99,99	0
55	MG	BA	3365	1/1	0.73	0.22	81,81,81,81	0
55	MG	BO	202	1/1	0.73	0.20	98,98,98,98	0
55	MG	BA	3323	1/1	0.73	0.59	73,73,73,73	0
55	MG	CA	1653	1/1	0.73	0.26	97,97,97,97	0
55	MG	BB	210	1/1	0.73	0.30	81,81,81,81	0
55	MG	CA	1684	1/1	0.73	0.26	101,101,101,101	0
55	MG	DA	3482	1/1	0.73	0.37	83,83,83,83	0
55	MG	CA	1694	1/1	0.73	0.16	80,80,80,80	0
55	MG	DB	218	1/1	0.73	0.13	107,107,107,107	0
55	MG	AA	1728	1/1	0.73	0.46	99,99,99,99	0
55	MG	BA	3263	1/1	0.73	0.45	80,80,80,80	0
55	MG	BA	3269	1/1	0.73	0.29	79,79,79,79	0
55	MG	BA	3473	1/1	0.73	0.30	92,92,92,92	0
55	MG	AA	1678	1/1	0.73	0.37	115,115,115,115	0
55	MG	AA	1746	1/1	0.73	0.32	93,93,93,93	0
55	MG	DA	3283	1/1	0.73	0.26	88,88,88,88	0
55	MG	BA	3324	1/1	0.73	0.43	105,105,105,105	0
55	MG	DA	3320	1/1	0.73	0.30	87,87,87,87	0
55	MG	DA	3404	1/1	0.74	0.26	119,119,119,119	0
55	MG	DA	3040	1/1	0.74	0.23	118,118,118,118	0
55	MG	BA	3540	1/1	0.74	0.44	83,83,83,83	0
55	MG	DA	3277	1/1	0.74	0.16	78,78,78,78	0
55	MG	DA	3481	1/1	0.74	0.14	79,79,79,79	0
55	MG	DB	219	1/1	0.74	0.12	94,94,94,94	0
55	MG	BA	3477	1/1	0.74	0.57	77,77,77,77	0
55	MG	DA	3088	1/1	0.74	0.26	62,62,62,62	0
55	MG	CA	1648	1/1	0.74	0.28	113,113,113,113	0
55	MG	BA	3352	1/1	0.74	0.40	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	DA	3114	1/1	0.74	0.38	91,91,91,91	0
55	MG	AA	1653	1/1	0.74	0.31	95,95,95,95	0
55	MG	BA	3547	1/1	0.74	0.29	77,77,77,77	0
55	MG	DA	3369	1/1	0.74	0.35	108,108,108,108	0
55	MG	AA	1775	1/1	0.74	0.45	129,129,129,129	0
55	MG	DA	3231	1/1	0.74	0.27	101,101,101,101	0
55	MG	DA	3316	1/1	0.74	0.17	102,102,102,102	0
55	MG	DA	3437	1/1	0.74	0.18	66,66,66,66	0
55	MG	BA	3245	1/1	0.74	0.47	107,107,107,107	0
55	MG	BA	3432	1/1	0.74	0.24	106,106,106,106	0
55	MG	AA	1695	1/1	0.75	0.20	128,128,128,128	0
55	MG	DA	3185	1/1	0.75	0.15	78,78,78,78	0
55	MG	DA	3270	1/1	0.75	0.36	76,76,76,76	0
55	MG	DA	3376	1/1	0.75	0.25	107,107,107,107	0
55	MG	AA	1816	1/1	0.75	0.25	95,95,95,95	0
55	MG	AA	1770	1/1	0.75	0.25	80,80,80,80	0
55	MG	DA	3461	1/1	0.75	0.24	97,97,97,97	0
55	MG	AA	1691	1/1	0.75	0.28	88,88,88,88	0
55	MG	DA	3248	1/1	0.75	0.19	95,95,95,95	0
55	MG	BA	3259	1/1	0.75	0.24	109,109,109,109	0
55	MG	DA	3153	1/1	0.75	0.10	88,88,88,88	0
55	MG	AA	1766	1/1	0.75	0.32	98,98,98,98	0
55	MG	AA	1690	1/1	0.75	0.18	98,98,98,98	0
55	MG	DA	3477	1/1	0.75	0.34	88,88,88,88	0
55	MG	BA	3309	1/1	0.75	0.46	77,77,77,77	0
55	MG	BA	3210	1/1	0.75	0.25	99,99,99,99	0
55	MG	DA	3314	1/1	0.75	0.15	95,95,95,95	0
55	MG	DA	3134	1/1	0.76	0.18	93,93,93,93	0
55	MG	CA	1615	1/1	0.76	0.27	106,106,106,106	0
55	MG	DA	3332	1/1	0.76	0.17	84,84,84,84	0
55	MG	B7	101	1/1	0.76	0.32	72,72,72,72	0
55	MG	AA	1817	1/1	0.76	0.17	61,61,61,61	0
55	MG	DA	3400	1/1	0.76	0.14	115,115,115,115	0
55	MG	DA	3392	1/1	0.76	0.22	126,126,126,126	0
55	MG	AA	1797	1/1	0.76	0.27	79,79,79,79	0
55	MG	DA	3327	1/1	0.76	0.23	93,93,93,93	0
55	MG	DA	3177	1/1	0.76	0.12	129,129,129,129	0
55	MG	BA	3275	1/1	0.76	0.35	60,60,60,60	0
55	MG	AA	1747	1/1	0.76	0.20	98,98,98,98	0
55	MG	DA	3225	1/1	0.76	0.45	102,102,102,102	0
55	MG	DA	3208	1/1	0.76	0.29	91,91,91,91	0
55	MG	DA	3358	1/1	0.76	0.45	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	AA	1803	1/1	0.76	0.28	89,89,89,89	0
55	MG	BA	3395	1/1	0.76	0.29	90,90,90,90	0
55	MG	BA	3385	1/1	0.76	0.18	86,86,86,86	0
55	MG	BA	3383	1/1	0.76	0.18	94,94,94,94	0
55	MG	DA	3442	1/1	0.76	0.30	98,98,98,98	0
55	MG	AA	1753	1/1	0.77	0.19	97,97,97,97	0
55	MG	BA	3065	1/1	0.77	0.31	82,82,82,82	0
55	MG	DA	3441	1/1	0.77	0.17	89,89,89,89	0
55	MG	BA	3075	1/1	0.77	0.40	75,75,75,75	0
55	MG	BA	3069	1/1	0.77	0.42	93,93,93,93	0
55	MG	DA	3099	1/1	0.77	0.51	83,83,83,83	0
55	MG	DA	3325	1/1	0.77	0.17	97,97,97,97	0
55	MG	DA	3209	1/1	0.77	0.36	96,96,96,96	0
55	MG	DA	3133	1/1	0.77	0.17	91,91,91,91	0
55	MG	AA	1759	1/1	0.77	0.14	66,66,66,66	0
55	MG	AA	1669	1/1	0.77	0.27	77,77,77,77	0
55	MG	CA	1746	1/1	0.77	0.20	87,87,87,87	0
55	MG	DA	3384	1/1	0.77	0.39	97,97,97,97	0
55	MG	DA	3354	1/1	0.77	0.25	83,83,83,83	0
55	MG	BB	211	1/1	0.77	0.22	109,109,109,109	0
55	MG	DA	3422	1/1	0.77	0.20	75,75,75,75	0
55	MG	AA	1704	1/1	0.77	0.24	110,110,110,110	0
55	MG	AA	1733	1/1	0.77	0.31	101,101,101,101	0
55	MG	CA	1734	1/1	0.77	0.13	80,80,80,80	0
55	MG	DA	3120	1/1	0.77	0.43	73,73,73,73	0
55	MG	DA	3468	1/1	0.77	0.15	101,101,101,101	0
55	MG	DA	3142	1/1	0.77	0.37	81,81,81,81	0
55	MG	DA	3480	1/1	0.77	0.20	109,109,109,109	0
55	MG	DA	3378	1/1	0.77	0.28	88,88,88,88	0
55	MG	DA	3322	1/1	0.77	0.32	99,99,99,99	0
55	MG	BA	3563	1/1	0.77	0.24	100,100,100,100	0
55	MG	AA	1772	1/1	0.78	0.58	131,131,131,131	0
55	MG	DA	3081	1/1	0.78	0.32	84,84,84,84	0
55	MG	BA	3270	1/1	0.78	0.36	96,96,96,96	0
55	MG	AA	1612	1/1	0.78	0.26	88,88,88,88	0
55	MG	CA	1771	1/1	0.78	0.19	117,117,117,117	0
55	MG	AA	1683	1/1	0.78	0.41	87,87,87,87	0
55	MG	BA	3238	1/1	0.78	0.32	75,75,75,75	0
55	MG	DA	3135	1/1	0.78	0.17	87,87,87,87	0
55	MG	DA	3387	1/1	0.78	0.26	102,102,102,102	0
55	MG	DA	3085	1/1	0.78	0.44	81,81,81,81	0
55	MG	AA	1800	1/1	0.78	0.43	131,131,131,131	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	BA	3474	1/1	0.78	0.37	72,72,72,72	0
55	MG	CA	1646	1/1	0.78	0.25	88,88,88,88	0
55	MG	AA	1635	1/1	0.78	0.18	81,81,81,81	0
55	MG	DA	3377	1/1	0.78	0.28	87,87,87,87	0
55	MG	BA	3106	1/1	0.78	0.22	89,89,89,89	0
55	MG	BA	3222	1/1	0.78	0.47	68,68,68,68	0
55	MG	AA	1731	1/1	0.78	0.11	90,90,90,90	0
55	MG	CA	1678	1/1	0.78	0.50	83,83,83,83	0
55	MG	CA	1666	1/1	0.78	0.16	90,90,90,90	0
55	MG	CA	1812	1/1	0.78	1.05	176,176,176,176	0
55	MG	BA	3487	1/1	0.78	0.49	100,100,100,100	0
55	MG	BA	3300	1/1	0.78	0.43	80,80,80,80	0
55	MG	DA	3278	1/1	0.79	0.25	100,100,100,100	0
55	MG	DA	3315	1/1	0.79	0.14	91,91,91,91	0
55	MG	CA	1699	1/1	0.79	0.33	87,87,87,87	0
55	MG	DA	3326	1/1	0.79	0.34	109,109,109,109	0
55	MG	DA	3374	1/1	0.79	0.19	92,92,92,92	0
55	MG	BA	3442	1/1	0.79	0.30	90,90,90,90	0
55	MG	BA	3512	1/1	0.79	0.32	90,90,90,90	0
55	MG	CA	1711	1/1	0.79	0.18	101,101,101,101	0
55	MG	AA	1768	1/1	0.79	0.48	71,71,71,71	0
55	MG	BA	3242	1/1	0.79	0.26	116,116,116,116	0
55	MG	DA	3401	1/1	0.79	0.12	75,75,75,75	0
55	MG	BA	3421	1/1	0.79	0.88	97,97,97,97	0
55	MG	CA	1798	1/1	0.79	0.39	74,74,74,74	0
55	MG	BA	3277	1/1	0.79	0.34	79,79,79,79	0
55	MG	BA	3461	1/1	0.79	0.34	98,98,98,98	0
55	MG	BA	3294	1/1	0.79	0.34	61,61,61,61	0
55	MG	DA	3259	1/1	0.79	0.30	92,92,92,92	0
55	MG	DA	3245	1/1	0.79	0.16	91,91,91,91	0
55	MG	DA	3243	1/1	0.79	0.26	97,97,97,97	0
55	MG	AA	1675	1/1	0.79	0.20	81,81,81,81	0
55	MG	CC	109	1/1	0.79	0.29	114,114,114,114	0
55	MG	DA	3488	1/1	0.79	0.23	100,100,100,100	0
55	MG	AA	1778	1/1	0.80	0.10	143,143,143,143	0
55	MG	CA	1660	1/1	0.80	0.13	85,85,85,85	0
55	MG	AA	1630	1/1	0.80	0.34	112,112,112,112	0
55	MG	BA	3450	1/1	0.80	0.30	82,82,82,82	0
55	MG	BA	3424	1/1	0.80	0.47	84,84,84,84	0
55	MG	CA	1655	1/1	0.80	0.11	85,85,85,85	0
55	MG	BA	3364	1/1	0.80	0.32	72,72,72,72	0
55	MG	CA	1736	1/1	0.80	1.03	143,143,143,143	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	CA	1688	1/1	0.80	0.21	95,95,95,95	0
55	MG	AA	1624	1/1	0.80	0.21	94,94,94,94	0
55	MG	DA	3458	1/1	0.80	0.34	75,75,75,75	0
55	MG	CA	1814	1/1	0.80	0.19	83,83,83,83	0
55	MG	DA	3307	1/1	0.80	0.32	99,99,99,99	0
55	MG	CA	1622	1/1	0.80	0.65	110,110,110,110	0
55	MG	CG	301	1/1	0.80	0.40	107,107,107,107	0
55	MG	AA	1623	1/1	0.80	0.34	63,63,63,63	0
55	MG	AA	1682	1/1	0.80	0.22	93,93,93,93	0
55	MG	BE	303	1/1	0.80	0.39	105,105,105,105	0
55	MG	DA	3286	1/1	0.80	0.33	78,78,78,78	0
55	MG	AA	1792	1/1	0.80	0.30	97,97,97,97	0
55	MG	BA	3194	1/1	0.80	0.27	74,74,74,74	0
55	MG	BA	3457	1/1	0.80	0.17	85,85,85,85	0
55	MG	AB	104	1/1	0.80	0.43	97,97,97,97	0
55	MG	BA	3561	1/1	0.80	0.29	84,84,84,84	0
55	MG	AC	106	1/1	0.80	0.39	102,102,102,102	0
55	MG	DA	3166	1/1	0.80	0.25	90,90,90,90	0
55	MG	BA	3295	1/1	0.80	0.19	92,92,92,92	0
55	MG	BA	3379	1/1	0.80	0.45	78,78,78,78	0
55	MG	BA	3162	1/1	0.80	0.28	67,67,67,67	0
55	MG	AA	1649	1/1	0.80	0.21	95,95,95,95	0
55	MG	AA	1654	1/1	0.81	0.28	77,77,77,77	0
55	MG	BA	3254	1/1	0.81	0.44	89,89,89,89	0
55	MG	DA	3318	1/1	0.81	0.28	77,77,77,77	0
55	MG	CA	1777	1/1	0.81	0.14	112,112,112,112	0
55	MG	BA	3253	1/1	0.81	0.47	92,92,92,92	0
55	MG	DA	3030	1/1	0.81	0.20	85,85,85,85	0
55	MG	BA	3322	1/1	0.81	0.38	81,81,81,81	0
55	MG	BA	3318	1/1	0.81	0.37	102,102,102,102	0
55	MG	BF	302	1/1	0.81	0.53	88,88,88,88	0
55	MG	BA	3097	1/1	0.81	0.20	59,59,59,59	0
55	MG	BA	3231	1/1	0.81	0.35	46,46,46,46	0
55	MG	DA	3273	1/1	0.81	0.10	77,77,77,77	0
55	MG	BA	3138	1/1	0.81	0.46	86,86,86,86	0
55	MG	D3	101	1/1	0.81	0.13	91,91,91,91	0
55	MG	CA	1750	1/1	0.81	0.26	86,86,86,86	0
55	MG	BA	3464	1/1	0.81	0.15	91,91,91,91	0
55	MG	DA	3258	1/1	0.81	0.13	87,87,87,87	0
55	MG	DA	3309	1/1	0.81	0.46	116,116,116,116	0
55	MG	CC	107	1/1	0.81	0.22	123,123,123,123	0
55	MG	DA	3140	1/1	0.81	0.30	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	B5	101	1/1	0.81	0.18	49,49,49,49	0
55	MG	CA	1677	1/1	0.81	0.19	107,107,107,107	0
55	MG	BA	3485	1/1	0.81	0.27	98,98,98,98	0
55	MG	DA	3280	1/1	0.81	0.42	91,91,91,91	0
55	MG	AA	1749	1/1	0.81	0.44	110,110,110,110	0
55	MG	BA	3252	1/1	0.81	0.42	107,107,107,107	0
55	MG	BA	3489	1/1	0.81	0.41	95,95,95,95	0
55	MG	BA	3233	1/1	0.81	0.36	66,66,66,66	0
55	MG	BA	3267	1/1	0.81	0.36	62,62,62,62	0
55	MG	AA	1744	1/1	0.81	0.38	79,79,79,79	0
55	MG	BA	3191	1/1	0.81	0.39	89,89,89,89	0
55	MG	BA	3239	1/1	0.82	0.20	69,69,69,69	0
55	MG	BA	3502	1/1	0.82	0.30	78,78,78,78	0
55	MG	BA	3151	1/1	0.82	0.57	97,97,97,97	0
55	MG	DA	3091	1/1	0.82	0.15	74,74,74,74	0
55	MG	BA	3315	1/1	0.82	0.44	93,93,93,93	0
55	MG	BA	3053	1/1	0.82	0.10	106,106,106,106	0
55	MG	AA	1798	1/1	0.82	0.31	84,84,84,84	0
55	MG	AA	1808	1/1	0.82	0.32	88,88,88,88	0
55	MG	DA	3269	1/1	0.82	0.30	78,78,78,78	0
55	MG	AA	1680	1/1	0.82	0.49	97,97,97,97	0
55	MG	BA	3107	1/1	0.82	0.19	81,81,81,81	0
55	MG	DA	3380	1/1	0.82	0.19	80,80,80,80	0
55	MG	BA	3414	1/1	0.82	0.36	100,100,100,100	0
55	MG	AA	1813	1/1	0.82	0.36	85,85,85,85	0
55	MG	CA	1751	1/1	0.82	0.24	90,90,90,90	0
55	MG	CC	108	1/1	0.82	0.22	95,95,95,95	0
55	MG	BA	3545	1/1	0.82	0.23	82,82,82,82	0
55	MG	AA	1685	1/1	0.82	0.34	85,85,85,85	0
55	MG	AA	1633	1/1	0.82	0.39	102,102,102,102	0
55	MG	DA	3139	1/1	0.82	0.28	53,53,53,53	0
55	MG	AA	1673	1/1	0.82	0.31	75,75,75,75	0
55	MG	DA	3282	1/1	0.82	0.30	64,64,64,64	0
55	MG	AA	1667	1/1	0.82	0.56	78,78,78,78	0
55	MG	BB	215	1/1	0.82	0.23	91,91,91,91	0
55	MG	BA	3505	1/1	0.82	0.23	61,61,61,61	0
55	MG	AA	1723	1/1	0.82	0.20	93,93,93,93	0
55	MG	DA	3257	1/1	0.82	0.41	77,77,77,77	0
55	MG	AA	1721	1/1	0.82	0.29	60,60,60,60	0
55	MG	BA	3217	1/1	0.82	0.34	40,40,40,40	0
55	MG	CA	1627	1/1	0.82	0.17	140,140,140,140	0
55	MG	DA	3271	1/1	0.82	0.21	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\AA^2$)	Q<0.9
55	MG	BA	3516	1/1	0.82	0.37	88,88,88,88	0
55	MG	BA	3459	1/1	0.82	0.36	81,81,81,81	0
55	MG	BA	3348	1/1	0.82	0.18	96,96,96,96	0
55	MG	BA	3091	1/1	0.83	0.44	73,73,73,73	0
55	MG	BA	3127	1/1	0.83	0.42	73,73,73,73	0
55	MG	BE	301	1/1	0.83	0.12	57,57,57,57	0
55	MG	DA	3416	1/1	0.83	0.49	77,77,77,77	0
55	MG	CA	1775	1/1	0.83	0.46	69,69,69,69	0
55	MG	DA	3412	1/1	0.83	0.29	92,92,92,92	0
55	MG	DA	3371	1/1	0.83	0.22	122,122,122,122	0
55	MG	DA	3038	1/1	0.83	0.21	73,73,73,73	0
55	MG	BA	3102	1/1	0.83	0.26	68,68,68,68	0
55	MG	DA	3267	1/1	0.83	0.47	80,80,80,80	0
55	MG	DA	3132	1/1	0.83	0.20	77,77,77,77	0
55	MG	AA	1629	1/1	0.83	0.12	95,95,95,95	0
55	MG	DA	3212	1/1	0.83	0.30	121,121,121,121	0
55	MG	BA	3427	1/1	0.83	0.45	97,97,97,97	0
55	MG	BA	3381	1/1	0.83	0.52	87,87,87,87	0
55	MG	DD	302	1/1	0.83	0.27	82,82,82,82	0
55	MG	BA	3229	1/1	0.83	0.38	65,65,65,65	0
55	MG	BA	3400	1/1	0.83	0.54	108,108,108,108	0
55	MG	DA	3127	1/1	0.83	0.36	73,73,73,73	0
55	MG	BA	3299	1/1	0.83	0.27	66,66,66,66	0
55	MG	AA	1699	1/1	0.83	0.16	99,99,99,99	0
55	MG	DA	3418	1/1	0.83	0.18	85,85,85,85	0
55	MG	CA	1611	1/1	0.83	0.35	82,82,82,82	0
55	MG	CA	1755	1/1	0.83	0.35	104,104,104,104	0
55	MG	DA	3363	1/1	0.83	0.21	78,78,78,78	0
55	MG	BA	3449	1/1	0.83	0.39	100,100,100,100	0
55	MG	CG	302	1/1	0.83	0.12	89,89,89,89	0
55	MG	BA	3498	1/1	0.83	0.27	40,40,40,40	0
55	MG	DA	3419	1/1	0.83	0.22	87,87,87,87	0
55	MG	BA	3206	1/1	0.83	0.26	68,68,68,68	0
55	MG	BA	3328	1/1	0.83	0.22	52,52,52,52	0
55	MG	BA	3287	1/1	0.83	0.28	60,60,60,60	0
55	MG	DA	3415	1/1	0.84	0.34	85,85,85,85	0
55	MG	AA	1782	1/1	0.84	0.12	118,118,118,118	0
55	MG	BA	3276	1/1	0.84	0.22	92,92,92,92	0
55	MG	BA	3247	1/1	0.84	0.32	97,97,97,97	0
55	MG	BA	3147	1/1	0.84	0.33	47,47,47,47	0
55	MG	BA	3198	1/1	0.84	0.18	74,74,74,74	0
55	MG	DA	3146	1/1	0.84	0.10	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	BA	3256	1/1	0.84	0.44	80,80,80,80	0
55	MG	CA	1774	1/1	0.84	0.22	75,75,75,75	0
55	MG	BA	3437	1/1	0.84	0.32	97,97,97,97	0
55	MG	BA	3172	1/1	0.84	0.44	74,74,74,74	0
55	MG	CA	1818	1/1	0.84	0.41	81,81,81,81	0
55	MG	BA	3121	1/1	0.84	0.33	72,72,72,72	0
55	MG	BA	3180	1/1	0.84	0.22	91,91,91,91	0
55	MG	AA	1794	1/1	0.84	0.49	112,112,112,112	0
55	MG	BA	3355	1/1	0.84	0.25	95,95,95,95	0
55	MG	BA	3443	1/1	0.84	0.23	125,125,125,125	0
55	MG	BA	3330	1/1	0.84	0.24	61,61,61,61	0
55	MG	BA	3359	1/1	0.84	0.49	78,78,78,78	0
55	MG	DA	3340	1/1	0.84	0.27	75,75,75,75	0
55	MG	DA	3215	1/1	0.84	0.31	83,83,83,83	0
55	MG	CA	1800	1/1	0.84	0.28	99,99,99,99	0
55	MG	BA	3346	1/1	0.84	0.53	69,69,69,69	0
55	MG	DB	220	1/1	0.84	0.13	121,121,121,121	0
55	MG	DA	3149	1/1	0.84	0.22	93,93,93,93	0
55	MG	DA	3126	1/1	0.84	0.17	63,63,63,63	0
55	MG	DA	3305	1/1	0.84	0.15	93,93,93,93	0
55	MG	BB	207	1/1	0.84	0.19	109,109,109,109	0
55	MG	DA	3298	1/1	0.84	0.28	80,80,80,80	0
55	MG	CA	1760	1/1	0.84	0.24	105,105,105,105	0
55	MG	AA	1693	1/1	0.84	0.31	72,72,72,72	0
55	MG	CA	1744	1/1	0.84	0.28	73,73,73,73	0
55	MG	CA	1726	1/1	0.84	0.10	73,73,73,73	0
55	MG	CA	1650	1/1	0.84	0.17	78,78,78,78	0
55	MG	DA	3190	1/1	0.84	0.33	66,66,66,66	0
55	MG	BA	3466	1/1	0.85	0.62	92,92,92,92	0
55	MG	CA	1783	1/1	0.85	0.13	87,87,87,87	0
55	MG	AA	1647	1/1	0.85	0.31	81,81,81,81	0
55	MG	BA	3064	1/1	0.85	0.31	87,87,87,87	0
55	MG	BA	3357	1/1	0.85	0.41	78,78,78,78	0
55	MG	DA	3466	1/1	0.85	0.17	81,81,81,81	0
55	MG	DA	3364	1/1	0.85	0.12	93,93,93,93	0
55	MG	DA	3233	1/1	0.85	0.33	90,90,90,90	0
55	MG	CA	1654	1/1	0.85	0.25	78,78,78,78	0
55	MG	AA	1701	1/1	0.85	0.57	87,87,87,87	0
55	MG	BA	3045	1/1	0.85	0.35	105,105,105,105	0
55	MG	BA	3419	1/1	0.85	0.49	80,80,80,80	0
55	MG	CA	1625	1/1	0.85	0.23	104,104,104,104	0
55	MG	BA	3418	1/1	0.85	0.28	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	DA	3333	1/1	0.85	0.31	95,95,95,95	0
55	MG	BA	3307	1/1	0.85	0.47	79,79,79,79	0
55	MG	CA	1686	1/1	0.85	0.24	77,77,77,77	0
55	MG	BA	3325	1/1	0.85	0.22	81,81,81,81	0
55	MG	AB	103	1/1	0.85	0.34	104,104,104,104	0
55	MG	BB	214	1/1	0.85	0.31	76,76,76,76	0
55	MG	AG	301	1/1	0.85	0.23	98,98,98,98	0
55	MG	BA	3368	1/1	0.85	0.29	59,59,59,59	0
55	MG	BA	3251	1/1	0.85	0.43	80,80,80,80	0
55	MG	AA	1711	1/1	0.85	0.17	97,97,97,97	0
55	MG	DA	3403	1/1	0.85	0.32	107,107,107,107	0
55	MG	BA	3297	1/1	0.85	0.21	86,86,86,86	0
55	MG	DB	203	1/1	0.85	0.09	111,111,111,111	0
55	MG	CA	1640	1/1	0.85	0.31	89,89,89,89	0
55	MG	AA	1640	1/1	0.85	0.35	71,71,71,71	0
55	MG	BA	3394	1/1	0.85	0.43	80,80,80,80	0
55	MG	DA	3184	1/1	0.85	0.36	78,78,78,78	0
55	MG	AA	1700	1/1	0.85	0.17	136,136,136,136	0
55	MG	BA	3310	1/1	0.85	0.29	76,76,76,76	0
55	MG	BA	3249	1/1	0.85	0.17	82,82,82,82	0
55	MG	BA	3265	1/1	0.85	0.14	89,89,89,89	0
55	MG	BA	3302	1/1	0.85	0.23	83,83,83,83	0
55	MG	CA	1787	1/1	0.86	0.45	84,84,84,84	0
55	MG	DA	3464	1/1	0.86	0.31	90,90,90,90	0
55	MG	BA	3123	1/1	0.86	0.33	81,81,81,81	0
55	MG	BA	3183	1/1	0.86	0.45	84,84,84,84	0
55	MG	DA	3224	1/1	0.86	0.20	75,75,75,75	0
55	MG	DA	3150	1/1	0.86	0.49	77,77,77,77	0
55	MG	DA	3434	1/1	0.86	0.19	73,73,73,73	0
55	MG	BA	3447	1/1	0.86	0.42	72,72,72,72	0
55	MG	CA	1784	1/1	0.86	0.11	92,92,92,92	0
55	MG	DA	3211	1/1	0.86	0.35	79,79,79,79	0
55	MG	CA	1618	1/1	0.86	0.18	95,95,95,95	0
55	MG	DA	3329	1/1	0.86	0.26	71,71,71,71	0
55	MG	B1	201	1/1	0.86	0.27	71,71,71,71	0
55	MG	B3	101	1/1	0.86	0.43	81,81,81,81	0
55	MG	CA	1730	1/1	0.86	0.15	79,79,79,79	0
55	MG	DA	3147	1/1	0.86	0.22	87,87,87,87	0
55	MG	AS	101	1/1	0.86	0.23	96,96,96,96	0
55	MG	BA	3112	1/1	0.86	0.48	73,73,73,73	0
55	MG	AA	1739	1/1	0.86	0.36	82,82,82,82	0
55	MG	DA	3213	1/1	0.86	0.18	103,103,103,103	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	DA	3104	1/1	0.86	0.34	62,62,62,62	0
55	MG	BA	3154	1/1	0.86	0.50	87,87,87,87	0
55	MG	DA	3352	1/1	0.86	0.27	122,122,122,122	0
55	MG	AA	1638	1/1	0.86	0.36	105,105,105,105	0
55	MG	DA	3375	1/1	0.86	0.13	86,86,86,86	0
55	MG	AA	1737	1/1	0.86	0.26	81,81,81,81	0
55	MG	BA	3219	1/1	0.86	0.33	68,68,68,68	0
55	MG	DA	3339	1/1	0.86	0.44	104,104,104,104	0
55	MG	CA	1628	1/1	0.86	0.21	123,123,123,123	0
55	MG	DA	3396	1/1	0.87	0.28	76,76,76,76	0
55	MG	DA	3338	1/1	0.87	0.33	69,69,69,69	0
55	MG	AA	1644	1/1	0.87	0.36	94,94,94,94	0
55	MG	DA	3197	1/1	0.87	0.27	48,48,48,48	0
55	MG	AA	1639	1/1	0.87	0.28	84,84,84,84	0
55	MG	CA	1685	1/1	0.87	0.36	91,91,91,91	0
55	MG	DA	3033	1/1	0.87	0.26	83,83,83,83	0
55	MG	BB	206	1/1	0.87	0.19	79,79,79,79	0
55	MG	CA	1789	1/1	0.87	0.14	71,71,71,71	0
55	MG	BA	3535	1/1	0.87	0.32	82,82,82,82	0
55	MG	DA	3095	1/1	0.87	0.27	89,89,89,89	0
55	MG	DB	205	1/1	0.87	0.33	73,73,73,73	0
55	MG	BA	3388	1/1	0.87	0.39	76,76,76,76	0
55	MG	BA	3071	1/1	0.87	0.27	63,63,63,63	0
55	MG	BA	3199	1/1	0.87	0.27	65,65,65,65	0
55	MG	CA	1785	1/1	0.87	0.40	155,155,155,155	0
55	MG	BA	3332	1/1	0.87	0.37	76,76,76,76	0
55	MG	BA	3135	1/1	0.87	0.41	69,69,69,69	0
55	MG	BA	3508	1/1	0.87	0.33	77,77,77,77	0
55	MG	DA	3265	1/1	0.87	0.36	76,76,76,76	0
55	MG	BA	3246	1/1	0.87	0.23	89,89,89,89	0
55	MG	BA	3090	1/1	0.87	0.26	40,40,40,40	0
55	MG	DA	3086	1/1	0.87	0.47	75,75,75,75	0
55	MG	DA	3287	1/1	0.87	0.46	120,120,120,120	0
55	MG	BA	3336	1/1	0.87	0.20	78,78,78,78	0
55	MG	CA	1649	1/1	0.87	0.42	77,77,77,77	0
55	MG	BA	3486	1/1	0.87	0.28	42,42,42,42	0
55	MG	DA	3292	1/1	0.87	0.39	98,98,98,98	0
55	MG	CA	1691	1/1	0.87	0.19	90,90,90,90	0
55	MG	BA	3342	1/1	0.87	0.25	66,66,66,66	0
55	MG	BA	3329	1/1	0.87	0.63	67,67,67,67	0
55	MG	BB	218	1/1	0.87	0.21	98,98,98,98	0
55	MG	BA	3511	1/1	0.87	0.15	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	BA	3409	1/1	0.87	0.38	98,98,98,98	0
55	MG	BA	3556	1/1	0.88	0.23	98,98,98,98	0
55	MG	AA	1709	1/1	0.88	0.24	56,56,56,56	0
55	MG	AA	1605	1/1	0.88	0.26	75,75,75,75	0
55	MG	CA	1668	1/1	0.88	0.42	72,72,72,72	0
55	MG	BA	3390	1/1	0.88	0.38	98,98,98,98	0
55	MG	DA	3323	1/1	0.88	0.91	104,104,104,104	0
55	MG	DA	3251	1/1	0.88	0.34	79,79,79,79	0
55	MG	CA	1735	1/1	0.88	0.41	119,119,119,119	0
55	MG	DA	3264	1/1	0.88	0.40	88,88,88,88	0
55	MG	BA	3098	1/1	0.88	0.38	88,88,88,88	0
55	MG	AA	1745	1/1	0.88	0.28	83,83,83,83	0
55	MG	BA	3350	1/1	0.88	0.48	92,92,92,92	0
55	MG	BA	3240	1/1	0.88	0.30	73,73,73,73	0
55	MG	DA	3173	1/1	0.88	0.27	90,90,90,90	0
55	MG	AB	101	1/1	0.88	0.18	92,92,92,92	0
55	MG	CA	1712	1/1	0.88	0.42	76,76,76,76	0
55	MG	BA	3360	1/1	0.88	0.38	81,81,81,81	0
55	MG	AA	1760	1/1	0.88	0.35	77,77,77,77	0
55	MG	BA	3567	1/1	0.88	0.21	99,99,99,99	0
55	MG	BA	3126	1/1	0.88	0.63	95,95,95,95	0
55	MG	DA	3201	1/1	0.88	0.33	76,76,76,76	0
55	MG	DA	3356	1/1	0.88	0.36	76,76,76,76	0
55	MG	BA	3431	1/1	0.88	0.18	66,66,66,66	0
55	MG	DA	3394	1/1	0.88	0.30	101,101,101,101	0
55	MG	BA	3185	1/1	0.88	0.17	46,46,46,46	0
55	MG	DA	3165	1/1	0.88	0.45	73,73,73,73	0
55	MG	BA	3220	1/1	0.88	0.28	70,70,70,70	0
55	MG	DA	3345	1/1	0.88	0.24	85,85,85,85	0
55	MG	BA	3559	1/1	0.88	0.26	86,86,86,86	0
55	MG	CA	1732	1/1	0.88	0.36	105,105,105,105	0
55	MG	BA	3278	1/1	0.88	0.69	92,92,92,92	0
55	MG	CA	1801	1/1	0.88	0.23	81,81,81,81	0
55	MG	DA	3436	1/1	0.88	0.16	66,66,66,66	0
55	MG	CA	1661	1/1	0.88	0.24	92,92,92,92	0
55	MG	DA	3235	1/1	0.88	0.33	69,69,69,69	0
55	MG	BA	3517	1/1	0.88	0.37	69,69,69,69	0
55	MG	DA	3311	1/1	0.88	0.20	109,109,109,109	0
55	MG	DB	213	1/1	0.88	0.15	99,99,99,99	0
55	MG	DA	3355	1/1	0.88	0.39	83,83,83,83	0
55	MG	AA	1732	1/1	0.88	0.32	95,95,95,95	0
55	MG	BA	3177	1/1	0.88	0.22	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	BA	3375	1/1	0.88	0.23	87,87,87,87	0
55	MG	CA	1656	1/1	0.88	0.33	72,72,72,72	0
55	MG	DA	3302	1/1	0.88	0.31	69,69,69,69	0
55	MG	BA	3405	1/1	0.88	0.21	82,82,82,82	0
55	MG	DA	3084	1/1	0.89	0.37	57,57,57,57	0
55	MG	DA	3077	1/1	0.89	0.38	72,72,72,72	0
55	MG	DA	3331	1/1	0.89	0.31	91,91,91,91	0
55	MG	BA	3179	1/1	0.89	0.40	72,72,72,72	0
55	MG	BA	3402	1/1	0.89	0.25	76,76,76,76	0
55	MG	BA	3488	1/1	0.89	0.30	137,137,137,137	0
55	MG	DA	3475	1/1	0.89	0.28	62,62,62,62	0
55	MG	BA	3554	1/1	0.89	0.28	48,48,48,48	0
55	MG	BA	3083	1/1	0.89	0.50	47,47,47,47	0
55	MG	BA	3536	1/1	0.89	0.12	37,37,37,37	0
55	MG	BA	3434	1/1	0.89	0.40	69,69,69,69	0
55	MG	DA	3016	1/1	0.89	0.28	78,78,78,78	0
55	MG	DA	3087	1/1	0.89	0.27	85,85,85,85	0
55	MG	BA	3225	1/1	0.89	0.37	68,68,68,68	0
55	MG	DA	3202	1/1	0.89	0.34	67,67,67,67	0
55	MG	BA	3351	1/1	0.89	0.25	88,88,88,88	0
55	MG	AA	1608	1/1	0.89	0.29	65,65,65,65	0
55	MG	CA	1629	1/1	0.89	0.21	115,115,115,115	0
55	MG	DA	3239	1/1	0.89	0.33	92,92,92,92	0
55	MG	DA	3473	1/1	0.89	0.15	56,56,56,56	0
55	MG	BA	3282	1/1	0.89	0.44	103,103,103,103	0
55	MG	BA	3304	1/1	0.89	0.37	80,80,80,80	0
55	MG	BF	303	1/1	0.89	0.45	78,78,78,78	0
55	MG	DA	3071	1/1	0.89	0.39	57,57,57,57	0
55	MG	BA	3285	1/1	0.89	0.41	102,102,102,102	0
55	MG	DA	3268	1/1	0.89	0.26	77,77,77,77	0
55	MG	AA	1742	1/1	0.89	0.27	88,88,88,88	0
55	MG	CA	1690	1/1	0.89	0.16	90,90,90,90	0
55	MG	DA	3075	1/1	0.89	0.31	57,57,57,57	0
55	MG	DA	3178	1/1	0.89	0.25	88,88,88,88	0
55	MG	DA	3440	1/1	0.89	0.09	81,81,81,81	0
55	MG	DA	3367	1/1	0.89	0.32	82,82,82,82	0
55	MG	BA	3168	1/1	0.89	0.36	47,47,47,47	0
55	MG	AA	1650	1/1	0.89	0.30	80,80,80,80	0
55	MG	BA	3216	1/1	0.89	0.26	53,53,53,53	0
55	MG	AA	1761	1/1	0.89	0.32	77,77,77,77	0
55	MG	BA	3080	1/1	0.89	0.29	64,64,64,64	0
55	MG	BA	3392	1/1	0.89	0.32	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	CA	1738	1/1	0.90	0.40	113,113,113,113	0
55	MG	AA	1677	1/1	0.90	0.42	73,73,73,73	0
55	MG	BA	3403	1/1	0.90	0.39	71,71,71,71	0
55	MG	CA	1770	1/1	0.90	0.38	82,82,82,82	0
55	MG	DA	3478	1/1	0.90	0.15	89,89,89,89	0
55	MG	DA	3017	1/1	0.90	0.26	90,90,90,90	0
55	MG	DA	3240	1/1	0.90	0.19	55,55,55,55	0
55	MG	BA	3074	1/1	0.90	0.17	91,91,91,91	0
55	MG	BA	3104	1/1	0.90	0.31	82,82,82,82	0
55	MG	DA	3074	1/1	0.90	0.35	65,65,65,65	0
55	MG	BA	3408	1/1	0.90	0.14	82,82,82,82	0
55	MG	BA	3086	1/1	0.90	0.32	56,56,56,56	0
55	MG	CA	1720	1/1	0.90	0.35	68,68,68,68	0
55	MG	BA	3207	1/1	0.90	0.55	70,70,70,70	0
55	MG	BB	212	1/1	0.90	0.45	74,74,74,74	0
55	MG	DA	3234	1/1	0.90	0.44	73,73,73,73	0
55	MG	BA	3026	1/1	0.90	0.32	43,43,43,43	0
55	MG	BA	3468	1/1	0.90	0.38	78,78,78,78	0
55	MG	CA	1765	1/1	0.90	0.22	115,115,115,115	0
55	MG	DA	3284	1/1	0.90	0.19	90,90,90,90	0
55	MG	DA	3060	1/1	0.90	0.33	67,67,67,67	0
55	MG	BB	216	1/1	0.90	0.41	63,63,63,63	0
55	MG	DA	3119	1/1	0.90	0.38	65,65,65,65	0
55	MG	AC	108	1/1	0.90	0.15	82,82,82,82	0
55	MG	BA	3362	1/1	0.90	0.21	84,84,84,84	0
55	MG	BA	3205	1/1	0.90	0.18	59,59,59,59	0
55	MG	CA	1766	1/1	0.90	0.17	114,114,114,114	0
55	MG	CA	1782	1/1	0.90	0.14	113,113,113,113	0
55	MG	BB	202	1/1	0.90	0.22	74,74,74,74	0
55	MG	CA	1794	1/1	0.90	0.10	67,67,67,67	0
55	MG	AA	1609	1/1	0.90	0.39	88,88,88,88	0
55	MG	BA	3049	1/1	0.90	0.23	75,75,75,75	0
55	MG	BA	3506	1/1	0.90	0.24	73,73,73,73	0
55	MG	CA	1662	1/1	0.90	0.43	84,84,84,84	0
55	MG	DA	3064	1/1	0.90	0.32	70,70,70,70	0
55	MG	BA	3175	1/1	0.90	0.30	62,62,62,62	0
55	MG	DA	3465	1/1	0.90	0.20	112,112,112,112	0
55	MG	DA	3141	1/1	0.90	0.29	101,101,101,101	0
55	MG	DA	3158	1/1	0.90	0.38	80,80,80,80	0
55	MG	CA	1717	1/1	0.90	0.39	73,73,73,73	0
55	MG	DA	3217	1/1	0.90	0.15	125,125,125,125	0
55	MG	DA	3143	1/1	0.90	0.31	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	DA	3485	1/1	0.90	0.34	84,84,84,84	0
55	MG	BA	3280	1/1	0.90	0.41	80,80,80,80	0
55	MG	DA	3156	1/1	0.90	0.27	78,78,78,78	0
55	MG	BA	3201	1/1	0.90	0.41	64,64,64,64	0
55	MG	DA	3117	1/1	0.90	0.25	61,61,61,61	0
55	MG	AA	1787	1/1	0.90	0.33	101,101,101,101	0
55	MG	AA	1740	1/1	0.90	0.45	76,76,76,76	0
55	MG	DA	3317	1/1	0.90	0.32	58,58,58,58	0
55	MG	DA	3052	1/1	0.90	0.16	78,78,78,78	0
55	MG	DA	3303	1/1	0.90	0.19	76,76,76,76	0
55	MG	BA	3458	1/1	0.90	0.32	91,91,91,91	0
55	MG	DA	3297	1/1	0.90	0.42	82,82,82,82	0
55	MG	AA	1790	1/1	0.90	0.27	79,79,79,79	0
55	MG	CC	101	1/1	0.90	0.33	77,77,77,77	0
55	MG	BA	3533	1/1	0.90	0.33	91,91,91,91	0
55	MG	BA	3321	1/1	0.90	0.46	88,88,88,88	0
55	MG	BA	3204	1/1	0.91	0.16	56,56,56,56	0
55	MG	DA	3230	1/1	0.91	0.32	74,74,74,74	0
55	MG	BA	3113	1/1	0.91	0.31	47,47,47,47	0
55	MG	BA	3507	1/1	0.91	0.29	79,79,79,79	0
55	MG	DB	214	1/1	0.91	0.10	95,95,95,95	0
55	MG	CA	1642	1/1	0.91	0.20	83,83,83,83	0
55	MG	BA	3227	1/1	0.91	0.43	64,64,64,64	0
55	MG	DA	3236	1/1	0.91	0.39	62,62,62,62	0
55	MG	DA	3138	1/1	0.91	0.35	54,54,54,54	0
55	MG	DA	3122	1/1	0.91	0.41	69,69,69,69	0
55	MG	BA	3542	1/1	0.91	0.36	85,85,85,85	0
55	MG	DA	3337	1/1	0.91	0.28	86,86,86,86	0
55	MG	BA	3417	1/1	0.91	0.58	86,86,86,86	0
55	MG	BA	3023	1/1	0.91	0.48	64,64,64,64	0
55	MG	DA	3216	1/1	0.91	0.33	90,90,90,90	0
55	MG	BA	3184	1/1	0.91	0.46	46,46,46,46	0
55	MG	BA	3093	1/1	0.91	0.35	57,57,57,57	0
55	MG	DA	3128	1/1	0.91	0.30	47,47,47,47	0
55	MG	BA	3052	1/1	0.91	0.24	66,66,66,66	0
55	MG	BA	3356	1/1	0.91	0.32	60,60,60,60	0
55	MG	DA	3424	1/1	0.91	0.24	83,83,83,83	0
55	MG	BA	3313	1/1	0.91	0.23	74,74,74,74	0
55	MG	DA	3223	1/1	0.91	0.16	81,81,81,81	0
55	MG	BA	3048	1/1	0.91	0.24	60,60,60,60	0
55	MG	BA	3257	1/1	0.91	0.29	87,87,87,87	0
55	MG	BA	3398	1/1	0.91	0.17	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	BA	3236	1/1	0.91	0.38	67,67,67,67	0
55	MG	BA	3562	1/1	0.91	0.42	91,91,91,91	0
55	MG	BA	3284	1/1	0.91	0.43	75,75,75,75	0
55	MG	DA	3025	1/1	0.91	0.13	70,70,70,70	0
55	MG	CA	1719	1/1	0.91	0.26	91,91,91,91	0
55	MG	AA	1734	1/1	0.91	0.44	93,93,93,93	0
55	MG	DA	3021	1/1	0.91	0.20	77,77,77,77	0
55	MG	CA	1754	1/1	0.91	0.37	92,92,92,92	0
55	MG	BA	3218	1/1	0.91	0.26	64,64,64,64	0
55	MG	AA	1774	1/1	0.91	0.52	69,69,69,69	0
55	MG	DA	3452	1/1	0.91	0.29	52,52,52,52	0
55	MG	CA	1705	1/1	0.91	0.20	101,101,101,101	0
55	MG	BA	3033	1/1	0.91	0.37	77,77,77,77	0
55	MG	CC	102	1/1	0.91	0.31	85,85,85,85	0
55	MG	CA	1632	1/1	0.91	0.17	53,53,53,53	0
55	MG	BA	3141	1/1	0.91	0.29	78,78,78,78	0
55	MG	BA	3481	1/1	0.91	0.22	97,97,97,97	0
55	MG	CA	1721	1/1	0.91	0.19	82,82,82,82	0
55	MG	DA	3214	1/1	0.91	0.30	76,76,76,76	0
55	MG	CA	1657	1/1	0.91	0.34	68,68,68,68	0
55	MG	DA	3203	1/1	0.91	0.30	74,74,74,74	0
55	MG	DA	3435	1/1	0.91	0.20	51,51,51,51	0
55	MG	DA	3289	1/1	0.91	0.39	62,62,62,62	0
55	MG	AA	1752	1/1	0.92	0.37	67,67,67,67	0
55	MG	DA	3431	1/1	0.92	0.24	69,69,69,69	0
55	MG	BA	3370	1/1	0.92	0.26	78,78,78,78	0
55	MG	DA	3241	1/1	0.92	0.32	75,75,75,75	0
55	MG	DA	3018	1/1	0.92	0.26	46,46,46,46	0
55	MG	BA	3129	1/1	0.92	0.42	50,50,50,50	0
55	MG	AA	1789	1/1	0.92	0.35	63,63,63,63	0
55	MG	DA	3037	1/1	0.92	0.12	71,71,71,71	0
55	MG	BA	3522	1/1	0.92	0.42	45,45,45,45	0
55	MG	AA	1676	1/1	0.92	0.35	89,89,89,89	0
55	MG	DA	3244	1/1	0.92	0.39	80,80,80,80	0
55	MG	DA	3115	1/1	0.92	0.45	64,64,64,64	0
55	MG	DA	3029	1/1	0.92	0.32	82,82,82,82	0
55	MG	BA	3553	1/1	0.92	0.27	49,49,49,49	0
55	MG	BA	3105	1/1	0.92	0.18	71,71,71,71	0
55	MG	CA	1636	1/1	0.92	0.31	53,53,53,53	0
55	MG	AA	1620	1/1	0.92	0.28	69,69,69,69	0
55	MG	AA	1668	1/1	0.92	0.43	68,68,68,68	0
55	MG	BA	3133	1/1	0.92	0.26	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	CA	1651	1/1	0.92	0.35	77,77,77,77	0
55	MG	DA	3447	1/1	0.92	0.27	92,92,92,92	0
55	MG	BA	3345	1/1	0.92	0.26	46,46,46,46	0
55	MG	CA	1723	1/1	0.92	0.20	90,90,90,90	0
55	MG	DA	3058	1/1	0.92	0.34	53,53,53,53	0
55	MG	BA	3272	1/1	0.92	0.22	59,59,59,59	0
55	MG	DB	201	1/1	0.92	0.18	92,92,92,92	0
55	MG	BA	3228	1/1	0.92	0.54	82,82,82,82	0
55	MG	CA	1681	1/1	0.92	0.35	89,89,89,89	0
55	MG	DA	3094	1/1	0.92	0.26	48,48,48,48	0
55	MG	AA	1769	1/1	0.92	0.18	95,95,95,95	0
55	MG	DA	3148	1/1	0.92	0.14	111,111,111,111	0
55	MG	CA	1624	1/1	0.92	0.17	93,93,93,93	0
55	MG	BA	3478	1/1	0.92	0.33	61,61,61,61	0
55	MG	BA	3308	1/1	0.92	0.12	63,63,63,63	0
55	MG	DA	3487	1/1	0.92	0.22	85,85,85,85	0
55	MG	CA	1635	1/1	0.92	0.29	72,72,72,72	0
55	MG	BA	3337	1/1	0.92	0.45	52,52,52,52	0
55	MG	DA	3361	1/1	0.92	0.10	89,89,89,89	0
55	MG	AA	1660	1/1	0.92	0.43	77,77,77,77	0
55	MG	DA	3429	1/1	0.93	0.31	54,54,54,54	0
55	MG	DA	3266	1/1	0.93	0.44	82,82,82,82	0
55	MG	DA	3453	1/1	0.93	0.41	65,65,65,65	0
55	MG	CA	1626	1/1	0.93	0.31	69,69,69,69	0
55	MG	BA	3298	1/1	0.93	0.40	66,66,66,66	0
55	MG	BA	3534	1/1	0.93	0.24	69,69,69,69	0
55	MG	DA	3103	1/1	0.93	0.36	60,60,60,60	0
55	MG	BA	3493	1/1	0.93	0.35	51,51,51,51	0
55	MG	AA	1679	1/1	0.93	0.42	83,83,83,83	0
55	MG	DA	3008	1/1	0.93	0.32	57,57,57,57	0
55	MG	D0	201	1/1	0.93	0.22	63,63,63,63	0
55	MG	DA	3106	1/1	0.93	0.33	57,57,57,57	0
55	MG	BA	3305	1/1	0.93	0.50	94,94,94,94	0
55	MG	DA	3195	1/1	0.93	0.28	82,82,82,82	0
55	MG	DA	3020	1/1	0.93	0.22	45,45,45,45	0
55	MG	AA	1793	1/1	0.93	0.20	87,87,87,87	0
55	MG	BA	3007	1/1	0.93	0.31	36,36,36,36	0
55	MG	BA	3047	1/1	0.93	0.20	46,46,46,46	0
55	MG	BA	3076	1/1	0.93	0.39	81,81,81,81	0
55	MG	BA	3196	1/1	0.93	0.22	103,103,103,103	0
55	MG	CA	1613	1/1	0.93	0.25	84,84,84,84	0
55	MG	BA	3067	1/1	0.93	0.27	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	BB	205	1/1	0.93	0.29	71,71,71,71	0
55	MG	DA	3048	1/1	0.93	0.36	76,76,76,76	0
55	MG	DA	3072	1/1	0.93	0.40	65,65,65,65	0
55	MG	DA	3123	1/1	0.93	0.43	50,50,50,50	0
55	MG	CA	1665	1/1	0.93	0.32	70,70,70,70	0
55	MG	AA	1614	1/1	0.93	0.29	92,92,92,92	0
55	MG	AA	1645	1/1	0.93	0.13	65,65,65,65	0
55	MG	CA	1631	1/1	0.93	0.27	65,65,65,65	0
55	MG	BA	3500	1/1	0.93	0.49	64,64,64,64	0
55	MG	CA	1802	1/1	0.93	0.24	73,73,73,73	0
55	MG	DA	3432	1/1	0.93	0.29	64,64,64,64	0
55	MG	DA	3057	1/1	0.93	0.31	56,56,56,56	0
55	MG	DA	3014	1/1	0.93	0.35	76,76,76,76	0
55	MG	DA	3220	1/1	0.93	0.31	64,64,64,64	0
55	MG	DA	3226	1/1	0.93	0.28	85,85,85,85	0
55	MG	DA	3460	1/1	0.93	0.27	116,116,116,116	0
55	MG	DA	3026	1/1	0.93	0.28	73,73,73,73	0
55	MG	AA	1616	1/1	0.93	0.10	110,110,110,110	0
55	MG	DA	3034	1/1	0.93	0.28	76,76,76,76	0
55	MG	BA	3028	1/1	0.93	0.33	52,52,52,52	0
55	MG	BA	3081	1/1	0.93	0.49	91,91,91,91	0
55	MG	AA	1705	1/1	0.93	0.31	81,81,81,81	0
55	MG	BA	3441	1/1	0.93	0.29	84,84,84,84	0
55	MG	BA	3057	1/1	0.93	0.21	46,46,46,46	0
55	MG	DA	3260	1/1	0.93	0.35	73,73,73,73	0
55	MG	BA	3214	1/1	0.93	0.42	58,58,58,58	0
55	MG	DA	3276	1/1	0.93	0.13	81,81,81,81	0
55	MG	BA	3010	1/1	0.93	0.38	45,45,45,45	0
55	MG	BA	3029	1/1	0.93	0.22	57,57,57,57	0
55	MG	DA	3022	1/1	0.93	0.27	74,74,74,74	0
55	MG	AA	1655	1/1	0.94	0.41	78,78,78,78	0
55	MG	DA	3348	1/1	0.94	0.19	56,56,56,56	0
55	MG	BA	3111	1/1	0.94	0.21	55,55,55,55	0
55	MG	DA	3160	1/1	0.94	0.34	59,59,59,59	0
55	MG	BA	3407	1/1	0.94	0.26	73,73,73,73	0
55	MG	AA	1636	1/1	0.94	0.28	95,95,95,95	0
55	MG	DA	3313	1/1	0.94	0.23	84,84,84,84	0
55	MG	DA	3449	1/1	0.94	0.28	66,66,66,66	0
55	MG	BA	3538	1/1	0.94	0.23	79,79,79,79	0
55	MG	BA	3094	1/1	0.94	0.37	68,68,68,68	0
55	MG	BA	3166	1/1	0.94	0.23	28,28,28,28	0
55	MG	DA	3272	1/1	0.94	0.46	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	CA	1614	1/1	0.94	0.29	79,79,79,79	0
55	MG	CA	1620	1/1	0.94	0.14	64,64,64,64	0
55	MG	BA	3153	1/1	0.94	0.47	78,78,78,78	0
55	MG	BA	3541	1/1	0.94	0.21	66,66,66,66	0
55	MG	DA	3068	1/1	0.94	0.31	54,54,54,54	0
55	MG	DA	3013	1/1	0.94	0.25	51,51,51,51	0
55	MG	BA	3131	1/1	0.94	0.38	41,41,41,41	0
55	MG	BA	3116	1/1	0.94	0.47	50,50,50,50	0
55	MG	BA	3070	1/1	0.94	0.28	68,68,68,68	0
55	MG	BA	3339	1/1	0.94	0.37	74,74,74,74	0
55	MG	DA	3028	1/1	0.94	0.30	73,73,73,73	0
55	MG	DA	3164	1/1	0.94	0.26	67,67,67,67	0
55	MG	AA	1603	1/1	0.94	0.25	65,65,65,65	0
55	MG	DA	3062	1/1	0.94	0.17	39,39,39,39	0
55	MG	BA	3532	1/1	0.94	0.41	54,54,54,54	0
55	MG	CA	1714	1/1	0.94	0.24	87,87,87,87	0
55	MG	CA	1606	1/1	0.94	0.19	65,65,65,65	0
55	MG	BA	3235	1/1	0.94	0.38	39,39,39,39	0
55	MG	DA	3110	1/1	0.94	0.14	61,61,61,61	0
55	MG	BA	3108	1/1	0.94	0.38	58,58,58,58	0
55	MG	CA	1659	1/1	0.94	0.41	75,75,75,75	0
55	MG	CA	1604	1/1	0.94	0.20	60,60,60,60	0
55	MG	DA	3083	1/1	0.94	0.10	65,65,65,65	0
55	MG	DA	3249	1/1	0.94	0.07	81,81,81,81	0
55	MG	DA	3182	1/1	0.94	0.27	47,47,47,47	0
55	MG	DA	3032	1/1	0.94	0.29	77,77,77,77	0
55	MG	DA	3069	1/1	0.94	0.42	76,76,76,76	0
55	MG	BA	3255	1/1	0.94	0.41	50,50,50,50	0
55	MG	DA	3175	1/1	0.94	0.38	60,60,60,60	0
55	MG	BA	3525	1/1	0.94	0.32	51,51,51,51	0
55	MG	DA	3151	1/1	0.94	0.33	78,78,78,78	0
55	MG	DA	3005	1/1	0.94	0.29	48,48,48,48	0
55	MG	CA	1607	1/1	0.94	0.13	70,70,70,70	0
55	MG	CA	1641	1/1	0.94	0.15	64,64,64,64	0
55	MG	DA	3385	1/1	0.94	0.17	86,86,86,86	0
55	MG	BA	3423	1/1	0.94	0.38	90,90,90,90	0
55	MG	DA	3152	1/1	0.94	0.29	63,63,63,63	0
55	MG	BA	3073	1/1	0.94	0.29	65,65,65,65	0
55	MG	CA	1617	1/1	0.94	0.37	83,83,83,83	0
55	MG	CA	1741	1/1	0.94	0.21	85,85,85,85	0
55	MG	CA	1795	1/1	0.94	0.41	73,73,73,73	0
55	MG	CA	1602	1/1	0.94	0.35	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	CA	1724	1/1	0.94	0.18	87,87,87,87	0
55	MG	BA	3560	1/1	0.94	0.38	69,69,69,69	0
55	MG	DA	3145	1/1	0.94	0.29	54,54,54,54	0
55	MG	DA	3155	1/1	0.94	0.14	90,90,90,90	0
55	MG	BA	3148	1/1	0.94	0.13	56,56,56,56	0
55	MG	D5	101	1/1	0.95	0.27	58,58,58,58	0
55	MG	BA	3043	1/1	0.95	0.39	78,78,78,78	0
55	MG	DA	3001	1/1	0.95	0.30	46,46,46,46	0
55	MG	BA	3158	1/1	0.95	0.40	66,66,66,66	0
55	MG	DA	3116	1/1	0.95	0.35	61,61,61,61	0
55	MG	BA	3170	1/1	0.95	0.31	54,54,54,54	0
55	MG	DA	3137	1/1	0.95	0.23	53,53,53,53	0
55	MG	BA	3156	1/1	0.95	0.35	61,61,61,61	0
55	MG	BA	3087	1/1	0.95	0.35	38,38,38,38	0
55	MG	AA	1602	1/1	0.95	0.28	71,71,71,71	0
55	MG	BA	3055	1/1	0.95	0.34	78,78,78,78	0
55	MG	BA	3384	1/1	0.95	0.66	85,85,85,85	0
55	MG	DA	3105	1/1	0.95	0.34	37,37,37,37	0
55	MG	DA	3237	1/1	0.95	0.27	79,79,79,79	0
55	MG	BA	3077	1/1	0.95	0.27	83,83,83,83	0
55	MG	BF	301	1/1	0.95	0.14	79,79,79,79	0
55	MG	BA	3002	1/1	0.95	0.38	40,40,40,40	0
55	MG	AA	1610	1/1	0.95	0.34	58,58,58,58	0
55	MG	BA	3167	1/1	0.95	0.39	45,45,45,45	0
55	MG	AA	1670	1/1	0.95	0.38	75,75,75,75	0
55	MG	CA	1679	1/1	0.95	0.23	80,80,80,80	0
55	MG	DA	3049	1/1	0.95	0.41	55,55,55,55	0
55	MG	DA	3046	1/1	0.95	0.11	100,100,100,100	0
55	MG	DA	3428	1/1	0.95	0.34	59,59,59,59	0
55	MG	AA	1652	1/1	0.95	0.43	72,72,72,72	0
55	MG	DA	3107	1/1	0.95	0.38	55,55,55,55	0
55	MG	DA	3196	1/1	0.95	0.22	45,45,45,45	0
55	MG	BA	3521	1/1	0.95	0.24	45,45,45,45	0
55	MG	BA	3146	1/1	0.95	0.36	62,62,62,62	0
55	MG	BA	3494	1/1	0.95	0.36	76,76,76,76	0
55	MG	DA	3200	1/1	0.95	0.37	55,55,55,55	0
55	MG	CA	1772	1/1	0.95	0.17	107,107,107,107	0
55	MG	BA	3019	1/1	0.95	0.31	45,45,45,45	0
55	MG	BA	3241	1/1	0.95	0.32	62,62,62,62	0
55	MG	DA	3253	1/1	0.95	0.28	77,77,77,77	0
55	MG	BA	3292	1/1	0.95	0.27	63,63,63,63	0
55	MG	DA	3113	1/1	0.95	0.23	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	BA	3136	1/1	0.95	0.15	53,53,53,53	0
55	MG	BA	3124	1/1	0.95	0.34	66,66,66,66	0
55	MG	DA	3080	1/1	0.95	0.27	73,73,73,73	0
55	MG	DA	3007	1/1	0.95	0.24	55,55,55,55	0
55	MG	DA	3027	1/1	0.95	0.13	47,47,47,47	0
55	MG	BA	3361	1/1	0.95	0.17	70,70,70,70	0
55	MG	BA	3117	1/1	0.95	0.41	52,52,52,52	0
55	MG	DA	3347	1/1	0.95	0.12	91,91,91,91	0
55	MG	DA	3053	1/1	0.95	0.28	72,72,72,72	0
55	MG	BA	3244	1/1	0.95	0.16	34,34,34,34	0
55	MG	BA	3103	1/1	0.95	0.49	76,76,76,76	0
55	MG	BA	3044	1/1	0.95	0.26	68,68,68,68	0
55	MG	BA	3497	1/1	0.95	0.28	30,30,30,30	0
55	MG	AA	1607	1/1	0.95	0.20	86,86,86,86	0
55	MG	DA	3047	1/1	0.95	0.34	67,67,67,67	0
55	MG	BA	3465	1/1	0.95	0.52	61,61,61,61	0
55	MG	CA	1769	1/1	0.95	0.30	67,67,67,67	0
55	MG	DB	202	1/1	0.95	0.14	91,91,91,91	0
55	MG	AA	1601	1/1	0.95	0.30	60,60,60,60	0
55	MG	DA	3111	1/1	0.95	0.23	45,45,45,45	0
55	MG	BA	3197	1/1	0.95	0.40	57,57,57,57	0
55	MG	AA	1662	1/1	0.95	0.23	41,41,41,41	0
55	MG	BA	3248	1/1	0.95	0.21	34,34,34,34	0
55	MG	BA	3520	1/1	0.96	0.38	40,40,40,40	0
55	MG	BA	3042	1/1	0.96	0.38	75,75,75,75	0
55	MG	BA	3164	1/1	0.96	0.40	47,47,47,47	0
55	MG	AA	1672	1/1	0.96	0.52	67,67,67,67	0
55	MG	BA	3182	1/1	0.96	0.50	45,45,45,45	0
55	MG	BA	3022	1/1	0.96	0.31	46,46,46,46	0
55	MG	BA	3208	1/1	0.96	0.55	55,55,55,55	0
55	MG	DA	3002	1/1	0.96	0.36	48,48,48,48	0
55	MG	BA	3072	1/1	0.96	0.35	67,67,67,67	0
55	MG	DA	3154	1/1	0.96	0.22	77,77,77,77	0
55	MG	BA	3499	1/1	0.96	0.48	38,38,38,38	0
55	MG	CA	1637	1/1	0.96	0.10	70,70,70,70	0
55	MG	DA	3341	1/1	0.96	0.33	56,56,56,56	0
55	MG	DA	3098	1/1	0.96	0.32	48,48,48,48	0
55	MG	DA	3112	1/1	0.96	0.28	63,63,63,63	0
55	MG	AA	1719	1/1	0.96	0.23	80,80,80,80	0
55	MG	DA	3015	1/1	0.96	0.33	64,64,64,64	0
55	MG	CA	1698	1/1	0.96	0.23	79,79,79,79	0
55	MG	BA	3354	1/1	0.96	0.44	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	AA	1665	1/1	0.96	0.17	52,52,52,52	0
55	MG	DA	3162	1/1	0.96	0.34	58,58,58,58	0
55	MG	BA	3311	1/1	0.96	0.38	68,68,68,68	0
55	MG	BA	3011	1/1	0.96	0.41	40,40,40,40	0
55	MG	BA	3159	1/1	0.96	0.37	57,57,57,57	0
55	MG	BA	3527	1/1	0.96	0.12	40,40,40,40	0
55	MG	DA	3109	1/1	0.96	0.36	55,55,55,55	0
55	MG	BA	3021	1/1	0.96	0.28	42,42,42,42	0
55	MG	DA	3204	1/1	0.96	0.13	48,48,48,48	0
55	MG	AA	1776	1/1	0.96	0.31	67,67,67,67	0
55	MG	AA	1674	1/1	0.96	0.32	56,56,56,56	0
55	MG	DA	3065	1/1	0.96	0.38	75,75,75,75	0
55	MG	DA	3191	1/1	0.96	0.46	55,55,55,55	0
55	MG	BA	3223	1/1	0.96	0.48	56,56,56,56	0
55	MG	BA	3050	1/1	0.96	0.31	65,65,65,65	0
55	MG	AA	1627	1/1	0.96	0.34	62,62,62,62	0
55	MG	BA	3119	1/1	0.96	0.39	61,61,61,61	0
55	MG	DA	3450	1/1	0.96	0.33	54,54,54,54	0
55	MG	DA	3433	1/1	0.96	0.37	50,50,50,50	0
55	MG	CA	1731	1/1	0.96	0.36	97,97,97,97	0
55	MG	BA	3039	1/1	0.96	0.28	55,55,55,55	0
55	MG	DA	3078	1/1	0.96	0.35	76,76,76,76	0
55	MG	BA	3327	1/1	0.96	0.30	69,69,69,69	0
55	MG	AA	1656	1/1	0.96	0.41	87,87,87,87	0
55	MG	CA	1633	1/1	0.96	0.37	61,61,61,61	0
55	MG	BA	3389	1/1	0.96	0.31	56,56,56,56	0
55	MG	CA	1608	1/1	0.96	0.23	74,74,74,74	0
55	MG	AA	1641	1/1	0.96	0.31	56,56,56,56	0
55	MG	DA	3180	1/1	0.96	0.25	48,48,48,48	0
55	MG	BA	3036	1/1	0.96	0.36	58,58,58,58	0
55	MG	BA	3363	1/1	0.96	0.37	57,57,57,57	0
55	MG	BA	3213	1/1	0.96	0.41	41,41,41,41	0
55	MG	AN	201	1/1	0.96	0.07	67,67,67,67	0
55	MG	BA	3387	1/1	0.96	0.10	88,88,88,88	0
55	MG	DA	3003	1/1	0.96	0.24	58,58,58,58	0
55	MG	DA	3247	1/1	0.96	0.34	58,58,58,58	0
55	MG	BA	3165	1/1	0.96	0.32	60,60,60,60	0
55	MG	BA	3060	1/1	0.96	0.22	51,51,51,51	0
55	MG	DA	3131	1/1	0.96	0.34	48,48,48,48	0
55	MG	AA	1606	1/1	0.96	0.07	77,77,77,77	0
55	MG	DA	3430	1/1	0.96	0.42	52,52,52,52	0
55	MG	AA	1604	1/1	0.97	0.35	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	DA	3063	1/1	0.97	0.25	45,45,45,45	0
55	MG	CA	1752	1/1	0.97	0.44	80,80,80,80	0
55	MG	DA	3144	1/1	0.97	0.47	66,66,66,66	0
55	MG	DA	3183	1/1	0.97	0.29	75,75,75,75	0
55	MG	DA	3006	1/1	0.97	0.29	50,50,50,50	0
55	MG	BA	3286	1/1	0.97	0.51	46,46,46,46	0
55	MG	AA	1710	1/1	0.97	0.22	56,56,56,56	0
55	MG	DA	3011	1/1	0.97	0.34	50,50,50,50	0
55	MG	AA	1698	1/1	0.97	0.48	76,76,76,76	0
55	MG	BA	3034	1/1	0.97	0.29	40,40,40,40	0
55	MG	BW	101	1/1	0.97	0.21	64,64,64,64	0
55	MG	BA	3526	1/1	0.97	0.39	41,41,41,41	0
55	MG	BA	3012	1/1	0.97	0.39	45,45,45,45	0
55	MG	DA	3293	1/1	0.97	0.48	89,89,89,89	0
55	MG	DA	3009	1/1	0.97	0.34	53,53,53,53	0
55	MG	BA	3008	1/1	0.97	0.38	44,44,44,44	0
55	MG	AA	1812	1/1	0.97	0.46	69,69,69,69	0
55	MG	BA	3084	1/1	0.97	0.37	37,37,37,37	0
55	MG	AA	1628	1/1	0.97	0.46	77,77,77,77	0
55	MG	BA	3003	1/1	0.97	0.34	50,50,50,50	0
55	MG	BA	3109	1/1	0.97	0.36	81,81,81,81	0
55	MG	DA	3041	1/1	0.97	0.41	47,47,47,47	0
55	MG	DA	3456	1/1	0.97	0.29	57,57,57,57	0
55	MG	BA	3027	1/1	0.97	0.24	41,41,41,41	0
55	MG	BA	3149	1/1	0.97	0.36	41,41,41,41	0
55	MG	DA	3193	1/1	0.97	0.50	48,48,48,48	0
55	MG	DA	3457	1/1	0.97	0.28	48,48,48,48	0
55	MG	BA	3017	1/1	0.97	0.41	58,58,58,58	0
55	MG	DA	3044	1/1	0.97	0.34	66,66,66,66	0
55	MG	DA	3043	1/1	0.97	0.28	69,69,69,69	0
55	MG	CA	1664	1/1	0.97	0.30	64,64,64,64	0
55	MG	BA	3518	1/1	0.97	0.49	36,36,36,36	0
55	MG	BA	3186	1/1	0.97	0.29	45,45,45,45	0
55	MG	BA	3144	1/1	0.97	0.42	39,39,39,39	0
55	MG	BA	3114	1/1	0.97	0.23	37,37,37,37	0
55	MG	CA	1728	1/1	0.97	0.45	58,58,58,58	0
55	MG	DA	3061	1/1	0.97	0.35	53,53,53,53	0
55	MG	BA	3015	1/1	0.97	0.39	35,35,35,35	0
55	MG	DA	3455	1/1	0.97	0.14	44,44,44,44	0
55	MG	BA	3038	1/1	0.97	0.23	33,33,33,33	0
55	MG	BA	3523	1/1	0.97	0.41	36,36,36,36	0
55	MG	BA	3115	1/1	0.97	0.44	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	BA	3143	1/1	0.97	0.19	43,43,43,43	0
55	MG	DA	3474	1/1	0.97	0.28	60,60,60,60	0
55	MG	DA	3042	1/1	0.97	0.38	51,51,51,51	0
55	MG	DA	3471	1/1	0.97	0.22	60,60,60,60	0
55	MG	BA	3377	1/1	0.97	0.41	64,64,64,64	0
56	ZN	AG	303	1/1	0.97	0.35	100,100,100,100	0
55	MG	DA	3472	1/1	0.97	0.24	53,53,53,53	0
55	MG	BA	3120	1/1	0.97	0.37	42,42,42,42	0
55	MG	BA	3006	1/1	0.97	0.44	58,58,58,58	0
56	ZN	CQ	101	1/1	0.97	0.17	118,118,118,118	0
55	MG	BA	3089	1/1	0.97	0.35	61,61,61,61	0
55	MG	DD	301	1/1	0.97	0.38	51,51,51,51	0
55	MG	BA	3088	1/1	0.97	0.43	57,57,57,57	0
55	MG	BA	3260	1/1	0.97	0.43	65,65,65,65	0
55	MG	BA	3492	1/1	0.97	0.39	54,54,54,54	0
55	MG	BA	3188	1/1	0.97	0.35	64,64,64,64	0
55	MG	AA	1659	1/1	0.97	0.40	46,46,46,46	0
55	MG	CA	1807	1/1	0.97	0.34	95,95,95,95	0
55	MG	BA	3273	1/1	0.97	0.34	73,73,73,73	0
55	MG	BA	3211	1/1	0.97	0.37	55,55,55,55	0
55	MG	DA	3470	1/1	0.98	0.33	54,54,54,54	0
55	MG	BA	3264	1/1	0.98	0.41	61,61,61,61	0
55	MG	DA	3118	1/1	0.98	0.36	55,55,55,55	0
55	MG	DA	3101	1/1	0.98	0.33	76,76,76,76	0
55	MG	BA	3490	1/1	0.98	0.37	36,36,36,36	0
55	MG	CA	1703	1/1	0.98	0.43	72,72,72,72	0
55	MG	BA	3221	1/1	0.98	0.39	59,59,59,59	0
55	MG	DA	3136	1/1	0.98	0.40	73,73,73,73	0
55	MG	B0	201	1/1	0.98	0.32	46,46,46,46	0
55	MG	BA	3519	1/1	0.98	0.38	24,24,24,24	0
55	MG	AA	1646	1/1	0.98	0.42	60,60,60,60	0
55	MG	BA	3551	1/1	0.98	0.30	64,64,64,64	0
55	MG	DA	3004	1/1	0.98	0.23	39,39,39,39	0
55	MG	BA	3001	1/1	0.98	0.50	55,55,55,55	0
55	MG	BA	3552	1/1	0.98	0.39	45,45,45,45	0
55	MG	BA	3085	1/1	0.98	0.42	38,38,38,38	0
56	ZN	CG	303	1/1	0.98	0.30	109,109,109,109	0
55	MG	DA	3045	1/1	0.98	0.43	71,71,71,71	0
55	MG	BA	3004	1/1	0.98	0.37	36,36,36,36	0
55	MG	BA	3152	1/1	0.98	0.42	58,58,58,58	0
55	MG	DA	3059	1/1	0.98	0.31	61,61,61,61	0
55	MG	DA	3055	1/1	0.98	0.41	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	BA	3261	1/1	0.98	0.47	57,57,57,57	0
55	MG	BA	3367	1/1	0.98	0.54	72,72,72,72	0
55	MG	DA	3408	1/1	0.98	0.23	66,66,66,66	0
55	MG	BA	3496	1/1	0.98	0.28	45,45,45,45	0
55	MG	BA	3142	1/1	0.98	0.13	49,49,49,49	0
55	MG	BA	3139	1/1	0.98	0.47	43,43,43,43	0
55	MG	BA	3130	1/1	0.98	0.43	50,50,50,50	0
55	MG	DA	3130	1/1	0.98	0.24	49,49,49,49	0
55	MG	BA	3024	1/1	0.98	0.39	44,44,44,44	0
55	MG	BA	3014	1/1	0.98	0.41	43,43,43,43	0
55	MG	DA	3067	1/1	0.98	0.17	50,50,50,50	0
55	MG	DA	3170	1/1	0.98	0.39	59,59,59,59	0
55	MG	BA	3032	1/1	0.98	0.31	41,41,41,41	0
55	MG	DA	3454	1/1	0.99	0.35	52,52,52,52	0
55	MG	DA	3097	1/1	0.99	0.33	53,53,53,53	0
55	MG	BE	302	1/1	0.99	0.43	40,40,40,40	0
55	MG	DA	3427	1/1	0.99	0.29	56,56,56,56	0
55	MG	BA	3529	1/1	0.99	0.49	42,42,42,42	0
55	MG	BA	3005	1/1	0.99	0.40	40,40,40,40	0
55	MG	BA	3491	1/1	0.99	0.35	41,41,41,41	0
55	MG	BA	3161	1/1	0.99	0.44	45,45,45,45	0
55	MG	BA	3173	1/1	0.99	0.40	58,58,58,58	0
55	MG	AA	1722	1/1	-	-	62,62,62,62	1
55	MG	BA	3391	1/1	0.13	0.52	112,112,112,112	0
55	MG	DA	3388	1/1	0.27	0.21	138,138,138,138	0
55	MG	AA	1748	1/1	0.37	0.29	116,116,116,116	0
55	MG	DA	3411	1/1	0.41	0.38	144,144,144,144	0
55	MG	AA	1621	1/1	0.41	0.28	102,102,102,102	0
55	MG	BA	3171	1/1	0.47	0.46	96,96,96,96	0
55	MG	CB	103	1/1	0.48	1.49	147,147,147,147	0
55	MG	DA	3395	1/1	0.48	0.29	87,87,87,87	0
55	MG	DA	3365	1/1	0.51	0.48	112,112,112,112	0
55	MG	DA	3082	1/1	0.51	0.21	91,91,91,91	0
55	MG	DA	3405	1/1	0.52	0.29	135,135,135,135	0
55	MG	BA	3100	1/1	0.53	0.41	93,93,93,93	0
55	MG	CA	1647	1/1	0.53	0.40	96,96,96,96	0
55	MG	D7	101	1/1	0.55	0.34	86,86,86,86	0
55	MG	AA	1780	1/1	0.56	0.24	103,103,103,103	0
55	MG	AA	1805	1/1	0.56	0.73	152,152,152,152	0
55	MG	DA	3360	1/1	0.58	0.15	97,97,97,97	0
55	MG	DA	3242	1/1	0.58	0.11	81,81,81,81	0
55	MG	BA	3234	1/1	0.60	0.26	107,107,107,107	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	BA	3416	1/1	0.60	0.30	98,98,98,98	0
55	MG	BA	3237	1/1	0.61	0.37	102,102,102,102	0
55	MG	AA	1767	1/1	0.63	0.22	116,116,116,116	0
55	MG	BA	3471	1/1	0.64	0.38	126,126,126,126	0
55	MG	AA	1795	1/1	0.64	0.37	113,113,113,113	0
55	MG	BA	3369	1/1	0.65	0.20	92,92,92,92	0
55	MG	AA	1617	1/1	0.68	0.35	76,76,76,76	0
55	MG	DA	3255	1/1	0.69	0.15	82,82,82,82	0
55	MG	CA	1791	1/1	0.71	0.20	80,80,80,80	0
55	MG	DA	3467	1/1	0.72	0.13	103,103,103,103	0
55	MG	DA	3210	1/1	0.74	0.38	77,77,77,77	0
55	MG	DA	3420	1/1	0.75	0.14	108,108,108,108	0
55	MG	BA	3504	1/1	0.75	0.51	88,88,88,88	0
55	MG	BA	3480	1/1	0.76	0.34	76,76,76,76	0
55	MG	BA	3250	1/1	0.77	0.23	90,90,90,90	0
55	MG	DA	3256	1/1	0.77	0.20	91,91,91,91	0
55	MG	CA	1638	1/1	0.78	0.33	68,68,68,68	0
55	MG	BA	3374	1/1	0.79	0.26	93,93,93,93	0
55	MG	DA	3066	1/1	0.79	0.30	76,76,76,76	0
55	MG	AA	1718	1/1	0.79	0.18	82,82,82,82	0
55	MG	DA	3207	1/1	0.80	0.44	83,83,83,83	0
55	MG	BA	3145	1/1	0.81	0.27	54,54,54,54	0
55	MG	DA	3306	1/1	0.81	0.34	96,96,96,96	0
55	MG	DA	3205	1/1	0.82	0.27	110,110,110,110	0
55	MG	DA	3051	1/1	0.83	0.13	87,87,87,87	0
55	MG	BA	3514	1/1	0.83	0.36	113,113,113,113	0
55	MG	BA	3200	1/1	0.84	0.24	81,81,81,81	0
55	MG	AA	1692	1/1	0.84	0.25	73,73,73,73	0
55	MG	CA	1779	1/1	0.84	0.27	109,109,109,109	0
55	MG	CA	1612	1/1	0.84	0.27	75,75,75,75	0
55	MG	DA	3362	1/1	0.85	0.31	150,150,150,150	0
55	MG	CD	101	1/1	0.85	0.13	145,145,145,145	0
55	MG	BA	3341	1/1	0.86	0.42	89,89,89,89	0
55	MG	BA	3460	1/1	0.86	0.36	97,97,97,97	0
55	MG	AA	1717	1/1	0.86	0.42	73,73,73,73	0
55	MG	DA	3031	1/1	0.87	0.17	70,70,70,70	0
55	MG	BA	3110	1/1	0.87	0.30	69,69,69,69	0
55	MG	DA	3285	1/1	0.88	0.37	79,79,79,79	0
55	MG	DA	3335	1/1	0.89	0.11	80,80,80,80	0
55	MG	DB	207	1/1	0.89	0.33	69,69,69,69	0
55	MG	DA	3102	1/1	0.90	0.35	72,72,72,72	0
55	MG	BA	3371	1/1	0.91	0.20	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	BA	3095	1/1	0.91	0.26	79,79,79,79	0
55	MG	DA	3090	1/1	0.91	0.27	71,71,71,71	0
55	MG	CA	1725	1/1	0.91	0.35	86,86,86,86	0
55	MG	BA	3061	1/1	0.91	0.33	73,73,73,73	0
55	MG	BB	213	1/1	0.92	0.24	101,101,101,101	0
55	MG	DA	3288	1/1	0.92	0.09	101,101,101,101	0
55	MG	DA	3169	1/1	0.92	0.26	92,92,92,92	0
55	MG	CA	1758	1/1	0.93	0.24	107,107,107,107	0
55	MG	BA	3056	1/1	0.93	0.31	57,57,57,57	0
55	MG	AA	1716	1/1	0.93	0.25	82,82,82,82	0
55	MG	DA	3096	1/1	0.93	0.44	47,47,47,47	0
55	MG	AA	1642	1/1	0.93	0.38	70,70,70,70	0
55	MG	BA	3150	1/1	0.93	0.49	49,49,49,49	0
55	MG	AA	1712	1/1	0.94	0.17	73,73,73,73	0
55	MG	BA	3054	1/1	0.94	0.30	52,52,52,52	0
55	MG	BA	3495	1/1	0.94	0.39	75,75,75,75	0
55	MG	BA	3018	1/1	0.94	0.41	44,44,44,44	0
55	MG	BA	3470	1/1	0.94	0.48	83,83,83,83	0
55	MG	DA	3056	1/1	0.95	0.44	52,52,52,52	0
55	MG	BA	3215	1/1	0.95	0.24	44,44,44,44	0
55	MG	DA	3129	1/1	0.96	0.38	65,65,65,65	0
55	MG	BA	3157	1/1	0.96	0.50	50,50,50,50	0
55	MG	CA	1616	1/1	0.96	0.23	87,87,87,87	0
55	MG	CA	1601	1/1	0.96	0.26	67,67,67,67	0
55	MG	DA	3108	1/1	0.96	0.41	54,54,54,54	0
55	MG	BA	3531	1/1	0.97	0.20	31,31,31,31	0
55	MG	DA	3070	1/1	0.97	0.33	49,49,49,49	0
55	MG	DA	3012	1/1	0.97	0.34	50,50,50,50	0
55	MG	DA	3010	1/1	0.97	0.31	53,53,53,53	0
55	MG	CA	1718	1/1	0.98	0.13	64,64,64,64	0
55	MG	CA	1634	1/1	0.98	0.45	58,58,58,58	0
55	MG	BA	3435	1/1	0.99	0.46	49,49,49,49	0
55	MG	BA	3312	1/1	-	-	62,62,62,62	1
55	MG	DA	3274	1/1	0.50	0.26	85,85,85,85	0
55	MG	BA	3410	1/1	0.79	0.23	84,84,84,84	0
55	MG	BA	3366	1/1	0.91	0.21	91,91,91,91	0
56	ZN	AQ	101	1/1	0.98	0.14	142,142,142,142	0

6.5 Other polymers ⓘ

There are no such residues in this entry.