wwPDB X-ray Structure Validation Summary Report (i)

Oct 10, 2023 – 08:20 AM EDT

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

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

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

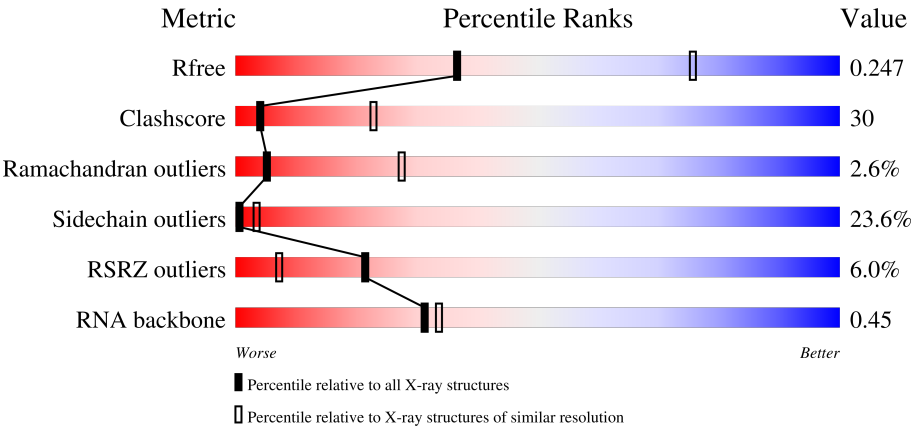
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	32% 48% 19% ·
1	CA	1506	30% 47% 22% ·
2	AE	256	4% 32% 46% 14% 7%
2	CE	256	10% 34% 41% 16% · 7%

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Mol	Chain	Length	Quality of chain
3	AF	239	14% 37% 38% 10% 14%
3	CF	239	25% 33% 39% 14% 14%
4	AG	208	6% 43% 42% 13%
4	CG	208	7% 40% 45% 15%
5	AH	162	5% 41% 41% 11% 7%
5	CH	162	4% 35% 48% 11% 7%
6	AI	101	14% 50% 42% 8%
6	CI	101	19% 52% 40% 8%
7	AJ	156	5% 54% 37% 8%
7	CJ	156	6% 50% 39% 10%
8	AK	138	45% 46% 9%
8	CK	138	% 41% 50% 9%
9	AL	128	% 40% 42% 17%
9	CL	128	3% 27% 59% 12%
10	AM	105	6% 36% 41% 16% 6%
10	CM	105	3% 23% 47% 24% 6%
11	AN	129	15% 45% 37% 10% 8%
11	CN	129	25% 53% 33% 6% 8%
12	AO	132	6% 45% 42% 8% 5%
12	CO	132	20% 40% 39% 15% 5%
13	AP	126	3% 33% 46% 12% 8%
13	CP	126	9% 29% 51% 13% 7%
14	AQ	61	36% 48% 11%
14	CQ	61	18% 25% 56% 16%
15	AR	89	2% 52% 38% 8%

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Mol	Chain	Length	Quality of chain
15	CR	89	2% 47% 43% 9%
16	AS	88	27% 50% 17% 5%
16	CS	88	48% 42% 6% 5%
17	AT	105	43% 45% 8% 5%
17	CT	105	57% 35% 5%
18	AU	88	14% 43% 30% 9% 18%
18	CU	88	14% 34% 36% 11% 18%
19	AV	93	2% 30% 40% 14% 16%
19	CV	93	13% 23% 44% 16% 16%
20	AW	106	33% 52% 8% 7%
20	CW	106	33% 47% 12% 7%
21	AX	27	41% 41% 11% 7%
21	CX	27	4% 37% 56% 7%
22	AB	87	33% 26% 33% 36% 5%
22	CB	87	63% 10% 39% 41% 9%
23	AC	77	18% 48% 26% 8%
23	AD	77	4% 16% 52% 32%
23	CC	77	18% 36% 35% 10%
23	CD	77	16% 17% 53% 30%
24	A1	10	20% 20% 40% 30% 10%
24	C1	10	20% 60% 40%
25	BA	2912	37% 44% 17%
25	DA	2912	2% 36% 45% 18%
26	BB	122	39% 37% 22%
26	DB	122	24% 47% 29%

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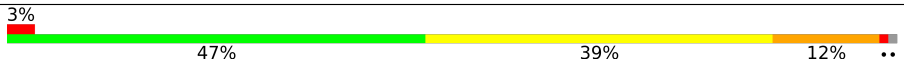
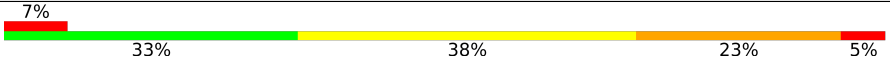
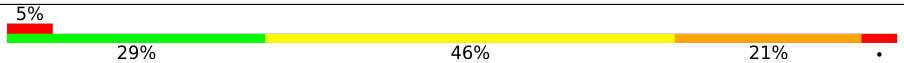
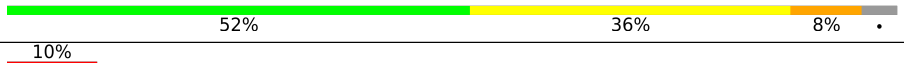
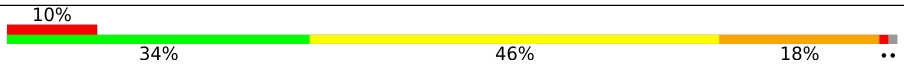
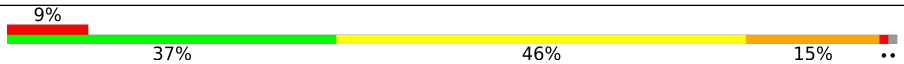
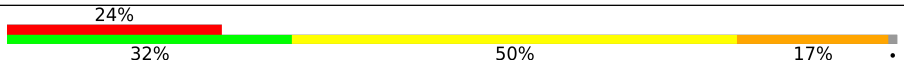
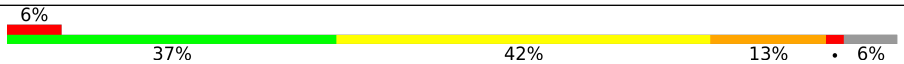
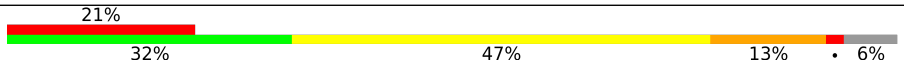
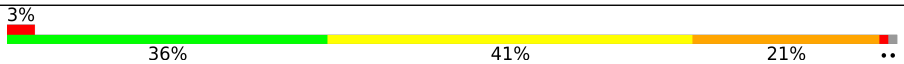
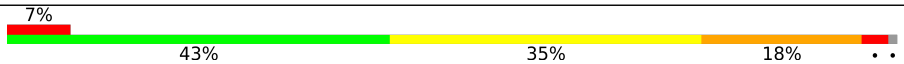
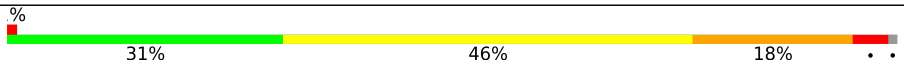
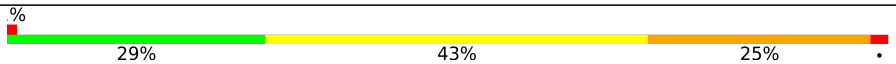
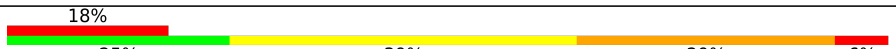
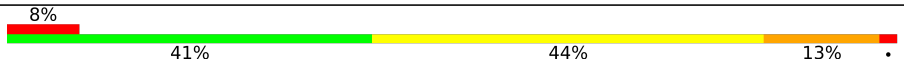
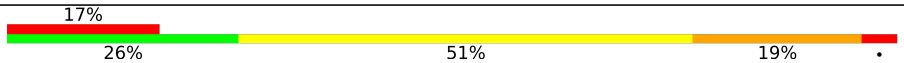
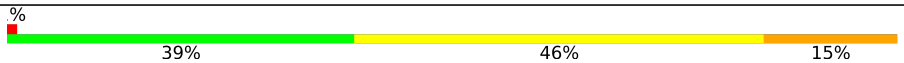
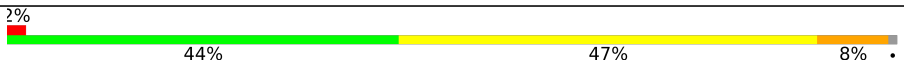
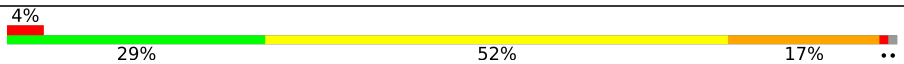
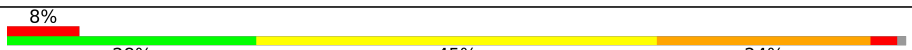
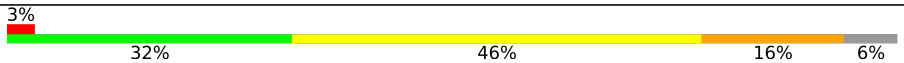
Mol	Chain	Length	Quality of chain
27	BD	276	
27	DD	276	
28	BE	206	
28	DE	206	
29	BF	210	
29	DF	210	
30	BG	182	
30	DG	182	
31	BH	180	
31	DH	180	
32	BK	148	
32	DK	148	
33	BM	140	
33	DM	140	
34	BN	122	
34	DN	122	
35	BO	150	
35	DO	150	
36	BP	141	
36	DP	141	
37	B0	118	
37	D0	118	
38	BQ	112	
38	DQ	112	
39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

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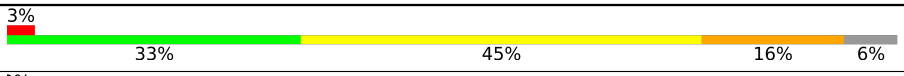
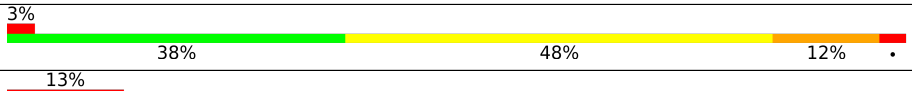
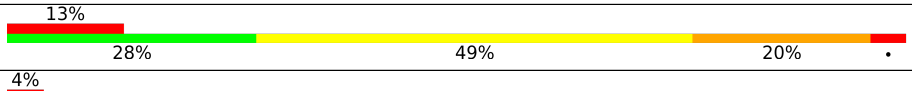
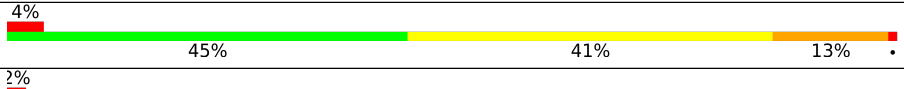
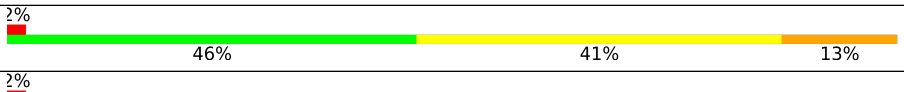
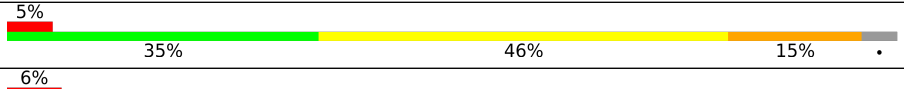
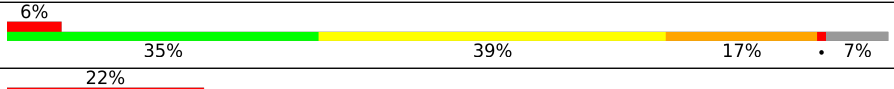
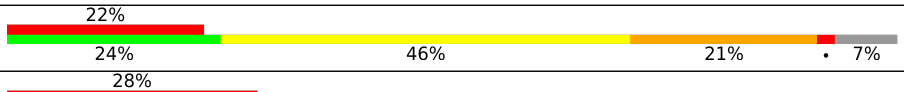
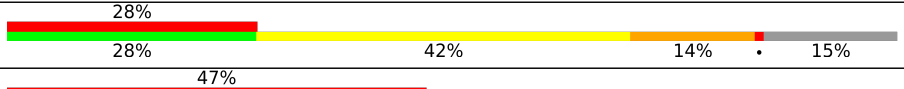
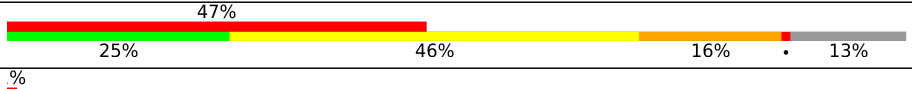
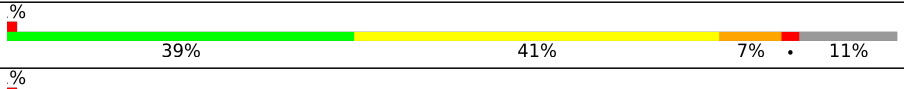
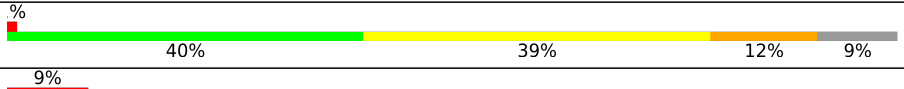
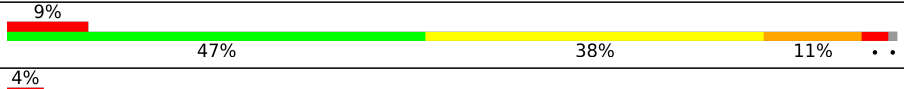
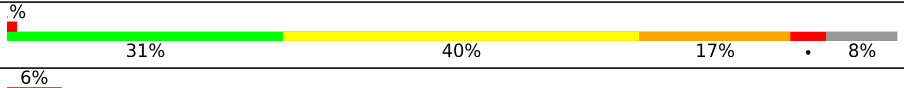
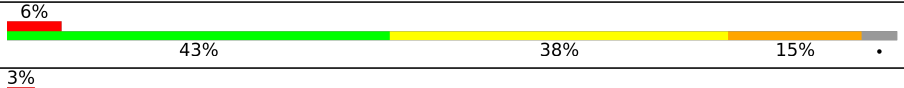
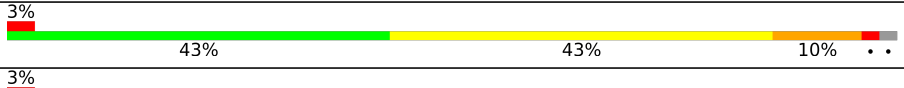
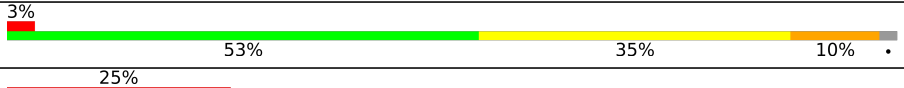
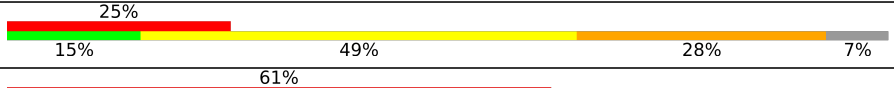
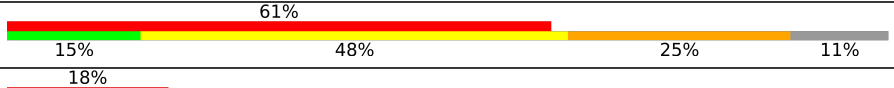
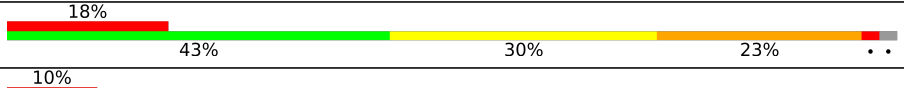
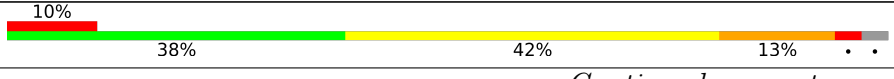
Mol	Chain	Length	Quality of chain
39	DR	146	
40	B1	118	
40	D1	118	
41	B2	101	
41	D2	101	
42	BS	113	
42	DS	113	
43	BT	96	
43	DT	96	
44	BU	110	
44	DU	110	
45	BV	206	
45	DV	206	
46	B3	85	
46	D3	85	
47	BZ	98	
47	DZ	98	
48	BW	72	
48	DW	72	
49	BX	60	
49	DX	60	
50	B4	71	
50	D4	71	
51	B5	60	
51	D5	60	

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Mol	Chain	Length	Quality of chain
52	B6	54	50% 50% 26% 17%
52	D6	54	56% 11% 50% 17% 6% 17%
53	B7	49	4% 63% 29% 6%
53	D7	49	6% 45% 45% 10%
54	B8	65	2% 23% 48% 22% 6%
54	D8	65	6% 31% 38% 22% 6%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	AA	1625	-	-	-	X
55	MG	AA	1662	-	-	-	X
55	MG	AA	1706	-	-	-	X
55	MG	AA	1727	-	-	-	X
55	MG	AA	1735	-	-	-	X
55	MG	AA	1755	-	-	-	X
55	MG	AA	1761	-	-	-	X
55	MG	AA	1772	-	-	-	X
55	MG	AA	1781	-	-	-	X
55	MG	AA	1807	-	-	-	X
55	MG	AA	1836	-	-	-	X
55	MG	BA	3069	-	-	-	X
55	MG	BA	3073	-	-	-	X
55	MG	BA	3121	-	-	-	X
55	MG	BA	3247	-	-	-	X
55	MG	BA	3317	-	-	-	X
55	MG	BA	3324	-	-	-	X
55	MG	BA	3325	-	-	-	X
55	MG	BA	3328	-	-	-	X
55	MG	BA	3334	-	-	-	X
55	MG	BA	3339	-	-	-	X
55	MG	BA	3349	-	-	-	X
55	MG	BA	3379	-	-	-	X
55	MG	BA	3388	-	-	-	X
55	MG	BA	3399	-	-	-	X
55	MG	BA	3408	-	-	-	X
55	MG	BA	3418	-	-	-	X

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

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

2 Entry composition (i)

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There are 4 discrepancies between the modelled and reference sequences:

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

- Molecule 24 is a RNA chain called MRNA.

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

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

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

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BA	161	U	-	EXPRESSION TAG	GB AP008226.1
BA	654A	A	G	CONFLICT	GB AP008226.1
BA	654E	C	G	CONFLICT	GB AP008226.1
BA	654P	G	C	CONFLICT	GB AP008226.1
BA	654T	A	C	CONFLICT	GB AP008226.1
BA	1058	U	G	CONFLICT	GB AP008226.1
BA	1080	A	C	CONFLICT	GB AP008226.1
DA	168	U	-	INSERTION	GB AP008226.1
DA	654A	A	G	CONFLICT	GB AP008226.1
DA	654E	C	G	CONFLICT	GB AP008226.1
DA	654P	G	C	CONFLICT	GB AP008226.1
DA	654T	A	C	CONFLICT	GB AP008226.1
DA	1058	U	G	CONFLICT	GB AP008226.1
DA	1080	A	C	CONFLICT	GB AP008226.1

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
55	AA	242	Total Mg 242 242	0	0
55	AG	1	Total Mg 1 1	0	0
55	AH	1	Total Mg 1 1	0	0
55	AN	2	Total Mg 2 2	0	0
55	AQ	1	Total Mg 1 1	0	0
55	AB	5	Total Mg 5 5	0	0
55	AC	9	Total Mg 9 9	0	0
55	AD	1	Total Mg 1 1	0	0
55	A1	2	Total Mg 2 2	0	0
55	BA	623	Total Mg 623 623	0	0
55	BB	17	Total Mg 17 17	0	0
55	BD	1	Total Mg 1 1	0	0
55	BE	5	Total Mg 5 5	0	0
55	BF	3	Total Mg 3 3	0	0
55	BO	2	Total Mg 2 2	0	0
55	B0	1	Total Mg 1 1	0	0
55	B1	1	Total Mg 1 1	0	0
55	B2	1	Total Mg 1 1	0	0
55	BU	2	Total Mg 2 2	0	0
55	B3	1	Total Mg 1 1	0	0
55	B5	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
55	B7	1	Total Mg 1 1	0	0
55	B8	1	Total Mg 1 1	0	0
55	CA	207	Total Mg 207 207	0	0
55	CG	2	Total Mg 2 2	0	0
55	CN	1	Total Mg 1 1	0	0
55	CS	1	Total Mg 1 1	0	0
55	CB	3	Total Mg 3 3	0	0
55	CC	8	Total Mg 8 8	0	0
55	DA	526	Total Mg 526 526	0	0
55	DB	14	Total Mg 14 14	0	0
55	DE	3	Total Mg 3 3	0	0
55	DP	1	Total Mg 1 1	0	0
55	DR	1	Total Mg 1 1	0	0
55	D1	2	Total Mg 2 2	0	0
55	DU	1	Total Mg 1 1	0	0
55	D3	1	Total Mg 1 1	0	0
55	D5	1	Total Mg 1 1	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

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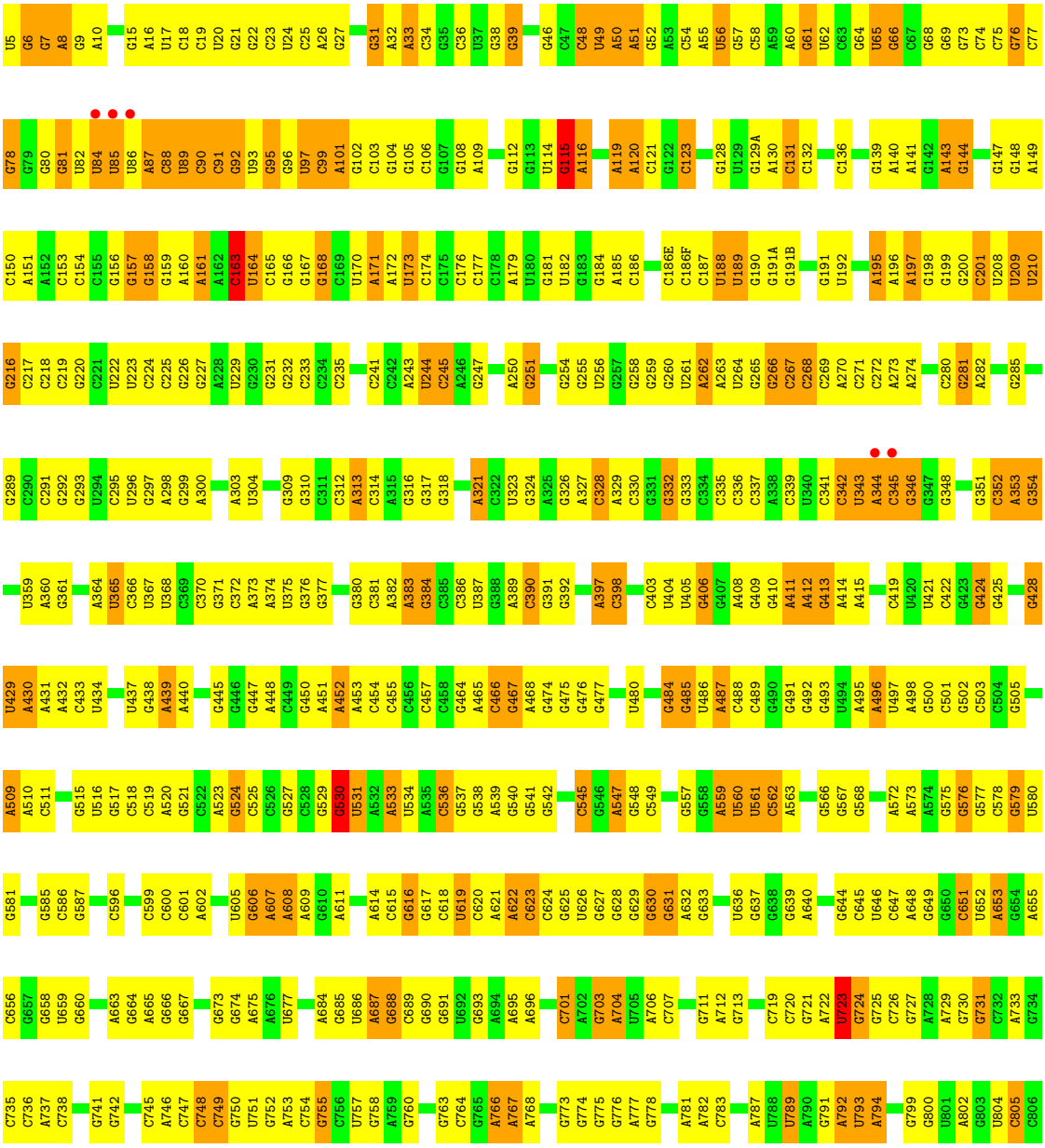
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	CG	1	Total Zn 1 1	0	0
56	CQ	1	Total Zn 1 1	0	0

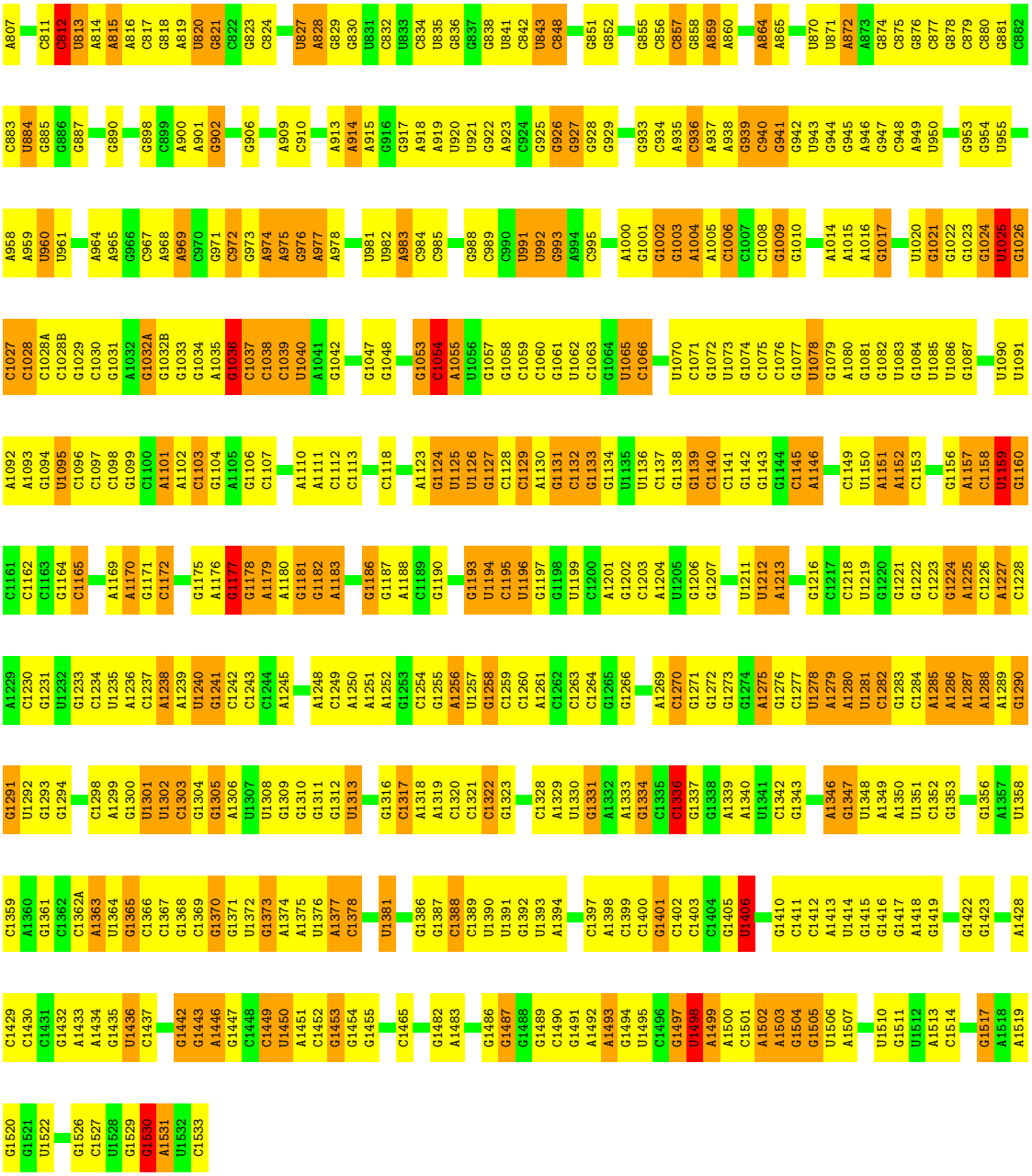
3 Residue-property plots (i)

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

- Molecule 1: 16S ribosomal RNA

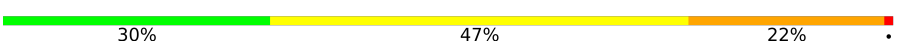
Chain AA: 32% 48% 19%

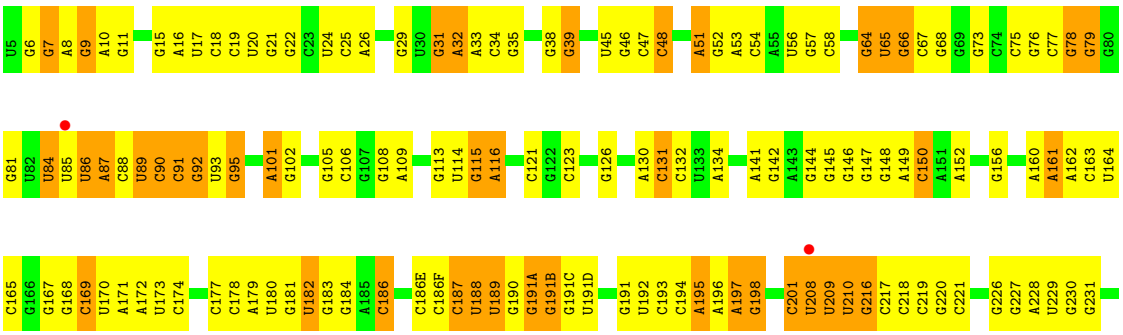


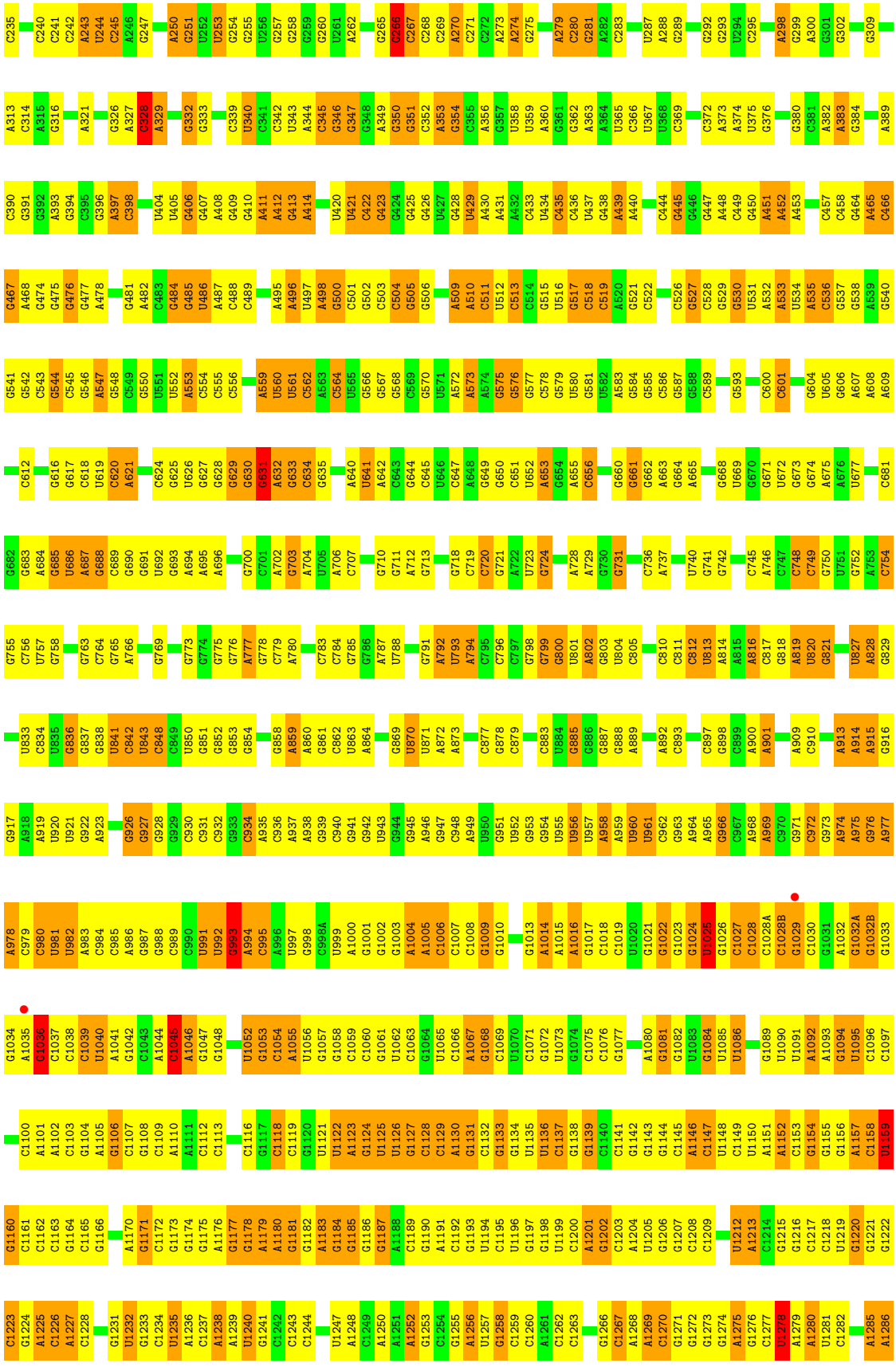


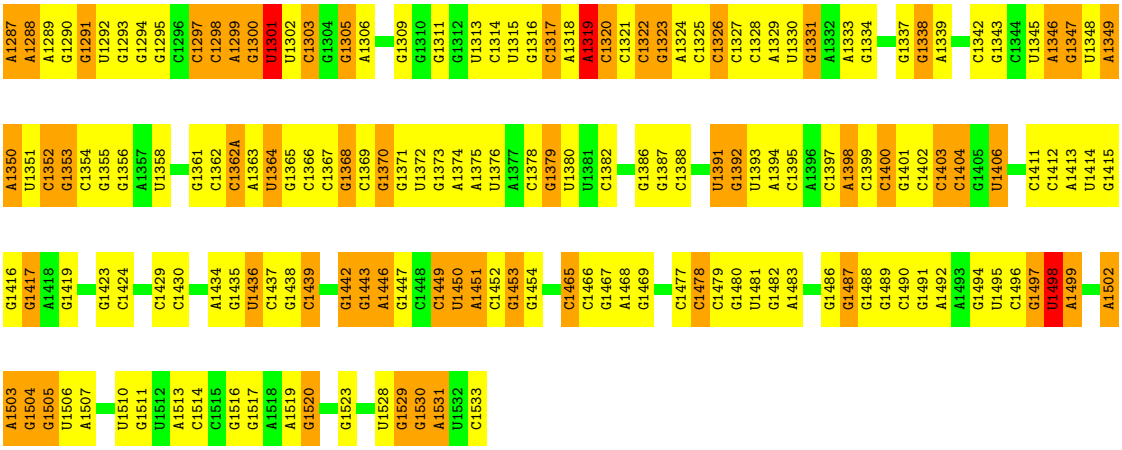
• Molecule 1: 16S ribosomal RNA

Chain CA:



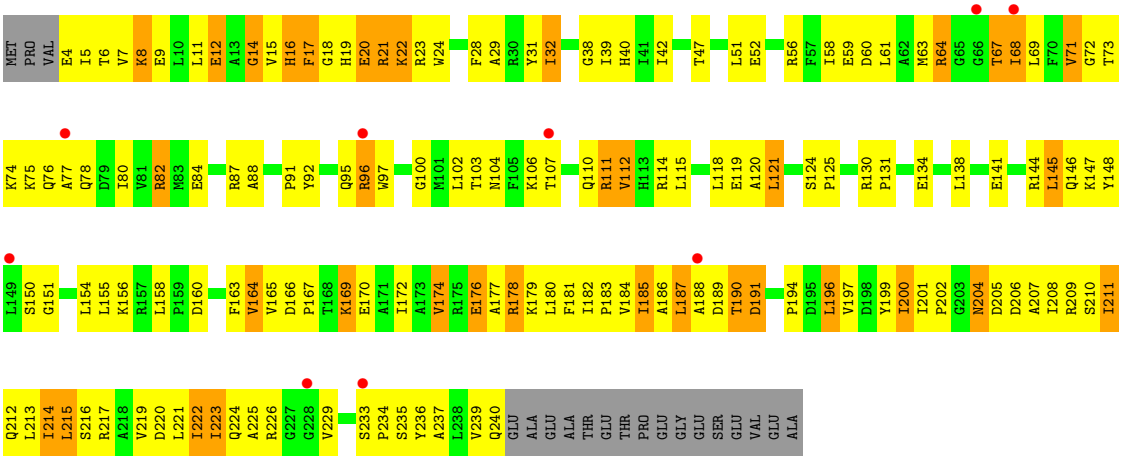






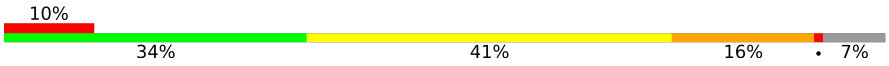
• Molecule 2: 30S RIBOSOMAL PROTEIN S2

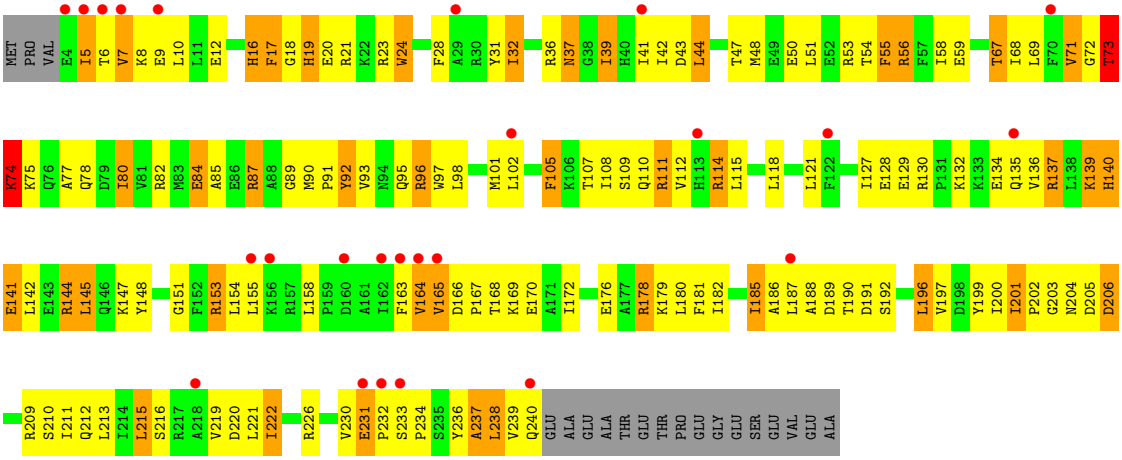
Chain AE:



• Molecule 2: 30S RIBOSOMAL PROTEIN S2

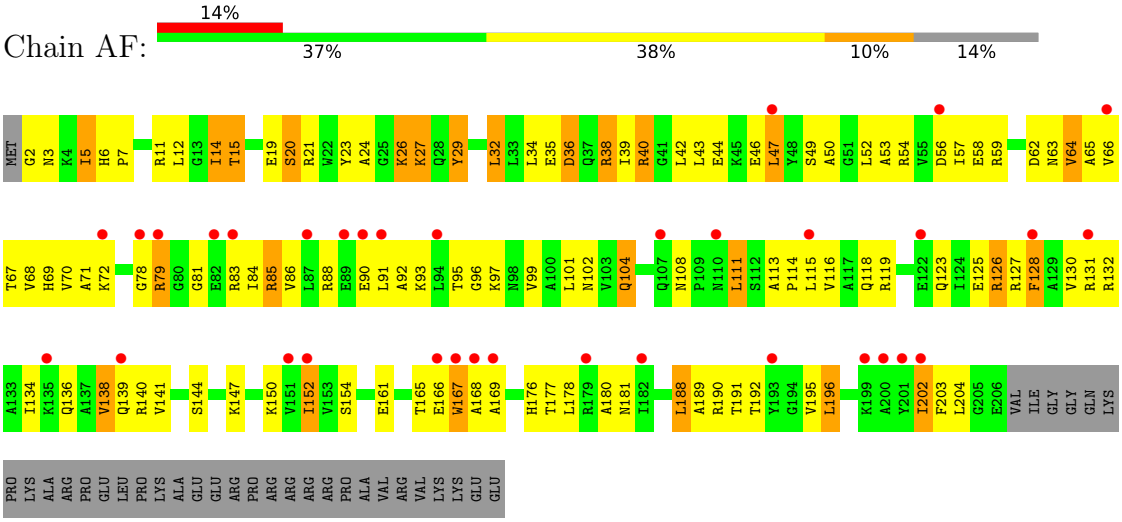
Chain CE:





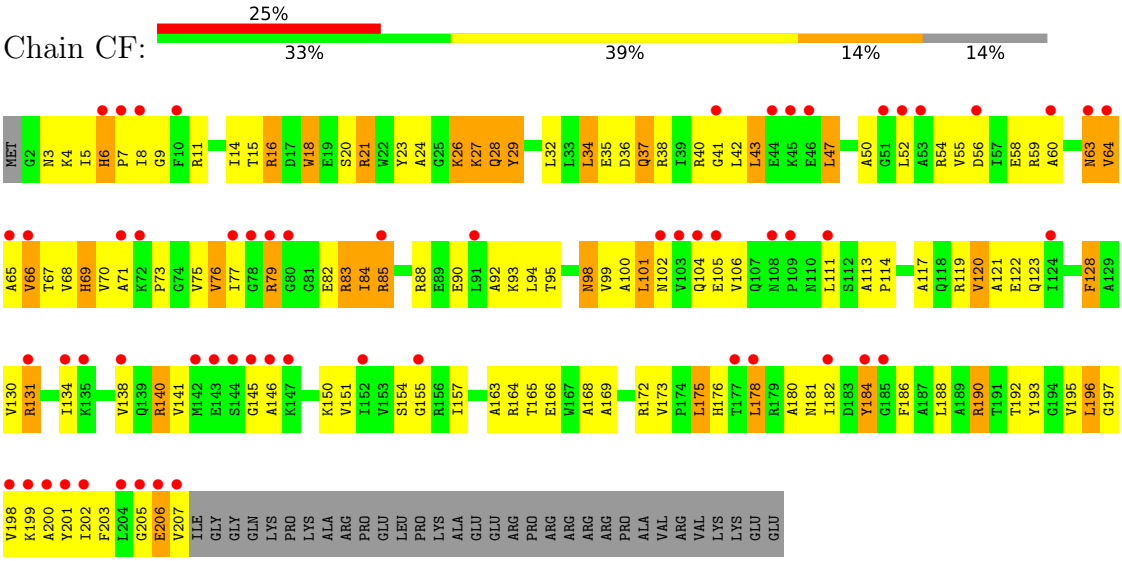
• Molecule 3: 30S RIBOSOMAL PROTEIN S3

Chain AF:



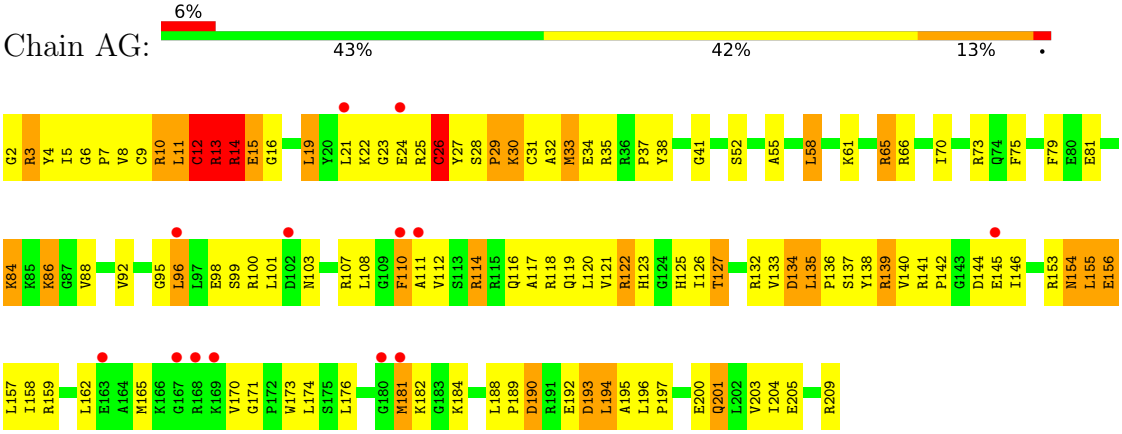
• Molecule 3: 30S RIBOSOMAL PROTEIN S3

Chain CF:



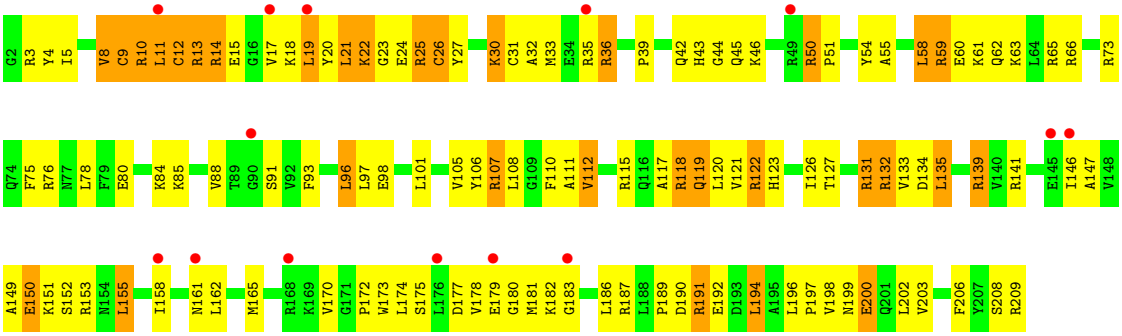
• Molecule 4: 30S RIBOSOMAL PROTEIN S4

Chain AG:



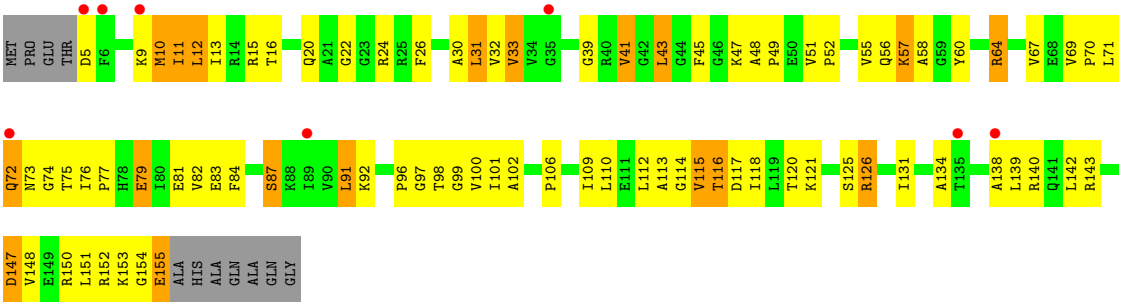
• Molecule 4: 30S RIBOSOMAL PROTEIN S4

Chain CG:



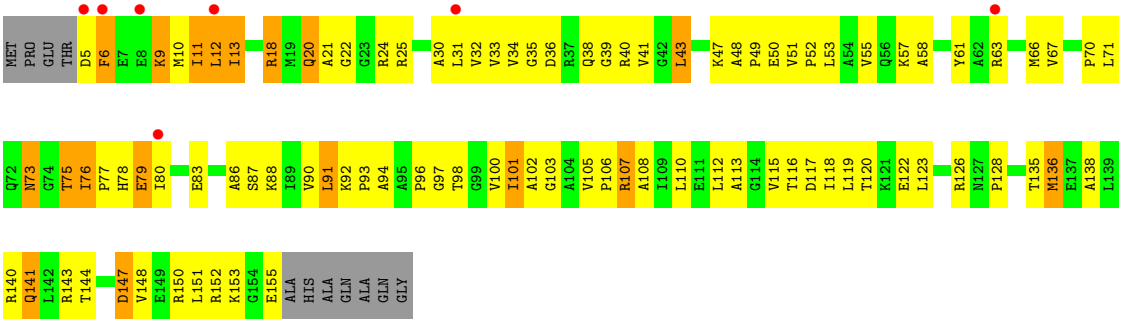
• Molecule 5: 30S RIBOSOMAL PROTEIN S5

Chain AH:



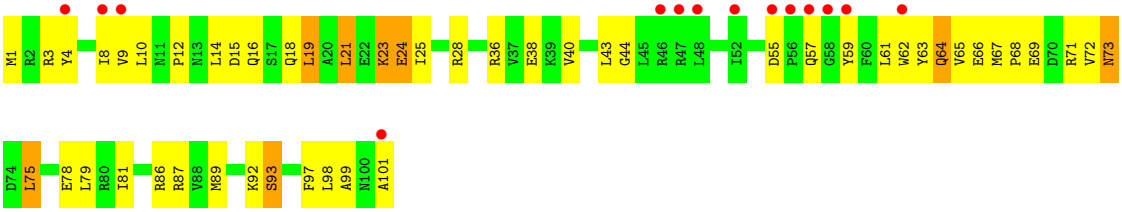
• Molecule 5: 30S RIBOSOMAL PROTEIN S5

Chain CH:



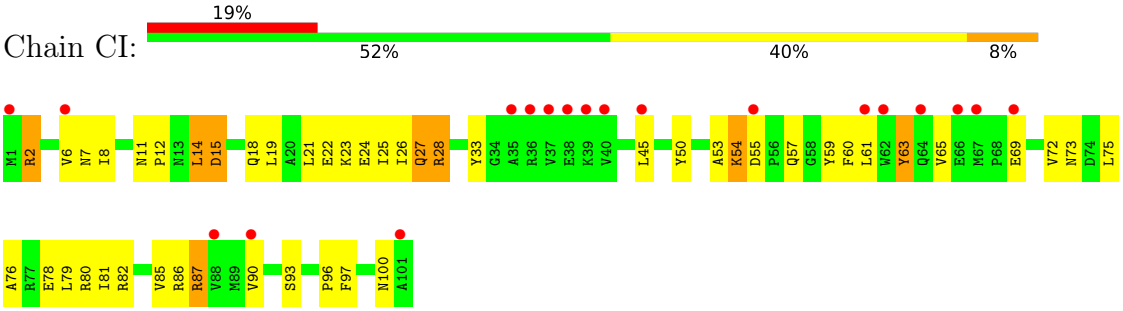
• Molecule 6: 30S RIBOSOMAL PROTEIN S6

Chain AI:



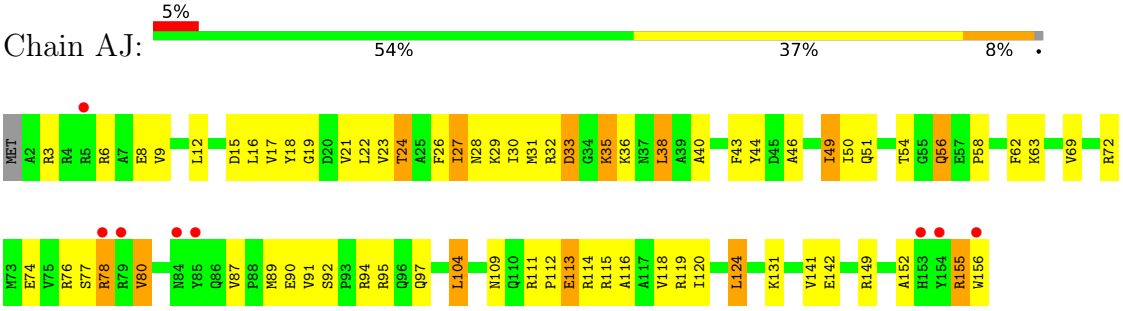
• Molecule 6: 30S RIBOSOMAL PROTEIN S6

Chain CI:



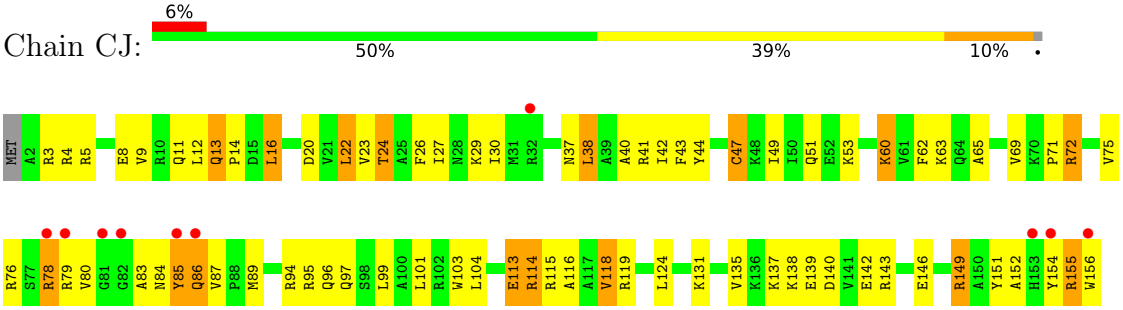
• Molecule 7: 30S RIBOSOMAL PROTEIN S7

Chain AJ:



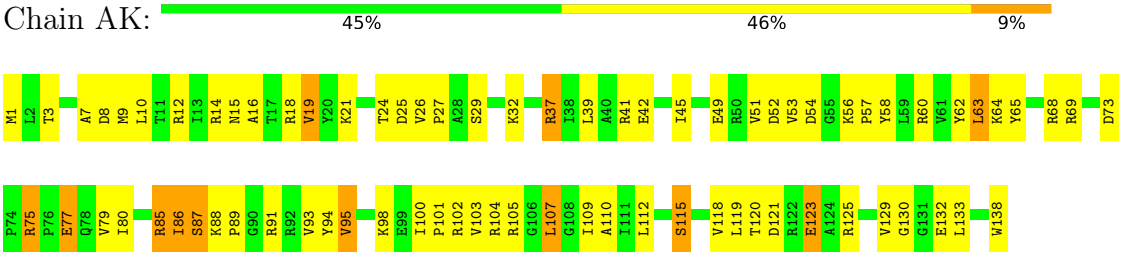
• Molecule 7: 30S RIBOSOMAL PROTEIN S7

Chain CJ:



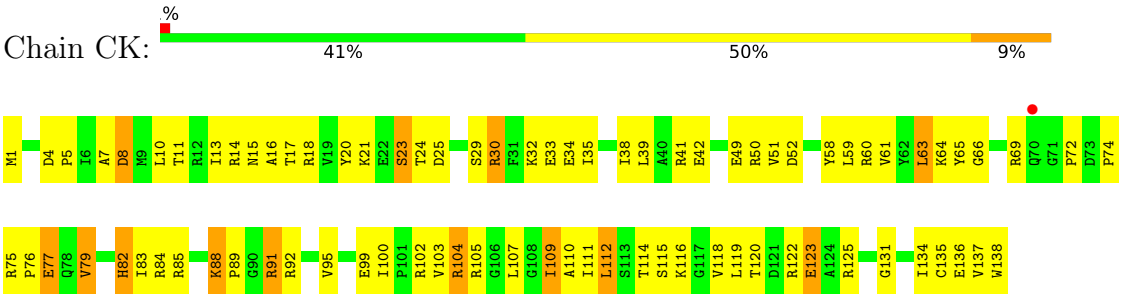
• Molecule 8: 30S RIBOSOMAL PROTEIN S8

Chain AK:



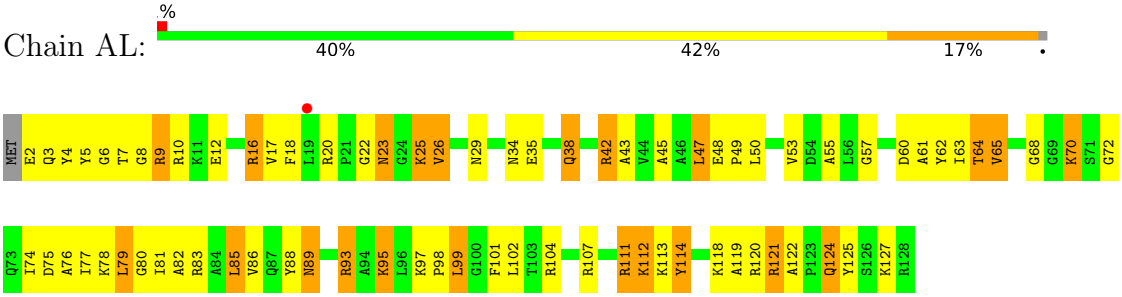
• Molecule 8: 30S RIBOSOMAL PROTEIN S8

Chain CK:



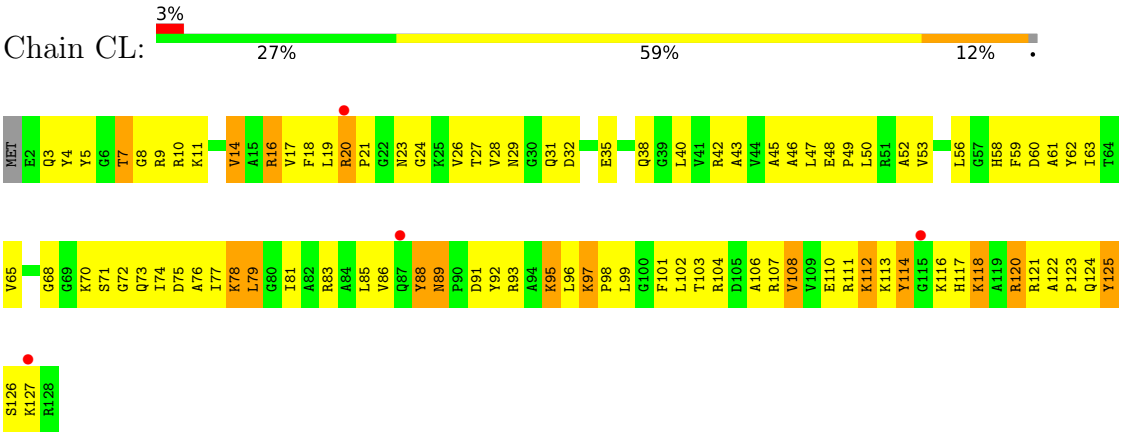
• Molecule 9: 30S RIBOSOMAL PROTEIN S9

Chain AL:



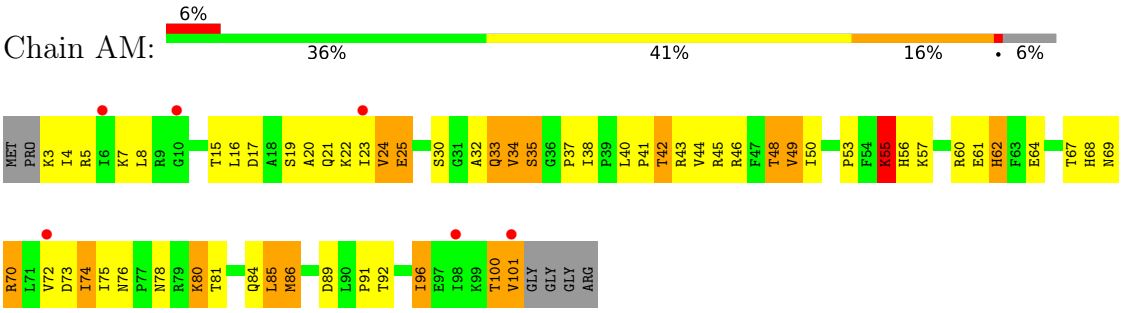
• Molecule 9: 30S RIBOSOMAL PROTEIN S9

Chain CL:



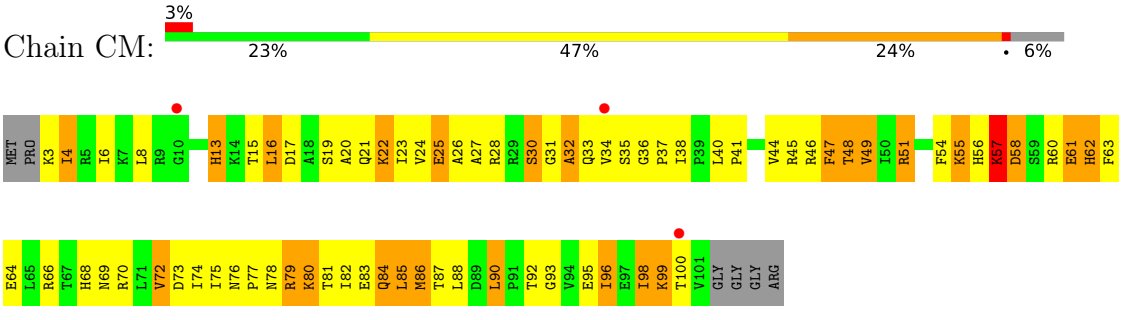
• Molecule 10: 30S RIBOSOMAL PROTEIN S10

Chain AM:



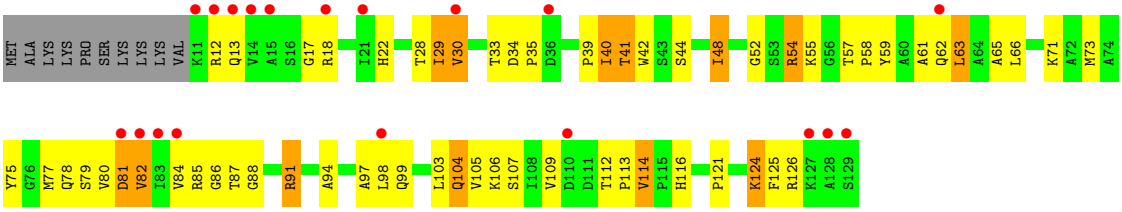
• Molecule 10: 30S RIBOSOMAL PROTEIN S10

Chain CM:



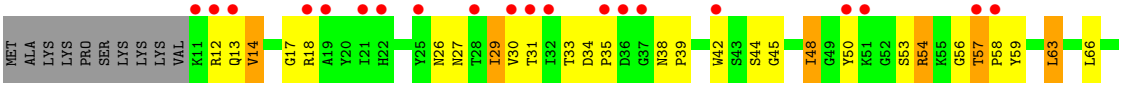
• Molecule 11: 30S RIBOSOMAL PROTEIN S11

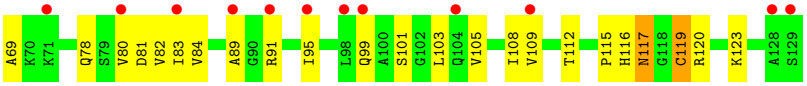
Chain AN:



• Molecule 11: 30S RIBOSOMAL PROTEIN S11

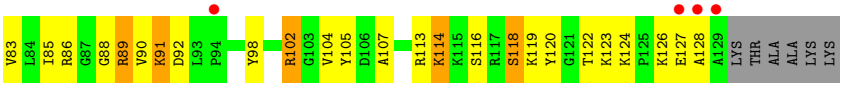
Chain CN:





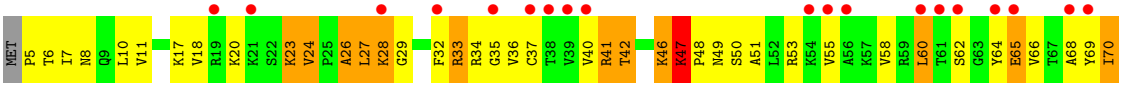
• Molecule 12: 30S RIBOSOMAL PROTEIN S12

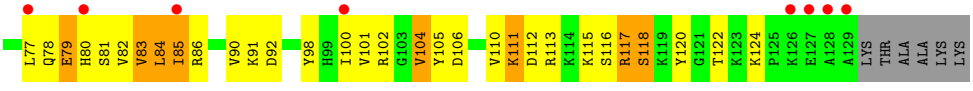
Chain AO:



• Molecule 12: 30S RIBOSOMAL PROTEIN S12

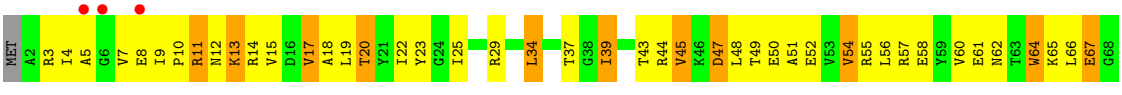
Chain CO:

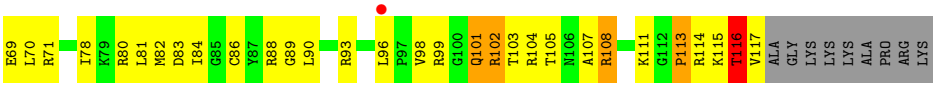




• Molecule 13: 30S RIBOSOMAL PROTEIN S13

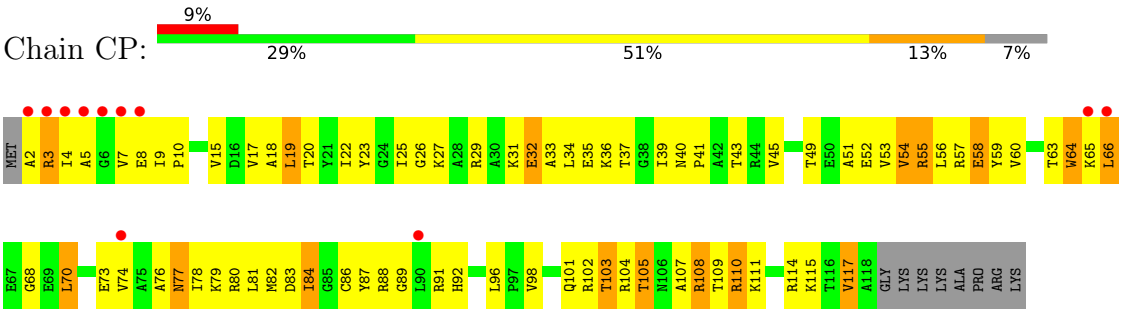
Chain AP:





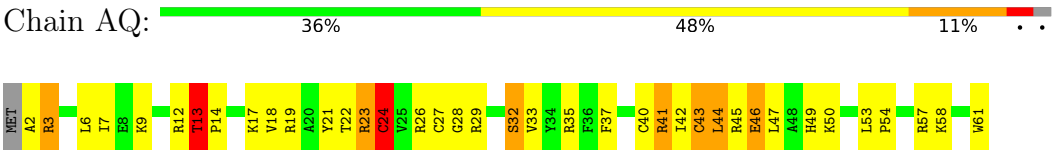
• Molecule 13: 30S RIBOSOMAL PROTEIN S13

Chain CP:



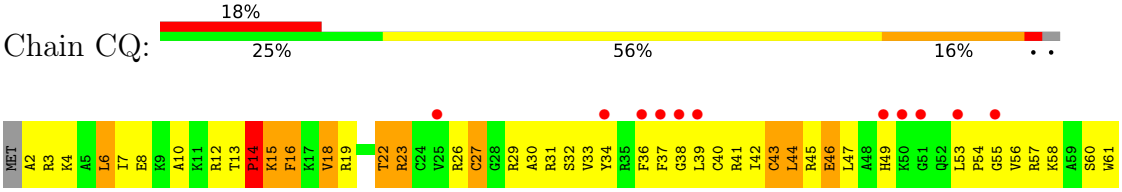
• Molecule 14: 30S RIBOSOMAL PROTEIN S14

Chain AQ:



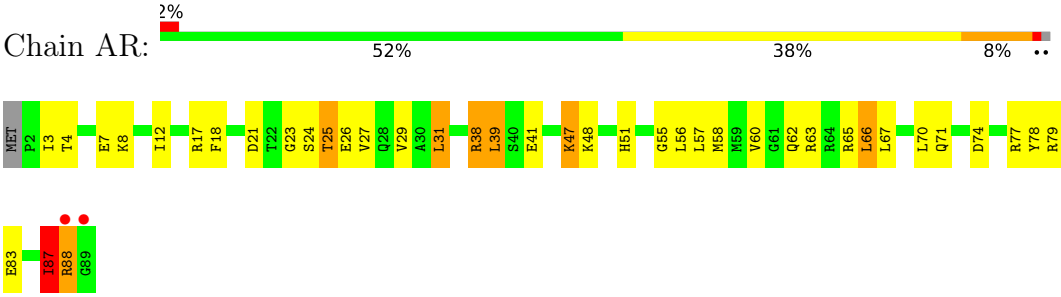
• Molecule 14: 30S RIBOSOMAL PROTEIN S14

Chain CQ:



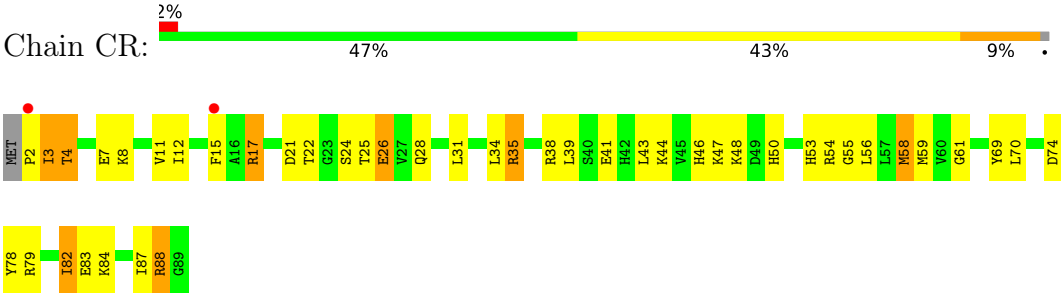
• Molecule 15: 30S RIBOSOMAL PROTEIN S15

Chain AR:



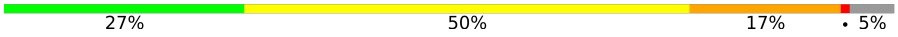
• Molecule 15: 30S RIBOSOMAL PROTEIN S15

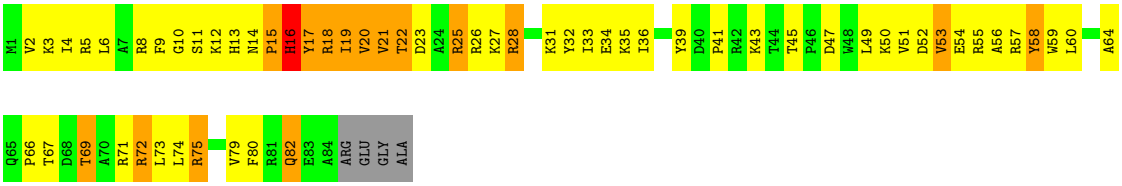
Chain CR:



• Molecule 16: 30S RIBOSOMAL PROTEIN S16

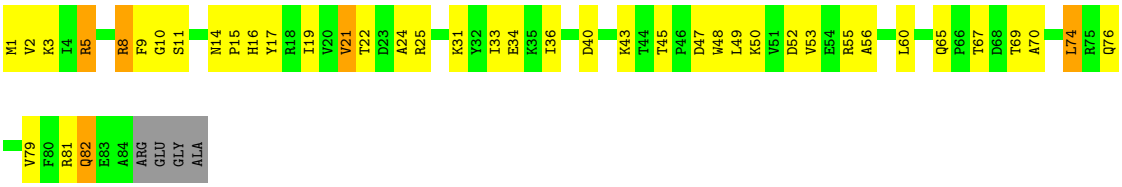
Chain AS:





• Molecule 16: 30S RIBOSOMAL PROTEIN S16

Chain CS:

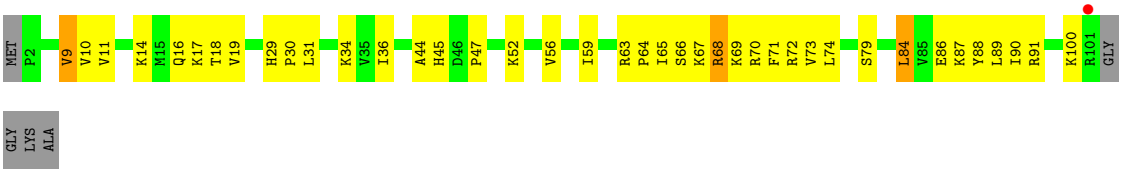


• Molecule 17: 30S RIBOSOMAL PROTEIN S17

Chain AT:

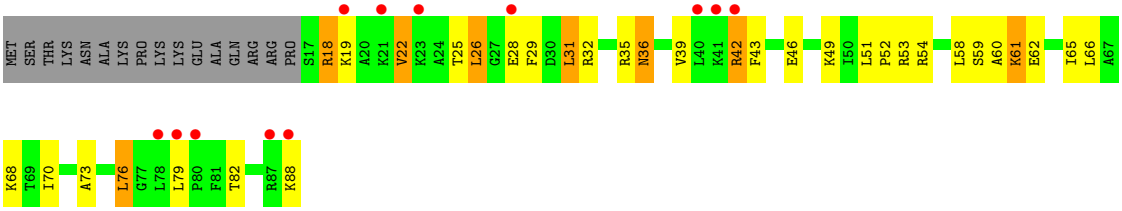
• Molecule 17: 30S RIBOSOMAL PROTEIN S17

Chain CT:



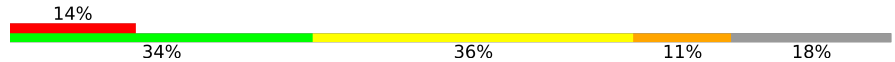
• Molecule 18: 30S RIBOSOMAL PROTEIN S18

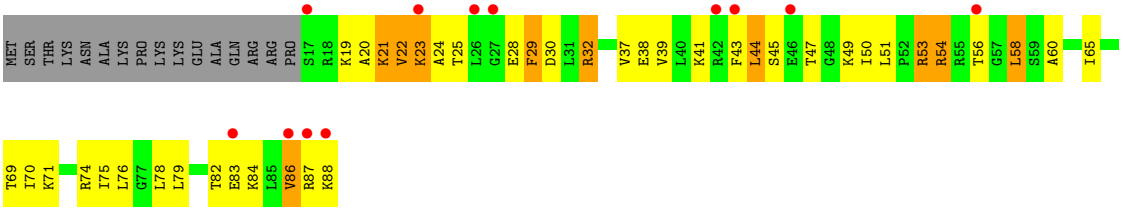
Chain AU:



• Molecule 18: 30S RIBOSOMAL PROTEIN S18

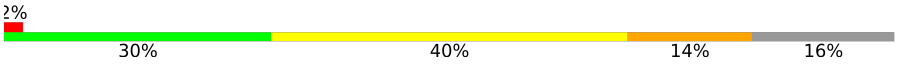
Chain CU:

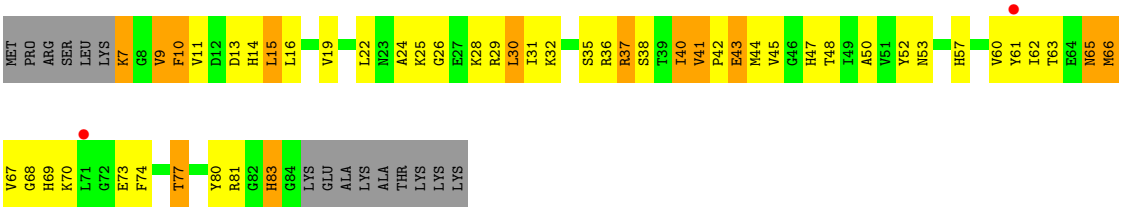




• Molecule 19: 30S RIBOSOMAL PROTEIN S19

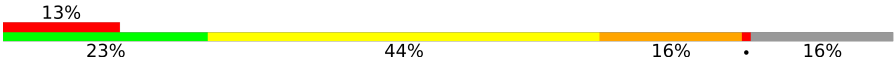
Chain AV:

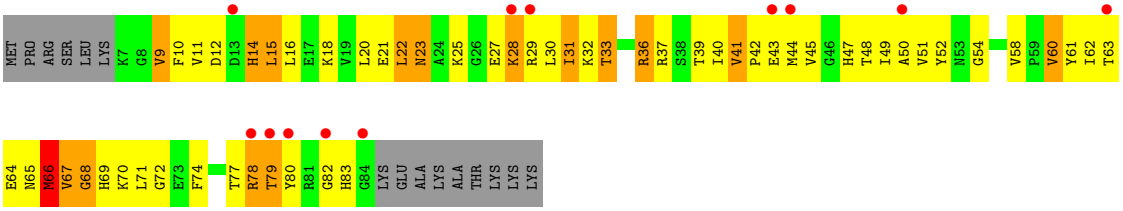




• Molecule 19: 30S RIBOSOMAL PROTEIN S19

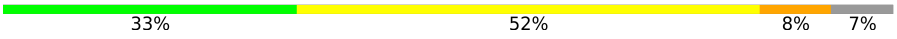
Chain CV:

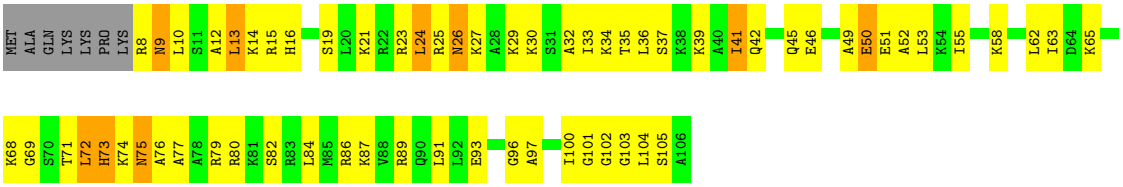




• Molecule 20: 30S RIBOSOMAL PROTEIN S20

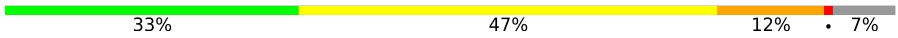
Chain AW:

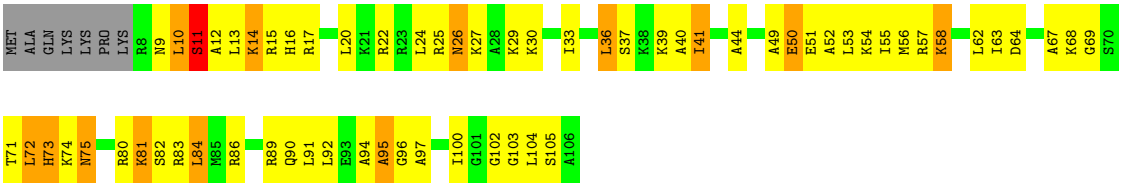




• Molecule 20: 30S RIBOSOMAL PROTEIN S20

Chain CW:



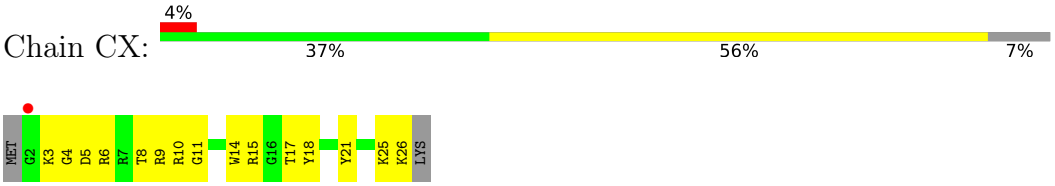


• Molecule 21: 30S RIBOSOMAL PROTEIN THX

Chain AX:

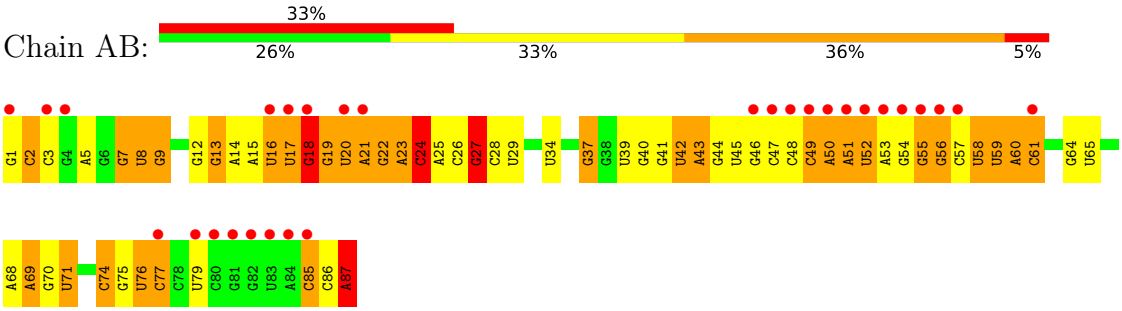
• Molecule 21: 30S RIBOSOMAL PROTEIN THX

Chain CX:



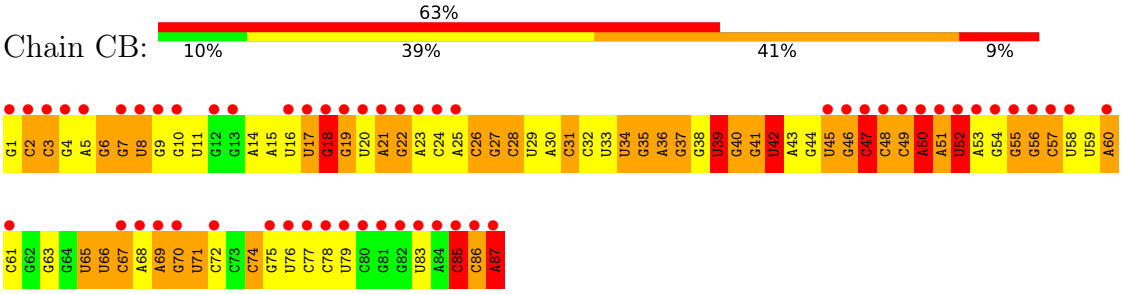
• Molecule 22: TRNA-LEU

Chain AB:



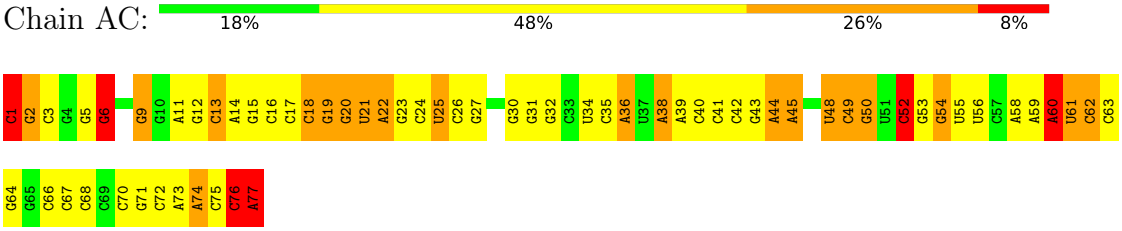
• Molecule 22: TRNA-LEU

Chain CB:



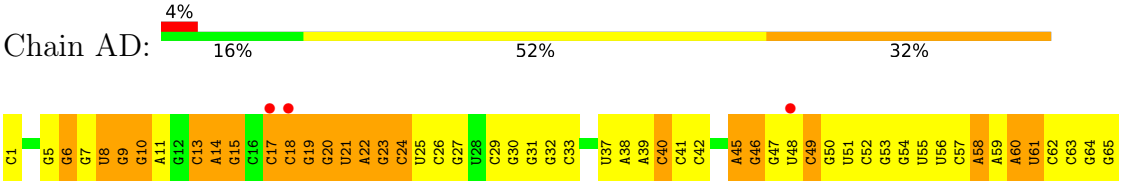
• Molecule 23: TRNA-FMET

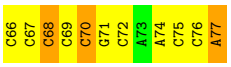
Chain AC:



• Molecule 23: TRNA-FMET

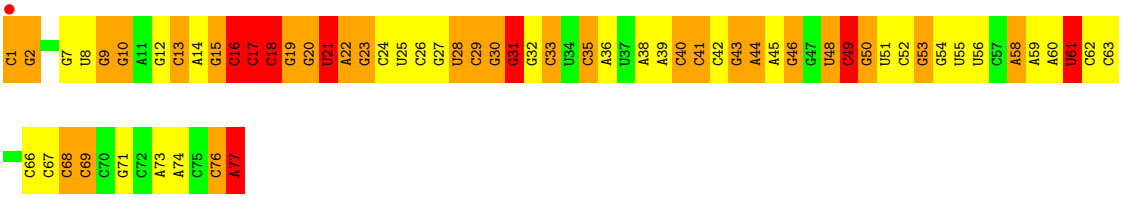
Chain AD:





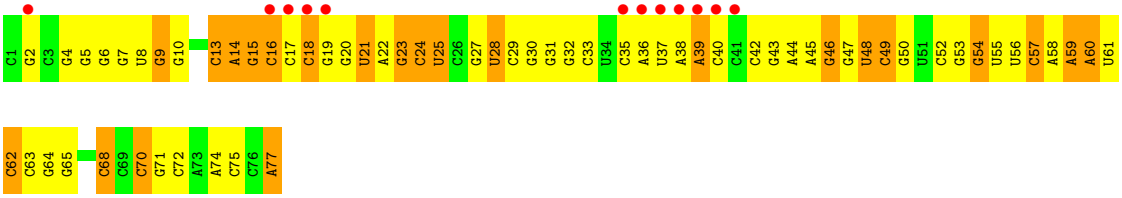
• Molecule 23: TRNA-FMET

Chain CC:



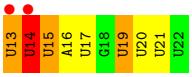
• Molecule 23: TRNA-FMET

Chain CD:



• Molecule 24: MRNA

Chain A1:

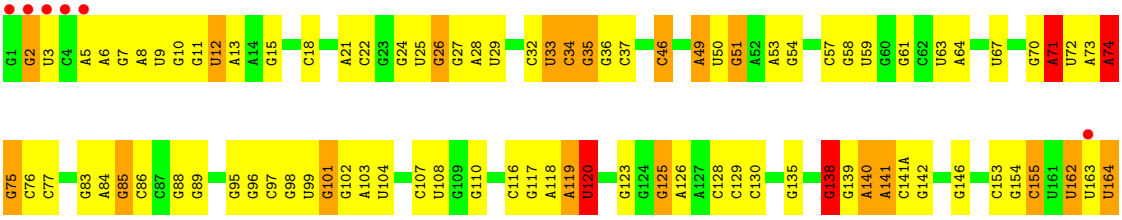


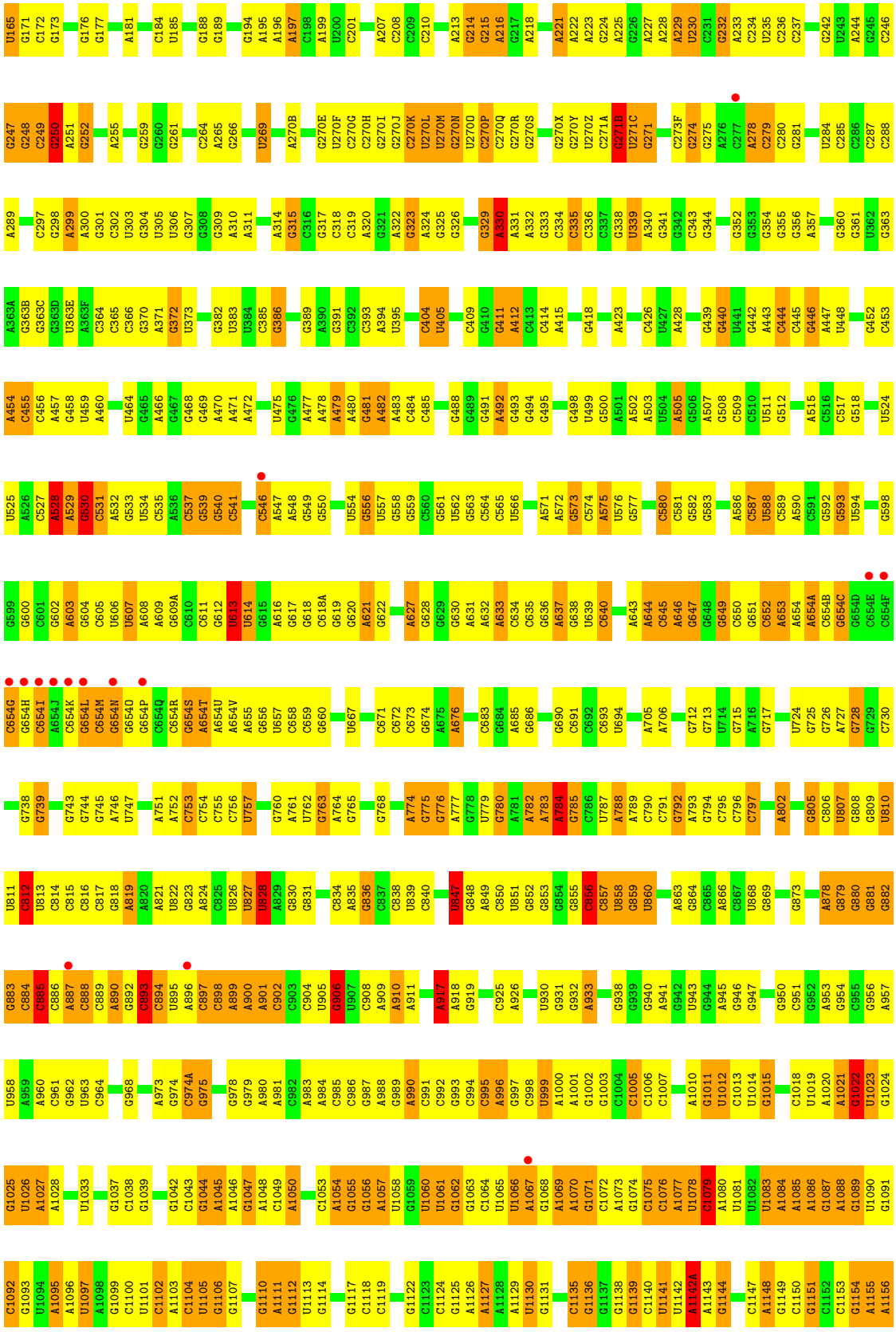
• Molecule 24: MRNA

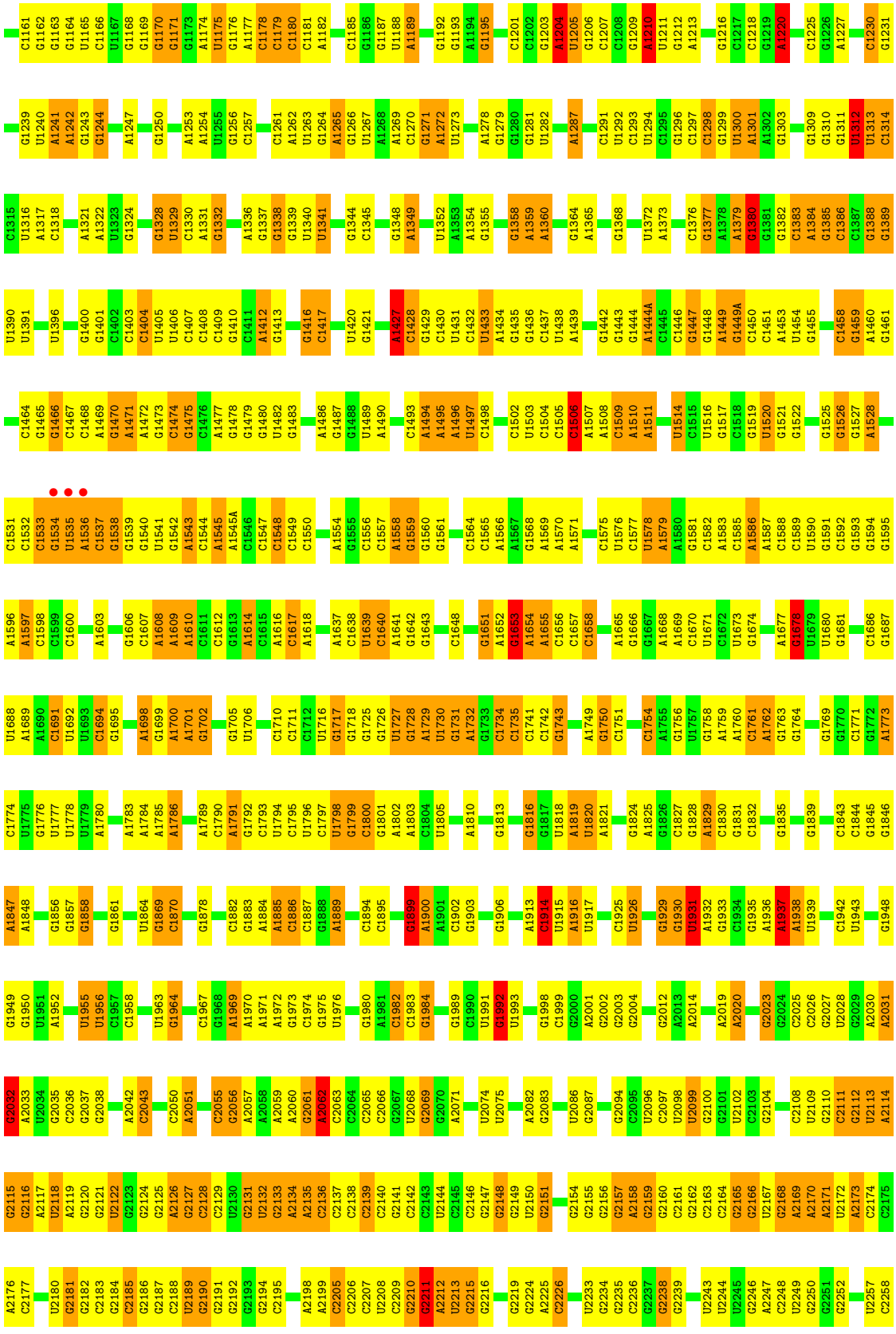
Chain C1:

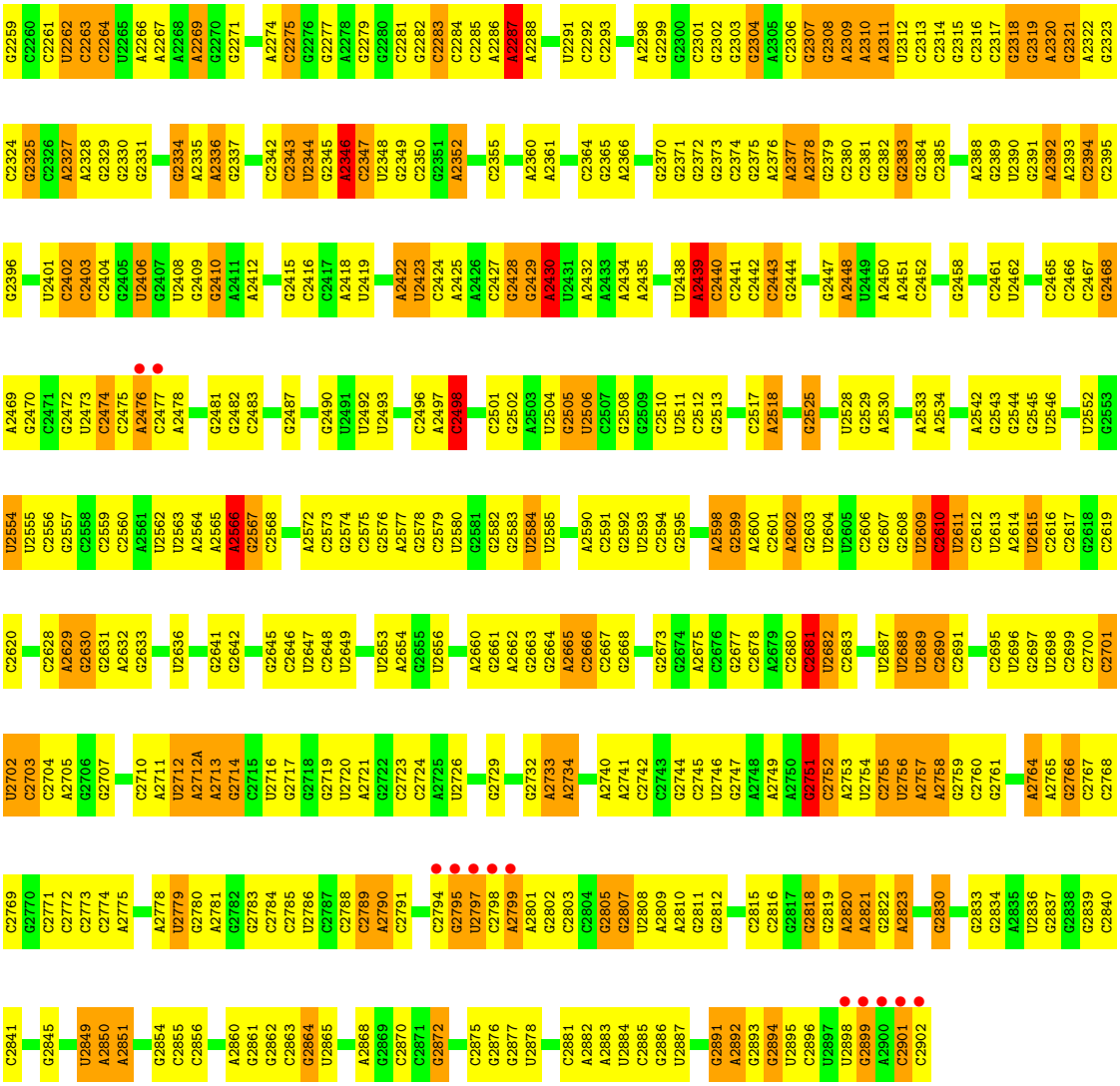
• Molecule 25: RNA (2912-MER)

Chain BA:

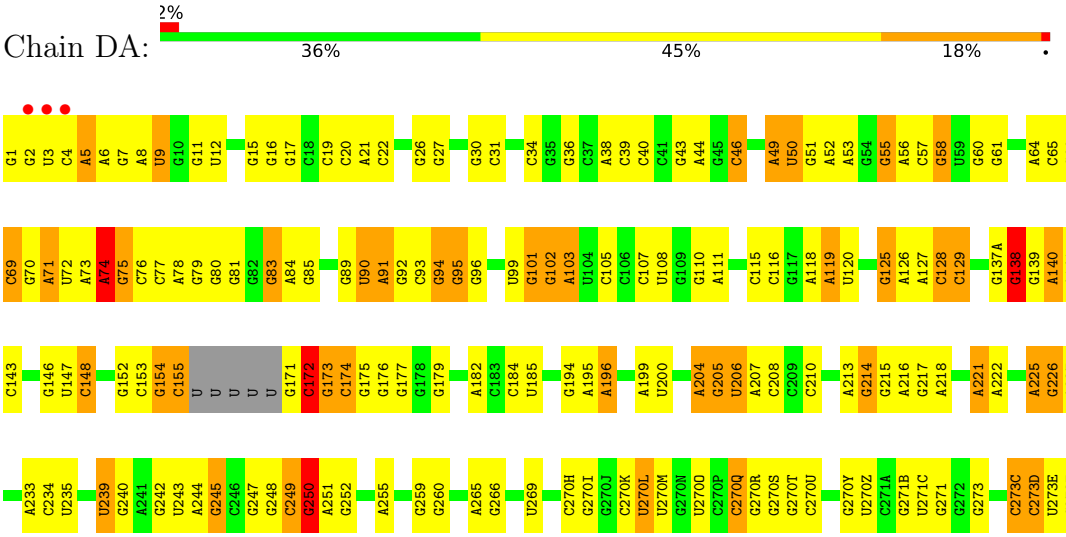


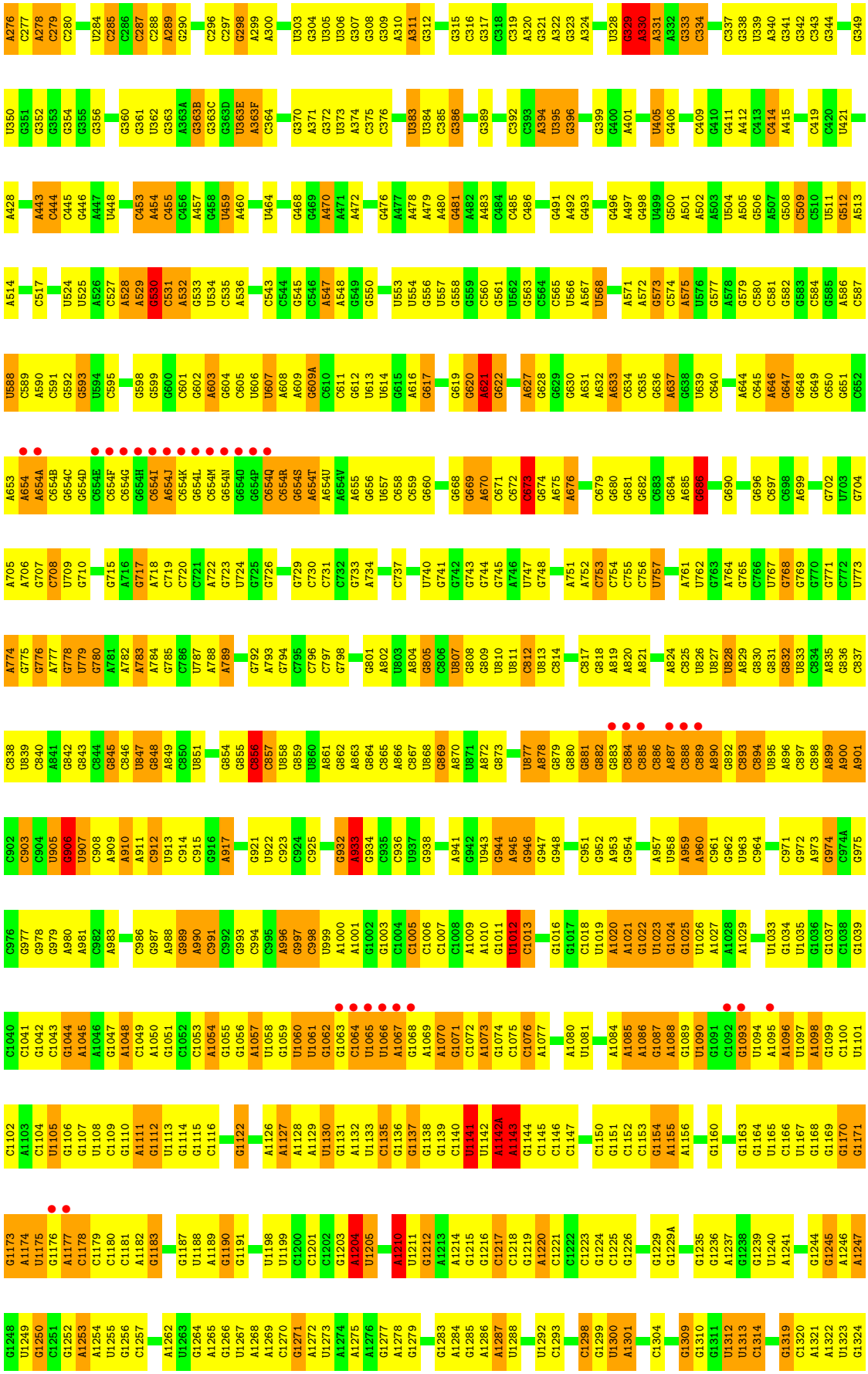


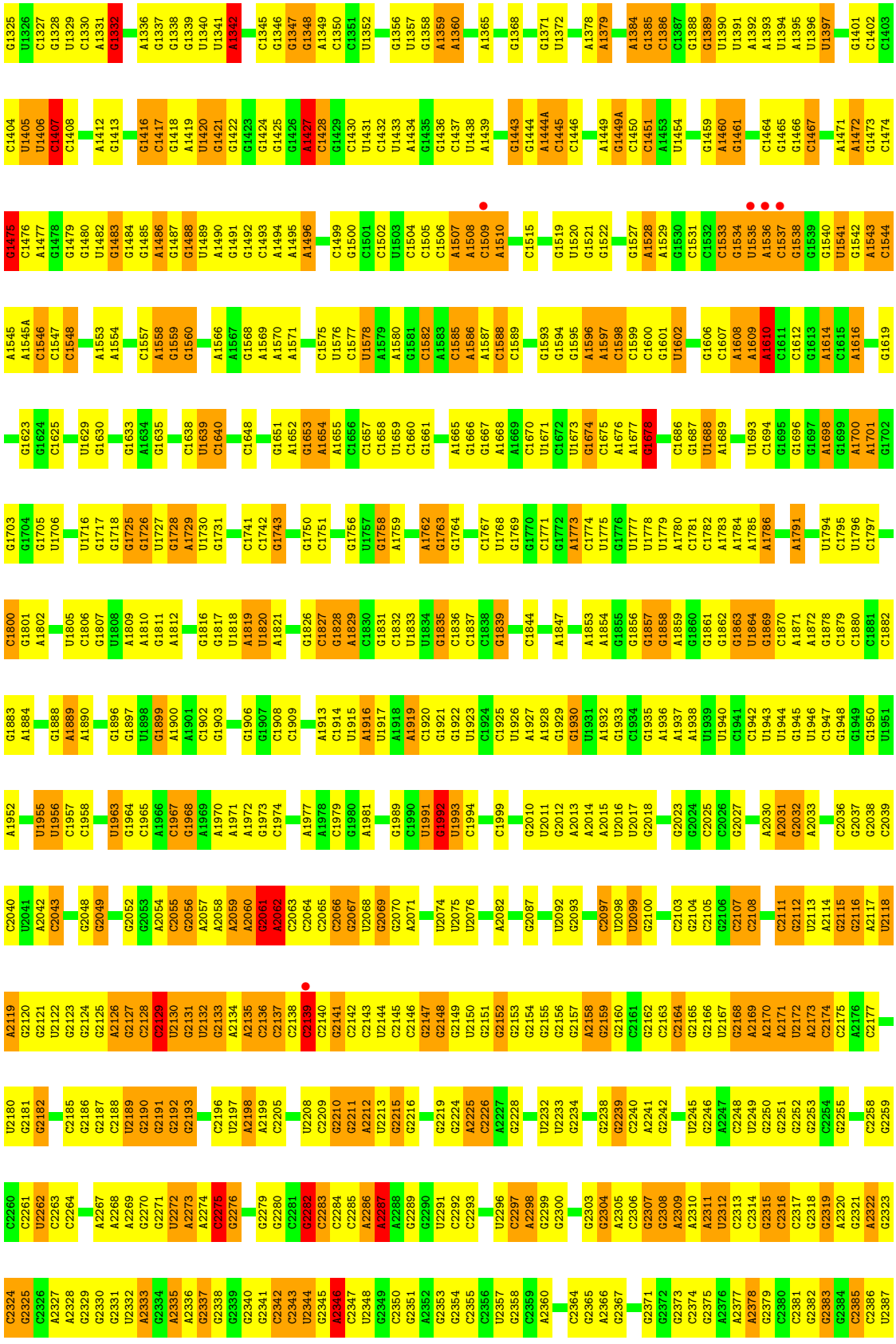




• Molecule 25: RNA (2912-MER)



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C1404 U1405 U1406 C1407 C1408 A1412 G1413 G1416 C1417 G1418 A1419 U1420 G1421 G1422 G1423 G1424 G1425 G1426 A1427 C1428 G1429 C1430 U1431 C1432 U1433 A1434 G1435 G1436 C1437 U1438 A1439 G1443 G1444 A1444A C1445 C1446 A1449 G1449A C1450 C1451 A1453 U1454 G1459 A1460 G1461 C1464 G1465 G1466 C1467 A1471 A1472 G1473 C1474
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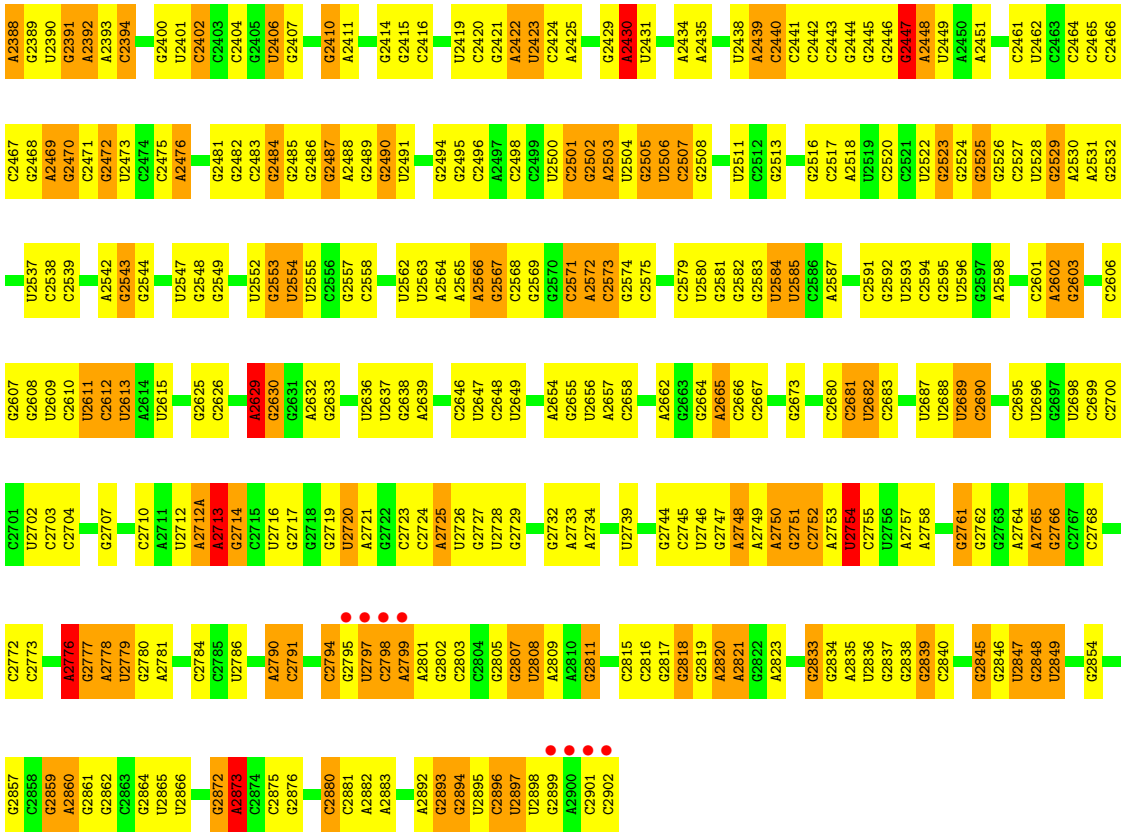
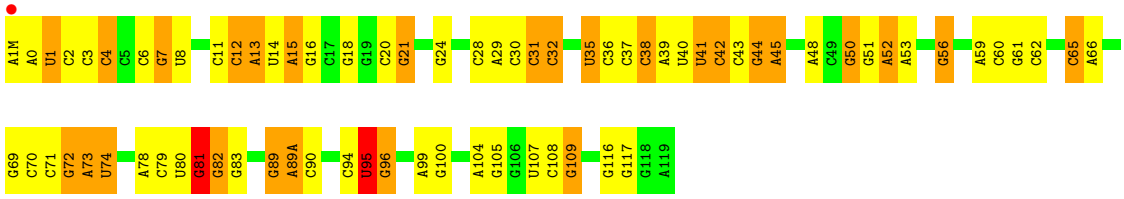
C2324 G2325 C2326 A2327 A2328 G2329 G2330 G2331 U2332 A2333 G2334 A2335 A2336 G2337 G2338 G2339 G2340 G2341 C2342 C2343 U2344 G2345 A2346 C2347 U2348 G2349 C2350 G2351 A2352 G2353 G2354 C2355 C2356 U2357 G2358 C2359 A2360 C2364 G2365 A2366 G2367 G2371 G2372 G2373 C2374 G2375 A2376 A2377 A2378 G2379 C2380 C2381 G2382 G2383 G2384 C2385 C2386 U2387



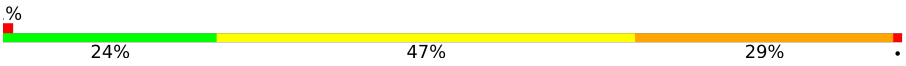
• Molecule 26: 5S RIBOSOMAL RNA

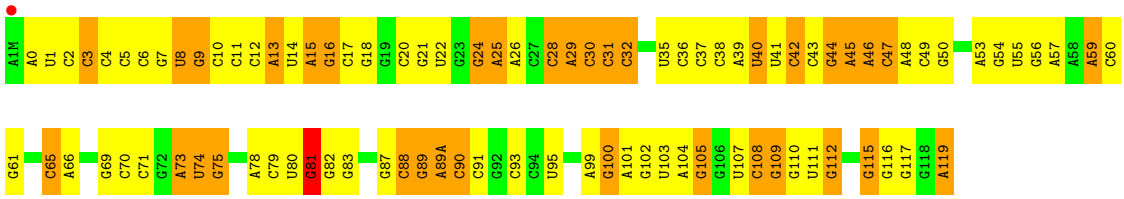
Chain BB:



• Molecule 26: 5S RIBOSOMAL RNA

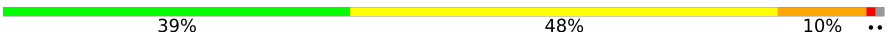
Chain DB:

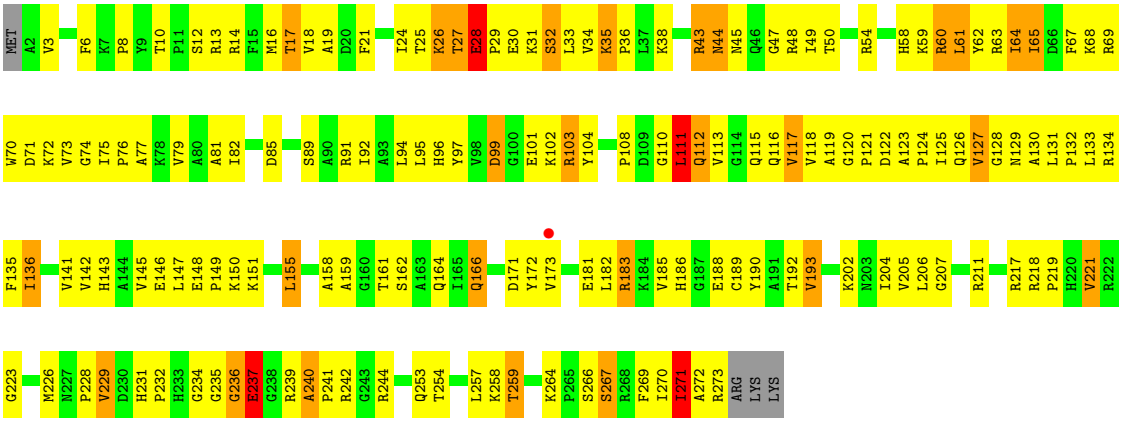




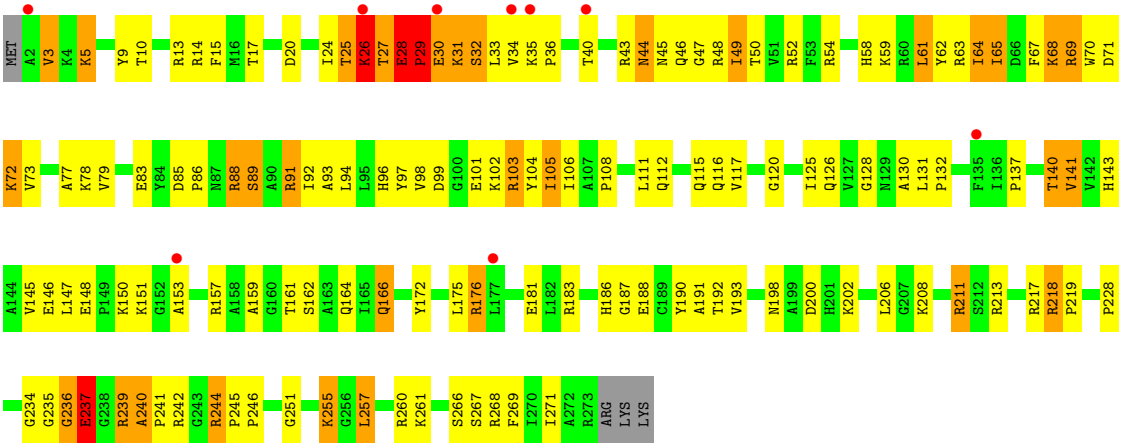
• Molecule 27: 50S ribosomal protein L2

Chain BD:

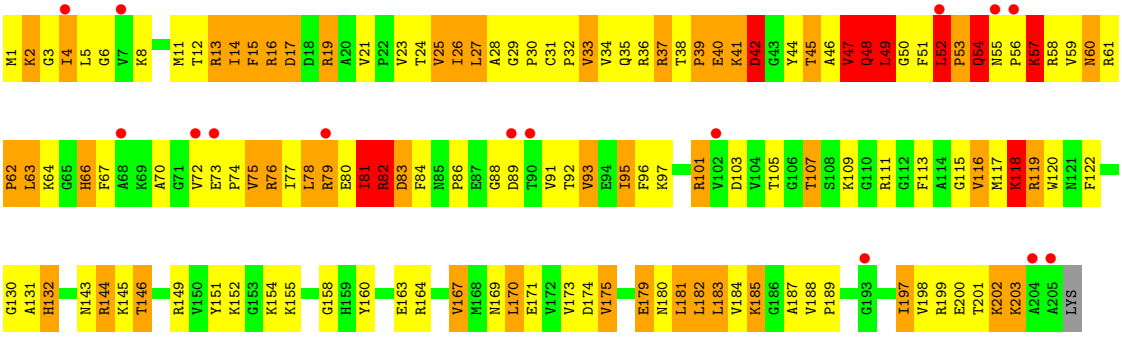




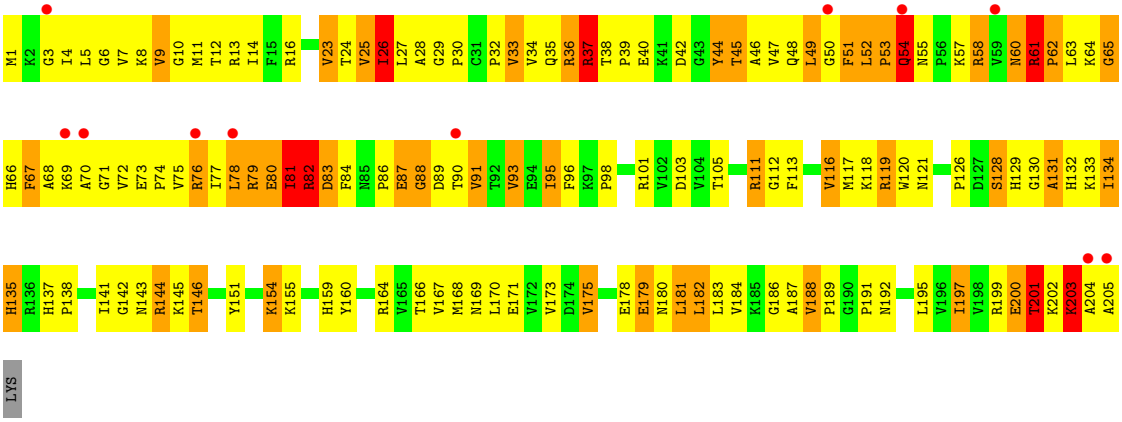
• Molecule 27: 50S ribosomal protein L2



• Molecule 28: 50S ribosomal protein L3

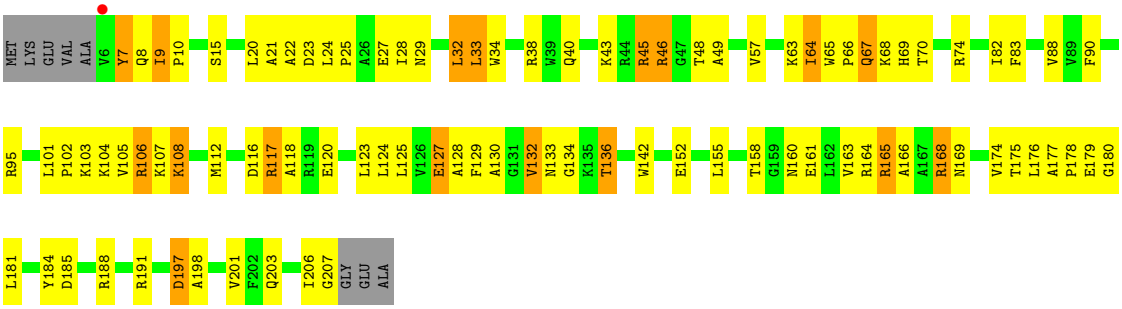


• Molecule 28: 50S ribosomal protein L3



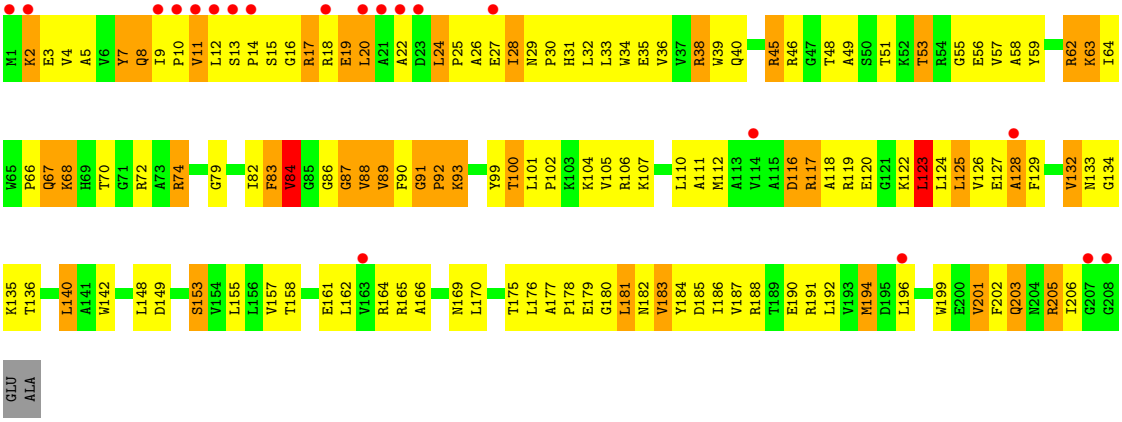
• Molecule 29: 50S ribosomal protein L4

Chain BF:



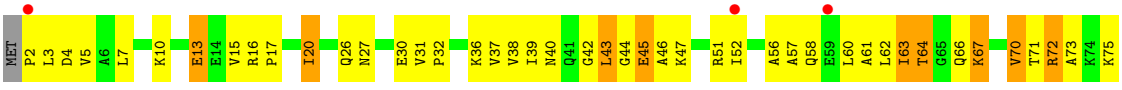
• Molecule 29: 50S ribosomal protein L4

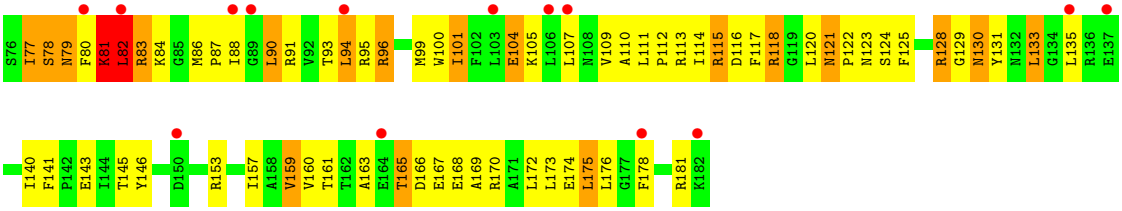
Chain DF:



• Molecule 30: 50S ribosomal protein L5

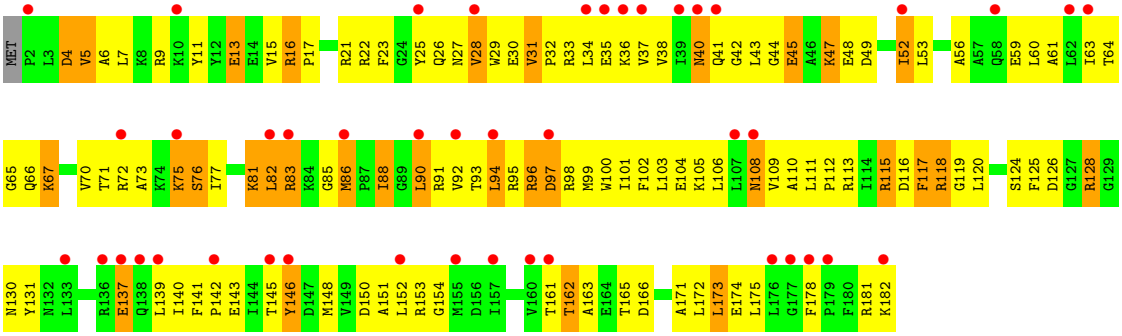
Chain BG:





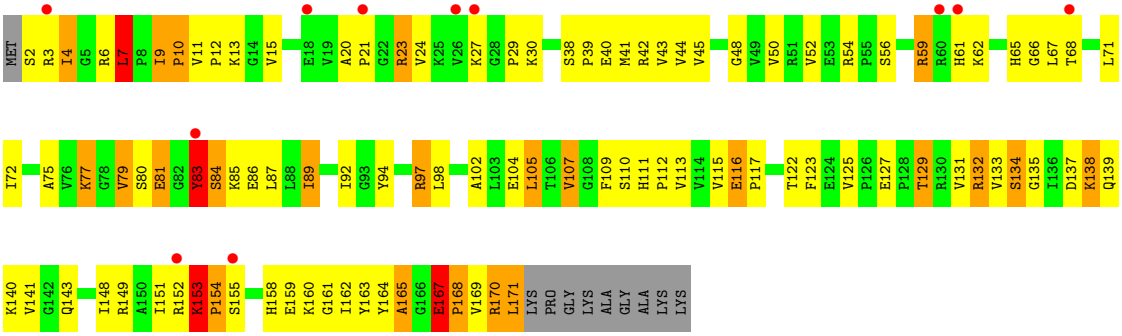
• Molecule 30: 50S ribosomal protein L5

Chain DG:



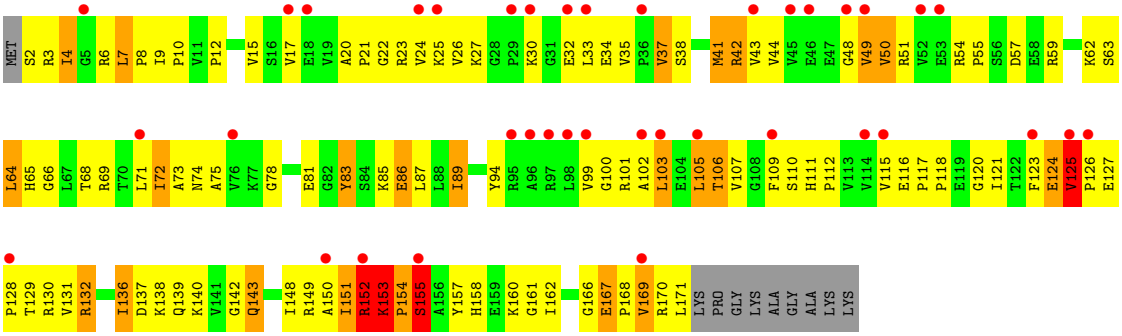
• Molecule 31: 50S ribosomal protein L6

Chain BH:



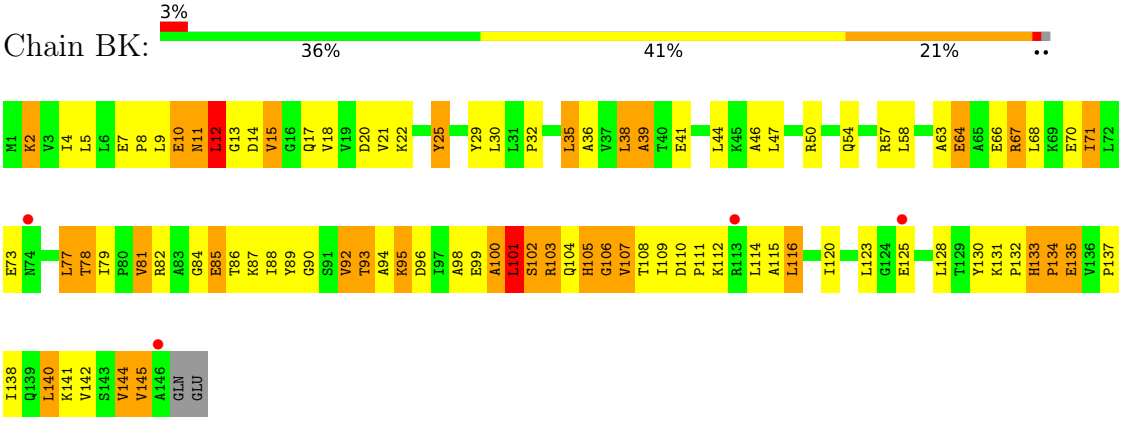
• Molecule 31: 50S ribosomal protein L6

Chain DH:



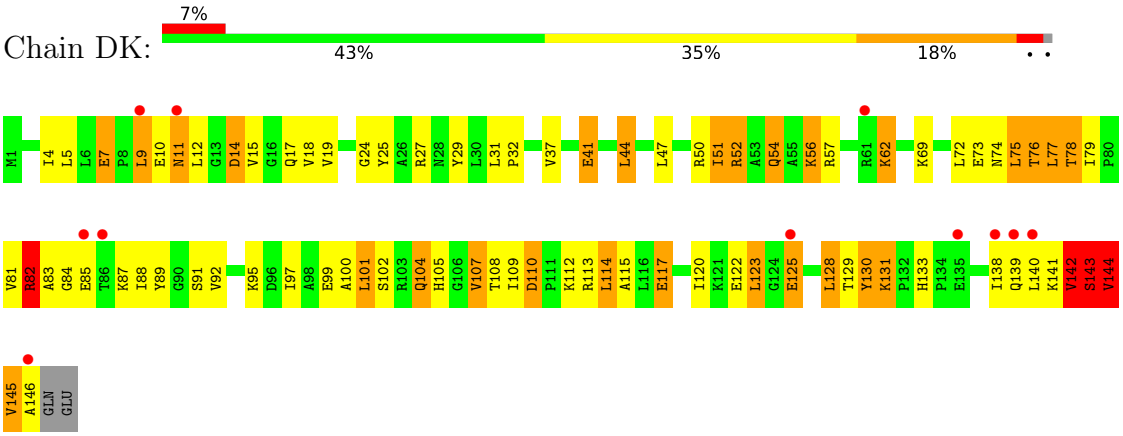
• Molecule 32: 50S ribosomal protein L9

Chain BK:



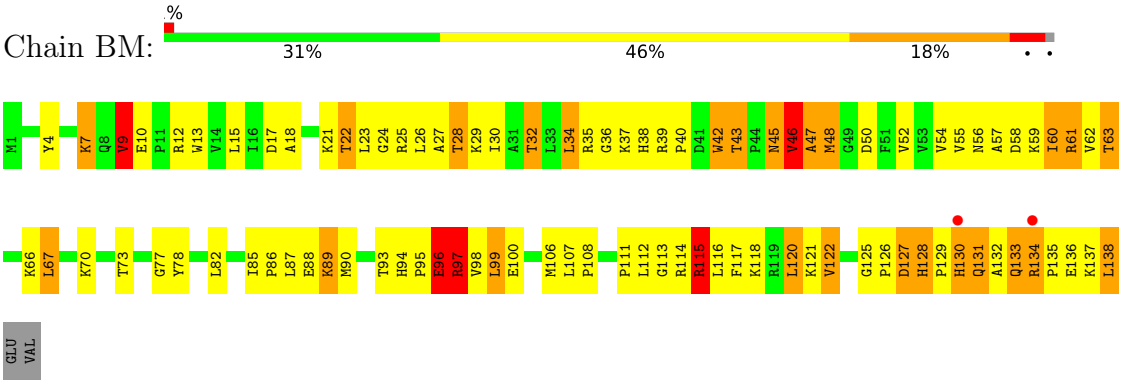
• Molecule 32: 50S ribosomal protein L9

Chain DK:



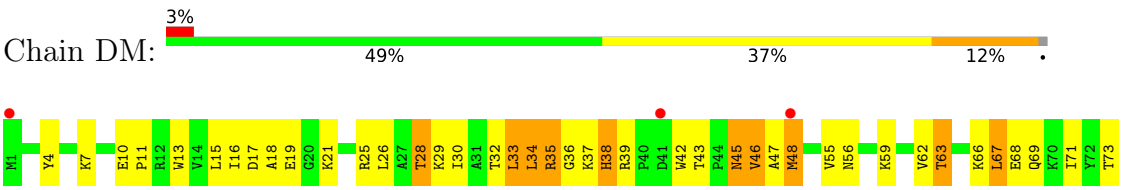
• Molecule 33: 50S ribosomal protein L13

Chain BM:



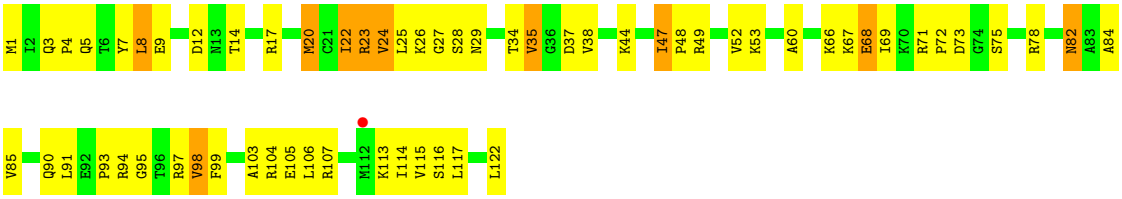
• Molecule 33: 50S ribosomal protein L13

Chain DM:



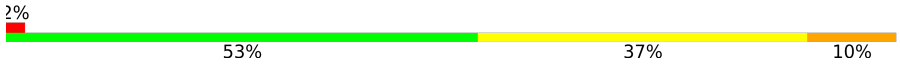
• Molecule 34: 50S ribosomal protein L14

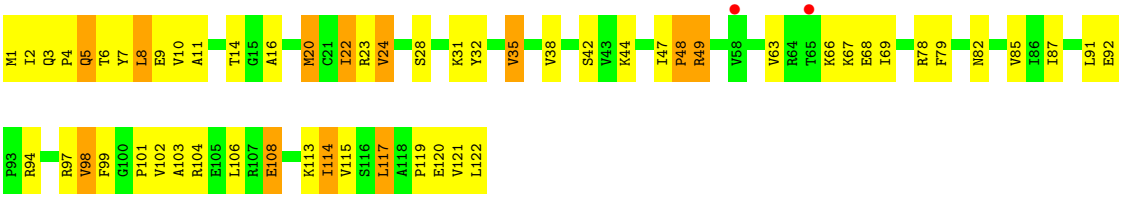
Chain BN:



• Molecule 34: 50S ribosomal protein L14

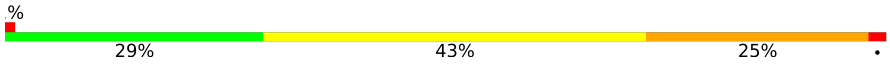
Chain DN:

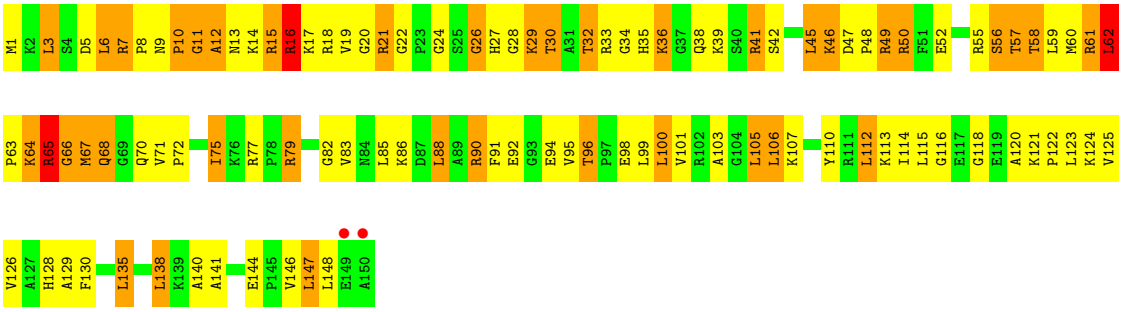




• Molecule 35: 50S ribosomal protein L15

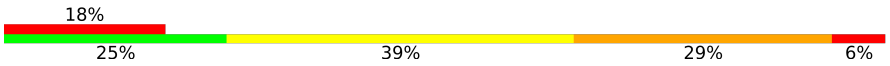
Chain BO:

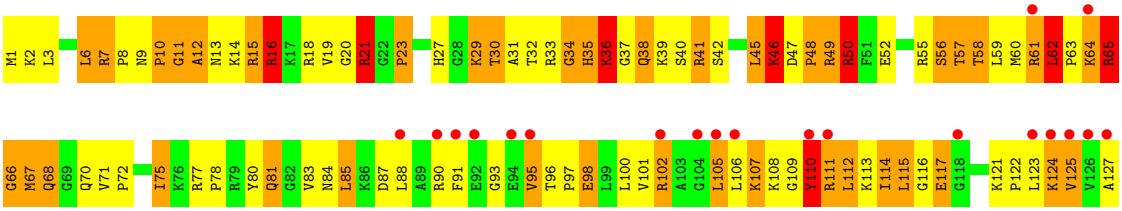


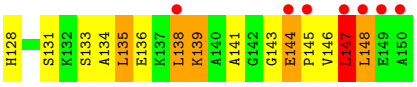


• Molecule 35: 50S ribosomal protein L15

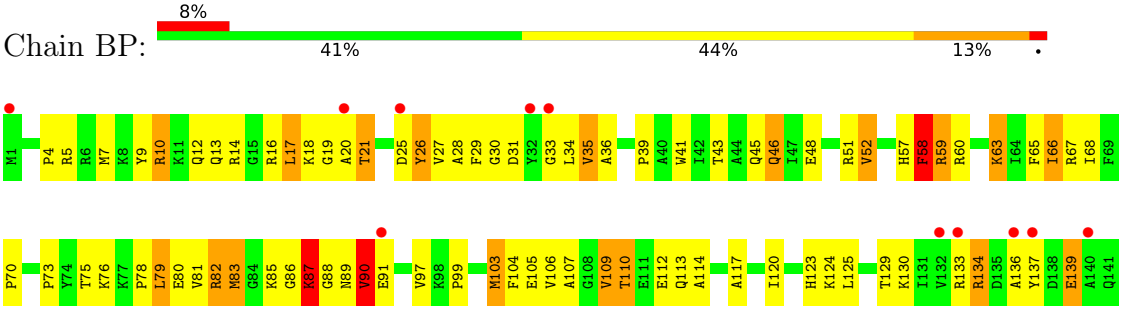
Chain DO:



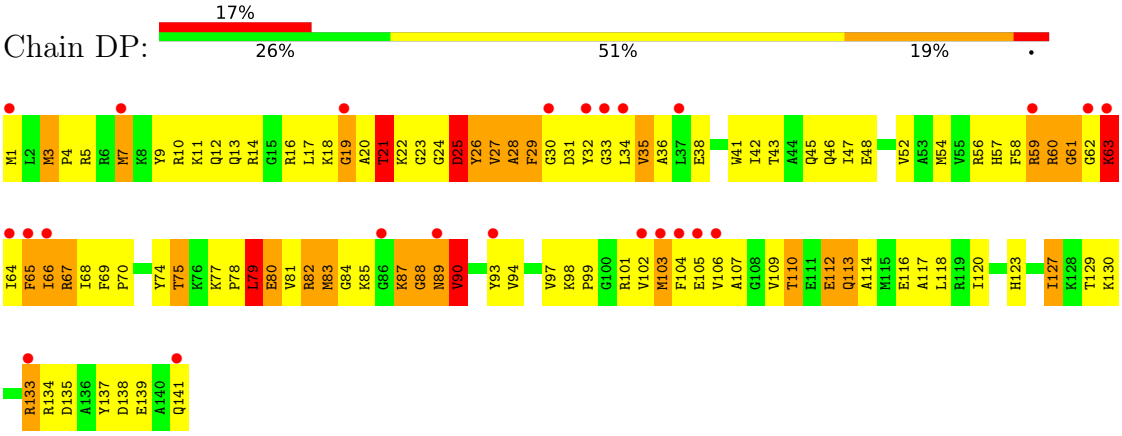




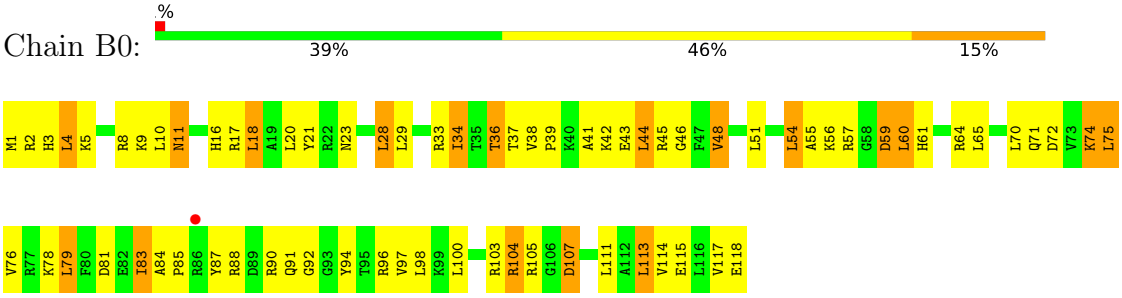
• Molecule 36: 50S ribosomal protein L16



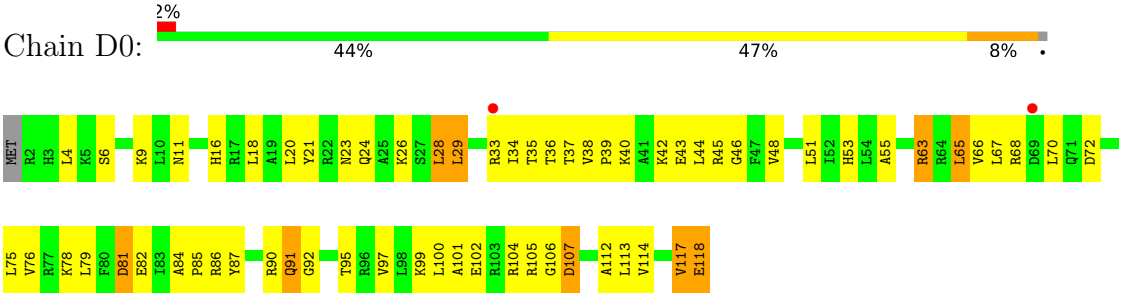
• Molecule 36: 50S ribosomal protein L16



• Molecule 37: 50S ribosomal protein L17

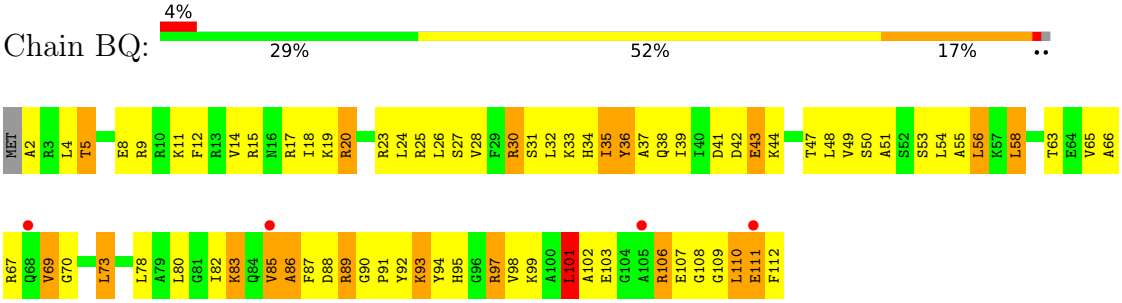


• Molecule 37: 50S ribosomal protein L17



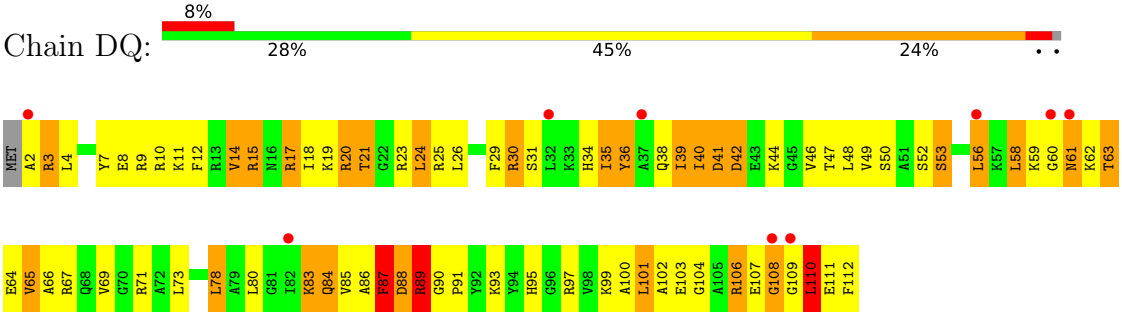
• Molecule 38: 50S ribosomal protein L18

Chain BQ:



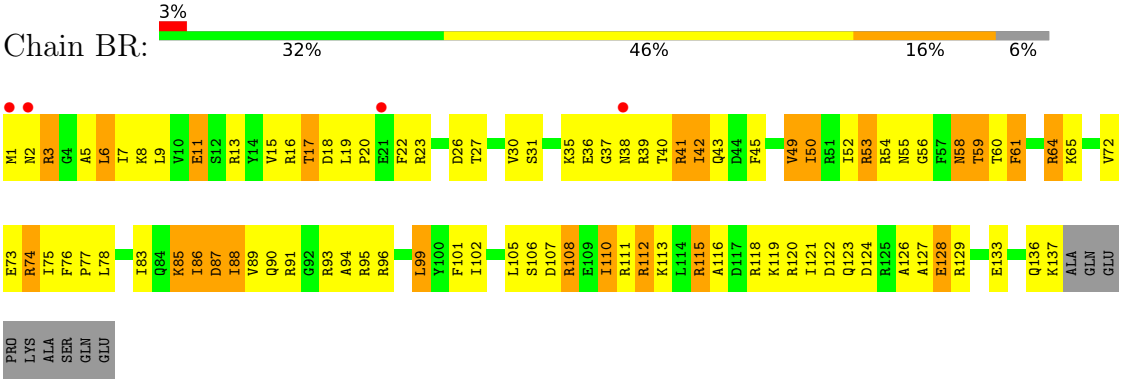
• Molecule 38: 50S ribosomal protein L18

Chain DQ:



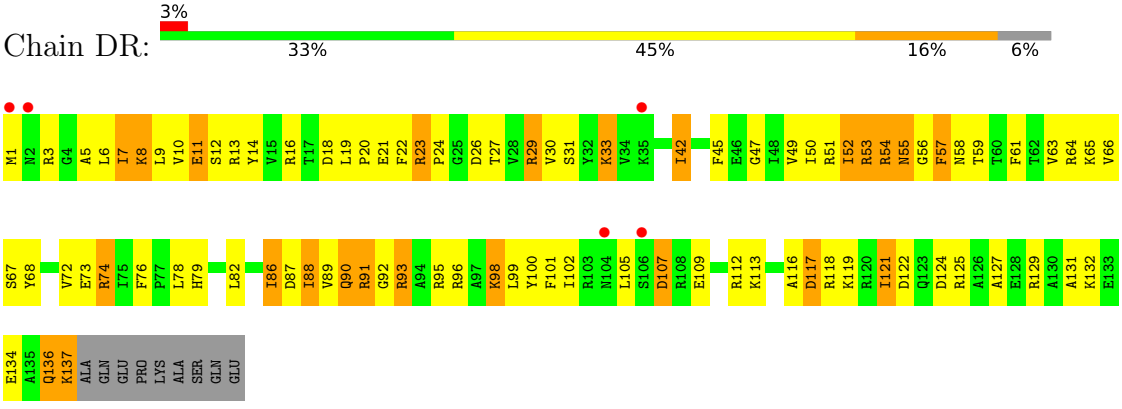
• Molecule 39: 50S ribosomal protein L19

Chain BR:



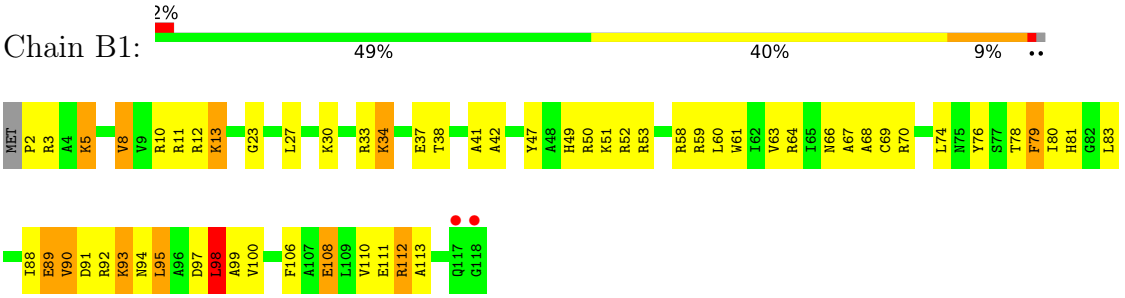
• Molecule 39: 50S ribosomal protein L19

Chain DR:



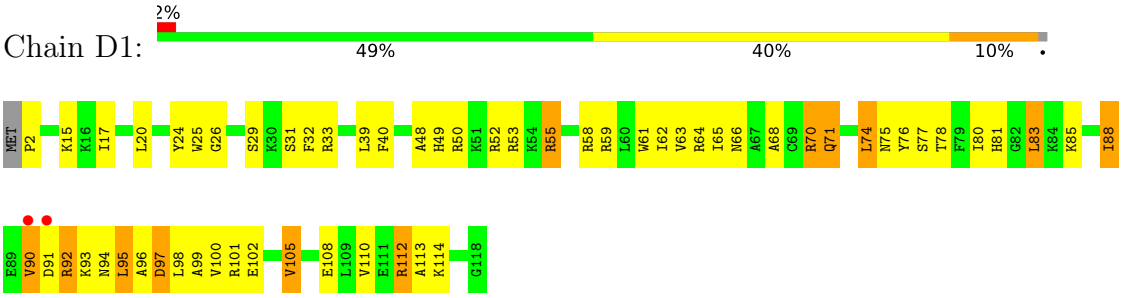
• Molecule 40: 50S ribosomal protein L20

Chain B1:



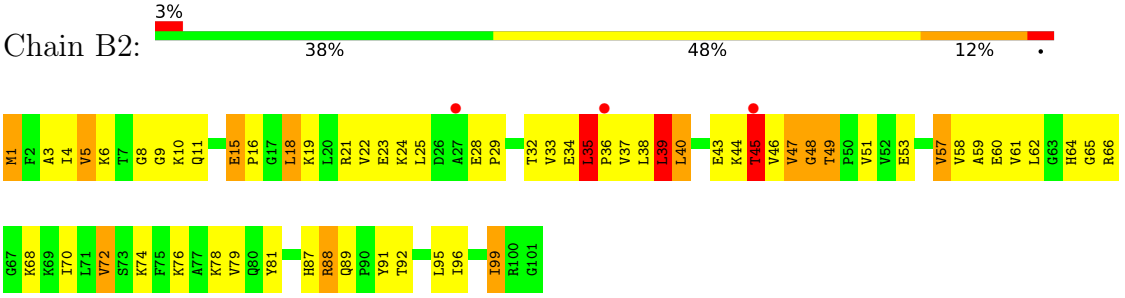
• Molecule 40: 50S ribosomal protein L20

Chain D1:



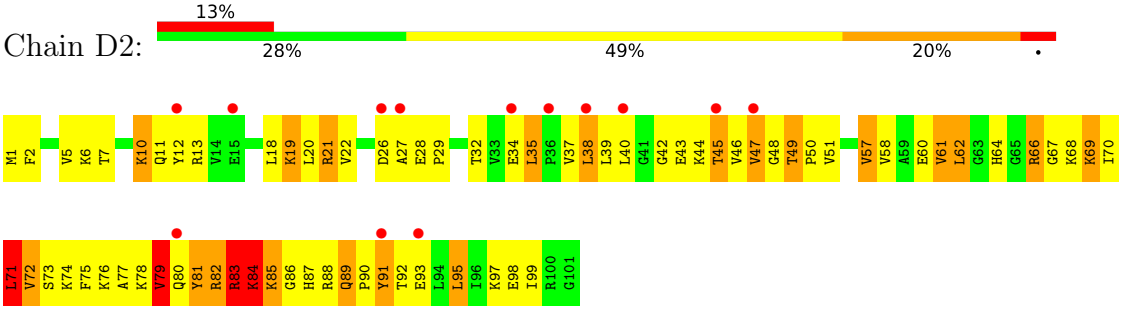
• Molecule 41: 50S ribosomal protein L21

Chain B2:



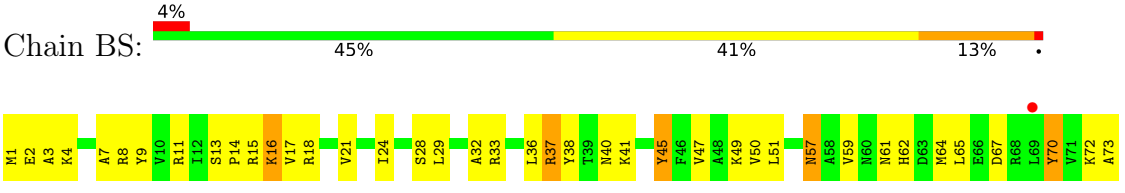
• Molecule 41: 50S ribosomal protein L21

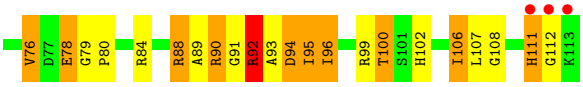
Chain D2:



• Molecule 42: 50S ribosomal protein L22

Chain BS:



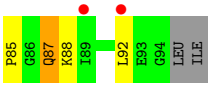


• Molecule 42: 50S ribosomal protein L22

Chain DS:

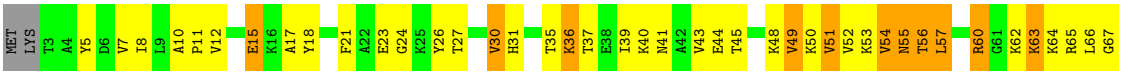
• Molecule 43: 50S ribosomal protein L23

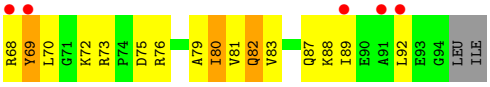
Chain BT:



• Molecule 43: 50S ribosomal protein L23

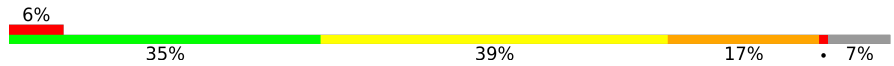
Chain DT:

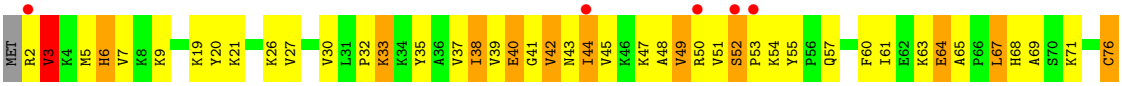




• Molecule 44: 50S ribosomal protein L24

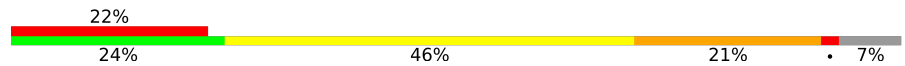
Chain BU:

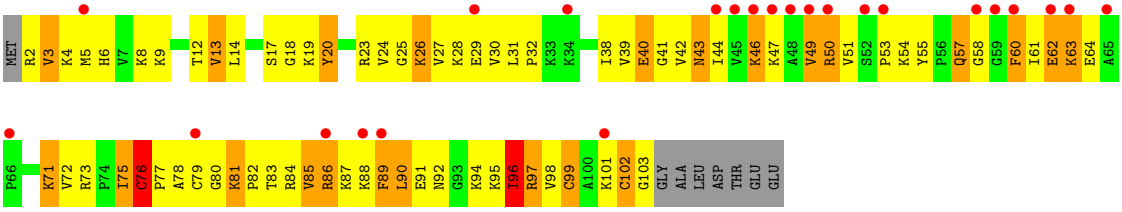




• Molecule 44: 50S ribosomal protein L24

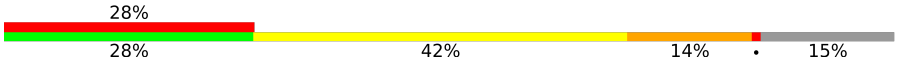
Chain DU:

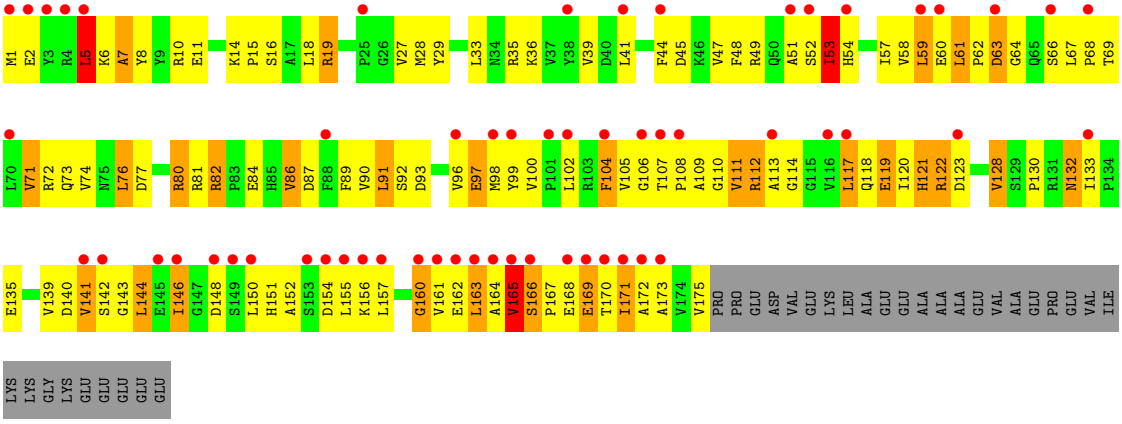




• Molecule 45: 50S ribosomal protein L25

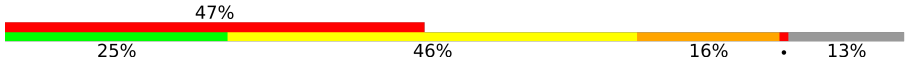
Chain BV:

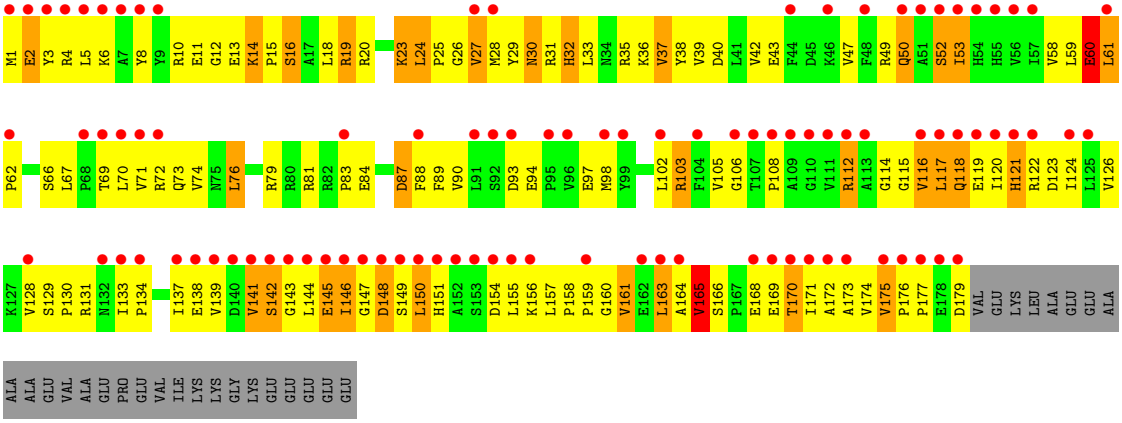




• Molecule 45: 50S ribosomal protein L25

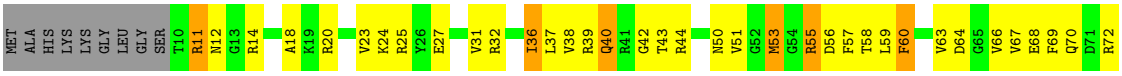
Chain DV:

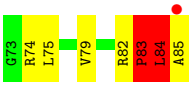




• Molecule 46: 50S ribosomal protein L27

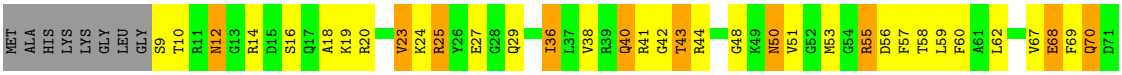
Chain B3:

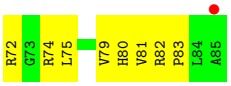




• Molecule 46: 50S ribosomal protein L27

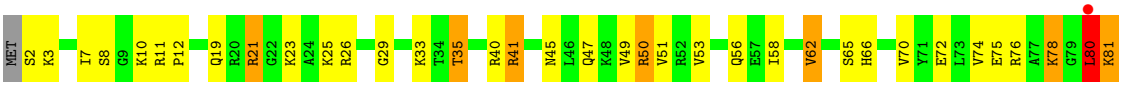
Chain D3:

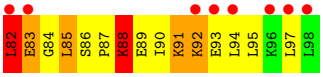




• Molecule 47: 50S ribosomal protein L28

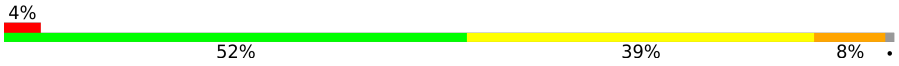
Chain BZ:

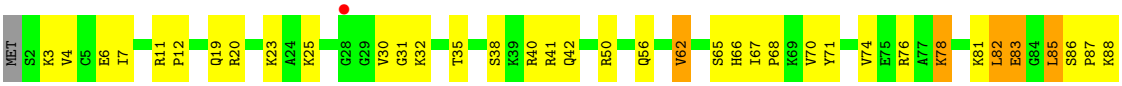


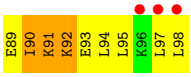


• Molecule 47: 50S ribosomal protein L28

Chain DZ:

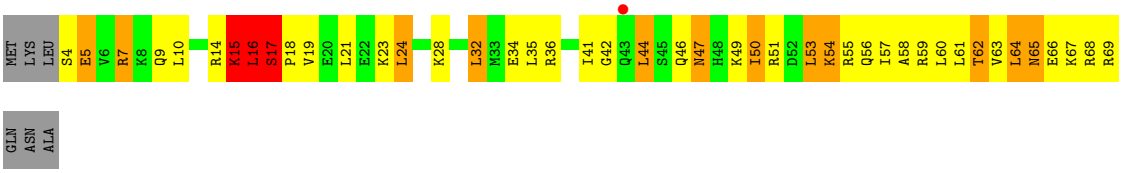






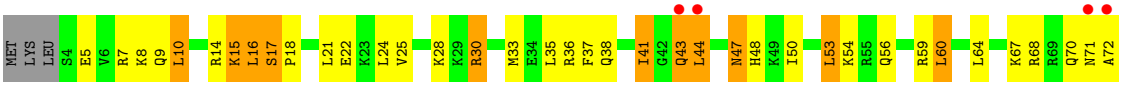
• Molecule 48: 50S ribosomal protein L29

Chain BW:

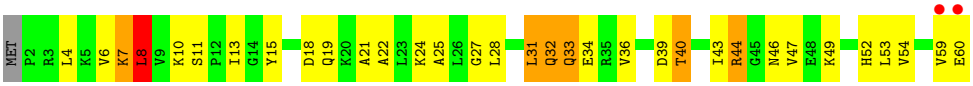


• Molecule 48: 50S ribosomal protein L29

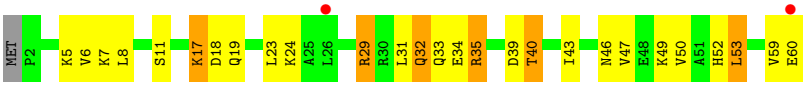
Chain DW:



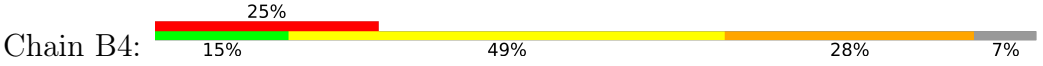
• Molecule 49: 50S ribosomal protein L30

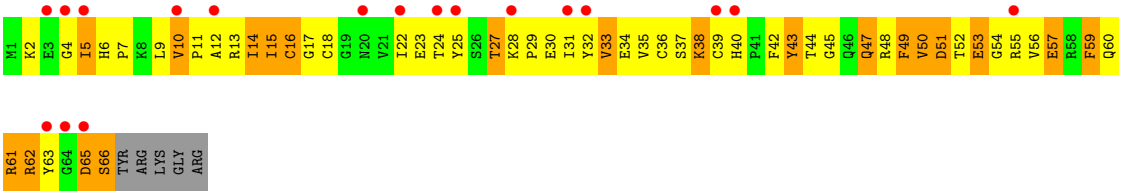


• Molecule 49: 50S ribosomal protein L30

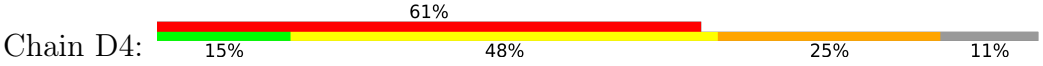


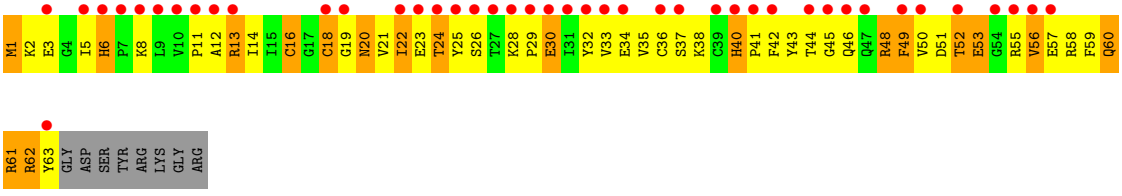
• Molecule 50: 50S ribosomal protein L31



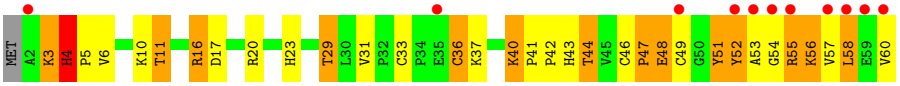


• Molecule 50: 50S ribosomal protein L31

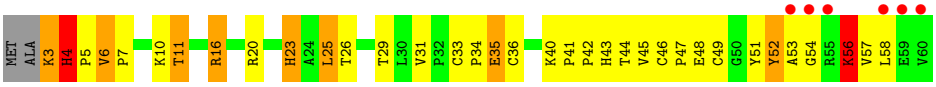




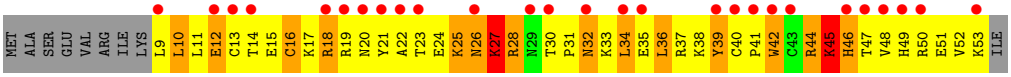
• Molecule 51: 50S ribosomal protein L32



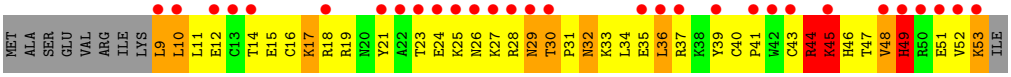
• Molecule 51: 50S ribosomal protein L32



• Molecule 52: 50S ribosomal protein L33

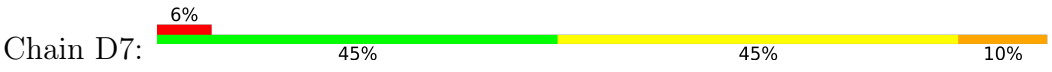


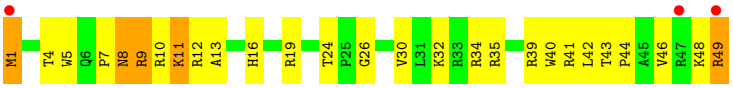
• Molecule 52: 50S ribosomal protein L33



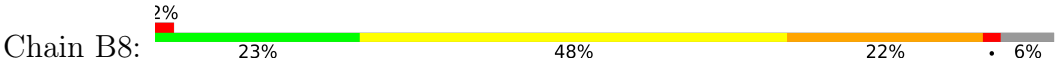
• Molecule 53: 50S ribosomal protein L34

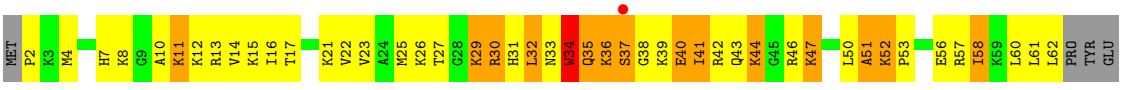
• Molecule 53: 50S ribosomal protein L34



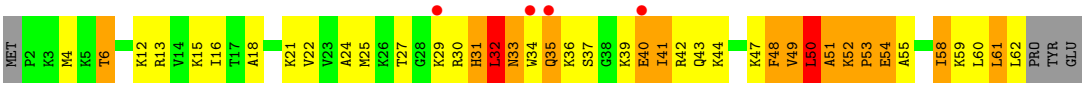


• Molecule 54: 50S ribosomal protein L35





• Molecule 54: 50S ribosomal protein L35



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	210.00Å 450.05Å 621.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	153.53 – 3.00 153.53 – 3.00	Depositor EDS
% Data completeness (in resolution range)	94.1 (153.53-3.00) 93.7 (153.53-3.00)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.44 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.7.1_743	Depositor
R, R_{free}	0.211 , 0.272 0.209 , 0.247	Depositor DCC
R_{free} test set	2000 reflections (0.17%)	wwPDB-VP
Wilson B-factor (Å^2)	77.4	Xtriage
Anisotropy	0.190	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 67.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	299552	wwPDB-VP
Average B, all atoms (Å^2)	100.0	wwPDB-VP

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

[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 (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	AA	0.44	5/36234 (0.0%)	0.91	68/56554 (0.1%)
1	CA	0.42	1/36237 (0.0%)	0.90	79/56558 (0.1%)
2	AE	0.29	0/1959	0.56	0/2642
2	CE	0.28	0/1959	0.53	0/2642
3	AF	0.33	0/1629	0.53	0/2195
3	CF	0.31	0/1636	0.54	0/2205
4	AG	0.49	2/1733 (0.1%)	0.62	1/2318 (0.0%)
4	CG	0.38	0/1733	0.61	0/2318
5	AH	0.35	0/1171	0.58	0/1576
5	CH	0.34	0/1171	0.56	0/1576
6	AI	0.33	0/856	0.55	0/1154
6	CI	0.32	0/856	0.54	0/1154
7	AJ	0.29	0/1276	0.50	0/1709
7	CJ	0.28	0/1276	0.45	0/1709
8	AK	0.33	0/1136	0.60	0/1527
8	CK	0.27	0/1136	0.51	0/1527
9	AL	0.29	0/1029	0.52	0/1379
9	CL	0.29	0/1029	0.53	0/1379
10	AM	0.31	0/814	0.59	1/1095 (0.1%)
10	CM	0.28	0/814	0.54	0/1095
11	AN	0.33	0/900	0.57	0/1213
11	CN	0.31	0/900	0.56	0/1213
12	AO	0.40	0/991	0.68	1/1327 (0.1%)
12	CO	0.35	0/991	0.60	0/1327
13	AP	0.30	0/938	0.57	0/1258
13	CP	0.28	0/943	0.52	0/1265
14	AQ	0.42	0/501	0.66	1/664 (0.2%)
14	CQ	0.29	0/501	0.58	0/664
15	AR	0.35	0/745	0.58	0/992
15	CR	0.30	0/745	0.51	0/992
16	AS	0.29	0/721	0.53	0/970
16	CS	0.31	0/721	0.58	0/970

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

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

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

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

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

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

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

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

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

There are no chirality outliers.

5 of 99 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	AE	14	GLY	Peptide
2	AE	194	PRO	Peptide
2	AE	71	VAL	Peptide
4	AG	29	PRO	Peptide
8	AK	102	ARG	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

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

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

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	B8	1	0	0	0	0
55	BA	623	0	0	0	0
55	BB	17	0	0	0	0
55	BD	1	0	0	0	0
55	BE	5	0	0	0	0
55	BF	3	0	0	0	0
55	BO	2	0	0	0	0
55	BU	2	0	0	0	0
55	CA	207	0	0	0	0
55	CB	3	0	0	0	0
55	CC	8	0	0	0	0
55	CG	2	0	0	0	0
55	CN	1	0	0	0	0
55	CS	1	0	0	0	0
55	D1	2	0	0	0	0
55	D3	1	0	0	0	0
55	D5	1	0	0	0	0
55	DA	526	0	0	0	0
55	DB	14	0	0	0	0
55	DE	3	0	0	0	0
55	DP	1	0	0	0	0
55	DR	1	0	0	0	0
55	DU	1	0	0	0	0
56	AG	1	0	0	0	0
56	AQ	1	0	0	0	0
56	CG	1	0	0	0	0
56	CQ	1	0	0	0	0
All	All	299552	0	200910	14872	3

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 30.

The worst 5 of 14872 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:625:G:H4'	16:AS:16:HIS:CD2	1.33	1.61
28:DE:46:ALA:CB	28:DE:82:ARG:HA	1.37	1.55
30:BG:83:ARG:H	30:BG:86:MET:CE	1.24	1.47
36:DP:26:TYR:CE1	36:DP:139:GLU:HB2	1.48	1.45
25:BA:1056:G:N2	25:BA:1103:A:H62	1.13	1.44

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:85:U:O2'	31:DH:100:GLY:O[3_555]	1.90	0.30
1:CA:86:U:O2'	25:DA:276:A:OP2[3_545]	2.02	0.18
6:AI:15:ASP:OD2	4:CG:27:TYR:OH[4_555]	2.17	0.03

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AE	235/256 (92%)	190 (81%)	45 (19%)	0	100	100
2	CE	235/256 (92%)	190 (81%)	41 (17%)	4 (2%)	9	39
3	AF	203/239 (85%)	179 (88%)	24 (12%)	0	100	100
3	CF	204/239 (85%)	179 (88%)	23 (11%)	2 (1%)	15	53
4	AG	206/208 (99%)	179 (87%)	24 (12%)	3 (2%)	10	42
4	CG	206/208 (99%)	179 (87%)	25 (12%)	2 (1%)	15	53
5	AH	149/162 (92%)	137 (92%)	10 (7%)	2 (1%)	12	45
5	CH	149/162 (92%)	139 (93%)	10 (7%)	0	100	100
6	AI	99/101 (98%)	92 (93%)	7 (7%)	0	100	100
6	CI	99/101 (98%)	94 (95%)	5 (5%)	0	100	100
7	AJ	153/156 (98%)	142 (93%)	11 (7%)	0	100	100
7	CJ	153/156 (98%)	143 (94%)	10 (6%)	0	100	100
8	AK	136/138 (99%)	123 (90%)	12 (9%)	1 (1%)	22	60
8	CK	136/138 (99%)	123 (90%)	13 (10%)	0	100	100
9	AL	125/128 (98%)	110 (88%)	15 (12%)	0	100	100
9	CL	125/128 (98%)	114 (91%)	11 (9%)	0	100	100
10	AM	97/105 (92%)	86 (89%)	11 (11%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
10	CM	97/105 (92%)	84 (87%)	9 (9%)	4 (4%)	3 16
11	AN	117/129 (91%)	102 (87%)	14 (12%)	1 (1%)	17 55
11	CN	117/129 (91%)	104 (89%)	13 (11%)	0	100 100
12	AO	123/132 (93%)	105 (85%)	16 (13%)	2 (2%)	9 40
12	CO	123/132 (93%)	105 (85%)	15 (12%)	3 (2%)	6 29
13	AP	114/126 (90%)	89 (78%)	23 (20%)	2 (2%)	8 37
13	CP	115/126 (91%)	96 (84%)	17 (15%)	2 (2%)	9 39
14	AQ	58/61 (95%)	49 (84%)	9 (16%)	0	100 100
14	CQ	58/61 (95%)	49 (84%)	8 (14%)	1 (2%)	9 39
15	AR	86/89 (97%)	74 (86%)	11 (13%)	1 (1%)	13 48
15	CR	86/89 (97%)	76 (88%)	10 (12%)	0	100 100
16	AS	82/88 (93%)	71 (87%)	8 (10%)	3 (4%)	3 19
16	CS	82/88 (93%)	75 (92%)	7 (8%)	0	100 100
17	AT	98/105 (93%)	91 (93%)	7 (7%)	0	100 100
17	CT	98/105 (93%)	91 (93%)	7 (7%)	0	100 100
18	AU	70/88 (80%)	64 (91%)	5 (7%)	1 (1%)	11 43
18	CU	70/88 (80%)	61 (87%)	9 (13%)	0	100 100
19	AV	76/93 (82%)	68 (90%)	6 (8%)	2 (3%)	5 27
19	CV	76/93 (82%)	60 (79%)	12 (16%)	4 (5%)	2 11
20	AW	97/106 (92%)	84 (87%)	13 (13%)	0	100 100
20	CW	97/106 (92%)	80 (82%)	16 (16%)	1 (1%)	15 53
21	AX	23/27 (85%)	22 (96%)	1 (4%)	0	100 100
21	CX	23/27 (85%)	21 (91%)	2 (9%)	0	100 100
27	BD	270/276 (98%)	243 (90%)	22 (8%)	5 (2%)	8 36
27	DD	270/276 (98%)	248 (92%)	15 (6%)	7 (3%)	5 27
28	BE	203/206 (98%)	149 (73%)	30 (15%)	24 (12%)	0 1
28	DE	203/206 (98%)	144 (71%)	41 (20%)	18 (9%)	1 3
29	BF	200/210 (95%)	179 (90%)	21 (10%)	0	100 100
29	DF	206/210 (98%)	168 (82%)	30 (15%)	8 (4%)	3 17
30	BG	179/182 (98%)	154 (86%)	20 (11%)	5 (3%)	5 25
30	DG	179/182 (98%)	150 (84%)	28 (16%)	1 (1%)	25 64

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
31	BH	168/180 (93%)	133 (79%)	28 (17%)	7 (4%)	3 16
31	DH	168/180 (93%)	125 (74%)	35 (21%)	8 (5%)	2 13
32	BK	144/148 (97%)	102 (71%)	32 (22%)	10 (7%)	1 6
32	DK	144/148 (97%)	113 (78%)	28 (19%)	3 (2%)	7 33
33	BM	136/140 (97%)	113 (83%)	16 (12%)	7 (5%)	2 12
33	DM	136/140 (97%)	119 (88%)	15 (11%)	2 (2%)	10 42
34	BN	120/122 (98%)	111 (92%)	9 (8%)	0	100 100
34	DN	120/122 (98%)	113 (94%)	6 (5%)	1 (1%)	19 57
35	BO	148/150 (99%)	107 (72%)	27 (18%)	14 (10%)	0 3
35	DO	148/150 (99%)	102 (69%)	24 (16%)	22 (15%)	0 1
36	BP	139/141 (99%)	109 (78%)	27 (19%)	3 (2%)	6 31
36	DP	139/141 (99%)	93 (67%)	30 (22%)	16 (12%)	0 2
37	B0	116/118 (98%)	101 (87%)	13 (11%)	2 (2%)	9 39
37	D0	115/118 (98%)	109 (95%)	6 (5%)	0	100 100
38	BQ	109/112 (97%)	86 (79%)	20 (18%)	3 (3%)	5 25
38	DQ	109/112 (97%)	87 (80%)	19 (17%)	3 (3%)	5 25
39	BR	135/146 (92%)	114 (84%)	21 (16%)	0	100 100
39	DR	135/146 (92%)	119 (88%)	14 (10%)	2 (2%)	10 42
40	B1	115/118 (98%)	103 (90%)	11 (10%)	1 (1%)	17 55
40	D1	115/118 (98%)	101 (88%)	14 (12%)	0	100 100
41	B2	99/101 (98%)	92 (93%)	5 (5%)	2 (2%)	7 34
41	D2	99/101 (98%)	78 (79%)	14 (14%)	7 (7%)	1 5
42	BS	111/113 (98%)	97 (87%)	10 (9%)	4 (4%)	3 19
42	DS	111/113 (98%)	103 (93%)	8 (7%)	0	100 100
43	BT	90/96 (94%)	84 (93%)	4 (4%)	2 (2%)	6 31
43	DT	90/96 (94%)	78 (87%)	10 (11%)	2 (2%)	6 31
44	BU	100/110 (91%)	80 (80%)	15 (15%)	5 (5%)	2 12
44	DU	100/110 (91%)	70 (70%)	24 (24%)	6 (6%)	1 9
45	BV	173/206 (84%)	129 (75%)	37 (21%)	7 (4%)	3 17
45	DV	177/206 (86%)	132 (75%)	35 (20%)	10 (6%)	2 10
46	B3	74/85 (87%)	67 (90%)	5 (7%)	2 (3%)	5 26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
46	D3	75/85 (88%)	69 (92%)	6 (8%)	0	100 100
47	BZ	95/98 (97%)	85 (90%)	7 (7%)	3 (3%)	4 22
47	DZ	95/98 (97%)	84 (88%)	10 (10%)	1 (1%)	14 50
48	BW	64/72 (89%)	58 (91%)	4 (6%)	2 (3%)	4 23
48	DW	67/72 (93%)	60 (90%)	6 (9%)	1 (2%)	10 42
49	BX	57/60 (95%)	52 (91%)	5 (9%)	0	100 100
49	DX	57/60 (95%)	53 (93%)	4 (7%)	0	100 100
50	B4	64/71 (90%)	41 (64%)	21 (33%)	2 (3%)	4 23
50	D4	61/71 (86%)	32 (52%)	28 (46%)	1 (2%)	9 40
51	B5	57/60 (95%)	49 (86%)	7 (12%)	1 (2%)	8 37
51	D5	56/60 (93%)	48 (86%)	7 (12%)	1 (2%)	8 37
52	B6	43/54 (80%)	27 (63%)	14 (33%)	2 (5%)	2 14
52	D6	43/54 (80%)	29 (67%)	10 (23%)	4 (9%)	0 3
53	B7	47/49 (96%)	44 (94%)	3 (6%)	0	100 100
53	D7	47/49 (96%)	45 (96%)	2 (4%)	0	100 100
54	B8	59/65 (91%)	47 (80%)	7 (12%)	5 (8%)	1 4
54	D8	59/65 (91%)	40 (68%)	12 (20%)	7 (12%)	0 1
All	All	11335/12052 (94%)	9588 (85%)	1457 (13%)	290 (3%)	5 27

5 of 290 Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	AE	205/220 (93%)	155 (76%)	50 (24%)	0 3
2	CE	205/220 (93%)	159 (78%)	46 (22%)	1 4
3	AF	159/188 (85%)	120 (76%)	39 (24%)	0 3
3	CF	160/188 (85%)	124 (78%)	36 (22%)	1 4
4	AG	180/180 (100%)	144 (80%)	36 (20%)	1 7
4	CG	180/180 (100%)	140 (78%)	40 (22%)	1 4
5	AH	116/123 (94%)	88 (76%)	28 (24%)	0 3
5	CH	116/123 (94%)	89 (77%)	27 (23%)	1 4
6	AI	90/90 (100%)	76 (84%)	14 (16%)	2 13
6	CI	90/90 (100%)	74 (82%)	16 (18%)	2 9
7	AJ	126/127 (99%)	104 (82%)	22 (18%)	2 10
7	CJ	126/127 (99%)	89 (71%)	37 (29%)	0 1
8	AK	119/119 (100%)	100 (84%)	19 (16%)	2 12
8	CK	119/119 (100%)	94 (79%)	25 (21%)	1 5
9	AL	98/99 (99%)	70 (71%)	28 (29%)	0 2
9	CL	98/99 (99%)	69 (70%)	29 (30%)	0 1
10	AM	89/92 (97%)	66 (74%)	23 (26%)	0 2
10	CM	89/92 (97%)	60 (67%)	29 (33%)	0 1
11	AN	90/99 (91%)	74 (82%)	16 (18%)	2 9
11	CN	90/99 (91%)	73 (81%)	17 (19%)	1 8
12	AO	104/109 (95%)	88 (85%)	16 (15%)	2 13
12	CO	104/109 (95%)	80 (77%)	24 (23%)	1 4
13	AP	94/101 (93%)	71 (76%)	23 (24%)	0 3
13	CP	94/101 (93%)	75 (80%)	19 (20%)	1 6
14	AQ	49/50 (98%)	33 (67%)	16 (33%)	0 1
14	CQ	49/50 (98%)	39 (80%)	10 (20%)	1 6
15	AR	79/80 (99%)	68 (86%)	11 (14%)	3 16
15	CR	79/80 (99%)	66 (84%)	13 (16%)	2 11
16	AS	72/74 (97%)	53 (74%)	19 (26%)	0 2
16	CS	72/74 (97%)	62 (86%)	10 (14%)	3 16
17	AT	95/97 (98%)	82 (86%)	13 (14%)	3 17
17	CT	95/97 (98%)	89 (94%)	6 (6%)	18 51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
18	AU	63/77 (82%)	50 (79%)	13 (21%)	1 6
18	CU	63/77 (82%)	48 (76%)	15 (24%)	0 3
19	AV	67/80 (84%)	47 (70%)	20 (30%)	0 1
19	CV	67/80 (84%)	53 (79%)	14 (21%)	1 5
20	AW	76/82 (93%)	60 (79%)	16 (21%)	1 5
20	CW	76/82 (93%)	55 (72%)	21 (28%)	0 2
21	AX	20/22 (91%)	17 (85%)	3 (15%)	3 14
21	CX	20/22 (91%)	20 (100%)	0	100 100
27	BD	214/218 (98%)	172 (80%)	42 (20%)	1 7
27	DD	214/218 (98%)	162 (76%)	52 (24%)	0 3
28	BE	165/166 (99%)	114 (69%)	51 (31%)	0 1
28	DE	165/166 (99%)	121 (73%)	44 (27%)	0 2
29	BF	161/166 (97%)	129 (80%)	32 (20%)	1 7
29	DF	165/166 (99%)	122 (74%)	43 (26%)	0 2
30	BG	155/156 (99%)	115 (74%)	40 (26%)	0 2
30	DG	155/156 (99%)	113 (73%)	42 (27%)	0 2
31	BH	142/148 (96%)	107 (75%)	35 (25%)	0 3
31	DH	142/148 (96%)	110 (78%)	32 (22%)	1 4
32	BK	122/124 (98%)	91 (75%)	31 (25%)	0 3
32	DK	122/124 (98%)	84 (69%)	38 (31%)	0 1
33	BM	117/119 (98%)	87 (74%)	30 (26%)	0 3
33	DM	117/119 (98%)	96 (82%)	21 (18%)	2 9
34	BN	100/100 (100%)	83 (83%)	17 (17%)	2 10
34	DN	100/100 (100%)	78 (78%)	22 (22%)	1 4
35	BO	116/116 (100%)	78 (67%)	38 (33%)	0 1
35	DO	116/116 (100%)	72 (62%)	44 (38%)	0 0
36	BP	111/111 (100%)	84 (76%)	27 (24%)	0 3
36	DP	111/111 (100%)	85 (77%)	26 (23%)	1 4
37	B0	101/101 (100%)	78 (77%)	23 (23%)	1 4
37	D0	100/101 (99%)	80 (80%)	20 (20%)	1 7
38	BQ	87/88 (99%)	65 (75%)	22 (25%)	0 3

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
54	B8	51/55 (93%)	40 (78%)	11 (22%)	1 5
54	D8	51/55 (93%)	41 (80%)	10 (20%)	1 7
All	All	9579/9996 (96%)	7317 (76%)	2262 (24%)	1 3

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

Mol	Chain	Res	Type
35	DO	105	LEU
37	D0	81	ASP
35	DO	100	LEU
44	DU	26	LYS
37	B0	48	VAL

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

Mol	Chain	Res	Type
48	BW	65	ASN
42	DS	61	ASN
6	CI	57	GLN
42	DS	57	ASN
46	D3	29	GLN

5.3.3 RNA (i)

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

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

5 of 2519 RNA backbone outliers are listed below:

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

5 of 208 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	CA	353	A
22	CB	21	A
25	DA	2602	A
1	CA	560	U
1	CA	1067	A

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	AA	1506/1506 (100%)	-0.57	5 (0%) 94 84	50, 98, 179, 234	0
1	CA	1506/1506 (100%)	-0.56	4 (0%) 94 84	62, 109, 181, 235	0
2	AE	237/256 (92%)	0.27	9 (3%) 40 16	103, 136, 174, 185	0
2	CE	237/256 (92%)	0.59	25 (10%) 6 2	114, 151, 185, 201	0
3	AF	205/239 (85%)	0.91	34 (16%) 1 0	84, 111, 144, 153	0
3	CF	206/239 (86%)	1.40	59 (28%) 0 0	118, 138, 166, 174	0
4	AG	208/208 (100%)	0.47	13 (6%) 20 6	80, 105, 129, 142	0
4	CG	208/208 (100%)	0.39	14 (6%) 17 5	77, 102, 123, 136	0
5	AH	151/162 (93%)	0.52	8 (5%) 26 10	74, 97, 118, 152	0
5	CH	151/162 (93%)	0.22	7 (4%) 32 12	91, 112, 134, 153	0
6	AI	101/101 (100%)	0.93	14 (13%) 2 1	76, 99, 115, 137	0
6	CI	101/101 (100%)	0.95	19 (18%) 1 0	74, 95, 116, 141	0
7	AJ	155/156 (99%)	-0.08	8 (5%) 27 10	99, 114, 145, 155	0
7	CJ	155/156 (99%)	0.27	10 (6%) 18 5	102, 122, 149, 156	0
8	AK	138/138 (100%)	-0.02	0 100 100	84, 103, 117, 122	0
8	CK	138/138 (100%)	-0.21	1 (0%) 87 69	94, 116, 128, 136	0
9	AL	127/128 (99%)	-0.31	1 (0%) 86 65	85, 133, 153, 160	0
9	CL	127/128 (99%)	-0.03	4 (3%) 49 21	107, 145, 160, 164	0
10	AM	99/105 (94%)	0.38	6 (6%) 21 7	81, 132, 162, 165	0
10	CM	99/105 (94%)	0.49	3 (3%) 50 22	111, 149, 165, 170	0
11	AN	119/129 (92%)	1.10	19 (15%) 1 1	64, 97, 128, 154	0
11	CN	119/129 (92%)	1.48	32 (26%) 0 0	79, 101, 134, 158	0
12	AO	125/132 (94%)	0.41	8 (6%) 19 6	63, 73, 105, 151	0
12	CO	125/132 (94%)	1.07	27 (21%) 0 0	75, 98, 124, 160	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	AP	116/126 (92%)	-0.14	4 (3%) 45 19	86, 117, 136, 145	0
13	CP	117/126 (92%)	0.44	11 (9%) 8 3	106, 146, 161, 164	0
14	AQ	60/61 (98%)	-0.12	0 100 100	86, 101, 115, 126	0
14	CQ	60/61 (98%)	0.94	11 (18%) 1 0	118, 132, 146, 153	0
15	AR	88/89 (98%)	0.04	2 (2%) 60 31	72, 93, 114, 117	0
15	CR	88/89 (98%)	0.03	2 (2%) 60 31	73, 104, 127, 133	0
16	AS	84/88 (95%)	-0.37	0 100 100	90, 107, 133, 165	0
16	CS	84/88 (95%)	-0.34	0 100 100	81, 96, 120, 153	0
17	AT	100/105 (95%)	-0.21	1 (1%) 82 59	82, 100, 118, 130	0
17	CT	100/105 (95%)	-0.24	1 (1%) 82 59	82, 102, 125, 137	0
18	AU	72/88 (81%)	1.10	12 (16%) 1 0	78, 99, 132, 159	0
18	CU	72/88 (81%)	1.08	12 (16%) 1 0	85, 106, 144, 157	0
19	AV	78/93 (83%)	0.19	2 (2%) 56 27	100, 122, 137, 144	0
19	CV	78/93 (83%)	0.78	12 (15%) 2 1	136, 154, 174, 177	0
20	AW	99/106 (93%)	-0.44	0 100 100	93, 115, 144, 155	0
20	CW	99/106 (93%)	-0.23	0 100 100	83, 109, 143, 157	0
21	AX	25/27 (92%)	-0.63	0 100 100	88, 109, 125, 147	0
21	CX	25/27 (92%)	0.03	1 (4%) 38 15	112, 133, 148, 160	0
22	AB	87/87 (100%)	1.67	29 (33%) 0 0	78, 145, 185, 196	0
22	CB	87/87 (100%)	4.00	55 (63%) 0 0	92, 148, 188, 200	0
23	AC	77/77 (100%)	-0.36	0 100 100	63, 100, 132, 147	0
23	AD	77/77 (100%)	0.15	3 (3%) 39 15	71, 218, 232, 234	0
23	CC	77/77 (100%)	-0.20	1 (1%) 77 51	73, 107, 141, 153	0
23	CD	77/77 (100%)	0.64	12 (15%) 2 1	77, 219, 231, 234	0
24	A1	10/10 (100%)	0.53	2 (20%) 1 0	67, 81, 112, 112	0
24	C1	10/10 (100%)	0.51	2 (20%) 1 0	81, 98, 118, 124	0
25	BA	2912/2912 (100%)	-0.30	36 (1%) 79 54	36, 66, 200, 234	0
25	DA	2907/2912 (99%)	-0.26	48 (1%) 70 41	45, 80, 220, 235	0
26	BB	122/122 (100%)	-0.60	1 (0%) 86 65	66, 91, 110, 169	0
26	DB	122/122 (100%)	-0.47	1 (0%) 86 65	84, 120, 141, 189	0
27	BD	272/276 (98%)	0.09	1 (0%) 92 79	35, 57, 79, 96	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
27	DD	272/276 (98%)	0.37	9 (3%) 46 20	42, 67, 88, 119	0
28	BE	205/206 (99%)	0.42	15 (7%) 15 4	42, 77, 123, 132	0
28	DE	205/206 (99%)	0.24	11 (5%) 25 9	52, 88, 137, 159	0
29	BF	202/210 (96%)	-0.13	1 (0%) 91 75	38, 70, 108, 123	0
29	DF	208/210 (99%)	0.59	20 (9%) 8 2	48, 94, 152, 175	0
30	BG	181/182 (99%)	0.69	17 (9%) 8 3	81, 101, 130, 142	0
30	DG	181/182 (99%)	1.21	44 (24%) 0 0	112, 135, 155, 162	0
31	BH	170/180 (94%)	0.45	11 (6%) 18 5	74, 104, 121, 146	0
31	DH	170/180 (94%)	1.06	38 (22%) 0 0	148, 188, 209, 218	0
32	BK	146/148 (98%)	0.22	4 (2%) 54 26	69, 121, 137, 142	0
32	DK	146/148 (98%)	0.38	11 (7%) 14 4	77, 120, 143, 150	0
33	BM	138/140 (98%)	0.09	2 (1%) 75 49	57, 81, 116, 129	0
33	DM	138/140 (98%)	0.11	4 (2%) 51 23	71, 102, 133, 143	0
34	BN	122/122 (100%)	0.35	1 (0%) 86 65	48, 67, 83, 97	0
34	DN	122/122 (100%)	0.42	2 (1%) 72 44	62, 82, 102, 118	0
35	BO	150/150 (100%)	-0.12	2 (1%) 77 51	42, 77, 106, 153	0
35	DO	150/150 (100%)	0.95	27 (18%) 1 0	44, 99, 135, 171	0
36	BP	141/141 (100%)	0.44	11 (7%) 13 4	52, 78, 99, 125	0
36	DP	141/141 (100%)	0.90	24 (17%) 1 0	58, 98, 129, 148	0
37	B0	118/118 (100%)	0.33	1 (0%) 86 65	50, 76, 94, 110	0
37	D0	117/118 (99%)	0.01	2 (1%) 70 41	50, 74, 97, 113	0
38	BQ	111/112 (99%)	0.36	4 (3%) 42 17	70, 88, 110, 127	0
38	DQ	111/112 (99%)	0.41	9 (8%) 12 3	83, 117, 139, 159	0
39	BR	137/146 (93%)	0.19	4 (2%) 51 23	60, 82, 134, 163	0
39	DR	137/146 (93%)	0.18	5 (3%) 42 17	69, 93, 154, 174	0
40	B1	117/118 (99%)	-0.19	2 (1%) 70 41	44, 70, 101, 132	0
40	D1	117/118 (99%)	0.23	2 (1%) 70 41	58, 89, 131, 152	0
41	B2	101/101 (100%)	0.08	3 (2%) 50 22	48, 92, 115, 132	0
41	D2	101/101 (100%)	0.78	13 (12%) 3 1	58, 115, 133, 142	0
42	BS	113/113 (100%)	0.05	4 (3%) 44 18	41, 65, 97, 147	0
42	DS	113/113 (100%)	0.06	2 (1%) 68 40	54, 69, 104, 148	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
43	BT	92/96 (95%)	0.10	2 (2%) 62 33	49, 63, 87, 104	0
43	DT	92/96 (95%)	0.21	5 (5%) 25 9	64, 80, 104, 121	0
44	BU	102/110 (92%)	0.37	7 (6%) 16 5	67, 92, 142, 159	0
44	DU	102/110 (92%)	1.12	24 (23%) 0 0	82, 109, 160, 176	0
45	BV	175/206 (84%)	1.67	58 (33%) 0 0	80, 117, 179, 183	0
45	DV	179/206 (86%)	2.69	96 (53%) 0 0	110, 151, 199, 206	0
46	B3	76/85 (89%)	-0.16	1 (1%) 77 51	52, 68, 83, 117	0
46	D3	77/85 (90%)	0.16	1 (1%) 77 51	65, 86, 108, 141	0
47	BZ	97/98 (98%)	0.27	9 (9%) 8 3	46, 64, 122, 151	0
47	DZ	97/98 (98%)	0.15	4 (4%) 37 14	54, 77, 126, 148	0
48	BW	66/72 (91%)	-0.00	1 (1%) 73 46	55, 73, 90, 120	0
48	DW	69/72 (95%)	0.27	4 (5%) 23 7	77, 100, 130, 167	0
49	BX	59/60 (98%)	0.11	2 (3%) 45 19	60, 75, 105, 120	0
49	DX	59/60 (98%)	0.62	2 (3%) 45 19	73, 98, 130, 153	0
50	B4	66/71 (92%)	1.49	18 (27%) 0 0	111, 146, 164, 173	0
50	D4	63/71 (88%)	3.03	43 (68%) 0 0	140, 176, 185, 191	0
51	B5	59/60 (98%)	0.93	11 (18%) 1 0	43, 80, 163, 168	0
51	D5	58/60 (96%)	0.43	6 (10%) 6 2	52, 78, 167, 178	0
52	B6	45/54 (83%)	2.85	27 (60%) 0 0	105, 134, 156, 160	0
52	D6	45/54 (83%)	3.12	30 (66%) 0 0	121, 156, 173, 176	0
53	B7	49/49 (100%)	-0.10	2 (4%) 37 14	35, 45, 88, 118	0
53	D7	49/49 (100%)	0.26	3 (6%) 21 7	44, 54, 112, 131	0
54	B8	61/65 (93%)	-0.04	1 (1%) 72 44	51, 64, 81, 102	0
54	D8	61/65 (93%)	0.60	4 (6%) 18 5	65, 79, 94, 123	0
All	All	21104/21634 (97%)	0.11	1258 (5%) 21 7	35, 96, 177, 235	0

The worst 5 of 1258 RSRZ outliers are listed below:

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

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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	CA	1714	1/1	0.18	0.60	92,92,92,92	0
55	MG	CA	1805	1/1	0.19	0.28	94,94,94,94	0
55	MG	DA	3315	1/1	0.23	0.28	108,108,108,108	0
55	MG	BA	3490	1/1	0.28	0.08	166,166,166,166	0
55	MG	CC	107	1/1	0.31	0.63	99,99,99,99	0
55	MG	DA	3487	1/1	0.37	0.39	95,95,95,95	0
55	MG	BA	3461	1/1	0.39	0.27	91,91,91,91	0
55	MG	BA	3547	1/1	0.41	0.41	77,77,77,77	0
55	MG	DA	3490	1/1	0.42	0.14	126,126,126,126	0
55	MG	BA	3334	1/1	0.43	0.56	96,96,96,96	0
55	MG	AD	101	1/1	0.45	0.39	101,101,101,101	0
55	MG	DB	213	1/1	0.45	0.16	94,94,94,94	0
55	MG	DA	3491	1/1	0.46	0.61	103,103,103,103	0
55	MG	CA	1751	1/1	0.46	0.27	94,94,94,94	0
55	MG	D1	202	1/1	0.46	0.46	89,89,89,89	0
55	MG	BA	3463	1/1	0.47	0.30	72,72,72,72	0
55	MG	CA	1689	1/1	0.48	0.29	89,89,89,89	0
55	MG	DA	3500	1/1	0.48	0.33	92,92,92,92	0
55	MG	AA	1758	1/1	0.49	0.35	85,85,85,85	0
55	MG	AH	201	1/1	0.49	0.39	99,99,99,99	0
55	MG	DA	3464	1/1	0.49	0.49	98,98,98,98	0
55	MG	BA	3580	1/1	0.50	0.21	71,71,71,71	0
55	MG	DA	3357	1/1	0.51	0.29	96,96,96,96	0
55	MG	AA	1700	1/1	0.51	0.21	99,99,99,99	0
55	MG	BA	3325	1/1	0.52	0.43	76,76,76,76	0
55	MG	AQ	101	1/1	0.52	0.15	88,88,88,88	0
55	MG	AA	1772	1/1	0.52	0.55	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	AA	1725	1/1	0.53	0.19	82,82,82,82	0
55	MG	DA	3441	1/1	0.53	0.10	137,137,137,137	0
55	MG	AA	1755	1/1	0.53	0.55	104,104,104,104	0
55	MG	AA	1751	1/1	0.54	0.29	98,98,98,98	0
55	MG	DA	3429	1/1	0.54	0.33	99,99,99,99	0
55	MG	DB	207	1/1	0.55	0.33	115,115,115,115	0
55	MG	DA	3304	1/1	0.55	0.37	85,85,85,85	0
55	MG	BA	3465	1/1	0.55	0.46	93,93,93,93	0
55	MG	BA	3151	1/1	0.56	0.27	83,83,83,83	0
55	MG	DA	3303	1/1	0.57	0.40	70,70,70,70	0
55	MG	AA	1715	1/1	0.57	0.27	115,115,115,115	0
55	MG	BA	3500	1/1	0.58	0.28	97,97,97,97	0
55	MG	BA	3075	1/1	0.58	0.27	110,110,110,110	0
55	MG	CA	1769	1/1	0.59	0.33	105,105,105,105	0
55	MG	BD	301	1/1	0.59	0.61	85,85,85,85	0
55	MG	BA	3379	1/1	0.59	0.45	82,82,82,82	0
55	MG	DA	3380	1/1	0.59	0.18	139,139,139,139	0
55	MG	DA	3064	1/1	0.59	0.43	101,101,101,101	0
55	MG	DA	3146	1/1	0.59	0.53	92,92,92,92	0
55	MG	CA	1763	1/1	0.59	0.47	91,91,91,91	0
55	MG	AA	1753	1/1	0.61	0.10	108,108,108,108	0
55	MG	DA	3010	1/1	0.61	0.40	97,97,97,97	0
55	MG	CS	101	1/1	0.61	0.30	87,87,87,87	0
55	MG	DA	3492	1/1	0.61	0.34	88,88,88,88	0
55	MG	DA	3042	1/1	0.62	0.50	81,81,81,81	0
55	MG	AA	1703	1/1	0.62	0.24	92,92,92,92	0
55	MG	AA	1777	1/1	0.62	0.39	90,90,90,90	0
55	MG	DA	3151	1/1	0.62	0.25	85,85,85,85	0
55	MG	AA	1727	1/1	0.62	0.86	87,87,87,87	0
55	MG	CA	1741	1/1	0.63	0.14	106,106,106,106	0
55	MG	AA	1731	1/1	0.63	0.30	103,103,103,103	0
55	MG	BA	3603	1/1	0.64	0.61	63,63,63,63	0
55	MG	DA	3522	1/1	0.64	0.48	78,78,78,78	0
55	MG	BA	3541	1/1	0.64	0.20	96,96,96,96	0
55	MG	DA	3447	1/1	0.64	0.46	82,82,82,82	0
55	MG	CA	1757	1/1	0.64	0.21	97,97,97,97	0
55	MG	DA	3119	1/1	0.65	0.44	98,98,98,98	0
55	MG	DA	3273	1/1	0.66	0.19	99,99,99,99	0
55	MG	CG	301	1/1	0.66	0.36	83,83,83,83	0
55	MG	BA	3420	1/1	0.66	0.34	94,94,94,94	0
55	MG	DA	3517	1/1	0.66	0.40	84,84,84,84	0
55	MG	DA	3461	1/1	0.66	0.23	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	CC	101	1/1	0.66	0.36	92,92,92,92	0
55	MG	CA	1664	1/1	0.66	0.29	99,99,99,99	0
55	MG	CA	1807	1/1	0.66	0.24	126,126,126,126	0
55	MG	DA	3402	1/1	0.67	0.32	101,101,101,101	0
55	MG	CA	1759	1/1	0.67	0.37	103,103,103,103	0
55	MG	DA	3494	1/1	0.67	0.21	75,75,75,75	0
55	MG	DA	3068	1/1	0.67	0.18	91,91,91,91	0
55	MG	DA	3507	1/1	0.67	0.44	91,91,91,91	0
55	MG	CA	1762	1/1	0.67	0.31	96,96,96,96	0
55	MG	DA	3120	1/1	0.67	0.26	90,90,90,90	0
55	MG	DA	3350	1/1	0.67	0.25	91,91,91,91	0
55	MG	BA	3484	1/1	0.67	0.23	117,117,117,117	0
55	MG	BA	3272	1/1	0.67	0.17	94,94,94,94	0
55	MG	DA	3459	1/1	0.68	0.28	86,86,86,86	0
55	MG	BA	3570	1/1	0.68	0.41	87,87,87,87	0
55	MG	AA	1680	1/1	0.68	0.29	80,80,80,80	0
55	MG	AA	1769	1/1	0.68	0.14	104,104,104,104	0
55	MG	DA	3028	1/1	0.68	0.22	101,101,101,101	0
55	MG	BA	3606	1/1	0.68	0.35	77,77,77,77	0
55	MG	AA	1630	1/1	0.68	0.16	101,101,101,101	0
55	MG	DA	3371	1/1	0.68	0.49	82,82,82,82	0
55	MG	BA	3349	1/1	0.68	0.42	97,97,97,97	0
55	MG	DA	3401	1/1	0.68	0.16	71,71,71,71	0
55	MG	AA	1720	1/1	0.68	0.19	93,93,93,93	0
55	MG	DA	3422	1/1	0.68	0.39	84,84,84,84	0
55	MG	CA	1696	1/1	0.68	0.37	91,91,91,91	0
55	MG	BA	3086	1/1	0.68	0.31	95,95,95,95	0
55	MG	AA	1804	1/1	0.68	0.11	74,74,74,74	0
55	MG	AB	103	1/1	0.69	0.30	111,111,111,111	0
55	MG	DA	3480	1/1	0.69	0.41	63,63,63,63	0
55	MG	CA	1660	1/1	0.69	0.17	85,85,85,85	0
55	MG	BA	3227	1/1	0.69	0.40	91,91,91,91	0
55	MG	BA	3472	1/1	0.69	0.61	89,89,89,89	0
55	MG	AA	1836	1/1	0.69	0.60	79,79,79,79	0
55	MG	DA	3020	1/1	0.69	0.32	85,85,85,85	0
55	MG	DA	3338	1/1	0.70	0.31	86,86,86,86	0
55	MG	BA	3415	1/1	0.70	0.37	84,84,84,84	0
55	MG	BA	3527	1/1	0.70	0.55	93,93,93,93	0
55	MG	AA	1621	1/1	0.70	0.19	108,108,108,108	0
55	MG	DA	3059	1/1	0.70	0.77	106,106,106,106	0
55	MG	AA	1770	1/1	0.70	0.25	102,102,102,102	0
55	MG	CA	1638	1/1	0.70	0.33	101,101,101,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	BA	3057	1/1	0.70	0.14	70,70,70,70	0
55	MG	DA	3335	1/1	0.70	0.21	61,61,61,61	0
55	MG	AA	1612	1/1	0.71	0.14	91,91,91,91	0
55	MG	AA	1781	1/1	0.71	0.43	94,94,94,94	0
55	MG	DA	3465	1/1	0.71	0.34	74,74,74,74	0
55	MG	BA	3397	1/1	0.71	0.24	81,81,81,81	0
55	MG	CA	1758	1/1	0.71	0.46	78,78,78,78	0
55	MG	BA	3087	1/1	0.71	0.38	77,77,77,77	0
55	MG	AA	1690	1/1	0.71	0.17	96,96,96,96	0
55	MG	CA	1630	1/1	0.71	0.45	91,91,91,91	0
55	MG	CA	1709	1/1	0.72	0.50	108,108,108,108	0
55	MG	DA	3290	1/1	0.72	0.31	79,79,79,79	0
55	MG	BA	3402	1/1	0.72	0.27	91,91,91,91	0
55	MG	CA	1632	1/1	0.72	0.30	95,95,95,95	0
55	MG	AA	1635	1/1	0.72	0.24	86,86,86,86	0
55	MG	DA	3320	1/1	0.72	0.15	76,76,76,76	0
55	MG	CA	1644	1/1	0.72	0.29	120,120,120,120	0
55	MG	AA	1681	1/1	0.72	0.33	80,80,80,80	0
55	MG	BA	3324	1/1	0.72	0.50	73,73,73,73	0
55	MG	DA	3353	1/1	0.72	0.75	93,93,93,93	0
55	MG	AA	1662	1/1	0.72	0.64	81,81,81,81	0
55	MG	BA	3399	1/1	0.72	0.58	90,90,90,90	0
55	MG	DA	3080	1/1	0.73	0.55	75,75,75,75	0
55	MG	DA	3344	1/1	0.73	0.33	95,95,95,95	0
55	MG	BA	3481	1/1	0.73	0.55	69,69,69,69	0
55	MG	AA	1826	1/1	0.73	0.12	101,101,101,101	0
55	MG	BA	3573	1/1	0.73	0.46	83,83,83,83	0
55	MG	AA	1782	1/1	0.73	0.19	96,96,96,96	0
55	MG	BA	3598	1/1	0.73	0.38	77,77,77,77	0
55	MG	DA	3396	1/1	0.73	0.25	82,82,82,82	0
55	MG	DA	3277	1/1	0.73	0.28	89,89,89,89	0
55	MG	BA	3354	1/1	0.73	0.21	72,72,72,72	0
55	MG	BA	3505	1/1	0.73	0.48	96,96,96,96	0
55	MG	DA	3508	1/1	0.73	0.70	80,80,80,80	0
55	MG	DA	3424	1/1	0.73	0.73	70,70,70,70	0
55	MG	BA	3232	1/1	0.73	0.31	72,72,72,72	0
55	MG	CA	1614	1/1	0.73	0.38	86,86,86,86	0
55	MG	DB	208	1/1	0.73	0.22	90,90,90,90	0
55	MG	DA	3067	1/1	0.73	0.35	94,94,94,94	0
55	MG	BA	3417	1/1	0.73	0.27	99,99,99,99	0
55	MG	BA	3121	1/1	0.74	0.48	57,57,57,57	0
55	MG	DA	3485	1/1	0.74	0.20	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	1645	1/1	0.74	0.22	86,86,86,86	0
55	MG	BA	3327	1/1	0.74	0.20	70,70,70,70	0
55	MG	AA	1807	1/1	0.74	0.60	98,98,98,98	0
55	MG	BB	208	1/1	0.74	0.25	74,74,74,74	0
55	MG	CA	1770	1/1	0.74	0.23	102,102,102,102	0
55	MG	BA	3467	1/1	0.74	0.32	78,78,78,78	0
55	MG	DA	3425	1/1	0.74	0.25	81,81,81,81	0
55	MG	BA	3282	1/1	0.74	0.09	83,83,83,83	0
55	MG	BA	3290	1/1	0.74	0.39	97,97,97,97	0
55	MG	DA	3088	1/1	0.74	0.24	96,96,96,96	0
55	MG	BA	3106	1/1	0.74	0.36	75,75,75,75	0
55	MG	BA	3431	1/1	0.74	0.71	88,88,88,88	0
55	MG	DB	211	1/1	0.74	0.41	93,93,93,93	0
55	MG	DA	3134	1/1	0.74	0.28	72,72,72,72	0
55	MG	CA	1641	1/1	0.74	0.29	66,66,66,66	0
55	MG	BA	3368	1/1	0.75	0.30	88,88,88,88	0
55	MG	DA	3404	1/1	0.75	0.30	61,61,61,61	0
55	MG	DA	3415	1/1	0.75	0.54	96,96,96,96	0
55	MG	BA	3059	1/1	0.75	0.38	91,91,91,91	0
55	MG	CA	1729	1/1	0.75	0.84	77,77,77,77	0
55	MG	CA	1637	1/1	0.75	0.34	79,79,79,79	0
55	MG	BA	3591	1/1	0.75	0.47	64,64,64,64	0
55	MG	CC	104	1/1	0.75	0.59	89,89,89,89	0
55	MG	BA	3466	1/1	0.75	0.44	97,97,97,97	0
55	MG	BA	3342	1/1	0.75	0.30	66,66,66,66	0
55	MG	BA	3534	1/1	0.75	0.30	79,79,79,79	0
55	MG	AA	1813	1/1	0.75	0.29	107,107,107,107	0
55	MG	BB	216	1/1	0.75	0.15	94,94,94,94	0
55	MG	BA	3446	1/1	0.75	0.19	92,92,92,92	0
55	MG	AA	1614	1/1	0.75	0.26	91,91,91,91	0
55	MG	DA	3366	1/1	0.76	0.43	83,83,83,83	0
55	MG	DA	3236	1/1	0.76	0.32	55,55,55,55	0
55	MG	BA	3408	1/1	0.76	0.45	87,87,87,87	0
55	MG	DA	3394	1/1	0.76	0.20	90,90,90,90	0
55	MG	AB	105	1/1	0.76	0.19	110,110,110,110	0
55	MG	AA	1822	1/1	0.76	0.14	107,107,107,107	0
55	MG	DA	3298	1/1	0.76	0.33	77,77,77,77	0
55	MG	DA	3493	1/1	0.76	0.55	82,82,82,82	0
55	MG	BE	304	1/1	0.76	0.37	80,80,80,80	0
55	MG	CA	1699	1/1	0.76	0.27	97,97,97,97	0
55	MG	BA	3418	1/1	0.76	0.41	78,78,78,78	0
55	MG	BA	3072	1/1	0.76	0.29	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	BA	3098	1/1	0.76	0.25	48,48,48,48	0
55	MG	BA	3583	1/1	0.76	0.50	86,86,86,86	0
55	MG	DA	3340	1/1	0.76	0.20	85,85,85,85	0
55	MG	BA	3073	1/1	0.76	0.42	82,82,82,82	0
55	MG	BA	3341	1/1	0.76	0.25	81,81,81,81	0
55	MG	BA	3462	1/1	0.76	0.27	87,87,87,87	0
55	MG	BA	3116	1/1	0.76	0.33	73,73,73,73	0
55	MG	DA	3312	1/1	0.77	0.29	85,85,85,85	0
55	MG	BA	3509	1/1	0.77	0.29	83,83,83,83	0
55	MG	AA	1820	1/1	0.77	0.30	75,75,75,75	0
55	MG	DA	3011	1/1	0.77	0.21	65,65,65,65	0
55	MG	BA	3247	1/1	0.77	0.48	70,70,70,70	0
55	MG	DA	3137	1/1	0.77	0.18	82,82,82,82	0
55	MG	AA	1616	1/1	0.77	0.18	94,94,94,94	0
55	MG	DA	3038	1/1	0.77	0.47	97,97,97,97	0
55	MG	BA	3339	1/1	0.77	0.58	88,88,88,88	0
55	MG	AA	1647	1/1	0.77	0.36	88,88,88,88	0
55	MG	BA	3069	1/1	0.77	0.45	77,77,77,77	0
55	MG	BA	3317	1/1	0.77	0.73	89,89,89,89	0
55	MG	AA	1706	1/1	0.77	0.46	74,74,74,74	0
55	MG	DA	3381	1/1	0.77	0.47	99,99,99,99	0
55	MG	DA	3078	1/1	0.77	0.37	89,89,89,89	0
55	MG	CA	1616	1/1	0.77	0.28	88,88,88,88	0
55	MG	BA	3412	1/1	0.78	0.35	78,78,78,78	0
55	MG	CA	1749	1/1	0.78	0.20	89,89,89,89	0
55	MG	BA	3385	1/1	0.78	0.16	87,87,87,87	0
55	MG	BA	3332	1/1	0.78	0.32	61,61,61,61	0
55	MG	BA	3367	1/1	0.78	0.26	82,82,82,82	0
55	MG	CA	1612	1/1	0.78	0.51	82,82,82,82	0
55	MG	CA	1683	1/1	0.78	0.41	87,87,87,87	0
55	MG	DA	3186	1/1	0.78	0.31	60,60,60,60	0
55	MG	DA	3029	1/1	0.78	0.27	79,79,79,79	0
55	MG	BA	3133	1/1	0.78	0.29	66,66,66,66	0
55	MG	DA	3393	1/1	0.78	0.52	69,69,69,69	0
55	MG	DA	3274	1/1	0.78	0.30	87,87,87,87	0
55	MG	BA	3054	1/1	0.78	0.25	80,80,80,80	0
55	MG	DA	3045	1/1	0.78	0.54	94,94,94,94	0
55	MG	DA	3058	1/1	0.78	0.31	76,76,76,76	0
55	MG	BA	3432	1/1	0.78	0.32	80,80,80,80	0
55	MG	DA	3406	1/1	0.78	0.73	86,86,86,86	0
55	MG	DA	3409	1/1	0.78	0.50	76,76,76,76	0
55	MG	CA	1797	1/1	0.78	0.32	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	DA	3524	1/1	0.78	0.28	105,105,105,105	0
55	MG	DA	3419	1/1	0.78	0.45	84,84,84,84	0
55	MG	CA	1702	1/1	0.78	0.41	78,78,78,78	0
55	MG	BA	3530	1/1	0.78	0.30	81,81,81,81	0
55	MG	BA	3442	1/1	0.78	0.37	76,76,76,76	0
55	MG	BA	3536	1/1	0.78	0.68	73,73,73,73	0
55	MG	AA	1761	1/1	0.79	0.41	113,113,113,113	0
55	MG	CA	1734	1/1	0.79	0.25	93,93,93,93	0
55	MG	BA	3533	1/1	0.79	0.57	72,72,72,72	0
55	MG	BA	3388	1/1	0.79	0.49	88,88,88,88	0
55	MG	AA	1679	1/1	0.79	0.28	86,86,86,86	0
55	MG	CA	1756	1/1	0.79	0.40	81,81,81,81	0
55	MG	DA	3057	1/1	0.79	0.35	83,83,83,83	0
55	MG	BA	3328	1/1	0.79	0.71	69,69,69,69	0
55	MG	AA	1708	1/1	0.79	0.40	91,91,91,91	0
55	MG	DA	3462	1/1	0.79	0.78	107,107,107,107	0
55	MG	BA	3563	1/1	0.79	0.19	82,82,82,82	0
55	MG	BA	3404	1/1	0.79	0.17	60,60,60,60	0
55	MG	AA	1735	1/1	0.79	0.46	79,79,79,79	0
55	MG	DA	3346	1/1	0.79	0.58	75,75,75,75	0
55	MG	CA	1766	1/1	0.79	0.30	85,85,85,85	0
55	MG	AA	1710	1/1	0.79	0.29	92,92,92,92	0
55	MG	AA	1696	1/1	0.79	0.29	88,88,88,88	0
55	MG	DA	3091	1/1	0.79	0.31	92,92,92,92	0
55	MG	AA	1754	1/1	0.79	0.19	95,95,95,95	0
55	MG	BA	3080	1/1	0.79	0.17	91,91,91,91	0
55	MG	DA	3123	1/1	0.79	0.25	83,83,83,83	0
55	MG	DA	3387	1/1	0.79	0.29	92,92,92,92	0
55	MG	AB	102	1/1	0.79	0.26	86,86,86,86	0
55	MG	AA	1786	1/1	0.79	0.19	86,86,86,86	0
55	MG	AA	1611	1/1	0.79	0.18	92,92,92,92	0
55	MG	BB	209	1/1	0.79	0.40	102,102,102,102	0
55	MG	BB	210	1/1	0.79	0.40	64,64,64,64	0
55	MG	BB	214	1/1	0.79	0.24	86,86,86,86	0
55	MG	DA	3251	1/1	0.79	0.27	74,74,74,74	0
55	MG	AA	1625	1/1	0.79	0.45	57,57,57,57	0
55	MG	DR	201	1/1	0.79	0.22	71,71,71,71	0
55	MG	BB	217	1/1	0.79	0.18	98,98,98,98	0
55	MG	AA	1652	1/1	0.80	0.44	81,81,81,81	0
55	MG	BA	3571	1/1	0.80	0.36	92,92,92,92	0
55	MG	AA	1617	1/1	0.80	0.50	69,69,69,69	0
55	MG	BA	3304	1/1	0.80	0.28	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	BA	3313	1/1	0.80	0.18	88,88,88,88	0
55	MG	CA	1667	1/1	0.80	0.16	102,102,102,102	0
55	MG	DA	3476	1/1	0.80	0.33	107,107,107,107	0
55	MG	DA	3479	1/1	0.80	0.11	99,99,99,99	0
55	MG	DA	3187	1/1	0.80	0.45	42,42,42,42	0
55	MG	CA	1669	1/1	0.80	0.19	60,60,60,60	0
55	MG	DA	3043	1/1	0.80	0.23	82,82,82,82	0
55	MG	CA	1604	1/1	0.80	0.17	81,81,81,81	0
55	MG	BA	3104	1/1	0.80	0.20	57,57,57,57	0
55	MG	AA	1785	1/1	0.80	0.40	96,96,96,96	0
55	MG	BA	3084	1/1	0.80	0.52	82,82,82,82	0
55	MG	DA	3297	1/1	0.80	0.23	83,83,83,83	0
55	MG	DA	3403	1/1	0.80	0.47	76,76,76,76	0
55	MG	CA	1771	1/1	0.80	0.42	76,76,76,76	0
55	MG	CA	1618	1/1	0.80	0.17	93,93,93,93	0
55	MG	DA	3512	1/1	0.80	0.48	75,75,75,75	0
55	MG	CA	1623	1/1	0.80	0.10	90,90,90,90	0
55	MG	DA	3070	1/1	0.80	0.28	78,78,78,78	0
55	MG	BA	3473	1/1	0.80	0.49	76,76,76,76	0
55	MG	CA	1727	1/1	0.80	0.45	94,94,94,94	0
55	MG	AA	1812	1/1	0.80	0.59	73,73,73,73	0
55	MG	BA	3403	1/1	0.80	0.66	93,93,93,93	0
55	MG	CA	1740	1/1	0.80	0.33	68,68,68,68	0
55	MG	DA	3431	1/1	0.80	0.43	91,91,91,91	0
55	MG	BA	3366	1/1	0.80	1.04	94,94,94,94	0
55	MG	AA	1840	1/1	0.81	0.47	87,87,87,87	0
55	MG	BA	3301	1/1	0.81	0.32	76,76,76,76	0
55	MG	CA	1661	1/1	0.81	0.22	87,87,87,87	0
55	MG	DA	3139	1/1	0.81	0.44	80,80,80,80	0
55	MG	CA	1777	1/1	0.81	0.30	88,88,88,88	0
55	MG	BA	3361	1/1	0.81	0.41	64,64,64,64	0
55	MG	DA	3417	1/1	0.81	0.22	81,81,81,81	0
55	MG	BA	3614	1/1	0.81	0.17	69,69,69,69	0
55	MG	AA	1705	1/1	0.81	0.31	83,83,83,83	0
55	MG	CA	1677	1/1	0.81	0.42	73,73,73,73	0
55	MG	CA	1681	1/1	0.81	0.52	72,72,72,72	0
55	MG	AA	1702	1/1	0.81	0.19	93,93,93,93	0
55	MG	BA	3526	1/1	0.81	0.39	86,86,86,86	0
55	MG	DA	3440	1/1	0.81	0.36	86,86,86,86	0
55	MG	CA	1693	1/1	0.81	0.54	76,76,76,76	0
55	MG	DA	3007	1/1	0.81	0.25	74,74,74,74	0
55	MG	DA	3448	1/1	0.81	0.71	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	AA	1730	1/1	0.81	0.43	78,78,78,78	0
55	MG	BA	3438	1/1	0.81	0.41	91,91,91,91	0
55	MG	DA	3302	1/1	0.81	0.57	95,95,95,95	0
55	MG	AA	1719	1/1	0.81	0.60	79,79,79,79	0
55	MG	AA	1790	1/1	0.81	0.24	98,98,98,98	0
55	MG	BA	3457	1/1	0.81	0.91	88,88,88,88	0
55	MG	DA	3478	1/1	0.81	0.32	80,80,80,80	0
55	MG	CA	1719	1/1	0.81	0.23	129,129,129,129	0
55	MG	B3	101	1/1	0.81	0.55	71,71,71,71	0
55	MG	DA	3330	1/1	0.81	0.14	81,81,81,81	0
55	MG	DA	3333	1/1	0.81	0.52	87,87,87,87	0
55	MG	BA	3175	1/1	0.81	0.52	69,69,69,69	0
55	MG	CA	1732	1/1	0.81	0.21	109,109,109,109	0
55	MG	BA	3546	1/1	0.81	0.16	87,87,87,87	0
55	MG	DA	3341	1/1	0.81	0.52	84,84,84,84	0
55	MG	AC	103	1/1	0.81	0.38	66,66,66,66	0
55	MG	BA	3330	1/1	0.81	0.29	79,79,79,79	0
55	MG	DA	3502	1/1	0.81	0.50	97,97,97,97	0
55	MG	AA	1698	1/1	0.81	0.33	72,72,72,72	0
55	MG	AA	1832	1/1	0.81	0.35	94,94,94,94	0
55	MG	CA	1755	1/1	0.81	0.49	92,92,92,92	0
55	MG	CA	1626	1/1	0.81	0.18	93,93,93,93	0
55	MG	DA	3072	1/1	0.81	0.44	112,112,112,112	0
55	MG	BA	3088	1/1	0.81	0.17	77,77,77,77	0
55	MG	BA	3579	1/1	0.81	0.13	92,92,92,92	0
55	MG	BA	3277	1/1	0.81	0.30	86,86,86,86	0
55	MG	BA	3409	1/1	0.81	0.20	68,68,68,68	0
55	MG	DA	3092	1/1	0.81	0.30	68,68,68,68	0
55	MG	AA	1806	1/1	0.81	0.28	81,81,81,81	0
55	MG	BA	3592	1/1	0.81	0.36	89,89,89,89	0
55	MG	DU	201	1/1	0.81	0.15	72,72,72,72	0
55	MG	CA	1798	1/1	0.82	0.21	85,85,85,85	0
55	MG	BA	3588	1/1	0.82	0.34	83,83,83,83	0
55	MG	DA	3337	1/1	0.82	0.46	89,89,89,89	0
55	MG	BA	3521	1/1	0.82	0.60	79,79,79,79	0
55	MG	CA	1624	1/1	0.82	0.36	88,88,88,88	0
55	MG	BA	3250	1/1	0.82	0.15	60,60,60,60	0
55	MG	CB	101	1/1	0.82	0.20	101,101,101,101	0
55	MG	CB	103	1/1	0.82	0.46	103,103,103,103	0
55	MG	DA	3473	1/1	0.82	0.48	96,96,96,96	0
55	MG	BA	3597	1/1	0.82	0.23	79,79,79,79	0
55	MG	BA	3365	1/1	0.82	0.33	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	DA	3136	1/1	0.82	0.34	76,76,76,76	0
55	MG	BA	3265	1/1	0.82	0.74	60,60,60,60	0
55	MG	AA	1688	1/1	0.82	0.21	72,72,72,72	0
55	MG	BA	3613	1/1	0.82	0.28	93,93,93,93	0
55	MG	AA	1689	1/1	0.82	0.26	115,115,115,115	0
55	MG	BA	3370	1/1	0.82	0.46	56,56,56,56	0
55	MG	DA	3025	1/1	0.82	1.38	84,84,84,84	0
55	MG	AA	1677	1/1	0.82	0.32	87,87,87,87	0
55	MG	AA	1768	1/1	0.82	0.36	101,101,101,101	0
55	MG	BA	3476	1/1	0.82	0.26	81,81,81,81	0
55	MG	BA	3161	1/1	0.82	0.22	56,56,56,56	0
55	MG	DA	3505	1/1	0.82	0.48	81,81,81,81	0
55	MG	AA	1637	1/1	0.82	0.18	98,98,98,98	0
55	MG	DA	3281	1/1	0.82	0.88	76,76,76,76	0
55	MG	BA	3398	1/1	0.82	0.44	70,70,70,70	0
55	MG	BA	3572	1/1	0.82	0.30	87,87,87,87	0
55	MG	BA	3496	1/1	0.82	0.26	96,96,96,96	0
55	MG	B7	101	1/1	0.82	0.46	67,67,67,67	0
55	MG	AA	1713	1/1	0.82	0.31	115,115,115,115	0
55	MG	AA	1791	1/1	0.82	0.11	109,109,109,109	0
55	MG	DB	210	1/1	0.82	0.37	71,71,71,71	0
55	MG	AA	1728	1/1	0.82	0.13	108,108,108,108	0
55	MG	CA	1787	1/1	0.82	0.13	87,87,87,87	0
55	MG	BA	3586	1/1	0.82	0.35	63,63,63,63	0
55	MG	DA	3327	1/1	0.82	0.34	61,61,61,61	0
55	MG	DA	3075	1/1	0.82	0.35	79,79,79,79	0
55	MG	DA	3449	1/1	0.83	0.38	87,87,87,87	0
55	MG	DA	3129	1/1	0.83	0.25	82,82,82,82	0
55	MG	AA	1819	1/1	0.83	0.35	87,87,87,87	0
55	MG	AA	1776	1/1	0.83	0.18	82,82,82,82	0
55	MG	AA	1749	1/1	0.83	0.21	81,81,81,81	0
55	MG	AA	1823	1/1	0.83	0.44	77,77,77,77	0
55	MG	AA	1824	1/1	0.83	0.56	86,86,86,86	0
55	MG	DA	3364	1/1	0.83	0.27	71,71,71,71	0
55	MG	BA	3595	1/1	0.83	0.18	65,65,65,65	0
55	MG	BA	3345	1/1	0.83	0.71	73,73,73,73	0
55	MG	AA	1766	1/1	0.83	0.16	79,79,79,79	0
55	MG	DA	3484	1/1	0.83	0.40	83,83,83,83	0
55	MG	DA	3197	1/1	0.83	0.70	70,70,70,70	0
55	MG	AC	106	1/1	0.83	0.56	89,89,89,89	0
55	MG	BA	3359	1/1	0.83	0.43	79,79,79,79	0
55	MG	BA	3309	1/1	0.83	0.19	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	1773	1/1	0.83	0.73	92,92,92,92	0
55	MG	BA	3185	1/1	0.83	0.36	76,76,76,76	0
55	MG	CA	1712	1/1	0.83	0.53	86,86,86,86	0
55	MG	BA	3193	1/1	0.83	0.51	85,85,85,85	0
55	MG	CA	1636	1/1	0.83	0.27	78,78,78,78	0
55	MG	DA	3503	1/1	0.83	0.65	80,80,80,80	0
55	MG	CA	1801	1/1	0.83	0.28	89,89,89,89	0
55	MG	CA	1720	1/1	0.83	0.49	102,102,102,102	0
55	MG	AA	1828	1/1	0.83	0.11	105,105,105,105	0
55	MG	AA	1711	1/1	0.83	0.28	89,89,89,89	0
55	MG	DA	3513	1/1	0.83	0.76	67,67,67,67	0
55	MG	BB	212	1/1	0.83	0.50	81,81,81,81	0
55	MG	DA	3519	1/1	0.83	0.47	85,85,85,85	0
55	MG	AA	1797	1/1	0.83	0.11	99,99,99,99	0
55	MG	DA	3084	1/1	0.83	0.29	88,88,88,88	0
55	MG	DB	205	1/1	0.83	0.35	69,69,69,69	0
55	MG	DB	206	1/1	0.83	0.28	90,90,90,90	0
55	MG	DA	3085	1/1	0.83	0.32	91,91,91,91	0
55	MG	AA	1815	1/1	0.83	0.46	84,84,84,84	0
55	MG	BA	3252	1/1	0.83	0.43	67,67,67,67	0
55	MG	DA	3432	1/1	0.83	0.29	69,69,69,69	0
55	MG	BA	3441	1/1	0.83	0.20	86,86,86,86	0
55	MG	CA	1662	1/1	0.83	0.24	90,90,90,90	0
55	MG	DA	3002	1/1	0.83	0.33	93,93,93,93	0
55	MG	DA	3004	1/1	0.83	0.48	99,99,99,99	0
55	MG	BA	3401	1/1	0.84	0.45	62,62,62,62	0
55	MG	CA	1772	1/1	0.84	0.29	72,72,72,72	0
55	MG	DA	3309	1/1	0.84	0.21	94,94,94,94	0
55	MG	BA	3110	1/1	0.84	0.52	59,59,59,59	0
55	MG	BA	3256	1/1	0.84	0.41	61,61,61,61	0
55	MG	AA	1684	1/1	0.84	0.18	90,90,90,90	0
55	MG	CA	1790	1/1	0.84	0.19	110,110,110,110	0
55	MG	CA	1791	1/1	0.84	0.30	79,79,79,79	0
55	MG	CA	1608	1/1	0.84	0.30	81,81,81,81	0
55	MG	BA	3120	1/1	0.84	0.42	56,56,56,56	0
55	MG	AB	101	1/1	0.84	0.28	90,90,90,90	0
55	MG	CA	1802	1/1	0.84	0.45	74,74,74,74	0
55	MG	DA	3468	1/1	0.84	0.42	92,92,92,92	0
55	MG	AA	1803	1/1	0.84	0.29	91,91,91,91	0
55	MG	DA	3475	1/1	0.84	0.35	88,88,88,88	0
55	MG	BA	3350	1/1	0.84	0.32	55,55,55,55	0
55	MG	DA	3477	1/1	0.84	0.60	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	DA	3342	1/1	0.84	0.42	82,82,82,82	0
55	MG	AA	1759	1/1	0.84	0.36	77,77,77,77	0
55	MG	BA	3295	1/1	0.84	0.44	81,81,81,81	0
55	MG	DA	3483	1/1	0.84	0.15	90,90,90,90	0
55	MG	DA	3347	1/1	0.84	0.12	75,75,75,75	0
55	MG	CA	1625	1/1	0.84	0.21	90,90,90,90	0
55	MG	CB	102	1/1	0.84	0.28	87,87,87,87	0
55	MG	DA	3356	1/1	0.84	0.29	67,67,67,67	0
55	MG	BA	3300	1/1	0.84	0.35	88,88,88,88	0
55	MG	CA	1629	1/1	0.84	0.16	98,98,98,98	0
55	MG	BA	3517	1/1	0.84	0.54	70,70,70,70	0
55	MG	AA	1618	1/1	0.84	0.27	82,82,82,82	0
55	MG	DA	3497	1/1	0.84	0.36	74,74,74,74	0
55	MG	CA	1737	1/1	0.84	0.28	99,99,99,99	0
55	MG	DA	3501	1/1	0.84	0.92	88,88,88,88	0
55	MG	BA	3166	1/1	0.84	0.62	72,72,72,72	0
55	MG	DA	3384	1/1	0.84	0.42	65,65,65,65	0
55	MG	AA	1683	1/1	0.84	0.20	87,87,87,87	0
55	MG	DA	3389	1/1	0.84	0.79	64,64,64,64	0
55	MG	BA	3607	1/1	0.84	0.34	96,96,96,96	0
55	MG	AA	1729	1/1	0.84	0.36	113,113,113,113	0
55	MG	BA	3191	1/1	0.84	0.21	81,81,81,81	0
55	MG	AA	1723	1/1	0.84	0.32	84,84,84,84	0
55	MG	DA	3247	1/1	0.84	0.20	87,87,87,87	0
55	MG	CA	1656	1/1	0.84	0.30	92,92,92,92	0
55	MG	BA	3222	1/1	0.84	0.33	89,89,89,89	0
55	MG	DA	3525	1/1	0.84	0.78	79,79,79,79	0
55	MG	BA	3537	1/1	0.84	0.42	89,89,89,89	0
55	MG	BA	3052	1/1	0.84	0.20	64,64,64,64	0
55	MG	AA	1724	1/1	0.84	0.20	84,84,84,84	0
55	MG	DA	3283	1/1	0.84	0.44	61,61,61,61	0
55	MG	DA	3287	1/1	0.84	0.64	65,65,65,65	0
55	MG	AA	1816	1/1	0.84	0.24	81,81,81,81	0
55	MG	DA	3051	1/1	0.84	0.27	85,85,85,85	0
55	MG	AA	1757	1/1	0.84	0.06	110,110,110,110	0
55	MG	DA	3427	1/1	0.84	0.28	76,76,76,76	0
55	MG	BA	3400	1/1	0.84	0.52	80,80,80,80	0
55	MG	BA	3215	1/1	0.85	0.48	74,74,74,74	0
55	MG	AA	1802	1/1	0.85	0.45	85,85,85,85	0
55	MG	DA	3292	1/1	0.85	0.24	89,89,89,89	0
55	MG	BA	3391	1/1	0.85	0.46	86,86,86,86	0
55	MG	BA	3392	1/1	0.85	0.39	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	DA	3400	1/1	0.85	0.40	89,89,89,89	0
55	MG	BB	201	1/1	0.85	0.43	92,92,92,92	0
55	MG	BA	3485	1/1	0.85	0.26	80,80,80,80	0
55	MG	BA	3089	1/1	0.85	0.33	88,88,88,88	0
55	MG	DA	3094	1/1	0.85	0.94	94,94,94,94	0
55	MG	DA	3117	1/1	0.85	0.38	78,78,78,78	0
55	MG	BA	3495	1/1	0.85	0.25	123,123,123,123	0
55	MG	CA	1711	1/1	0.85	0.38	90,90,90,90	0
55	MG	BA	3134	1/1	0.85	0.18	81,81,81,81	0
55	MG	AA	1709	1/1	0.85	0.19	70,70,70,70	0
55	MG	DA	3131	1/1	0.85	0.25	79,79,79,79	0
55	MG	BA	3154	1/1	0.85	0.30	55,55,55,55	0
55	MG	CA	1780	1/1	0.85	0.32	88,88,88,88	0
55	MG	CA	1783	1/1	0.85	0.47	100,100,100,100	0
55	MG	AA	1651	1/1	0.85	0.56	71,71,71,71	0
55	MG	DA	3140	1/1	0.85	0.28	78,78,78,78	0
55	MG	DA	3509	1/1	0.85	0.41	64,64,64,64	0
55	MG	BA	3514	1/1	0.85	0.31	71,71,71,71	0
55	MG	BA	3164	1/1	0.85	0.68	86,86,86,86	0
55	MG	AA	1839	1/1	0.85	0.37	74,74,74,74	0
55	MG	CA	1659	1/1	0.85	0.20	110,110,110,110	0
55	MG	AA	1793	1/1	0.85	0.39	73,73,73,73	0
55	MG	B8	101	1/1	0.85	0.19	97,97,97,97	0
55	MG	DA	3237	1/1	0.85	0.27	83,83,83,83	0
55	MG	DA	3460	1/1	0.85	0.46	72,72,72,72	0
55	MG	DA	3061	1/1	0.85	0.56	74,74,74,74	0
55	MG	DA	3361	1/1	0.85	0.71	79,79,79,79	0
55	MG	BA	3112	1/1	0.85	0.28	77,77,77,77	0
55	MG	DB	209	1/1	0.85	0.20	92,92,92,92	0
55	MG	AA	1640	1/1	0.85	0.33	90,90,90,90	0
55	MG	DA	3467	1/1	0.85	0.40	61,61,61,61	0
55	MG	BA	3411	1/1	0.85	0.30	68,68,68,68	0
55	MG	CA	1753	1/1	0.85	0.26	123,123,123,123	0
55	MG	AC	105	1/1	0.85	0.50	93,93,93,93	0
55	MG	BA	3206	1/1	0.85	0.38	75,75,75,75	0
55	MG	CA	1672	1/1	0.86	0.75	75,75,75,75	0
55	MG	DA	3005	1/1	0.86	0.48	77,77,77,77	0
55	MG	AA	1626	1/1	0.86	0.46	69,69,69,69	0
55	MG	CA	1761	1/1	0.86	0.40	92,92,92,92	0
55	MG	DA	3466	1/1	0.86	0.63	78,78,78,78	0
55	MG	BA	3348	1/1	0.86	0.29	61,61,61,61	0
55	MG	BA	3394	1/1	0.86	0.19	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	BA	3396	1/1	0.86	0.19	82,82,82,82	0
55	MG	BA	3523	1/1	0.86	0.60	70,70,70,70	0
55	MG	BA	3310	1/1	0.86	0.37	57,57,57,57	0
55	MG	DA	3363	1/1	0.86	0.79	79,79,79,79	0
55	MG	DA	3164	1/1	0.86	0.45	47,47,47,47	0
55	MG	DA	3183	1/1	0.86	0.51	57,57,57,57	0
55	MG	DA	3367	1/1	0.86	0.43	82,82,82,82	0
55	MG	DA	3370	1/1	0.86	0.10	67,67,67,67	0
55	MG	CA	1698	1/1	0.86	0.09	107,107,107,107	0
55	MG	DA	3041	1/1	0.86	0.41	86,86,86,86	0
55	MG	DA	3486	1/1	0.86	0.32	68,68,68,68	0
55	MG	AA	1674	1/1	0.86	0.33	98,98,98,98	0
55	MG	AC	107	1/1	0.86	0.28	94,94,94,94	0
55	MG	BA	3356	1/1	0.86	0.51	70,70,70,70	0
55	MG	DA	3049	1/1	0.86	0.28	74,74,74,74	0
55	MG	BA	3357	1/1	0.86	0.56	81,81,81,81	0
55	MG	BA	3358	1/1	0.86	0.37	74,74,74,74	0
55	MG	BA	3140	1/1	0.86	0.25	58,58,58,58	0
55	MG	BA	3622	1/1	0.86	0.47	59,59,59,59	0
55	MG	AA	1795	1/1	0.86	0.23	73,73,73,73	0
55	MG	DA	3062	1/1	0.86	0.27	72,72,72,72	0
55	MG	CA	1796	1/1	0.86	0.40	102,102,102,102	0
55	MG	CA	1723	1/1	0.86	0.07	86,86,86,86	0
55	MG	BA	3362	1/1	0.86	0.24	48,48,48,48	0
55	MG	AA	1834	1/1	0.86	0.48	97,97,97,97	0
55	MG	DA	3413	1/1	0.86	0.29	94,94,94,94	0
55	MG	BA	3551	1/1	0.86	0.40	87,87,87,87	0
55	MG	CA	1804	1/1	0.86	0.30	75,75,75,75	0
55	MG	DA	3077	1/1	0.86	0.11	64,64,64,64	0
55	MG	BA	3285	1/1	0.86	0.35	72,72,72,72	0
55	MG	DA	3306	1/1	0.86	0.54	65,65,65,65	0
55	MG	BA	3565	1/1	0.86	0.28	77,77,77,77	0
55	MG	BA	3083	1/1	0.86	0.12	62,62,62,62	0
55	MG	CG	302	1/1	0.86	0.14	101,101,101,101	0
55	MG	DA	3430	1/1	0.86	0.58	62,62,62,62	0
55	MG	BA	3291	1/1	0.86	0.39	72,72,72,72	0
55	MG	CA	1745	1/1	0.86	0.12	91,91,91,91	0
55	MG	AA	1716	1/1	0.86	0.22	92,92,92,92	0
55	MG	BA	3371	1/1	0.86	0.31	70,70,70,70	0
55	MG	DA	3098	1/1	0.86	0.46	68,68,68,68	0
55	MG	DB	212	1/1	0.86	0.26	88,88,88,88	0
55	MG	B2	201	1/1	0.86	0.42	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	BA	3240	1/1	0.86	0.54	88,88,88,88	0
55	MG	AA	1638	1/1	0.86	0.31	104,104,104,104	0
55	MG	AA	1682	1/1	0.86	0.16	91,91,91,91	0
55	MG	CA	1774	1/1	0.87	0.13	104,104,104,104	0
55	MG	DA	3026	1/1	0.87	0.43	95,95,95,95	0
55	MG	DA	3482	1/1	0.87	0.45	81,81,81,81	0
55	MG	AA	1656	1/1	0.87	0.43	87,87,87,87	0
55	MG	DA	3319	1/1	0.87	0.40	74,74,74,74	0
55	MG	BA	3497	1/1	0.87	0.21	71,71,71,71	0
55	MG	AA	1778	1/1	0.87	0.14	106,106,106,106	0
55	MG	CA	1784	1/1	0.87	0.23	81,81,81,81	0
55	MG	CA	1725	1/1	0.87	0.24	86,86,86,86	0
55	MG	BA	3455	1/1	0.87	0.24	76,76,76,76	0
55	MG	BA	3578	1/1	0.87	0.35	81,81,81,81	0
55	MG	BA	3506	1/1	0.87	0.37	78,78,78,78	0
55	MG	BA	3319	1/1	0.87	0.28	65,65,65,65	0
55	MG	AA	1817	1/1	0.87	0.21	85,85,85,85	0
55	MG	DA	3168	1/1	0.87	0.29	49,49,49,49	0
55	MG	BA	3584	1/1	0.87	0.18	72,72,72,72	0
55	MG	BA	3375	1/1	0.87	0.25	50,50,50,50	0
55	MG	BA	3378	1/1	0.87	0.56	76,76,76,76	0
55	MG	CA	1601	1/1	0.87	0.31	96,96,96,96	0
55	MG	DA	3434	1/1	0.87	0.15	74,74,74,74	0
55	MG	DA	3438	1/1	0.87	0.25	87,87,87,87	0
55	MG	AA	1830	1/1	0.87	0.30	73,73,73,73	0
55	MG	AA	1752	1/1	0.87	0.27	78,78,78,78	0
55	MG	CA	1611	1/1	0.87	0.89	93,93,93,93	0
55	MG	DA	3515	1/1	0.87	0.63	82,82,82,82	0
55	MG	BA	3387	1/1	0.87	0.40	73,73,73,73	0
55	MG	BA	3471	1/1	0.87	0.31	72,72,72,72	0
55	MG	DA	3520	1/1	0.87	0.83	76,76,76,76	0
55	MG	DA	3455	1/1	0.87	0.29	69,69,69,69	0
55	MG	DA	3523	1/1	0.87	0.91	81,81,81,81	0
55	MG	AA	1633	1/1	0.87	0.25	74,74,74,74	0
55	MG	CA	1691	1/1	0.87	0.33	78,78,78,78	0
55	MG	DB	204	1/1	0.87	0.28	82,82,82,82	0
55	MG	AA	1835	1/1	0.87	0.29	87,87,87,87	0
55	MG	BA	3475	1/1	0.87	0.31	83,83,83,83	0
55	MG	AA	1742	1/1	0.87	0.17	78,78,78,78	0
55	MG	BA	3479	1/1	0.87	0.46	82,82,82,82	0
55	MG	DA	3291	1/1	0.87	0.59	65,65,65,65	0
55	MG	CA	1768	1/1	0.87	0.41	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	AA	1639	1/1	0.87	0.31	91,91,91,91	0
55	MG	BA	3090	1/1	0.87	0.47	49,49,49,49	0
55	MG	BA	3364	1/1	0.87	0.45	82,82,82,82	0
55	MG	BA	3203	1/1	0.87	0.33	85,85,85,85	0
55	MG	BA	3266	1/1	0.87	0.41	77,77,77,77	0
55	MG	DA	3023	1/1	0.87	0.44	57,57,57,57	0
55	MG	DA	3220	1/1	0.88	0.36	66,66,66,66	0
55	MG	BA	3445	1/1	0.88	0.35	79,79,79,79	0
55	MG	BA	3503	1/1	0.88	0.20	65,65,65,65	0
55	MG	CA	1615	1/1	0.88	0.22	81,81,81,81	0
55	MG	DA	3428	1/1	0.88	0.58	84,84,84,84	0
55	MG	AA	1821	1/1	0.88	0.23	75,75,75,75	0
55	MG	DA	3263	1/1	0.88	0.86	82,82,82,82	0
55	MG	BA	3448	1/1	0.88	0.43	100,100,100,100	0
55	MG	BA	3507	1/1	0.88	0.30	89,89,89,89	0
55	MG	AA	1737	1/1	0.88	0.55	83,83,83,83	0
55	MG	DA	3435	1/1	0.88	0.11	72,72,72,72	0
55	MG	DA	3436	1/1	0.88	0.30	98,98,98,98	0
55	MG	DA	3015	1/1	0.88	0.69	89,89,89,89	0
55	MG	DA	3439	1/1	0.88	0.33	62,62,62,62	0
55	MG	BA	3510	1/1	0.88	0.15	108,108,108,108	0
55	MG	BA	3511	1/1	0.88	0.15	89,89,89,89	0
55	MG	DA	3442	1/1	0.88	0.22	91,91,91,91	0
55	MG	BA	3267	1/1	0.88	0.30	61,61,61,61	0
55	MG	CA	1742	1/1	0.88	0.15	97,97,97,97	0
55	MG	BA	3114	1/1	0.88	0.20	74,74,74,74	0
55	MG	DA	3454	1/1	0.88	0.37	92,92,92,92	0
55	MG	CA	1747	1/1	0.88	0.26	94,94,94,94	0
55	MG	DA	3034	1/1	0.88	0.33	62,62,62,62	0
55	MG	AA	1739	1/1	0.88	0.07	93,93,93,93	0
55	MG	DA	3040	1/1	0.88	0.14	81,81,81,81	0
55	MG	CA	1634	1/1	0.88	0.45	77,77,77,77	0
55	MG	BA	3118	1/1	0.88	0.42	61,61,61,61	0
55	MG	BA	3204	1/1	0.88	0.34	78,78,78,78	0
55	MG	AC	109	1/1	0.88	0.41	82,82,82,82	0
55	MG	BA	3211	1/1	0.88	0.46	39,39,39,39	0
55	MG	CA	1643	1/1	0.88	0.49	82,82,82,82	0
55	MG	DA	3471	1/1	0.88	0.43	80,80,80,80	0
55	MG	BA	3531	1/1	0.88	0.36	53,53,53,53	0
55	MG	CA	1760	1/1	0.88	0.27	91,91,91,91	0
55	MG	BA	3621	1/1	0.88	0.15	63,63,63,63	0
55	MG	CA	1648	1/1	0.88	0.42	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	BA	3532	1/1	0.88	0.22	85,85,85,85	0
55	MG	CA	1657	1/1	0.88	0.27	95,95,95,95	0
55	MG	CA	1767	1/1	0.88	0.46	77,77,77,77	0
55	MG	DA	3481	1/1	0.88	0.41	96,96,96,96	0
55	MG	BA	3623	1/1	0.88	0.40	60,60,60,60	0
55	MG	AA	1675	1/1	0.88	0.45	80,80,80,80	0
55	MG	BB	204	1/1	0.88	0.31	78,78,78,78	0
55	MG	AA	1743	1/1	0.88	0.11	107,107,107,107	0
55	MG	AA	1744	1/1	0.88	0.13	117,117,117,117	0
55	MG	BA	3231	1/1	0.88	0.50	73,73,73,73	0
55	MG	AA	1745	1/1	0.88	0.56	67,67,67,67	0
55	MG	AA	1693	1/1	0.88	0.16	87,87,87,87	0
55	MG	CA	1673	1/1	0.88	0.53	64,64,64,64	0
55	MG	BA	3424	1/1	0.88	0.65	72,72,72,72	0
55	MG	DA	3090	1/1	0.88	0.33	86,86,86,86	0
55	MG	CA	1679	1/1	0.88	0.37	85,85,85,85	0
55	MG	BA	3482	1/1	0.88	0.39	57,57,57,57	0
55	MG	BA	3094	1/1	0.88	0.56	78,78,78,78	0
55	MG	CA	1686	1/1	0.88	0.42	73,73,73,73	0
55	MG	DA	3368	1/1	0.88	0.72	73,73,73,73	0
55	MG	DA	3504	1/1	0.88	0.34	65,65,65,65	0
55	MG	AA	1694	1/1	0.88	0.12	91,91,91,91	0
55	MG	BE	305	1/1	0.88	0.42	71,71,71,71	0
55	MG	DA	3376	1/1	0.88	0.53	82,82,82,82	0
55	MG	DA	3377	1/1	0.88	0.22	98,98,98,98	0
55	MG	BF	302	1/1	0.88	0.22	72,72,72,72	0
55	MG	CA	1800	1/1	0.88	0.32	78,78,78,78	0
55	MG	DA	3383	1/1	0.88	0.47	87,87,87,87	0
55	MG	DA	3125	1/1	0.88	0.43	45,45,45,45	0
55	MG	BA	3569	1/1	0.88	0.54	85,85,85,85	0
55	MG	CA	1697	1/1	0.88	0.30	65,65,65,65	0
55	MG	CA	1803	1/1	0.88	0.30	96,96,96,96	0
55	MG	BA	3489	1/1	0.88	0.24	70,70,70,70	0
55	MG	DA	3395	1/1	0.88	0.47	69,69,69,69	0
55	MG	BA	3395	1/1	0.88	0.31	72,72,72,72	0
55	MG	DA	3526	1/1	0.88	0.31	68,68,68,68	0
55	MG	DB	203	1/1	0.88	0.33	66,66,66,66	0
55	MG	DA	3399	1/1	0.88	0.45	76,76,76,76	0
55	MG	CA	1700	1/1	0.88	0.47	77,77,77,77	0
55	MG	AC	102	1/1	0.88	0.67	93,93,93,93	0
55	MG	CA	1707	1/1	0.88	0.57	98,98,98,98	0
55	MG	AA	1613	1/1	0.88	0.07	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	BA	3574	1/1	0.88	0.53	78,78,78,78	0
55	MG	DA	3405	1/1	0.88	0.47	79,79,79,79	0
55	MG	BA	3575	1/1	0.88	0.35	71,71,71,71	0
55	MG	DA	3175	1/1	0.88	0.34	83,83,83,83	0
55	MG	CA	1713	1/1	0.88	0.57	102,102,102,102	0
55	MG	DB	214	1/1	0.88	0.19	96,96,96,96	0
55	MG	DE	302	1/1	0.88	0.27	65,65,65,65	0
55	MG	CA	1609	1/1	0.88	0.16	115,115,115,115	0
55	MG	BA	3444	1/1	0.88	0.50	78,78,78,78	0
55	MG	CC	105	1/1	0.88	0.59	82,82,82,82	0
55	MG	DA	3307	1/1	0.89	0.26	77,77,77,77	0
55	MG	BA	3210	1/1	0.89	0.20	74,74,74,74	0
55	MG	BF	303	1/1	0.89	0.48	66,66,66,66	0
55	MG	BO	202	1/1	0.89	0.23	37,37,37,37	0
55	MG	CA	1684	1/1	0.89	0.61	85,85,85,85	0
55	MG	AA	1712	1/1	0.89	0.38	78,78,78,78	0
55	MG	CA	1687	1/1	0.89	0.17	89,89,89,89	0
55	MG	DA	3328	1/1	0.89	0.34	47,47,47,47	0
55	MG	CA	1781	1/1	0.89	0.05	117,117,117,117	0
55	MG	AA	1787	1/1	0.89	0.47	96,96,96,96	0
55	MG	AA	1722	1/1	0.89	0.46	68,68,68,68	0
55	MG	BA	3223	1/1	0.89	0.27	92,92,92,92	0
55	MG	BA	3416	1/1	0.89	0.18	87,87,87,87	0
55	MG	BA	3225	1/1	0.89	0.17	65,65,65,65	0
55	MG	BA	3494	1/1	0.89	0.77	76,76,76,76	0
55	MG	AN	202	1/1	0.89	0.32	82,82,82,82	0
55	MG	AA	1773	1/1	0.89	0.26	87,87,87,87	0
55	MG	BA	3314	1/1	0.89	0.58	64,64,64,64	0
55	MG	CA	1704	1/1	0.89	0.28	99,99,99,99	0
55	MG	BA	3425	1/1	0.89	0.51	91,91,91,91	0
55	MG	DA	3351	1/1	0.89	0.28	79,79,79,79	0
55	MG	DA	3352	1/1	0.89	0.65	64,64,64,64	0
55	MG	BA	3502	1/1	0.89	0.26	67,67,67,67	0
55	MG	A1	102	1/1	0.89	0.42	86,86,86,86	0
55	MG	BA	3034	1/1	0.89	0.34	41,41,41,41	0
55	MG	DA	3112	1/1	0.89	0.35	81,81,81,81	0
55	MG	BA	3435	1/1	0.89	0.28	65,65,65,65	0
55	MG	BA	3589	1/1	0.89	0.31	41,41,41,41	0
55	MG	CA	1715	1/1	0.89	0.25	104,104,104,104	0
55	MG	BA	3323	1/1	0.89	0.32	66,66,66,66	0
55	MG	AA	1615	1/1	0.89	0.55	105,105,105,105	0
55	MG	DA	3369	1/1	0.89	0.27	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	BA	3249	1/1	0.89	0.29	30,30,30,30	0
55	MG	DA	3488	1/1	0.89	0.58	86,86,86,86	0
55	MG	BA	3381	1/1	0.89	0.44	90,90,90,90	0
55	MG	BA	3053	1/1	0.89	0.28	95,95,95,95	0
55	MG	AA	1734	1/1	0.89	0.19	96,96,96,96	0
55	MG	BA	3447	1/1	0.89	0.49	71,71,71,71	0
55	MG	AA	1631	1/1	0.89	0.21	66,66,66,66	0
55	MG	BA	3331	1/1	0.89	0.42	65,65,65,65	0
55	MG	CA	1639	1/1	0.89	0.36	95,95,95,95	0
55	MG	DA	3150	1/1	0.89	0.34	68,68,68,68	0
55	MG	BA	3260	1/1	0.89	0.42	47,47,47,47	0
55	MG	DA	3391	1/1	0.89	0.23	78,78,78,78	0
55	MG	DA	3154	1/1	0.89	0.32	69,69,69,69	0
55	MG	BA	3619	1/1	0.89	0.33	69,69,69,69	0
55	MG	BA	3167	1/1	0.89	0.38	73,73,73,73	0
55	MG	DA	3173	1/1	0.89	0.22	60,60,60,60	0
55	MG	BA	3103	1/1	0.89	0.49	52,52,52,52	0
55	MG	DA	3511	1/1	0.89	0.43	76,76,76,76	0
55	MG	CA	1647	1/1	0.89	0.51	61,61,61,61	0
55	MG	DA	3018	1/1	0.89	0.28	77,77,77,77	0
55	MG	DA	3019	1/1	0.89	0.92	90,90,90,90	0
55	MG	AB	104	1/1	0.89	0.35	82,82,82,82	0
55	MG	BA	3270	1/1	0.89	0.22	76,76,76,76	0
55	MG	BA	3060	1/1	0.89	0.17	64,64,64,64	0
55	MG	BA	3273	1/1	0.89	0.41	94,94,94,94	0
55	MG	DA	3408	1/1	0.89	0.11	73,73,73,73	0
55	MG	DA	3027	1/1	0.89	0.23	77,77,77,77	0
55	MG	DA	3412	1/1	0.89	0.33	89,89,89,89	0
55	MG	BA	3061	1/1	0.89	0.54	61,61,61,61	0
55	MG	DB	201	1/1	0.89	0.37	81,81,81,81	0
55	MG	BA	3539	1/1	0.89	0.26	74,74,74,74	0
55	MG	AA	1673	1/1	0.89	0.47	78,78,78,78	0
55	MG	DA	3037	1/1	0.89	0.33	98,98,98,98	0
55	MG	CA	1663	1/1	0.89	0.35	81,81,81,81	0
55	MG	BA	3543	1/1	0.89	0.41	80,80,80,80	0
55	MG	CA	1665	1/1	0.89	0.17	83,83,83,83	0
55	MG	AA	1718	1/1	0.89	0.58	82,82,82,82	0
55	MG	CA	1668	1/1	0.89	0.42	79,79,79,79	0
55	MG	BA	3289	1/1	0.89	0.56	60,60,60,60	0
55	MG	DA	3047	1/1	0.89	0.42	76,76,76,76	0
55	MG	DA	3048	1/1	0.89	0.49	75,75,75,75	0
55	MG	BA	3548	1/1	0.89	0.48	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	AA	1643	1/1	0.89	0.62	85,85,85,85	0
55	MG	DA	3053	1/1	0.89	0.62	62,62,62,62	0
55	MG	D1	201	1/1	0.89	0.39	71,71,71,71	0
55	MG	DA	3055	1/1	0.89	0.54	68,68,68,68	0
55	MG	BA	3552	1/1	0.89	0.30	102,102,102,102	0
55	MG	AA	1668	1/1	0.90	0.63	76,76,76,76	0
55	MG	BA	3132	1/1	0.90	0.41	71,71,71,71	0
55	MG	DA	3279	1/1	0.90	0.24	84,84,84,84	0
55	MG	DA	3385	1/1	0.90	0.70	62,62,62,62	0
55	MG	DA	3076	1/1	0.90	0.37	86,86,86,86	0
55	MG	BA	3449	1/1	0.90	0.36	80,80,80,80	0
55	MG	BA	3451	1/1	0.90	0.48	65,65,65,65	0
55	MG	AA	1774	1/1	0.90	0.13	91,91,91,91	0
55	MG	CA	1688	1/1	0.90	0.34	71,71,71,71	0
55	MG	CA	1628	1/1	0.90	0.21	101,101,101,101	0
55	MG	AA	1692	1/1	0.90	0.13	115,115,115,115	0
55	MG	DA	3398	1/1	0.90	0.40	74,74,74,74	0
55	MG	BB	202	1/1	0.90	0.14	79,79,79,79	0
55	MG	AA	1678	1/1	0.90	0.35	74,74,74,74	0
55	MG	CA	1633	1/1	0.90	0.28	91,91,91,91	0
55	MG	BA	3281	1/1	0.90	0.54	72,72,72,72	0
55	MG	CA	1635	1/1	0.90	0.78	86,86,86,86	0
55	MG	BA	3321	1/1	0.90	0.41	77,77,77,77	0
55	MG	BA	3322	1/1	0.90	0.63	64,64,64,64	0
55	MG	BA	3144	1/1	0.90	0.29	48,48,48,48	0
55	MG	DA	3496	1/1	0.90	0.24	83,83,83,83	0
55	MG	BA	3516	1/1	0.90	0.86	78,78,78,78	0
55	MG	DA	3498	1/1	0.90	0.24	85,85,85,85	0
55	MG	AA	1624	1/1	0.90	0.28	79,79,79,79	0
55	MG	CA	1778	1/1	0.90	0.40	96,96,96,96	0
55	MG	BA	3421	1/1	0.90	0.35	62,62,62,62	0
55	MG	DA	3032	1/1	0.90	0.12	76,76,76,76	0
55	MG	BA	3423	1/1	0.90	0.56	61,61,61,61	0
55	MG	DA	3332	1/1	0.90	0.39	76,76,76,76	0
55	MG	BA	3393	1/1	0.90	0.51	81,81,81,81	0
55	MG	BA	3581	1/1	0.90	0.33	69,69,69,69	0
55	MG	DA	3336	1/1	0.90	0.41	87,87,87,87	0
55	MG	CA	1785	1/1	0.90	0.24	105,105,105,105	0
55	MG	AA	1653	1/1	0.90	0.53	81,81,81,81	0
55	MG	CA	1654	1/1	0.90	0.31	99,99,99,99	0
55	MG	DA	3514	1/1	0.90	0.68	59,59,59,59	0
55	MG	CA	1655	1/1	0.90	0.37	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	BA	3360	1/1	0.90	0.14	84,84,84,84	0
55	MG	AA	1808	1/1	0.90	0.54	76,76,76,76	0
55	MG	BA	3587	1/1	0.90	0.32	64,64,64,64	0
55	MG	AA	1809	1/1	0.90	0.36	63,63,63,63	0
55	MG	DA	3348	1/1	0.90	0.60	73,73,73,73	0
55	MG	DA	3437	1/1	0.90	0.20	87,87,87,87	0
55	MG	BA	3437	1/1	0.90	0.42	67,67,67,67	0
55	MG	BA	3292	1/1	0.90	0.40	85,85,85,85	0
55	MG	DA	3179	1/1	0.90	0.32	70,70,70,70	0
55	MG	DB	202	1/1	0.90	0.18	98,98,98,98	0
55	MG	BA	3535	1/1	0.90	0.44	80,80,80,80	0
55	MG	BA	3593	1/1	0.90	0.26	80,80,80,80	0
55	MG	CA	1606	1/1	0.90	0.35	87,87,87,87	0
55	MG	DA	3358	1/1	0.90	0.53	88,88,88,88	0
55	MG	BA	3439	1/1	0.90	0.36	71,71,71,71	0
55	MG	DA	3060	1/1	0.90	0.85	73,73,73,73	0
55	MG	DA	3225	1/1	0.90	0.59	73,73,73,73	0
55	MG	DA	3230	1/1	0.90	0.16	59,59,59,59	0
55	MG	BA	3257	1/1	0.90	0.25	64,64,64,64	0
55	MG	BA	3217	1/1	0.90	0.31	52,52,52,52	0
55	MG	AA	1664	1/1	0.90	0.20	45,45,45,45	0
55	MG	BA	3336	1/1	0.90	0.47	66,66,66,66	0
55	MG	DA	3253	1/1	0.90	0.17	87,87,87,87	0
55	MG	DA	3373	1/1	0.90	0.43	79,79,79,79	0
55	MG	BA	3544	1/1	0.90	0.40	72,72,72,72	0
55	MG	DA	3269	1/1	0.90	0.42	84,84,84,84	0
55	MG	BA	3038	1/1	0.90	0.40	56,56,56,56	0
55	MG	BA	3234	1/1	0.91	0.43	86,86,86,86	0
55	MG	AA	1767	1/1	0.91	0.22	96,96,96,96	0
55	MG	BA	3582	1/1	0.91	0.42	86,86,86,86	0
55	MG	CA	1794	1/1	0.91	0.34	74,74,74,74	0
55	MG	DA	3314	1/1	0.91	0.47	76,76,76,76	0
55	MG	DA	3073	1/1	0.91	0.52	80,80,80,80	0
55	MG	DA	3318	1/1	0.91	0.22	63,63,63,63	0
55	MG	BA	3246	1/1	0.91	0.40	68,68,68,68	0
55	MG	BA	3302	1/1	0.91	0.41	26,26,26,26	0
55	MG	BA	3513	1/1	0.91	0.41	90,90,90,90	0
55	MG	BA	3303	1/1	0.91	0.38	72,72,72,72	0
55	MG	DA	3451	1/1	0.91	0.47	75,75,75,75	0
55	MG	BA	3459	1/1	0.91	0.42	70,70,70,70	0
55	MG	BA	3460	1/1	0.91	0.13	83,83,83,83	0
55	MG	AA	1607	1/1	0.91	0.22	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	3305	1/1	0.91	0.42	70,70,70,70	0
55	MG	BA	3524	1/1	0.91	0.19	66,66,66,66	0
55	MG	CA	1627	1/1	0.91	0.31	88,88,88,88	0
55	MG	BA	3179	1/1	0.91	0.44	64,64,64,64	0
55	MG	DA	3093	1/1	0.91	0.20	80,80,80,80	0
55	MG	BA	3596	1/1	0.91	0.46	55,55,55,55	0
55	MG	AA	1644	1/1	0.91	0.16	62,62,62,62	0
55	MG	DA	3343	1/1	0.91	0.36	95,95,95,95	0
55	MG	CA	1718	1/1	0.91	0.07	92,92,92,92	0
55	MG	CA	1631	1/1	0.91	0.11	81,81,81,81	0
55	MG	BA	3187	1/1	0.91	0.48	73,73,73,73	0
55	MG	BA	3601	1/1	0.91	0.20	85,85,85,85	0
55	MG	DA	3349	1/1	0.91	0.29	63,63,63,63	0
55	MG	AA	1697	1/1	0.91	0.41	84,84,84,84	0
55	MG	BA	3469	1/1	0.91	0.30	60,60,60,60	0
55	MG	DA	3128	1/1	0.91	0.34	77,77,77,77	0
55	MG	BA	3470	1/1	0.91	0.31	88,88,88,88	0
55	MG	DA	3355	1/1	0.91	0.50	77,77,77,77	0
55	MG	CC	108	1/1	0.91	0.56	106,106,106,106	0
55	MG	BA	3609	1/1	0.91	0.65	70,70,70,70	0
55	MG	DA	3003	1/1	0.91	0.29	64,64,64,64	0
55	MG	DA	3359	1/1	0.91	0.36	76,76,76,76	0
55	MG	CA	1733	1/1	0.91	0.43	69,69,69,69	0
55	MG	BA	3611	1/1	0.91	0.52	87,87,87,87	0
55	MG	DA	3489	1/1	0.91	0.16	71,71,71,71	0
55	MG	BA	3122	1/1	0.91	0.30	37,37,37,37	0
55	MG	CA	1640	1/1	0.91	0.33	81,81,81,81	0
55	MG	BA	3318	1/1	0.91	0.53	75,75,75,75	0
55	MG	BA	3617	1/1	0.91	0.72	71,71,71,71	0
55	MG	DA	3152	1/1	0.91	0.07	67,67,67,67	0
55	MG	DA	3017	1/1	0.91	0.37	75,75,75,75	0
55	MG	BA	3618	1/1	0.91	0.47	73,73,73,73	0
55	MG	BA	3127	1/1	0.91	0.59	53,53,53,53	0
55	MG	BA	3474	1/1	0.91	0.43	80,80,80,80	0
55	MG	AA	1810	1/1	0.91	0.45	67,67,67,67	0
55	MG	CA	1652	1/1	0.91	0.33	71,71,71,71	0
55	MG	BA	3540	1/1	0.91	0.30	61,61,61,61	0
55	MG	BA	3205	1/1	0.91	0.33	80,80,80,80	0
55	MG	BA	3542	1/1	0.91	0.48	72,72,72,72	0
55	MG	DA	3506	1/1	0.91	0.40	78,78,78,78	0
55	MG	DA	3188	1/1	0.91	0.60	56,56,56,56	0
55	MG	AA	1771	1/1	0.91	0.11	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	BA	3065	1/1	0.91	0.34	91,91,91,91	0
55	MG	AA	1801	1/1	0.91	0.49	84,84,84,84	0
55	MG	DA	3226	1/1	0.91	0.41	62,62,62,62	0
55	MG	BA	3071	1/1	0.91	0.23	70,70,70,70	0
55	MG	BA	3145	1/1	0.91	0.35	74,74,74,74	0
55	MG	BA	3487	1/1	0.91	0.10	94,94,94,94	0
55	MG	DA	3242	1/1	0.91	0.58	63,63,63,63	0
55	MG	DA	3518	1/1	0.91	0.41	83,83,83,83	0
55	MG	BA	3488	1/1	0.91	0.36	80,80,80,80	0
55	MG	BA	3553	1/1	0.91	0.21	78,78,78,78	0
55	MG	BA	3556	1/1	0.91	0.51	58,58,58,58	0
55	MG	DA	3259	1/1	0.91	0.26	72,72,72,72	0
55	MG	DA	3044	1/1	0.91	0.29	73,73,73,73	0
55	MG	DA	3266	1/1	0.91	0.50	55,55,55,55	0
55	MG	BA	3278	1/1	0.91	0.42	81,81,81,81	0
55	MG	BA	3219	1/1	0.91	0.43	76,76,76,76	0
55	MG	DA	3407	1/1	0.91	0.42	73,73,73,73	0
55	MG	BA	3566	1/1	0.91	0.29	88,88,88,88	0
55	MG	BA	3146	1/1	0.91	0.38	59,59,59,59	0
55	MG	DA	3050	1/1	0.91	0.68	66,66,66,66	0
55	MG	AA	1704	1/1	0.91	0.11	83,83,83,83	0
55	MG	BA	3335	1/1	0.91	0.35	58,58,58,58	0
55	MG	DA	3285	1/1	0.91	0.25	50,50,50,50	0
55	MG	BU	202	1/1	0.91	0.12	55,55,55,55	0
55	MG	DA	3056	1/1	0.91	0.44	81,81,81,81	0
55	MG	AA	1829	1/1	0.91	0.55	77,77,77,77	0
55	MG	AA	1764	1/1	0.91	0.17	79,79,79,79	0
55	MG	DA	3293	1/1	0.91	0.48	75,75,75,75	0
55	MG	DA	3294	1/1	0.91	0.23	64,64,64,64	0
55	MG	AA	1831	1/1	0.91	0.45	90,90,90,90	0
55	MG	AA	1663	1/1	0.91	0.27	47,47,47,47	0
55	MG	BA	3344	1/1	0.91	0.36	55,55,55,55	0
55	MG	BA	3293	1/1	0.91	0.26	65,65,65,65	0
55	MG	CA	1786	1/1	0.91	0.26	73,73,73,73	0
55	MG	BA	3549	1/1	0.92	0.34	68,68,68,68	0
55	MG	BA	3477	1/1	0.92	0.46	95,95,95,95	0
55	MG	CA	1776	1/1	0.92	0.50	71,71,71,71	0
55	MG	BE	301	1/1	0.92	0.39	59,59,59,59	0
55	MG	BA	3414	1/1	0.92	0.13	72,72,72,72	0
55	MG	BA	3174	1/1	0.92	0.81	71,71,71,71	0
55	MG	DA	3300	1/1	0.92	0.27	81,81,81,81	0
55	MG	DA	3063	1/1	0.92	0.53	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	AA	1645	1/1	0.92	0.47	50,50,50,50	0
55	MG	CA	1782	1/1	0.92	0.38	93,93,93,93	0
55	MG	CA	1678	1/1	0.92	0.23	70,70,70,70	0
55	MG	BA	3559	1/1	0.92	0.17	81,81,81,81	0
55	MG	BA	3483	1/1	0.92	0.34	68,68,68,68	0
55	MG	CA	1682	1/1	0.92	0.38	86,86,86,86	0
55	MG	DA	3313	1/1	0.92	0.29	85,85,85,85	0
55	MG	DA	3444	1/1	0.92	0.17	73,73,73,73	0
55	MG	DA	3074	1/1	0.92	0.18	70,70,70,70	0
55	MG	AA	1699	1/1	0.92	0.26	64,64,64,64	0
55	MG	CA	1788	1/1	0.92	0.33	84,84,84,84	0
55	MG	CA	1789	1/1	0.92	0.58	71,71,71,71	0
55	MG	AA	1805	1/1	0.92	0.35	65,65,65,65	0
55	MG	DA	3322	1/1	0.92	0.54	70,70,70,70	0
55	MG	DA	3458	1/1	0.92	0.60	92,92,92,92	0
55	MG	DA	3324	1/1	0.92	0.20	78,78,78,78	0
55	MG	BA	3419	1/1	0.92	0.53	85,85,85,85	0
55	MG	DA	3082	1/1	0.92	0.38	91,91,91,91	0
55	MG	AA	1661	1/1	0.92	0.34	48,48,48,48	0
55	MG	BA	3311	1/1	0.92	0.30	83,83,83,83	0
55	MG	DA	3086	1/1	0.92	0.20	114,114,114,114	0
55	MG	BA	3081	1/1	0.92	0.30	75,75,75,75	0
55	MG	CA	1602	1/1	0.92	0.28	80,80,80,80	0
55	MG	BA	3363	1/1	0.92	0.56	67,67,67,67	0
55	MG	CA	1694	1/1	0.92	0.47	97,97,97,97	0
55	MG	CA	1605	1/1	0.92	0.38	76,76,76,76	0
55	MG	AA	1717	1/1	0.92	0.40	74,74,74,74	0
55	MG	CA	1607	1/1	0.92	0.43	85,85,85,85	0
55	MG	BA	3426	1/1	0.92	0.49	85,85,85,85	0
55	MG	BA	3315	1/1	0.92	0.34	78,78,78,78	0
55	MG	CA	1701	1/1	0.92	0.42	88,88,88,88	0
55	MG	CA	1610	1/1	0.92	0.27	97,97,97,97	0
55	MG	BA	3194	1/1	0.92	0.42	68,68,68,68	0
55	MG	BA	3501	1/1	0.92	0.24	55,55,55,55	0
55	MG	CA	1708	1/1	0.92	0.09	97,97,97,97	0
55	MG	BA	3434	1/1	0.92	0.51	75,75,75,75	0
55	MG	DA	3130	1/1	0.92	0.18	60,60,60,60	0
55	MG	BA	3195	1/1	0.92	0.49	47,47,47,47	0
55	MG	BA	3048	1/1	0.92	0.54	77,77,77,77	0
55	MG	BA	3085	1/1	0.92	0.17	73,73,73,73	0
55	MG	BA	3130	1/1	0.92	0.43	44,44,44,44	0
55	MG	BA	3372	1/1	0.92	0.27	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	BA	3271	1/1	0.92	0.20	35,35,35,35	0
55	MG	AA	1825	1/1	0.92	0.24	93,93,93,93	0
55	MG	BA	3512	1/1	0.92	0.27	69,69,69,69	0
55	MG	BA	3208	1/1	0.92	0.10	45,45,45,45	0
55	MG	AA	1701	1/1	0.92	0.19	70,70,70,70	0
55	MG	DA	3009	1/1	0.92	0.53	68,68,68,68	0
55	MG	BA	3384	1/1	0.92	0.24	73,73,73,73	0
55	MG	AA	1788	1/1	0.92	0.52	77,77,77,77	0
55	MG	DA	3014	1/1	0.92	0.56	74,74,74,74	0
55	MG	BA	3518	1/1	0.92	0.23	70,70,70,70	0
55	MG	BA	3520	1/1	0.92	0.46	44,44,44,44	0
55	MG	BA	3214	1/1	0.92	0.56	67,67,67,67	0
55	MG	DA	3185	1/1	0.92	0.35	74,74,74,74	0
55	MG	BA	3602	1/1	0.92	0.25	67,67,67,67	0
55	MG	AA	1756	1/1	0.92	0.22	69,69,69,69	0
55	MG	AA	1628	1/1	0.92	0.35	69,69,69,69	0
55	MG	DA	3192	1/1	0.92	0.48	62,62,62,62	0
55	MG	DA	3510	1/1	0.92	0.32	85,85,85,85	0
55	MG	BA	3333	1/1	0.92	0.47	80,80,80,80	0
55	MG	BA	3458	1/1	0.92	0.12	82,82,82,82	0
55	MG	BA	3288	1/1	0.92	0.46	76,76,76,76	0
55	MG	AA	1650	1/1	0.92	0.49	71,71,71,71	0
55	MG	DA	3392	1/1	0.92	0.42	68,68,68,68	0
55	MG	DA	3516	1/1	0.92	0.33	105,105,105,105	0
55	MG	DA	3229	1/1	0.92	0.50	62,62,62,62	0
55	MG	AA	1654	1/1	0.92	0.44	75,75,75,75	0
55	MG	DA	3231	1/1	0.92	0.43	72,72,72,72	0
55	MG	DA	3030	1/1	0.92	0.40	74,74,74,74	0
55	MG	DA	3397	1/1	0.92	0.29	60,60,60,60	0
55	MG	BA	3615	1/1	0.92	0.41	81,81,81,81	0
55	MG	BA	3338	1/1	0.92	0.21	71,71,71,71	0
55	MG	BA	3101	1/1	0.92	0.64	63,63,63,63	0
55	MG	DA	3248	1/1	0.92	0.48	75,75,75,75	0
55	MG	AA	1760	1/1	0.92	0.69	78,78,78,78	0
55	MG	CA	1649	1/1	0.92	0.29	64,64,64,64	0
55	MG	DA	3255	1/1	0.92	0.28	75,75,75,75	0
55	MG	BA	3159	1/1	0.92	0.51	58,58,58,58	0
55	MG	BA	3343	1/1	0.92	0.30	60,60,60,60	0
55	MG	BA	3468	1/1	0.92	0.32	77,77,77,77	0
55	MG	AA	1748	1/1	0.92	0.42	84,84,84,84	0
55	MG	BA	3296	1/1	0.92	0.40	53,53,53,53	0
55	MG	DA	3410	1/1	0.92	0.39	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	1765	1/1	0.92	0.25	101,101,101,101	0
55	MG	BA	3347	1/1	0.92	0.43	68,68,68,68	0
55	MG	DA	3414	1/1	0.92	0.31	85,85,85,85	0
55	MG	BA	3299	1/1	0.92	0.49	89,89,89,89	0
55	MG	DA	3416	1/1	0.92	0.49	59,59,59,59	0
55	MG	BA	3105	1/1	0.92	0.32	75,75,75,75	0
55	MG	BA	3545	1/1	0.92	0.38	69,69,69,69	0
55	MG	BA	3070	1/1	0.92	0.13	63,63,63,63	0
55	MG	BA	3351	1/1	0.92	0.96	78,78,78,78	0
55	MG	AA	1732	1/1	0.92	0.33	92,92,92,92	0
55	MG	DA	3325	1/1	0.93	0.54	73,73,73,73	0
55	MG	DA	3326	1/1	0.93	0.36	70,70,70,70	0
55	MG	BA	3156	1/1	0.93	0.29	40,40,40,40	0
55	MG	BA	3316	1/1	0.93	0.50	69,69,69,69	0
55	MG	AA	1636	1/1	0.93	0.28	87,87,87,87	0
55	MG	DA	3138	1/1	0.93	0.20	70,70,70,70	0
55	MG	CA	1620	1/1	0.93	0.46	64,64,64,64	0
55	MG	BA	3616	1/1	0.93	0.38	58,58,58,58	0
55	MG	DA	3445	1/1	0.93	0.33	78,78,78,78	0
55	MG	DA	3143	1/1	0.93	0.28	58,58,58,58	0
55	MG	DA	3031	1/1	0.93	0.22	72,72,72,72	0
55	MG	AA	1605	1/1	0.93	0.40	82,82,82,82	0
55	MG	BA	3056	1/1	0.93	0.21	54,54,54,54	0
55	MG	BA	3558	1/1	0.93	0.14	63,63,63,63	0
55	MG	CA	1775	1/1	0.93	0.40	72,72,72,72	0
55	MG	AA	1629	1/1	0.93	0.12	86,86,86,86	0
55	MG	BA	3279	1/1	0.93	0.09	70,70,70,70	0
55	MG	DA	3172	1/1	0.93	0.10	88,88,88,88	0
55	MG	AA	1775	1/1	0.93	0.12	79,79,79,79	0
55	MG	AA	1685	1/1	0.93	0.29	88,88,88,88	0
55	MG	AA	1687	1/1	0.93	0.32	72,72,72,72	0
55	MG	BB	203	1/1	0.93	0.42	65,65,65,65	0
55	MG	AA	1738	1/1	0.93	0.54	79,79,79,79	0
55	MG	BB	205	1/1	0.93	0.35	74,74,74,74	0
55	MG	CA	1703	1/1	0.93	0.27	94,94,94,94	0
55	MG	DA	3469	1/1	0.93	0.60	80,80,80,80	0
55	MG	BB	206	1/1	0.93	0.34	86,86,86,86	0
55	MG	BA	3413	1/1	0.93	0.52	78,78,78,78	0
55	MG	BA	3067	1/1	0.93	0.23	48,48,48,48	0
55	MG	DA	3207	1/1	0.93	0.57	66,66,66,66	0
55	MG	DA	3208	1/1	0.93	0.47	74,74,74,74	0
55	MG	DA	3360	1/1	0.93	0.39	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	DA	3212	1/1	0.93	0.60	48,48,48,48	0
55	MG	DA	3362	1/1	0.93	0.61	53,53,53,53	0
55	MG	BA	3093	1/1	0.93	0.27	57,57,57,57	0
55	MG	DA	3224	1/1	0.93	0.47	66,66,66,66	0
55	MG	DA	3365	1/1	0.93	0.53	58,58,58,58	0
55	MG	BA	3236	1/1	0.93	0.44	52,52,52,52	0
55	MG	BA	3369	1/1	0.93	0.30	73,73,73,73	0
55	MG	BA	3519	1/1	0.93	0.31	80,80,80,80	0
55	MG	BA	3239	1/1	0.93	0.27	74,74,74,74	0
55	MG	BA	3011	1/1	0.93	0.29	42,42,42,42	0
55	MG	CA	1716	1/1	0.93	0.25	79,79,79,79	0
55	MG	DA	3372	1/1	0.93	0.36	65,65,65,65	0
55	MG	CA	1717	1/1	0.93	0.18	106,106,106,106	0
55	MG	BA	3012	1/1	0.93	0.28	45,45,45,45	0
55	MG	BA	3374	1/1	0.93	0.40	71,71,71,71	0
55	MG	DA	3378	1/1	0.93	0.50	63,63,63,63	0
55	MG	DA	3066	1/1	0.93	0.53	65,65,65,65	0
55	MG	BA	3099	1/1	0.93	0.58	67,67,67,67	0
55	MG	CA	1721	1/1	0.93	0.20	80,80,80,80	0
55	MG	DA	3069	1/1	0.93	0.44	60,60,60,60	0
55	MG	BA	3377	1/1	0.93	0.74	62,62,62,62	0
55	MG	DA	3071	1/1	0.93	0.24	81,81,81,81	0
55	MG	CA	1806	1/1	0.93	0.48	96,96,96,96	0
55	MG	DA	3267	1/1	0.93	0.36	64,64,64,64	0
55	MG	DA	3268	1/1	0.93	0.48	69,69,69,69	0
55	MG	CA	1651	1/1	0.93	0.35	90,90,90,90	0
55	MG	BA	3298	1/1	0.93	0.27	65,65,65,65	0
55	MG	CA	1653	1/1	0.93	0.17	77,77,77,77	0
55	MG	BO	201	1/1	0.93	0.36	62,62,62,62	0
55	MG	BA	3135	1/1	0.93	0.49	72,72,72,72	0
55	MG	B1	201	1/1	0.93	0.30	47,47,47,47	0
55	MG	BA	3429	1/1	0.93	0.12	75,75,75,75	0
55	MG	DA	3081	1/1	0.93	0.51	64,64,64,64	0
55	MG	CA	1739	1/1	0.93	0.56	75,75,75,75	0
55	MG	CA	1658	1/1	0.93	0.45	91,91,91,91	0
55	MG	BA	3198	1/1	0.93	0.17	45,45,45,45	0
55	MG	BA	3340	1/1	0.93	0.30	77,77,77,77	0
55	MG	BA	3200	1/1	0.93	0.39	62,62,62,62	0
55	MG	DA	3089	1/1	0.93	0.54	82,82,82,82	0
55	MG	BA	3032	1/1	0.93	0.52	49,49,49,49	0
55	MG	AA	1833	1/1	0.93	0.44	88,88,88,88	0
55	MG	BA	3486	1/1	0.93	0.41	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	CA	1752	1/1	0.93	0.18	70,70,70,70	0
55	MG	BA	3389	1/1	0.93	0.23	59,59,59,59	0
55	MG	BA	3258	1/1	0.93	0.29	45,45,45,45	0
55	MG	DA	3111	1/1	0.93	0.26	52,52,52,52	0
55	MG	BA	3600	1/1	0.93	0.34	66,66,66,66	0
55	MG	DA	3308	1/1	0.93	0.38	97,97,97,97	0
55	MG	AA	1779	1/1	0.93	0.36	72,72,72,72	0
55	MG	DA	3418	1/1	0.93	0.41	78,78,78,78	0
55	MG	DA	3310	1/1	0.93	0.49	71,71,71,71	0
55	MG	DA	3421	1/1	0.93	0.32	62,62,62,62	0
55	MG	AA	1608	1/1	0.93	0.26	64,64,64,64	0
55	MG	BA	3149	1/1	0.93	0.20	80,80,80,80	0
55	MG	AA	1740	1/1	0.93	0.18	75,75,75,75	0
55	MG	DA	3426	1/1	0.93	0.42	58,58,58,58	0
55	MG	DA	3124	1/1	0.93	0.57	54,54,54,54	0
55	MG	DA	3316	1/1	0.93	0.33	61,61,61,61	0
55	MG	BA	3268	1/1	0.93	0.58	67,67,67,67	0
55	MG	BA	3108	1/1	0.93	0.36	86,86,86,86	0
55	MG	CA	1680	1/1	0.93	0.55	68,68,68,68	0
55	MG	DA	3321	1/1	0.93	0.57	66,66,66,66	0
55	MG	CA	1613	1/1	0.93	0.28	68,68,68,68	0
55	MG	BA	3499	1/1	0.93	0.39	68,68,68,68	0
55	MG	AA	1838	1/1	0.94	0.41	61,61,61,61	0
55	MG	DA	3423	1/1	0.94	0.89	75,75,75,75	0
55	MG	DA	3305	1/1	0.94	0.36	77,77,77,77	0
55	MG	AA	1655	1/1	0.94	0.47	88,88,88,88	0
55	MG	AA	1648	1/1	0.94	0.52	78,78,78,78	0
55	MG	AA	1676	1/1	0.94	0.38	70,70,70,70	0
55	MG	BA	3297	1/1	0.94	0.22	58,58,58,58	0
55	MG	BA	3464	1/1	0.94	0.51	77,77,77,77	0
55	MG	BA	3612	1/1	0.94	0.44	66,66,66,66	0
55	MG	DA	3099	1/1	0.94	0.27	40,40,40,40	0
55	MG	DA	3105	1/1	0.94	0.36	45,45,45,45	0
55	MG	AA	1666	1/1	0.94	0.52	62,62,62,62	0
55	MG	BA	3346	1/1	0.94	0.33	51,51,51,51	0
55	MG	CA	1724	1/1	0.94	0.51	84,84,84,84	0
55	MG	BA	3242	1/1	0.94	0.44	50,50,50,50	0
55	MG	BA	3006	1/1	0.94	0.43	38,38,38,38	0
55	MG	AA	1799	1/1	0.94	0.33	78,78,78,78	0
55	MG	CA	1730	1/1	0.94	0.19	106,106,106,106	0
55	MG	DA	3323	1/1	0.94	0.14	42,42,42,42	0
55	MG	BA	3405	1/1	0.94	0.47	56,56,56,56	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	0.94	0.36	80,80,80,80	0
55	MG	DA	3127	1/1	0.94	0.40	74,74,74,74	0
55	MG	AA	1814	1/1	0.94	0.32	83,83,83,83	0
55	MG	CA	1642	1/1	0.94	0.20	91,91,91,91	0
55	MG	CA	1735	1/1	0.94	0.20	89,89,89,89	0
55	MG	BA	3620	1/1	0.94	0.28	68,68,68,68	0
55	MG	DA	3450	1/1	0.94	0.33	88,88,88,88	0
55	MG	DA	3012	1/1	0.94	0.50	66,66,66,66	0
55	MG	DA	3453	1/1	0.94	0.24	66,66,66,66	0
55	MG	BA	3136	1/1	0.94	0.16	74,74,74,74	0
55	MG	DA	3334	1/1	0.94	0.56	68,68,68,68	0
55	MG	BA	3353	1/1	0.94	0.44	52,52,52,52	0
55	MG	BA	3197	1/1	0.94	0.53	46,46,46,46	0
55	MG	BA	3016	1/1	0.94	0.53	39,39,39,39	0
55	MG	CA	1743	1/1	0.94	0.49	80,80,80,80	0
55	MG	DA	3339	1/1	0.94	0.32	66,66,66,66	0
55	MG	BA	3306	1/1	0.94	0.25	67,67,67,67	0
55	MG	BA	3307	1/1	0.94	0.48	39,39,39,39	0
55	MG	DA	3148	1/1	0.94	0.48	75,75,75,75	0
55	MG	DA	3024	1/1	0.94	0.32	108,108,108,108	0
55	MG	CA	1748	1/1	0.94	0.16	87,87,87,87	0
55	MG	BA	3308	1/1	0.94	0.32	61,61,61,61	0
55	MG	BA	3141	1/1	0.94	0.48	35,35,35,35	0
55	MG	BA	3143	1/1	0.94	0.68	72,72,72,72	0
55	MG	BA	3550	1/1	0.94	0.24	93,93,93,93	0
55	MG	BA	3025	1/1	0.94	0.36	42,42,42,42	0
55	MG	BA	3312	1/1	0.94	0.48	57,57,57,57	0
55	MG	BB	211	1/1	0.94	0.29	92,92,92,92	0
55	MG	DA	3033	1/1	0.94	0.25	62,62,62,62	0
55	MG	BA	3263	1/1	0.94	0.64	54,54,54,54	0
55	MG	DA	3035	1/1	0.94	0.26	62,62,62,62	0
55	MG	BB	213	1/1	0.94	0.45	66,66,66,66	0
55	MG	BA	3422	1/1	0.94	0.26	78,78,78,78	0
55	MG	DA	3039	1/1	0.94	0.34	85,85,85,85	0
55	MG	BA	3264	1/1	0.94	0.21	30,30,30,30	0
55	MG	AA	1603	1/1	0.94	0.33	63,63,63,63	0
55	MG	DA	3198	1/1	0.94	0.31	47,47,47,47	0
55	MG	BA	3560	1/1	0.94	0.56	78,78,78,78	0
55	MG	BA	3562	1/1	0.94	0.30	79,79,79,79	0
55	MG	AA	1721	1/1	0.94	0.29	77,77,77,77	0
55	MG	DA	3214	1/1	0.94	0.44	40,40,40,40	0
55	MG	BA	3148	1/1	0.94	0.41	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	BA	3493	1/1	0.94	0.37	63,63,63,63	0
55	MG	CA	1670	1/1	0.94	0.49	56,56,56,56	0
55	MG	BA	3568	1/1	0.94	0.39	83,83,83,83	0
55	MG	BA	3427	1/1	0.94	0.41	65,65,65,65	0
55	MG	BA	3037	1/1	0.94	0.38	44,44,44,44	0
55	MG	BA	3430	1/1	0.94	0.27	57,57,57,57	0
55	MG	DA	3374	1/1	0.94	0.41	62,62,62,62	0
55	MG	DA	3375	1/1	0.94	0.69	88,88,88,88	0
55	MG	DA	3054	1/1	0.94	0.62	58,58,58,58	0
55	MG	BA	3150	1/1	0.94	0.44	36,36,36,36	0
55	MG	BA	3498	1/1	0.94	0.33	85,85,85,85	0
55	MG	DA	3379	1/1	0.94	0.44	85,85,85,85	0
55	MG	BA	3076	1/1	0.94	0.33	68,68,68,68	0
55	MG	B5	101	1/1	0.94	0.35	45,45,45,45	0
55	MG	AA	1695	1/1	0.94	0.23	90,90,90,90	0
55	MG	CA	1779	1/1	0.94	0.33	72,72,72,72	0
55	MG	BA	3577	1/1	0.94	0.18	73,73,73,73	0
55	MG	DA	3386	1/1	0.94	0.48	61,61,61,61	0
55	MG	BA	3047	1/1	0.94	0.41	74,74,74,74	0
55	MG	DA	3388	1/1	0.94	0.29	74,74,74,74	0
55	MG	DA	3261	1/1	0.94	0.49	58,58,58,58	0
55	MG	DA	3262	1/1	0.94	0.46	48,48,48,48	0
55	MG	BA	3218	1/1	0.94	0.54	48,48,48,48	0
55	MG	AA	1672	1/1	0.94	0.33	87,87,87,87	0
55	MG	BA	3115	1/1	0.94	0.27	87,87,87,87	0
55	MG	BA	3440	1/1	0.94	0.44	74,74,74,74	0
55	MG	BA	3280	1/1	0.94	0.52	50,50,50,50	0
55	MG	DA	3270	1/1	0.94	0.28	83,83,83,83	0
55	MG	DA	3272	1/1	0.94	0.28	64,64,64,64	0
55	MG	AA	1747	1/1	0.94	0.40	88,88,88,88	0
55	MG	BA	3224	1/1	0.94	0.11	55,55,55,55	0
55	MG	DA	3276	1/1	0.94	0.52	68,68,68,68	0
55	MG	BA	3165	1/1	0.94	0.56	61,61,61,61	0
55	MG	BA	3386	1/1	0.94	0.50	59,59,59,59	0
55	MG	BA	3286	1/1	0.94	0.28	66,66,66,66	0
55	MG	DA	3282	1/1	0.94	0.44	69,69,69,69	0
55	MG	BA	3590	1/1	0.94	0.34	63,63,63,63	0
55	MG	BA	3287	1/1	0.94	0.39	62,62,62,62	0
55	MG	BA	3515	1/1	0.94	0.21	72,72,72,72	0
55	MG	DA	3289	1/1	0.94	0.43	90,90,90,90	0
55	MG	BA	3226	1/1	0.94	0.41	50,50,50,50	0
55	MG	BA	3450	1/1	0.94	0.18	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	CA	1705	1/1	0.94	0.47	80,80,80,80	0
55	MG	AA	1641	1/1	0.94	0.37	57,57,57,57	0
55	MG	BA	3454	1/1	0.94	0.36	92,92,92,92	0
55	MG	DA	3083	1/1	0.94	0.49	85,85,85,85	0
55	MG	BA	3337	1/1	0.94	0.30	72,72,72,72	0
55	MG	BA	3599	1/1	0.94	0.47	69,69,69,69	0
55	MG	BA	3228	1/1	0.94	0.62	72,72,72,72	0
55	MG	AA	1736	1/1	0.94	0.46	90,90,90,90	0
56	ZN	CQ	101	1/1	0.94	0.14	120,120,120,120	0
55	MG	BA	3049	1/1	0.95	0.40	68,68,68,68	0
55	MG	BA	3153	1/1	0.95	0.44	52,52,52,52	0
55	MG	BA	3050	1/1	0.95	0.48	39,39,39,39	0
55	MG	AA	1667	1/1	0.95	0.33	68,68,68,68	0
55	MG	DA	3036	1/1	0.95	0.21	99,99,99,99	0
55	MG	AA	1658	1/1	0.95	0.65	49,49,49,49	0
55	MG	DA	3153	1/1	0.95	0.31	70,70,70,70	0
55	MG	AA	1669	1/1	0.95	0.43	68,68,68,68	0
55	MG	DA	3163	1/1	0.95	0.59	62,62,62,62	0
55	MG	BA	3522	1/1	0.95	0.48	82,82,82,82	0
55	MG	DA	3165	1/1	0.95	0.59	65,65,65,65	0
55	MG	DA	3167	1/1	0.95	0.40	70,70,70,70	0
55	MG	DA	3331	1/1	0.95	0.55	50,50,50,50	0
55	MG	AA	1746	1/1	0.95	0.41	84,84,84,84	0
55	MG	DA	3170	1/1	0.95	0.44	68,68,68,68	0
55	MG	BA	3235	1/1	0.95	0.39	54,54,54,54	0
55	MG	BA	3525	1/1	0.95	0.29	77,77,77,77	0
55	MG	AA	1827	1/1	0.95	0.28	87,87,87,87	0
55	MG	DA	3176	1/1	0.95	0.55	65,65,65,65	0
55	MG	BA	3237	1/1	0.95	0.49	57,57,57,57	0
55	MG	BA	3528	1/1	0.95	0.44	76,76,76,76	0
55	MG	DA	3452	1/1	0.95	0.21	83,83,83,83	0
55	MG	DA	3046	1/1	0.95	0.34	65,65,65,65	0
55	MG	BA	3529	1/1	0.95	0.38	68,68,68,68	0
55	MG	BA	3107	1/1	0.95	0.43	36,36,36,36	0
55	MG	DA	3456	1/1	0.95	0.36	83,83,83,83	0
55	MG	CA	1617	1/1	0.95	0.24	93,93,93,93	0
55	MG	DA	3189	1/1	0.95	0.50	41,41,41,41	0
55	MG	DA	3345	1/1	0.95	0.39	64,64,64,64	0
55	MG	DA	3190	1/1	0.95	0.57	61,61,61,61	0
55	MG	BA	3410	1/1	0.95	0.72	62,62,62,62	0
55	MG	BA	3352	1/1	0.95	0.35	76,76,76,76	0
55	MG	CA	1621	1/1	0.95	0.36	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	DA	3199	1/1	0.95	0.48	61,61,61,61	0
55	MG	DA	3205	1/1	0.95	0.54	67,67,67,67	0
55	MG	DA	3206	1/1	0.95	0.53	65,65,65,65	0
55	MG	CA	1622	1/1	0.95	0.33	95,95,95,95	0
55	MG	DA	3470	1/1	0.95	0.11	80,80,80,80	0
55	MG	AC	104	1/1	0.95	0.47	56,56,56,56	0
55	MG	BA	3169	1/1	0.95	0.60	63,63,63,63	0
55	MG	BA	3170	1/1	0.95	0.48	55,55,55,55	0
55	MG	DA	3216	1/1	0.95	0.30	49,49,49,49	0
55	MG	AA	1762	1/1	0.95	0.21	80,80,80,80	0
55	MG	BA	3248	1/1	0.95	0.35	53,53,53,53	0
55	MG	AA	1780	1/1	0.95	0.26	86,86,86,86	0
55	MG	BA	3177	1/1	0.95	0.51	57,57,57,57	0
55	MG	DA	3228	1/1	0.95	0.47	44,44,44,44	0
55	MG	CA	1793	1/1	0.95	0.34	91,91,91,91	0
55	MG	BA	3064	1/1	0.95	0.29	49,49,49,49	0
55	MG	BA	3478	1/1	0.95	0.23	63,63,63,63	0
55	MG	BA	3180	1/1	0.95	0.40	37,37,37,37	0
55	MG	AA	1763	1/1	0.95	0.58	53,53,53,53	0
55	MG	DA	3238	1/1	0.95	0.42	60,60,60,60	0
55	MG	AC	108	1/1	0.95	0.40	85,85,85,85	0
55	MG	DA	3243	1/1	0.95	0.51	79,79,79,79	0
55	MG	AA	1670	1/1	0.95	0.38	63,63,63,63	0
55	MG	AA	1765	1/1	0.95	0.51	84,84,84,84	0
55	MG	DA	3249	1/1	0.95	0.40	72,72,72,72	0
55	MG	DA	3250	1/1	0.95	0.39	63,63,63,63	0
55	MG	A1	101	1/1	0.95	0.17	66,66,66,66	0
55	MG	AA	1671	1/1	0.95	0.12	67,67,67,67	0
55	MG	BA	3125	1/1	0.95	0.53	52,52,52,52	0
55	MG	DA	3258	1/1	0.95	0.32	37,37,37,37	0
55	MG	DA	3499	1/1	0.95	0.21	61,61,61,61	0
55	MG	BA	3003	1/1	0.95	0.44	47,47,47,47	0
55	MG	AA	1659	1/1	0.95	0.75	69,69,69,69	0
55	MG	AA	1610	1/1	0.95	0.49	51,51,51,51	0
55	MG	BA	3491	1/1	0.95	0.53	42,42,42,42	0
55	MG	BA	3492	1/1	0.95	0.43	77,77,77,77	0
55	MG	CA	1728	1/1	0.95	0.66	69,69,69,69	0
55	MG	BA	3373	1/1	0.95	0.44	64,64,64,64	0
55	MG	CA	1646	1/1	0.95	0.37	76,76,76,76	0
55	MG	CA	1731	1/1	0.95	0.58	72,72,72,72	0
55	MG	CC	103	1/1	0.95	1.01	72,72,72,72	0
55	MG	AA	1622	1/1	0.95	0.23	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	AA	1642	1/1	0.95	0.68	72,72,72,72	0
55	MG	DA	3275	1/1	0.95	0.36	76,76,76,76	0
55	MG	BA	3436	1/1	0.95	0.23	59,59,59,59	0
55	MG	BA	3564	1/1	0.95	0.61	84,84,84,84	0
55	MG	CA	1736	1/1	0.95	0.73	79,79,79,79	0
55	MG	BA	3082	1/1	0.95	0.36	64,64,64,64	0
55	MG	BA	3274	1/1	0.95	0.17	46,46,46,46	0
55	MG	BB	215	1/1	0.95	0.26	82,82,82,82	0
55	MG	BA	3326	1/1	0.95	0.34	52,52,52,52	0
55	MG	BA	3275	1/1	0.95	0.21	73,73,73,73	0
55	MG	DA	3521	1/1	0.95	0.58	69,69,69,69	0
55	MG	AA	1623	1/1	0.95	0.74	65,65,65,65	0
55	MG	DA	3100	1/1	0.95	0.44	44,44,44,44	0
55	MG	CA	1744	1/1	0.95	0.27	79,79,79,79	0
55	MG	AA	1620	1/1	0.95	0.28	66,66,66,66	0
55	MG	DA	3013	1/1	0.95	0.53	56,56,56,56	0
55	MG	BA	3443	1/1	0.95	0.14	77,77,77,77	0
55	MG	AA	1818	1/1	0.95	0.60	76,76,76,76	0
55	MG	DA	3016	1/1	0.95	0.43	78,78,78,78	0
55	MG	DA	3411	1/1	0.95	0.19	70,70,70,70	0
55	MG	DA	3122	1/1	0.95	0.49	46,46,46,46	0
55	MG	BF	301	1/1	0.95	0.07	73,73,73,73	0
55	MG	AA	1796	1/1	0.95	0.14	75,75,75,75	0
55	MG	AA	1726	1/1	0.95	0.48	81,81,81,81	0
55	MG	BA	3576	1/1	0.95	0.41	74,74,74,74	0
55	MG	DA	3022	1/1	0.95	0.55	60,60,60,60	0
55	MG	BA	3508	1/1	0.95	0.41	59,59,59,59	0
55	MG	BA	3040	1/1	0.95	0.36	54,54,54,54	0
55	MG	BA	3284	1/1	0.95	0.45	56,56,56,56	0
55	MG	BA	3043	1/1	0.95	0.25	32,32,32,32	0
55	MG	BA	3147	1/1	0.95	0.15	55,55,55,55	0
55	MG	BA	3044	1/1	0.95	0.33	62,62,62,62	0
55	MG	AA	1798	1/1	0.95	0.25	58,58,58,58	0
55	MG	CA	1675	1/1	0.95	0.48	62,62,62,62	0
55	MG	AA	1714	1/1	0.95	0.32	107,107,107,107	0
55	MG	DA	3317	1/1	0.95	0.22	81,81,81,81	0
55	MG	DA	3232	1/1	0.96	0.42	44,44,44,44	0
55	MG	DA	3234	1/1	0.96	0.43	52,52,52,52	0
55	MG	AA	1800	1/1	0.96	0.31	82,82,82,82	0
55	MG	BA	3428	1/1	0.96	0.36	68,68,68,68	0
55	MG	DA	3021	1/1	0.96	0.48	51,51,51,51	0
55	MG	DA	3241	1/1	0.96	0.47	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	BA	3480	1/1	0.96	0.51	50,50,50,50	0
55	MG	AA	1811	1/1	0.96	0.50	67,67,67,67	0
55	MG	DA	3244	1/1	0.96	0.46	71,71,71,71	0
55	MG	BA	3096	1/1	0.96	0.50	56,56,56,56	0
55	MG	DA	3108	1/1	0.96	0.33	54,54,54,54	0
55	MG	DA	3457	1/1	0.96	0.76	65,65,65,65	0
55	MG	DA	3109	1/1	0.96	0.23	65,65,65,65	0
55	MG	DA	3110	1/1	0.96	0.33	58,58,58,58	0
55	MG	BA	3380	1/1	0.96	0.17	65,65,65,65	0
55	MG	BA	3176	1/1	0.96	0.51	48,48,48,48	0
55	MG	BA	3097	1/1	0.96	0.36	59,59,59,59	0
55	MG	AA	1649	1/1	0.96	0.37	79,79,79,79	0
55	MG	AA	1646	1/1	0.96	0.41	67,67,67,67	0
55	MG	DA	3121	1/1	0.96	0.17	64,64,64,64	0
55	MG	BA	3238	1/1	0.96	0.56	41,41,41,41	0
55	MG	BA	3184	1/1	0.96	0.23	39,39,39,39	0
55	MG	BA	3100	1/1	0.96	0.37	42,42,42,42	0
55	MG	BU	201	1/1	0.96	0.25	81,81,81,81	0
55	MG	BA	3241	1/1	0.96	0.49	60,60,60,60	0
55	MG	BA	3137	1/1	0.96	0.37	47,47,47,47	0
55	MG	BA	3243	1/1	0.96	0.48	48,48,48,48	0
55	MG	DA	3271	1/1	0.96	0.47	58,58,58,58	0
55	MG	BA	3138	1/1	0.96	0.47	46,46,46,46	0
55	MG	AA	1792	1/1	0.96	0.21	55,55,55,55	0
55	MG	BA	3008	1/1	0.96	0.49	37,37,37,37	0
55	MG	BA	3604	1/1	0.96	0.11	61,61,61,61	0
55	MG	CA	1722	1/1	0.96	0.38	75,75,75,75	0
55	MG	BA	3605	1/1	0.96	0.51	47,47,47,47	0
55	MG	DA	3278	1/1	0.96	0.51	42,42,42,42	0
55	MG	BA	3142	1/1	0.96	0.37	51,51,51,51	0
55	MG	BA	3010	1/1	0.96	0.41	46,46,46,46	0
55	MG	DA	3382	1/1	0.96	0.52	78,78,78,78	0
55	MG	BA	3251	1/1	0.96	0.39	68,68,68,68	0
55	MG	CA	1795	1/1	0.96	0.29	76,76,76,76	0
55	MG	AA	1837	1/1	0.96	0.53	73,73,73,73	0
55	MG	BA	3253	1/1	0.96	0.26	51,51,51,51	0
55	MG	BA	3254	1/1	0.96	0.34	43,43,43,43	0
55	MG	CA	1666	1/1	0.96	0.29	71,71,71,71	0
55	MG	BA	3452	1/1	0.96	0.40	41,41,41,41	0
55	MG	BA	3078	1/1	0.96	0.37	65,65,65,65	0
55	MG	DA	3495	1/1	0.96	0.20	63,63,63,63	0
55	MG	DA	3156	1/1	0.96	0.69	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	DA	3159	1/1	0.96	0.26	37,37,37,37	0
55	MG	DA	3295	1/1	0.96	0.37	50,50,50,50	0
55	MG	BA	3201	1/1	0.96	0.64	66,66,66,66	0
55	MG	AA	1733	1/1	0.96	0.60	71,71,71,71	0
55	MG	DA	3299	1/1	0.96	0.33	38,38,38,38	0
55	MG	CA	1671	1/1	0.96	0.56	49,49,49,49	0
55	MG	DA	3301	1/1	0.96	0.34	63,63,63,63	0
55	MG	BA	3406	1/1	0.96	0.51	82,82,82,82	0
55	MG	CA	1738	1/1	0.96	0.41	63,63,63,63	0
55	MG	DA	3169	1/1	0.96	0.31	69,69,69,69	0
55	MG	AA	1686	1/1	0.96	0.36	85,85,85,85	0
55	MG	CA	1674	1/1	0.96	0.11	70,70,70,70	0
55	MG	CN	201	1/1	0.96	0.15	74,74,74,74	0
55	MG	DA	3174	1/1	0.96	0.57	44,44,44,44	0
55	MG	BA	3109	1/1	0.96	0.32	70,70,70,70	0
55	MG	AA	1741	1/1	0.96	0.31	67,67,67,67	0
55	MG	DA	3311	1/1	0.96	0.41	73,73,73,73	0
55	MG	BA	3026	1/1	0.96	0.31	47,47,47,47	0
55	MG	DA	3181	1/1	0.96	0.49	50,50,50,50	0
55	MG	BA	3209	1/1	0.96	0.47	39,39,39,39	0
55	MG	DA	3184	1/1	0.96	0.65	61,61,61,61	0
55	MG	BA	3113	1/1	0.96	0.53	57,57,57,57	0
55	MG	CA	1746	1/1	0.96	0.61	57,57,57,57	0
55	MG	BA	3152	1/1	0.96	0.51	40,40,40,40	0
55	MG	BA	3058	1/1	0.96	0.32	62,62,62,62	0
55	MG	CC	106	1/1	0.96	0.60	96,96,96,96	0
55	MG	BA	3031	1/1	0.96	0.36	33,33,33,33	0
55	MG	AA	1606	1/1	0.96	0.07	91,91,91,91	0
55	MG	DA	3193	1/1	0.96	0.69	63,63,63,63	0
55	MG	DA	3001	1/1	0.96	0.46	67,67,67,67	0
55	MG	CA	1685	1/1	0.96	0.37	93,93,93,93	0
55	MG	BA	3117	1/1	0.96	0.49	60,60,60,60	0
55	MG	BB	207	1/1	0.96	0.18	83,83,83,83	0
55	MG	AN	201	1/1	0.96	0.17	68,68,68,68	0
55	MG	DA	3329	1/1	0.96	0.35	44,44,44,44	0
55	MG	BA	3221	1/1	0.96	0.37	60,60,60,60	0
55	MG	DA	3008	1/1	0.96	0.38	70,70,70,70	0
55	MG	CA	1690	1/1	0.96	0.36	68,68,68,68	0
55	MG	BA	3062	1/1	0.96	0.29	56,56,56,56	0
55	MG	CA	1692	1/1	0.96	0.49	82,82,82,82	0
55	MG	DA	3217	1/1	0.96	0.40	55,55,55,55	0
55	MG	DA	3218	1/1	0.96	0.41	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	AA	1632	1/1	0.96	0.25	67,67,67,67	0
55	MG	AA	1789	1/1	0.96	0.29	74,74,74,74	0
55	MG	DA	3087	1/1	0.96	0.50	63,63,63,63	0
55	MG	DE	303	1/1	0.96	0.35	56,56,56,56	0
55	MG	CA	1695	1/1	0.96	0.50	87,87,87,87	0
55	MG	CA	1764	1/1	0.96	0.54	72,72,72,72	0
55	MG	BA	3124	1/1	0.96	0.52	45,45,45,45	0
55	MG	BA	3168	1/1	0.96	0.36	49,49,49,49	0
55	MG	BA	3092	1/1	0.96	0.46	32,32,32,32	0
55	MG	DA	3177	1/1	0.97	0.34	74,74,74,74	0
55	MG	DA	3178	1/1	0.97	0.75	59,59,59,59	0
55	MG	BA	3102	1/1	0.97	0.28	66,66,66,66	0
55	MG	BA	3433	1/1	0.97	0.15	70,70,70,70	0
55	MG	BA	3329	1/1	0.97	0.40	65,65,65,65	0
55	MG	AC	101	1/1	0.97	0.48	53,53,53,53	0
55	MG	DA	3006	1/1	0.97	0.48	71,71,71,71	0
55	MG	BA	3178	1/1	0.97	0.36	36,36,36,36	0
55	MG	BA	3383	1/1	0.97	0.22	71,71,71,71	0
55	MG	DA	3433	1/1	0.97	0.53	57,57,57,57	0
55	MG	BA	3020	1/1	0.97	0.47	41,41,41,41	0
55	MG	BA	3021	1/1	0.97	0.53	41,41,41,41	0
55	MG	BA	3181	1/1	0.97	0.35	39,39,39,39	0
55	MG	DA	3191	1/1	0.97	0.55	46,46,46,46	0
55	MG	BA	3182	1/1	0.97	0.33	43,43,43,43	0
55	MG	BA	3555	1/1	0.97	0.23	38,38,38,38	0
55	MG	DA	3195	1/1	0.97	0.76	70,70,70,70	0
55	MG	DA	3196	1/1	0.97	0.46	50,50,50,50	0
55	MG	BA	3183	1/1	0.97	0.30	47,47,47,47	0
55	MG	BA	3557	1/1	0.97	0.47	77,77,77,77	0
55	MG	BA	3077	1/1	0.97	0.45	54,54,54,54	0
55	MG	DA	3200	1/1	0.97	0.45	44,44,44,44	0
55	MG	DA	3446	1/1	0.97	0.50	75,75,75,75	0
55	MG	DA	3202	1/1	0.97	0.43	47,47,47,47	0
55	MG	DA	3204	1/1	0.97	0.39	51,51,51,51	0
55	MG	BA	3051	1/1	0.97	0.23	74,74,74,74	0
55	MG	BA	3186	1/1	0.97	0.42	36,36,36,36	0
55	MG	BA	3561	1/1	0.97	0.31	74,74,74,74	0
55	MG	BA	3022	1/1	0.97	0.45	30,30,30,30	0
55	MG	DA	3209	1/1	0.97	0.50	66,66,66,66	0
55	MG	DA	3210	1/1	0.97	0.42	63,63,63,63	0
55	MG	BA	3188	1/1	0.97	0.37	60,60,60,60	0
55	MG	DA	3096	1/1	0.97	0.58	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	DA	3215	1/1	0.97	0.42	42,42,42,42	0
55	MG	AA	1794	1/1	0.97	0.21	84,84,84,84	0
55	MG	BA	3504	1/1	0.97	0.33	45,45,45,45	0
55	MG	BA	3192	1/1	0.97	0.33	34,34,34,34	0
55	MG	DA	3219	1/1	0.97	0.24	70,70,70,70	0
55	MG	DA	3103	1/1	0.97	0.40	50,50,50,50	0
55	MG	DA	3221	1/1	0.97	0.70	63,63,63,63	0
55	MG	DA	3222	1/1	0.97	0.50	60,60,60,60	0
55	MG	BA	3567	1/1	0.97	0.23	80,80,80,80	0
55	MG	DA	3107	1/1	0.97	0.36	53,53,53,53	0
55	MG	AA	1657	1/1	0.97	0.45	50,50,50,50	0
55	MG	DA	3227	1/1	0.97	0.72	50,50,50,50	0
55	MG	BA	3244	1/1	0.97	0.33	58,58,58,58	0
55	MG	BA	3111	1/1	0.97	0.33	59,59,59,59	0
55	MG	BA	3453	1/1	0.97	0.57	60,60,60,60	0
55	MG	BA	3055	1/1	0.97	0.43	57,57,57,57	0
55	MG	DA	3113	1/1	0.97	0.55	43,43,43,43	0
55	MG	DA	3233	1/1	0.97	0.42	52,52,52,52	0
55	MG	DA	3354	1/1	0.97	0.41	73,73,73,73	0
55	MG	BA	3028	1/1	0.97	0.41	46,46,46,46	0
55	MG	BA	3456	1/1	0.97	0.50	78,78,78,78	0
55	MG	BA	3030	1/1	0.97	0.54	44,44,44,44	0
55	MG	BA	3199	1/1	0.97	0.42	49,49,49,49	0
55	MG	DA	3239	1/1	0.97	0.36	45,45,45,45	0
55	MG	BA	3001	1/1	0.97	0.48	47,47,47,47	0
55	MG	AA	1750	1/1	0.97	0.54	62,62,62,62	0
55	MG	BE	302	1/1	0.97	0.23	56,56,56,56	0
55	MG	BE	303	1/1	0.97	0.40	44,44,44,44	0
55	MG	DA	3245	1/1	0.97	0.51	60,60,60,60	0
55	MG	DA	3246	1/1	0.97	0.43	53,53,53,53	0
55	MG	DA	3126	1/1	0.97	0.26	41,41,41,41	0
55	MG	BA	3202	1/1	0.97	0.39	51,51,51,51	0
55	MG	BA	3407	1/1	0.97	0.26	59,59,59,59	0
55	MG	BA	3033	1/1	0.97	0.38	38,38,38,38	0
55	MG	BA	3355	1/1	0.97	0.57	46,46,46,46	0
55	MG	DA	3252	1/1	0.97	0.32	64,64,64,64	0
55	MG	BA	3005	1/1	0.97	0.49	43,43,43,43	0
55	MG	DA	3254	1/1	0.97	0.55	50,50,50,50	0
55	MG	DA	3132	1/1	0.97	0.31	53,53,53,53	0
55	MG	DA	3256	1/1	0.97	0.44	49,49,49,49	0
55	MG	DA	3257	1/1	0.97	0.33	49,49,49,49	0
55	MG	BA	3119	1/1	0.97	0.38	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	DA	3135	1/1	0.97	0.42	49,49,49,49	0
55	MG	BA	3585	1/1	0.97	0.38	60,60,60,60	0
55	MG	BA	3035	1/1	0.97	0.27	37,37,37,37	0
55	MG	CA	1799	1/1	0.97	0.31	96,96,96,96	0
55	MG	DA	3264	1/1	0.97	0.65	59,59,59,59	0
55	MG	DA	3265	1/1	0.97	0.41	50,50,50,50	0
55	MG	BA	3259	1/1	0.97	0.25	40,40,40,40	0
55	MG	BA	3063	1/1	0.97	0.13	43,43,43,43	0
55	MG	DA	3141	1/1	0.97	0.52	38,38,38,38	0
55	MG	BA	3160	1/1	0.97	0.42	42,42,42,42	0
55	MG	DA	3145	1/1	0.97	0.51	60,60,60,60	0
55	MG	AA	1601	1/1	0.97	0.36	56,56,56,56	0
55	MG	DA	3390	1/1	0.97	0.35	75,75,75,75	0
55	MG	BA	3162	1/1	0.97	0.52	45,45,45,45	0
55	MG	DA	3149	1/1	0.97	0.62	57,57,57,57	0
55	MG	BA	3213	1/1	0.97	0.56	49,49,49,49	0
55	MG	AA	1634	1/1	0.97	0.29	62,62,62,62	0
55	MG	BA	3594	1/1	0.97	0.55	79,79,79,79	0
55	MG	BA	3095	1/1	0.97	0.47	37,37,37,37	0
55	MG	CA	1603	1/1	0.97	0.35	77,77,77,77	0
55	MG	DA	3155	1/1	0.97	0.46	46,46,46,46	0
55	MG	DA	3280	1/1	0.97	0.57	46,46,46,46	0
55	MG	BA	3066	1/1	0.97	0.31	62,62,62,62	0
55	MG	DA	3157	1/1	0.97	0.69	47,47,47,47	0
55	MG	DA	3158	1/1	0.97	0.59	44,44,44,44	0
55	MG	DA	3284	1/1	0.97	0.33	56,56,56,56	0
55	MG	BA	3129	1/1	0.97	0.44	52,52,52,52	0
55	MG	DA	3286	1/1	0.97	0.14	47,47,47,47	0
55	MG	DA	3160	1/1	0.97	0.40	49,49,49,49	0
55	MG	DA	3288	1/1	0.97	0.37	47,47,47,47	0
55	MG	DA	3161	1/1	0.97	0.44	45,45,45,45	0
55	MG	DA	3162	1/1	0.97	0.38	66,66,66,66	0
55	MG	BA	3320	1/1	0.97	0.27	62,62,62,62	0
55	MG	AA	1784	1/1	0.97	0.47	66,66,66,66	0
55	MG	BA	3220	1/1	0.97	0.45	44,44,44,44	0
55	MG	DA	3166	1/1	0.97	0.45	58,58,58,58	0
55	MG	CA	1676	1/1	0.97	0.44	55,55,55,55	0
55	MG	CC	102	1/1	0.97	0.52	73,73,73,73	0
55	MG	AA	1665	1/1	0.97	0.75	70,70,70,70	0
55	MG	AA	1602	1/1	0.97	0.33	79,79,79,79	0
55	MG	BA	3276	1/1	0.97	0.23	74,74,74,74	0
55	MG	DP	201	1/1	0.97	0.35	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	BA	3046	1/1	0.97	0.38	39,39,39,39	0
55	MG	DA	3420	1/1	0.97	0.31	67,67,67,67	0
55	MG	CA	1750	1/1	0.97	0.48	79,79,79,79	0
55	MG	BA	3376	1/1	0.97	0.44	73,73,73,73	0
55	MG	D3	101	1/1	0.97	0.43	66,66,66,66	0
56	ZN	AG	302	1/1	0.97	0.34	95,95,95,95	0
55	MG	BA	3014	1/1	0.97	0.48	53,53,53,53	0
55	MG	AA	1619	1/1	0.98	0.40	63,63,63,63	0
55	MG	BA	3004	1/1	0.98	0.46	35,35,35,35	0
55	MG	DA	3472	1/1	0.98	0.69	71,71,71,71	0
55	MG	BA	3024	1/1	0.98	0.38	27,27,27,27	0
55	MG	DA	3079	1/1	0.98	0.38	54,54,54,54	0
55	MG	BA	3229	1/1	0.98	0.12	50,50,50,50	0
55	MG	DA	3235	1/1	0.98	0.42	48,48,48,48	0
55	MG	BA	3230	1/1	0.98	0.59	56,56,56,56	0
55	MG	BA	3189	1/1	0.98	0.39	49,49,49,49	0
55	MG	BA	3190	1/1	0.98	0.33	63,63,63,63	0
55	MG	BA	3123	1/1	0.98	0.21	51,51,51,51	0
55	MG	DA	3240	1/1	0.98	0.55	42,42,42,42	0
55	MG	CA	1619	1/1	0.98	0.49	61,61,61,61	0
55	MG	AA	1627	1/1	0.98	0.32	53,53,53,53	0
55	MG	BA	3155	1/1	0.98	0.18	45,45,45,45	0
55	MG	BA	3283	1/1	0.98	0.38	49,49,49,49	0
55	MG	AA	1841	1/1	0.98	0.38	59,59,59,59	0
55	MG	BA	3157	1/1	0.98	0.60	45,45,45,45	0
55	MG	BA	3196	1/1	0.98	0.32	33,33,33,33	0
55	MG	BA	3158	1/1	0.98	0.32	41,41,41,41	0
55	MG	BA	3382	1/1	0.98	0.39	43,43,43,43	0
55	MG	BA	3126	1/1	0.98	0.42	46,46,46,46	0
55	MG	DA	3095	1/1	0.98	0.44	49,49,49,49	0
55	MG	BA	3007	1/1	0.98	0.54	53,53,53,53	0
55	MG	DA	3171	1/1	0.98	0.34	63,63,63,63	0
55	MG	DA	3097	1/1	0.98	0.29	52,52,52,52	0
55	MG	BA	3128	1/1	0.98	0.50	46,46,46,46	0
55	MG	AA	1842	1/1	0.98	0.46	59,59,59,59	0
55	MG	BA	3245	1/1	0.98	0.55	49,49,49,49	0
55	MG	DA	3101	1/1	0.98	0.33	43,43,43,43	0
55	MG	DA	3102	1/1	0.98	0.37	51,51,51,51	0
55	MG	BA	3163	1/1	0.98	0.58	50,50,50,50	0
55	MG	DA	3104	1/1	0.98	0.40	43,43,43,43	0
55	MG	DA	3180	1/1	0.98	0.59	52,52,52,52	0
55	MG	BA	3294	1/1	0.98	0.35	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	DA	3106	1/1	0.98	0.41	48,48,48,48	0
55	MG	BA	3390	1/1	0.98	0.31	60,60,60,60	0
55	MG	BA	3538	1/1	0.98	0.55	66,66,66,66	0
55	MG	BA	3009	1/1	0.98	0.33	36,36,36,36	0
55	MG	AG	301	1/1	0.98	0.57	81,81,81,81	0
55	MG	BA	3079	1/1	0.98	0.41	55,55,55,55	0
55	MG	AA	1660	1/1	0.98	0.62	53,53,53,53	0
55	MG	CA	1754	1/1	0.98	0.32	86,86,86,86	0
55	MG	DA	3116	1/1	0.98	0.40	74,74,74,74	0
55	MG	BA	3207	1/1	0.98	0.57	41,41,41,41	0
55	MG	DA	3118	1/1	0.98	0.35	71,71,71,71	0
55	MG	DA	3194	1/1	0.98	0.43	73,73,73,73	0
55	MG	AA	1707	1/1	0.98	0.58	50,50,50,50	0
55	MG	BA	3013	1/1	0.98	0.43	34,34,34,34	0
55	MG	BA	3036	1/1	0.98	0.54	44,44,44,44	0
55	MG	DA	3052	1/1	0.98	0.45	71,71,71,71	0
55	MG	BA	3255	1/1	0.98	0.38	46,46,46,46	0
55	MG	B0	201	1/1	0.98	0.32	51,51,51,51	0
55	MG	DA	3201	1/1	0.98	0.25	47,47,47,47	0
55	MG	BA	3172	1/1	0.98	0.36	34,34,34,34	0
55	MG	BA	3212	1/1	0.98	0.61	43,43,43,43	0
55	MG	AA	1783	1/1	0.98	0.60	67,67,67,67	0
55	MG	CA	1650	1/1	0.98	0.26	102,102,102,102	0
55	MG	BA	3139	1/1	0.98	0.39	35,35,35,35	0
55	MG	BA	3015	1/1	0.98	0.35	38,38,38,38	0
55	MG	BA	3261	1/1	0.98	0.62	52,52,52,52	0
55	MG	CA	1710	1/1	0.98	0.29	106,106,106,106	0
55	MG	DA	3211	1/1	0.98	0.49	42,42,42,42	0
55	MG	DA	3133	1/1	0.98	0.38	42,42,42,42	0
55	MG	BA	3554	1/1	0.98	0.47	45,45,45,45	0
55	MG	BA	3039	1/1	0.98	0.30	42,42,42,42	0
55	MG	DA	3065	1/1	0.98	0.41	74,74,74,74	0
55	MG	AA	1691	1/1	0.98	0.49	50,50,50,50	0
55	MG	BA	3041	1/1	0.98	0.31	46,46,46,46	0
55	MG	BA	3610	1/1	0.98	0.43	61,61,61,61	0
55	MG	BA	3042	1/1	0.98	0.34	41,41,41,41	0
55	MG	BA	3017	1/1	0.98	0.46	25,25,25,25	0
55	MG	BA	3091	1/1	0.98	0.52	35,35,35,35	0
55	MG	DA	3223	1/1	0.98	0.47	52,52,52,52	0
55	MG	DA	3144	1/1	0.98	0.29	60,60,60,60	0
55	MG	BA	3269	1/1	0.98	0.45	61,61,61,61	0
55	MG	BA	3002	1/1	0.98	0.47	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MG	DA	3147	1/1	0.98	0.38	53,53,53,53	0
55	MG	D5	2001	1/1	0.98	0.41	46,46,46,46	0
55	MG	BA	3045	1/1	0.98	0.41	45,45,45,45	0
56	ZN	AQ	102	1/1	0.98	0.09	122,122,122,122	0
56	ZN	CG	303	1/1	0.98	0.31	118,118,118,118	0
55	MG	BA	3068	1/1	0.98	0.34	75,75,75,75	0
55	MG	DA	3213	1/1	0.99	0.48	41,41,41,41	0
55	MG	BA	3233	1/1	0.99	0.41	48,48,48,48	0
55	MG	BA	3019	1/1	0.99	0.44	66,66,66,66	0
55	MG	BA	3074	1/1	0.99	0.47	49,49,49,49	0
55	MG	DA	3474	1/1	0.99	0.60	83,83,83,83	0
55	MG	BA	3262	1/1	0.99	0.57	33,33,33,33	0
55	MG	BA	3131	1/1	0.99	0.32	59,59,59,59	0
55	MG	AA	1604	1/1	0.99	0.33	67,67,67,67	0
55	MG	CA	1706	1/1	0.99	0.42	87,87,87,87	0
55	MG	AA	1609	1/1	0.99	0.41	78,78,78,78	0
55	MG	DA	3296	1/1	0.99	0.66	51,51,51,51	0
55	MG	DA	3114	1/1	0.99	0.56	54,54,54,54	0
55	MG	DA	3115	1/1	0.99	0.52	49,49,49,49	0
55	MG	CA	1792	1/1	0.99	0.62	70,70,70,70	0
55	MG	BA	3027	1/1	0.99	0.54	36,36,36,36	0
55	MG	DE	301	1/1	0.99	0.38	41,41,41,41	0
55	MG	BA	3171	1/1	0.99	0.54	61,61,61,61	0
55	MG	DA	3203	1/1	0.99	0.27	48,48,48,48	0
55	MG	CA	1726	1/1	0.99	0.62	75,75,75,75	0
55	MG	DA	3182	1/1	0.99	0.81	44,44,44,44	0
55	MG	BA	3216	1/1	0.99	0.32	33,33,33,33	0
55	MG	BA	3018	1/1	0.99	0.35	54,54,54,54	0
55	MG	DA	3463	1/1	0.99	0.20	73,73,73,73	0
55	MG	DA	3142	1/1	0.99	0.52	40,40,40,40	0
55	MG	BA	3173	1/1	0.99	0.59	52,52,52,52	0
55	MG	BA	3029	1/1	0.99	0.42	35,35,35,35	0
55	MG	BA	3608	1/1	0.99	0.37	39,39,39,39	0
55	MG	DA	3260	1/1	0.99	0.62	41,41,41,41	0
55	MG	BA	3023	1/1	0.99	0.36	45,45,45,45	0

6.5 Other polymers (i)

There are no such residues in this entry.