



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 13, 2024 – 05:44 PM EST

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

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

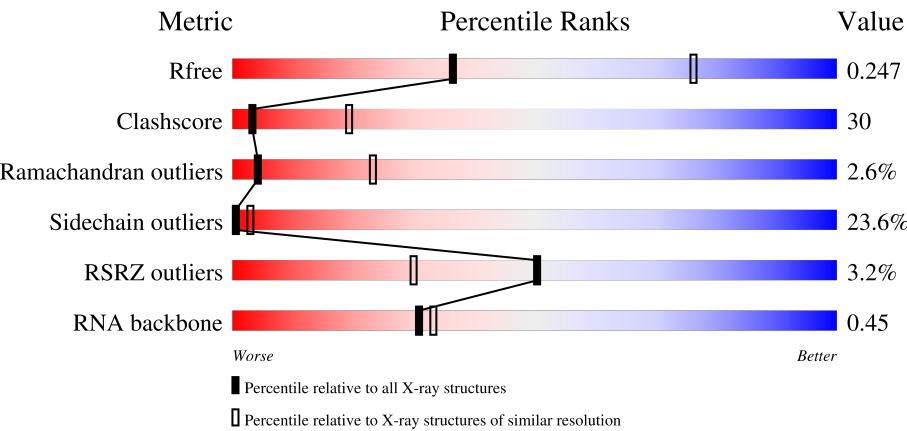
1 Overall quality at a glance i

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}	164625	2511 (3.00-3.00)
Clashscore	180529	2866 (3.00-3.00)
Ramachandran outliers	177936	2778 (3.00-3.00)
Sidechain outliers	177891	2781 (3.00-3.00)
RSRZ outliers	164620	2523 (3.00-3.00)
RNA backbone	3690	1019 (3.20-2.80)

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

Mol	Chain	Length	Quality of chain
1	AA	1506	
1	CA	1506	
2	AE	256	
2	CE	256	

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

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

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

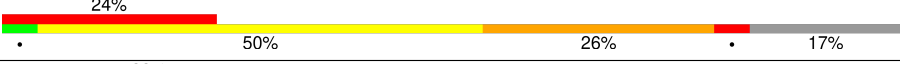
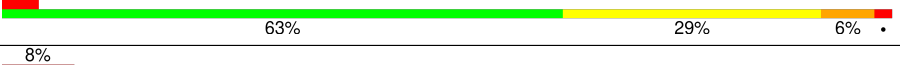
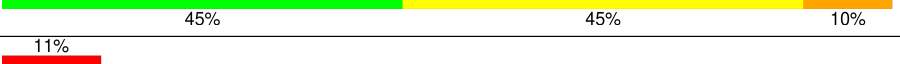
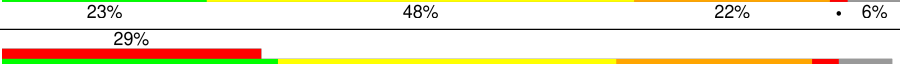
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Mol	Chain	Length	Quality of chain
39	DR	146	
40	B1	118	
40	D1	118	
41	B2	101	
41	D2	101	
42	BS	113	
42	DS	113	
43	BT	96	
43	DT	96	
44	BU	110	
44	DU	110	
45	BV	206	
45	DV	206	
46	B3	85	
46	D3	85	
47	BZ	98	
47	DZ	98	
48	BW	72	
48	DW	72	
49	BX	60	
49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

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	AA	1643	-	-	-	X
55	MG	AA	1747	-	-	-	X
55	MG	AA	1748	-	-	-	X
55	MG	AA	1761	-	-	-	X
55	MG	AA	1807	-	-	-	X
55	MG	AA	1818	-	-	-	X
55	MG	AA	1831	-	-	-	X
55	MG	BA	3164	-	-	-	X
55	MG	BA	3379	-	-	-	X
55	MG	BA	3400	-	-	-	X
55	MG	BA	3403	-	-	-	X
55	MG	CA	1601	-	-	-	X
55	MG	CA	1622	-	-	-	X
55	MG	CA	1638	-	-	-	X
55	MG	CA	1639	-	-	-	X
55	MG	CA	1684	-	-	-	X
55	MG	CA	1694	-	-	-	X
55	MG	CA	1707	-	-	-	X
55	MG	CA	1713	-	-	-	X
55	MG	CA	1755	-	-	-	X
55	MG	CA	1761	-	-	-	X
55	MG	DA	3019	-	-	-	X
55	MG	DA	3025	-	-	-	X
55	MG	DA	3026	-	-	-	X
55	MG	DA	3073	-	-	-	X
55	MG	DA	3080	-	-	-	X
55	MG	DA	3089	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	DA	3146	-	-	-	X
55	MG	DA	3302	-	-	-	X
55	MG	DA	3342	-	-	-	X
55	MG	DA	3363	-	-	-	X
55	MG	DA	3376	-	-	-	X
55	MG	DA	3381	-	-	-	X
55	MG	DA	3458	-	-	-	X
55	MG	DA	3481	-	-	-	X
55	MG	DA	3491	-	-	-	X
55	MG	DA	3501	-	-	-	X
55	MG	DA	3503	-	-	-	X
55	MG	DA	3507	-	-	-	X

2 Entry composition

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There are 4 discrepancies between the modelled and reference sequences:

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

- Molecule 24 is a RNA chain called MRNA.

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

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

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

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BA	161	U	-	expression tag	GB AP008226.1
BA	654A	A	G	conflict	GB AP008226.1
BA	654E	C	G	conflict	GB AP008226.1
BA	654P	G	C	conflict	GB AP008226.1
BA	654T	A	C	conflict	GB AP008226.1
BA	1058	U	G	conflict	GB AP008226.1
BA	1080	A	C	conflict	GB AP008226.1
DA	168	U	-	insertion	GB AP008226.1
DA	654A	A	G	conflict	GB AP008226.1
DA	654E	C	G	conflict	GB AP008226.1
DA	654P	G	C	conflict	GB AP008226.1
DA	654T	A	C	conflict	GB AP008226.1
DA	1058	U	G	conflict	GB AP008226.1
DA	1080	A	C	conflict	GB AP008226.1

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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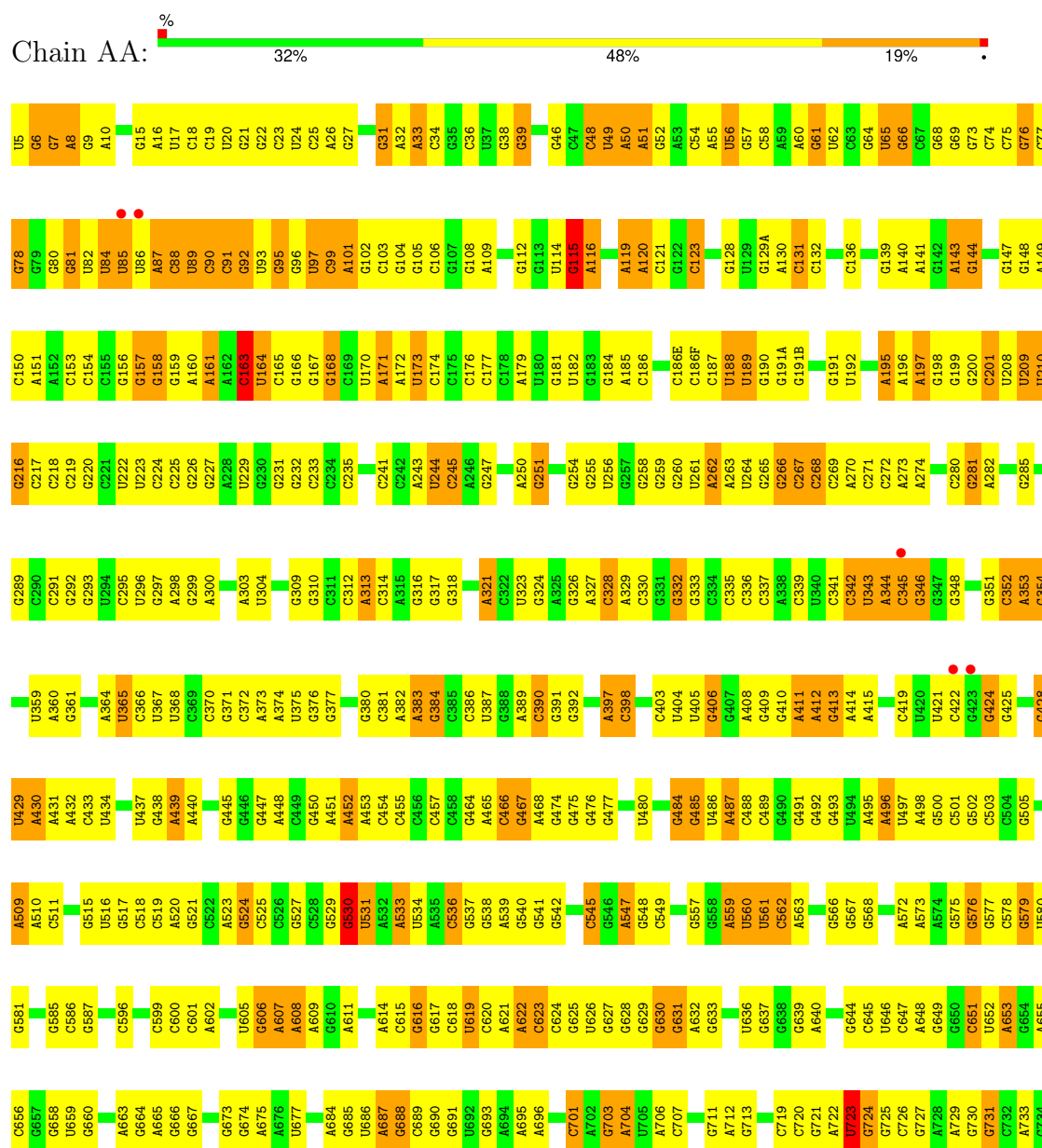
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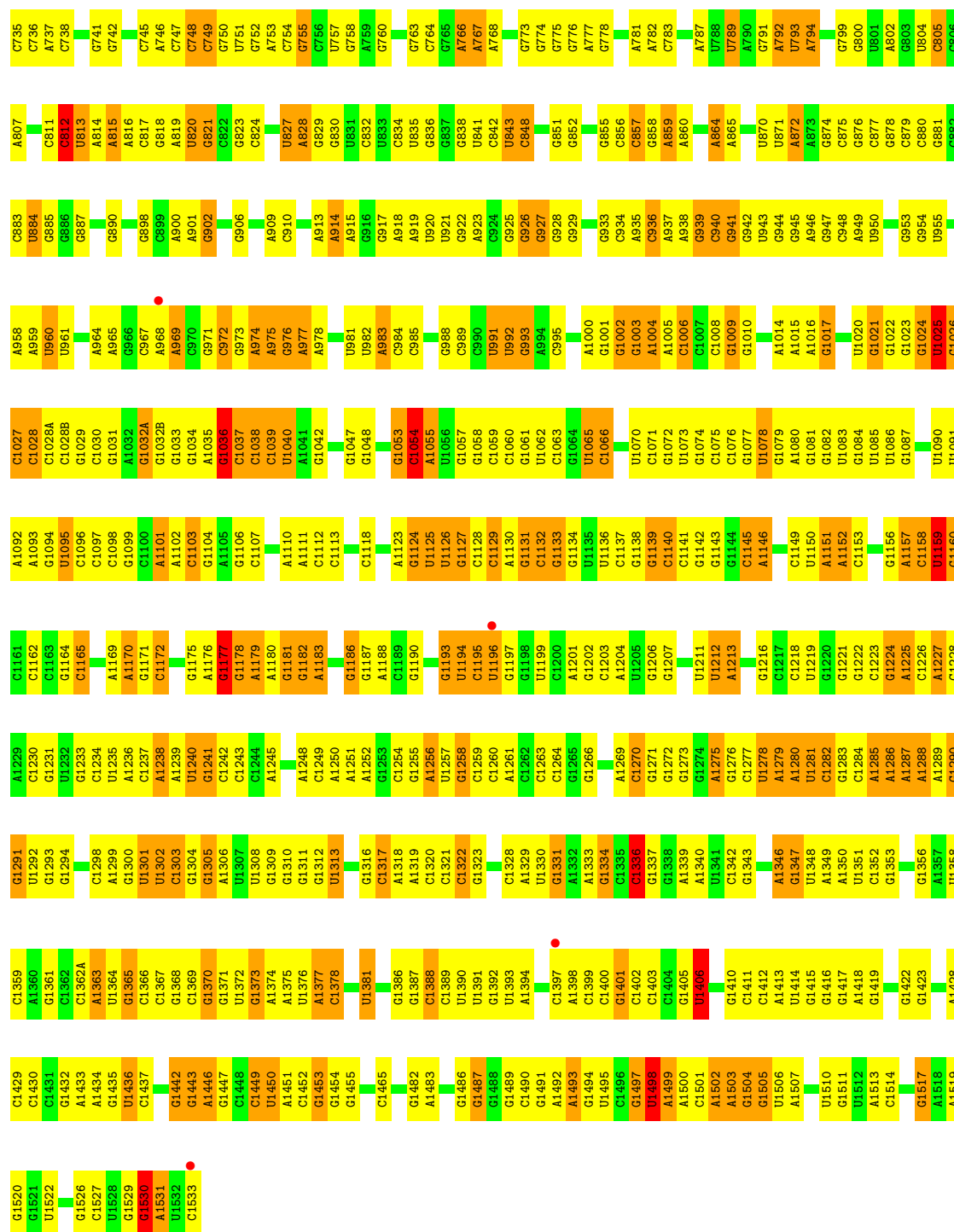
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	CG	1	Total 1	Zn 1	0	0
56	CQ	1	Total 1	Zn 1	0	0

3 Residue-property plots

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.

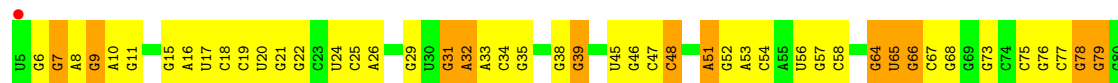
• Molecule 1: 16S ribosomal RNA



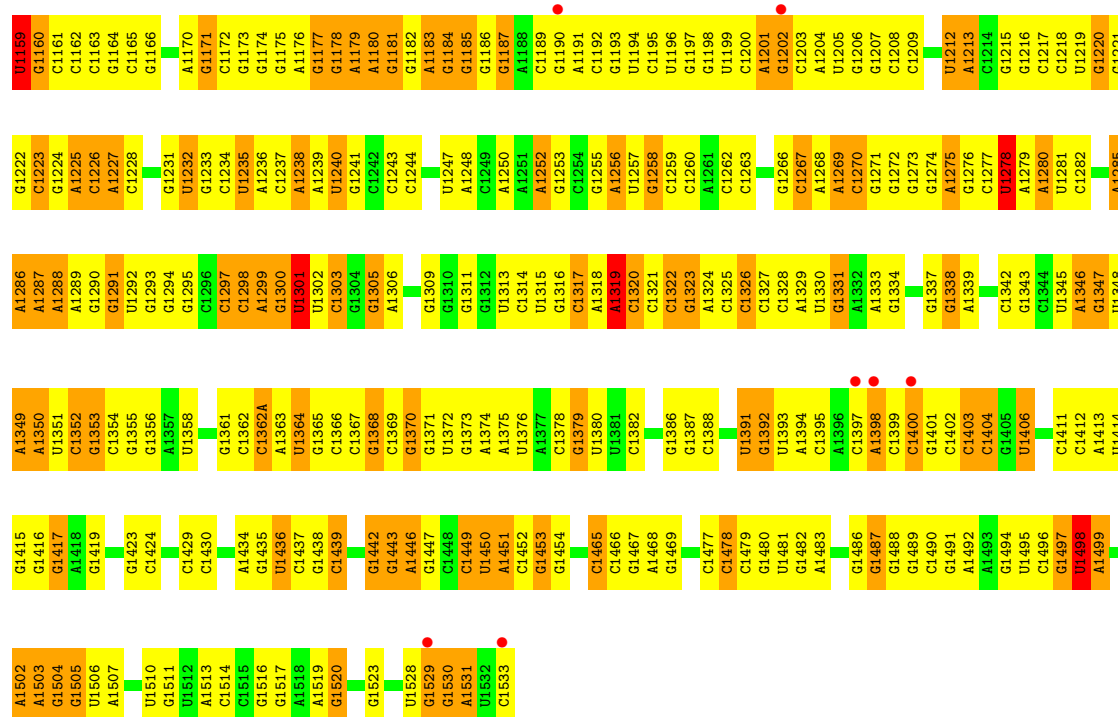


● Molecule 1: 16S ribosomal RNA

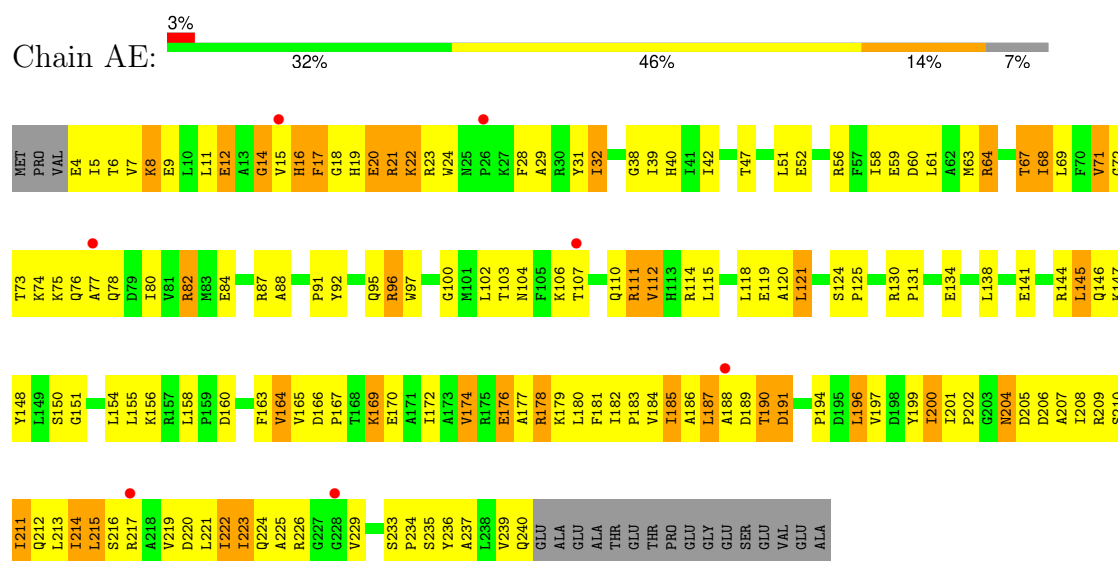
Chain CA: 30% 47% 22%



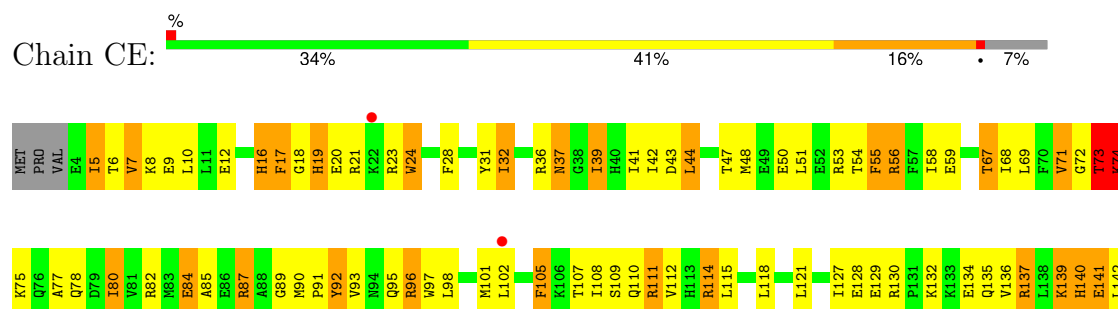
G1097	G1033	A977	G916	G829	G755	G632	G541	G467	C390	A313	C235	C165	G81
G1034	G1034	A978	G917	U833	C756	G612	G542	A468	C391	C314	C236	G166	U82
A1035	A1035	C979	A918	U834	G757	G616	G543	A469	G392	A315	C240	G167	U84
G1036	G1036	C980	A919	C834	G758	G685	G544	C475	A393	G316	C241	G168	U85
C1037	C1037	U981	U920	U835	U686	G617	C545	C476	G394	C242	C242	C169	U86
C1038	C1038	U982	U921	U836	U687	C618	G546	C477	C395	A321	U170	U170	A87
C1039	C1039	U983	U922	U837	C764	U619	G547	A478	G396	U244	U244	A171	C88
A984	A984	C984	A923	C838	C765	C620	G548	A479	A397	G326	C245	A172	U89
C985	C985	U841	A924	U842	A766	A621	C549	G481	C398	A327	C246	U173	C90
A1041	A1041	C842	G926	C843	G767	G624	G550	A482	U404	A328	C247	C174	C91
G1042	G1042	U843	G927	U844	G768	G625	U551	A483	U405	A329	A250	C177	U93
A1044	A1044	C848	G928	C849	G769	G626	U552	C484	G406	C251	C251	C178	G95
C990	C990	U850	C929	C850	G773	U627	A553	C485	G407	G332	U252	A179	
U991	U991	G851	C930	U851	G774	G628	C554	U486	A408	G333	U253	U180	A101
C992	C992	G852	C931	C852	G775	G629	C555	A487	G409	U343	G254	G181	G102
G993	G993	G853	C932	C853	G776	G630	C556	C488	G410	C339	G255	U182	
C994	C994	G854	C933	C854	A777	G631	A559	C489	A411	U340	U256	G183	G105
A994	A994	C934	G934	C855	A778	G632	U560	G501	A412	G342	U257	G184	C106
C995	C995	A935	A935	C856	C779	A632	U561	G502	G422	C343	G258	A185	G107
A996	A996	C936	C936	C857	A780	G633	U562	C503	G423	U344	G259	C186	G108
G998	G998	U937	U937	C858	C783	G634	C563	G504	A414	C345	G260	A109	
C998A	C998A	A860	A938	C859	U705	G641	A563	G505	U420	G346	U261	C186E	U114
U999	U999	C861	C940	C862	U706	U642	A564	G506	G421	G347	G262	C187	G113
A1000	A1000	U863	G941	U863	C707	U643	A565	C507	A420	G348	A262	U188	G115
G1001	G1001	A864	A942	A864	G707	U644	U566	C508	U421	G349	G265	G116	
G1002	G1002	C869	G943	C869	G710	U645	G567	C509	G422	G350	G266	A116	
C1003	C1003	U870	G944	U870	G711	U646	G568	C510	G423	G351	G267	G190	
A1004	A1004	U871	G945	U871	A712	U647	C569	G512	G424	G352	G268	G191A	C121
A1005	A1005	A946	A946	A946	G713	U648	G570	G513	G425	C352	C269	G191B	G122
C1006	C1006	A872	G947	A872	U723	U649	U571	C514	C433	A353	G270	G191C	C123
C1007	C1007	A873	U724	A873	G724	U650	A572	C515	U434	G354	A270	G191D	
C1008	C1008	C877	G795	C877	G725	U651	A573	C516	U435	G355	C271	G126	
G1009	G1009	C878	C796	C878	A728	U652	A574	C517	A430	A356	C272	G191	A130
G1010	G1010	C879	G797	C879	A729	C651	G575	C518	U431	G357	A273	U192	C131
G1013	G1013	C883	G800	C883	U801	U653	G576	C519	C432	U358	G275	C193	C132
A1014	A1014	U884	U801	U884	A802	A654	G577	C520	U433	A360	G279	A195	U133
A1015	A1015	C885	U802	C885	A803	U655	U580	C521	C436	G362	C280	A196	A134
C1016	C1016	U886	G803	U886	U804	C656	G581	C522	U437	A363	A281	A197	
G1017	G1017	C887	U804	C887	G730	U657	U582	C523	G438	A364	A282	G198	A141
C1018	C1018	G887	C805	G887	G731	U658	A583	C524	A439	U365	C283	G201	A143
A1019	A1019	C888	C805	C888	G732	U659	G584	C525	A440	C366	U287	U208	A144
U1020	U1020	A889	G809	A889	A736	U660	G585	C526	C444	U367	A288	U209	G145
G1021	G1021	C890	C810	C890	A737	U661	G586	C527	G445	U368	G289	G216	G146
C1022	C1022	C891	C811	C891	U740	U662	G587	C528	G446	C369	G290	G217	G147
G1023	G1023	C892	C812	C892	G741	U663	G588	C529	G447	C372	G291	C218	G148
U1024	U1024	C893	U813	C893	G742	U664	C589	G530	C449	A373	U292	C219	A149
G1025	G1025	C894	U814	C894	G743	U665	G593	G531	G450	A374	C295	G220	C150
C1026	C1026	A895	A815	A895	C745	U666	G594	C532	A451	U375	C296	A151	A152
G1027	G1027	C896	A816	C896	A746	U667	C600	C533	A452	G376	A298	G221	G156
C1028	C1028	A900	C817	A900	C747	U668	C601	U534	A453	C380	G299	G226	G157
A1028A	A1028A	A901	C818	A901	C748	U669	G604	A535	G454	C381	G300	G227	A160
C970	C970	C819	U819	C819	C749	U670	U605	C536	C457	A382	A301	G228	A161
G971	G971	A909	U820	A909	C750	U671	G606	C537	C458	G383	G302	U229	C162
C972	C972	C910	U821	C910	U751	U672	G607	G538	G464	A384	G303	G230	A163
G973	G973	A913	U822	A913	U752	U673	G608	A539	A465	G385	G304	G231	U164
A974	A974	U914	U823	A974	C753	U674	A609	G540	C466				
A975	A975	A915	A828	A915	C754	C681							

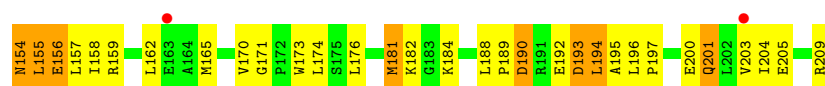


• Molecule 2: 30S RIBOSOMAL PROTEIN S2

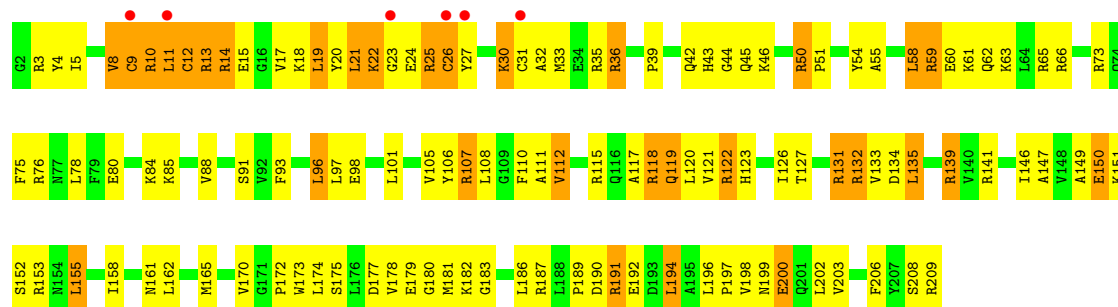


• Molecule 2: 30S RIBOSOMAL PROTEIN S2

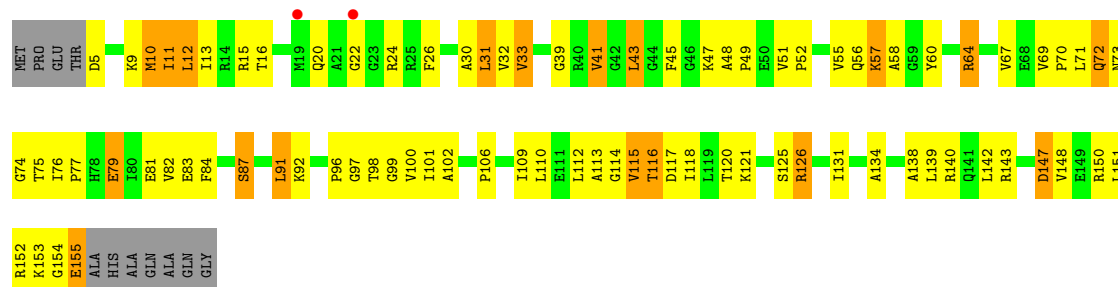
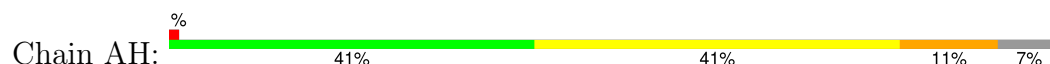




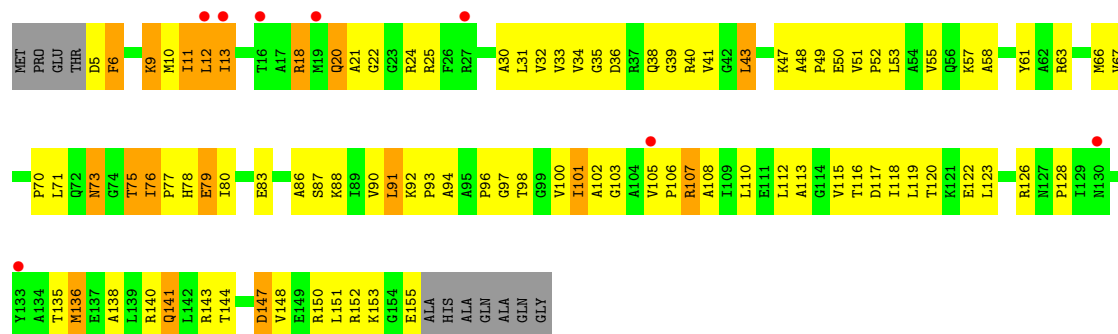
• Molecule 4: 30S RIBOSOMAL PROTEIN S4



• Molecule 5: 30S RIBOSOMAL PROTEIN S5



• Molecule 5: 30S RIBOSOMAL PROTEIN S5

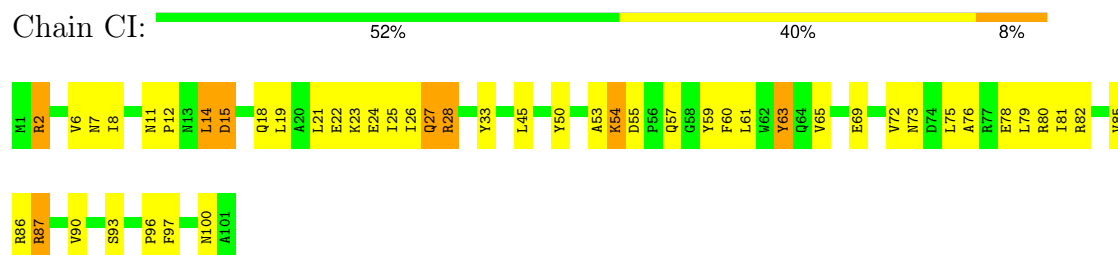


• Molecule 6: 30S RIBOSOMAL PROTEIN S6

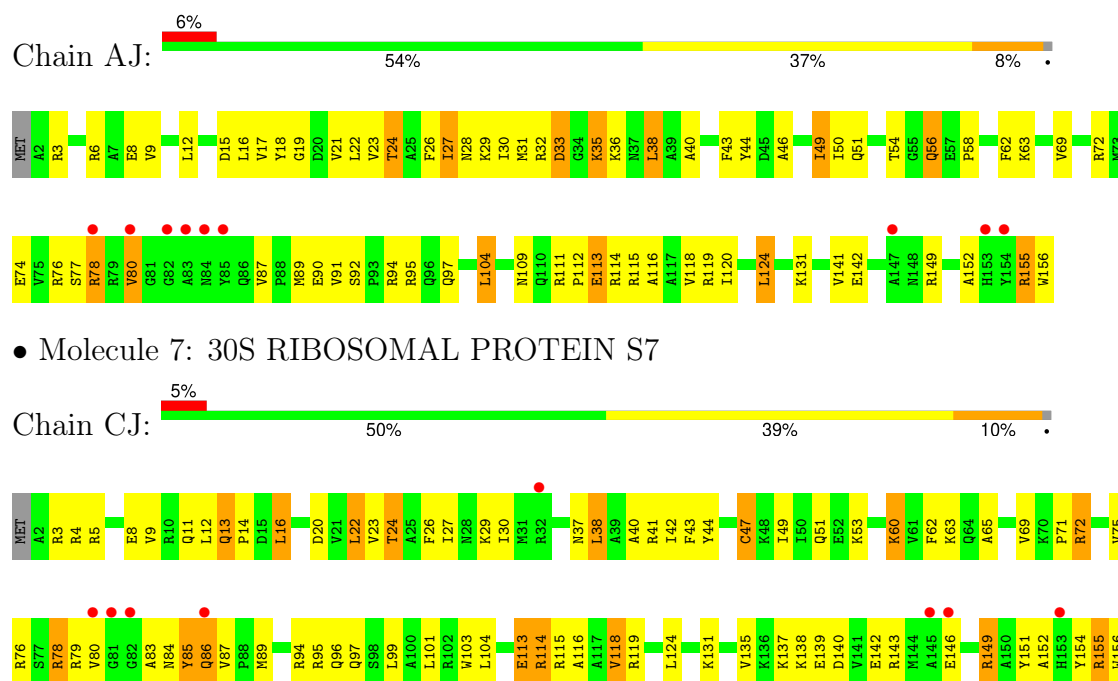




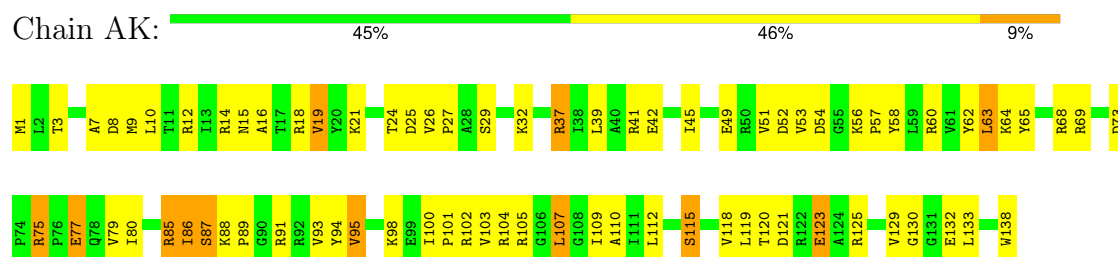
• Molecule 6: 30S RIBOSOMAL PROTEIN S6



• Molecule 7: 30S RIBOSOMAL PROTEIN S7

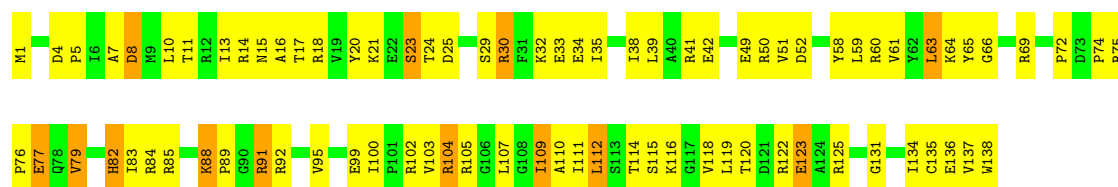


• Molecule 8: 30S RIBOSOMAL PROTEIN S8



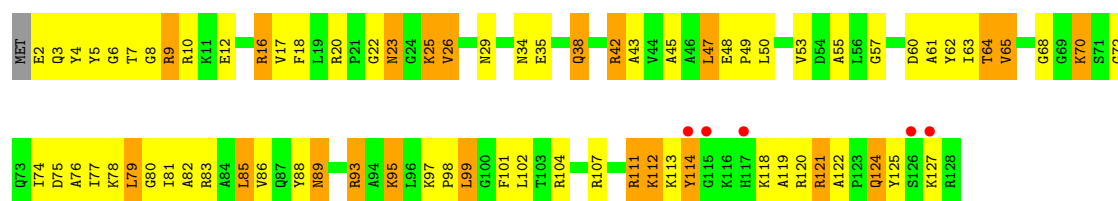
• Molecule 8: 30S RIBOSOMAL PROTEIN S8

Chain CK: 




• Molecule 9: 30S RIBOSOMAL PROTEIN S9

Chain AL: 



• Molecule 9: 30S RIBOSOMAL PROTEIN S9

Chain CL: 



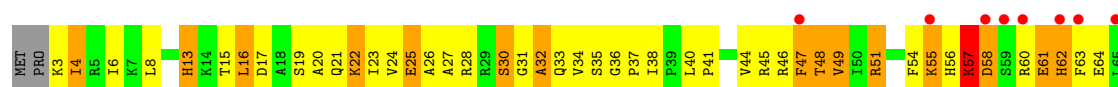
• Molecule 10: 30S RIBOSOMAL PROTEIN S10

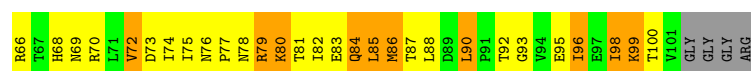
Chain AM: 



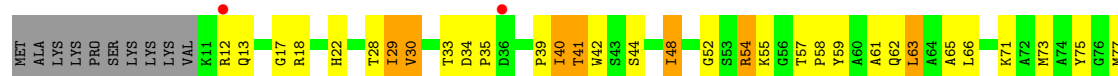
• Molecule 10: 30S RIBOSOMAL PROTEIN S10

Chain CM: 





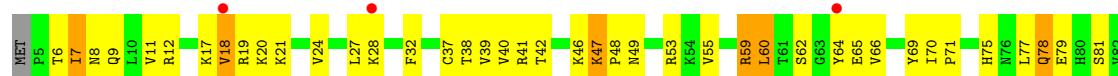
• Molecule 11: 30S RIBOSOMAL PROTEIN S11



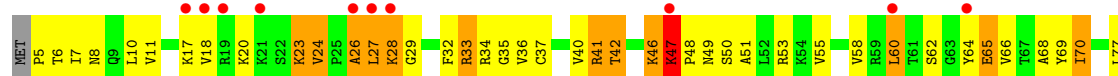
• Molecule 11: 30S RIBOSOMAL PROTEIN S11



• Molecule 12: 30S RIBOSOMAL PROTEIN S12

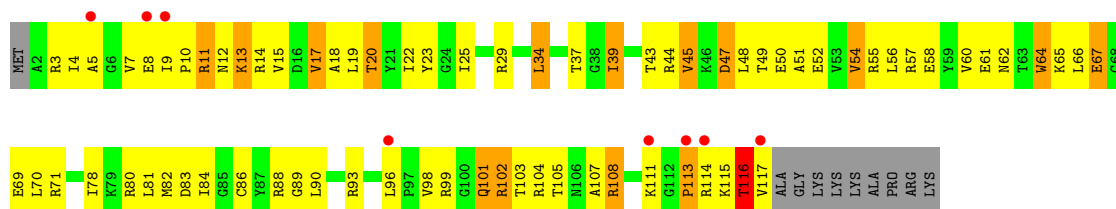


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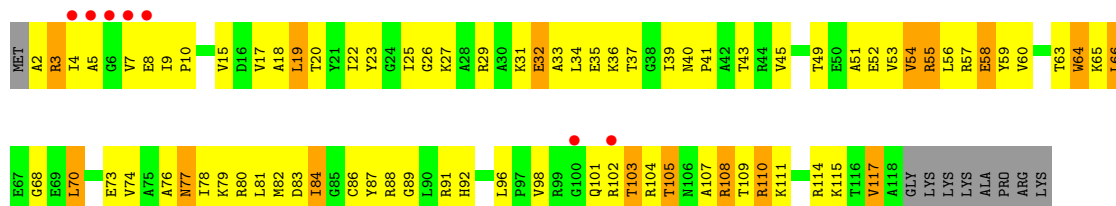


• Molecule 13: 30S RIBOSOMAL PROTEIN S13

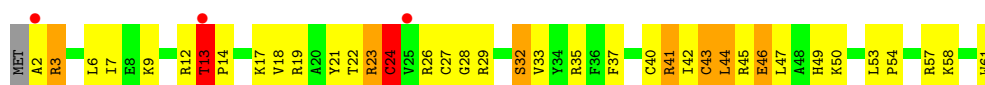




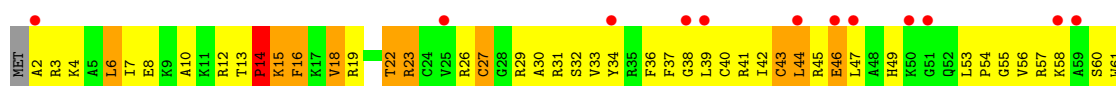
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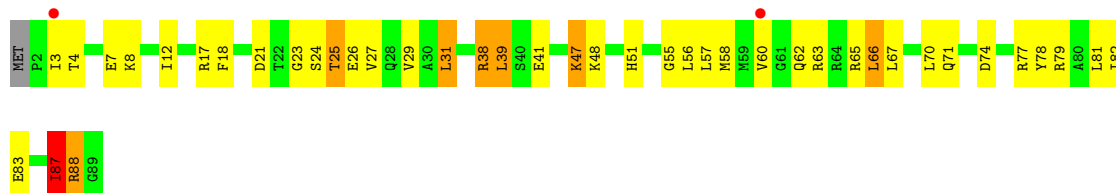
• Molecule 14: 30S RIBOSOMAL PROTEIN S14



• Molecule 14: 30S RIBOSOMAL PROTEIN S14



• Molecule 15: 30S RIBOSOMAL PROTEIN S15

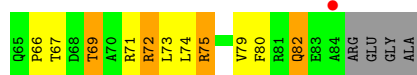


• Molecule 15: 30S RIBOSOMAL PROTEIN S15

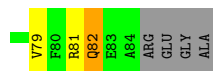
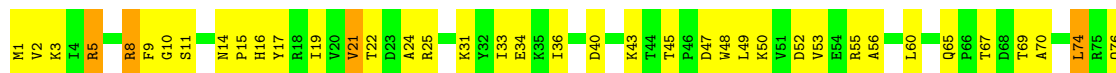




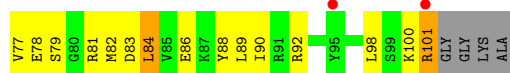
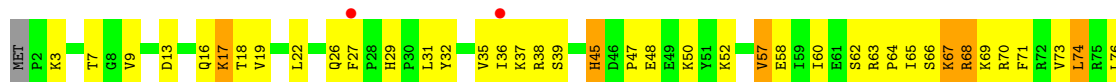
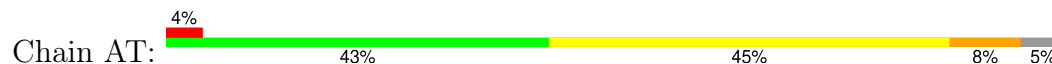
• Molecule 16: 30S RIBOSOMAL PROTEIN S16



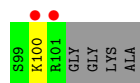
• Molecule 16: 30S RIBOSOMAL PROTEIN S16



• Molecule 17: 30S RIBOSOMAL PROTEIN S17

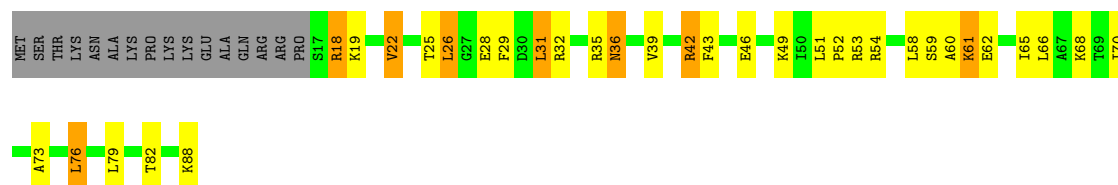


• Molecule 17: 30S RIBOSOMAL PROTEIN S17

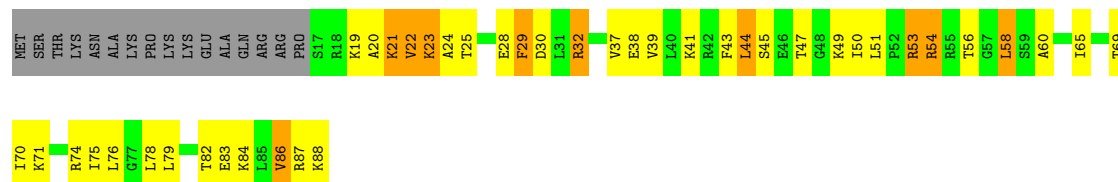


• Molecule 18: 30S RIBOSOMAL PROTEIN S18

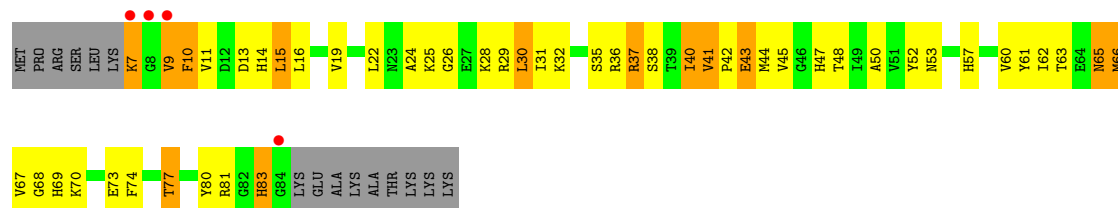




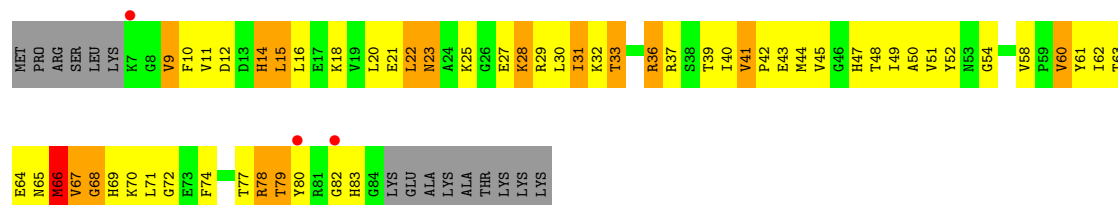
• Molecule 18: 30S RIBOSOMAL PROTEIN S18



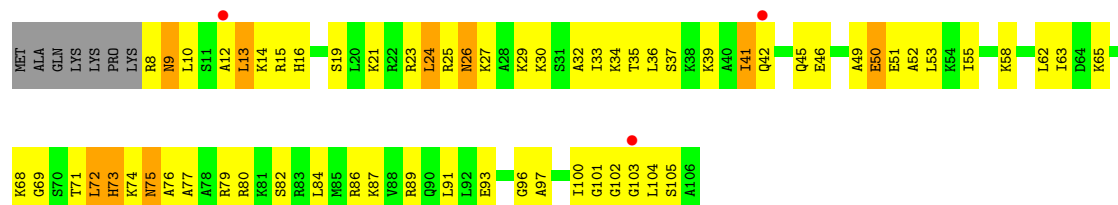
• Molecule 19: 30S RIBOSOMAL PROTEIN S19



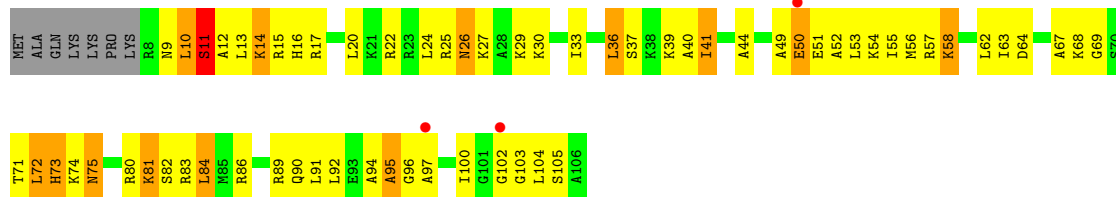
• Molecule 19: 30S RIBOSOMAL PROTEIN S19



• Molecule 20: 30S RIBOSOMAL PROTEIN S20



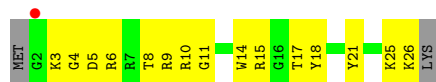
• Molecule 20: 30S RIBOSOMAL PROTEIN S20



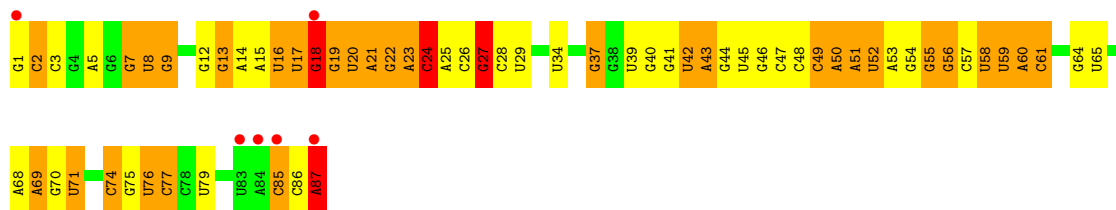
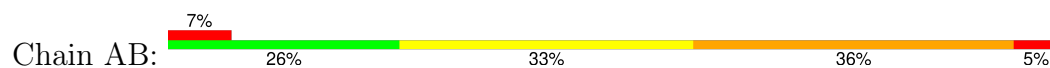
• Molecule 21: 30S RIBOSOMAL PROTEIN THX



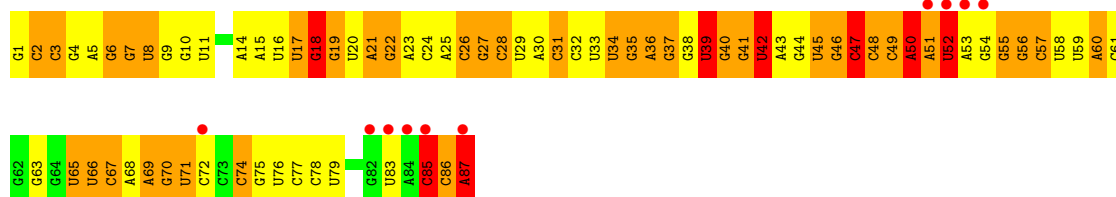
• Molecule 21: 30S RIBOSOMAL PROTEIN THX



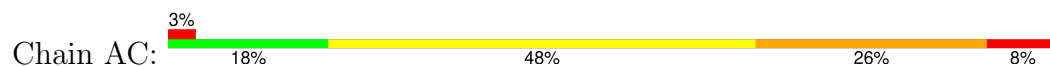
• Molecule 22: TRNA-LEU

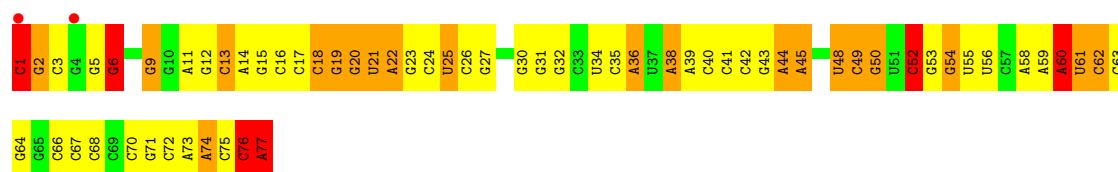


• Molecule 22: TRNA-LEU

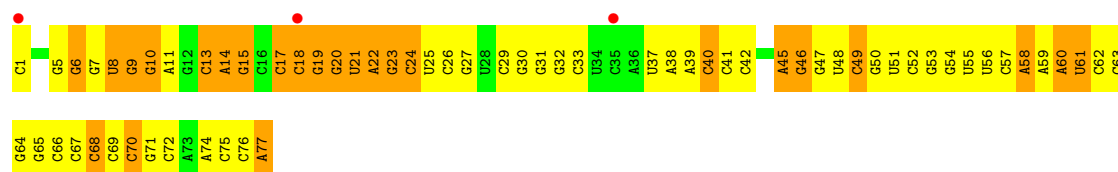
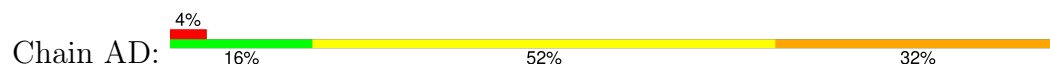


• Molecule 23: TRNA-FMET

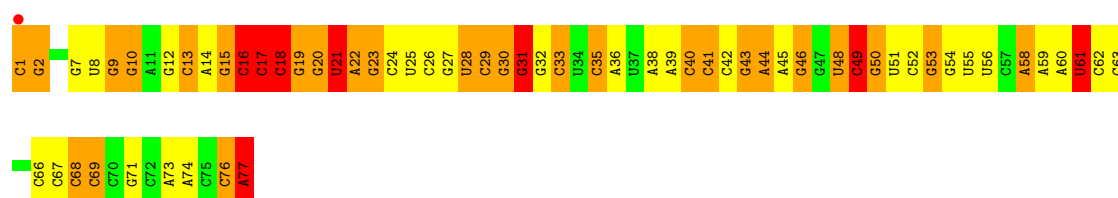
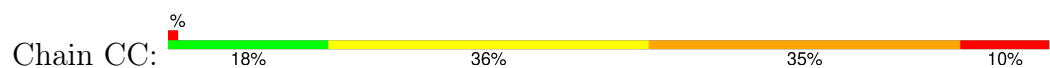




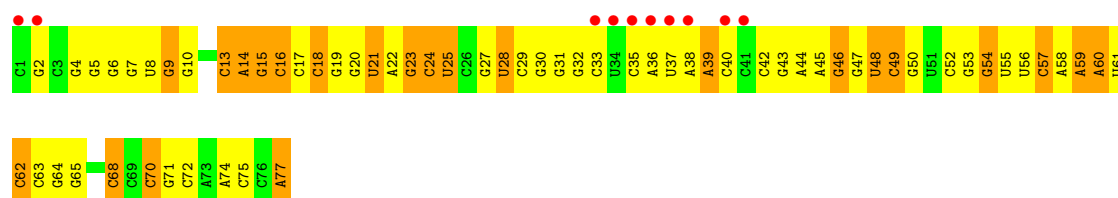
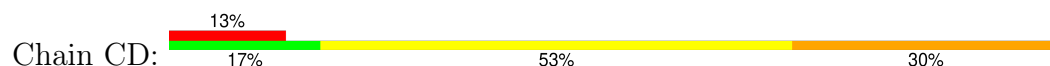
• Molecule 23: TRNA-FMET



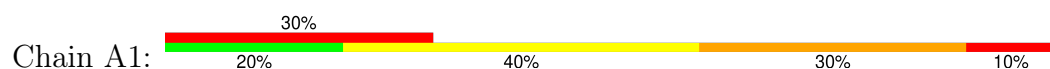
• Molecule 23: TRNA-FMET



• Molecule 23: TRNA-FMET



• Molecule 24: MRNA



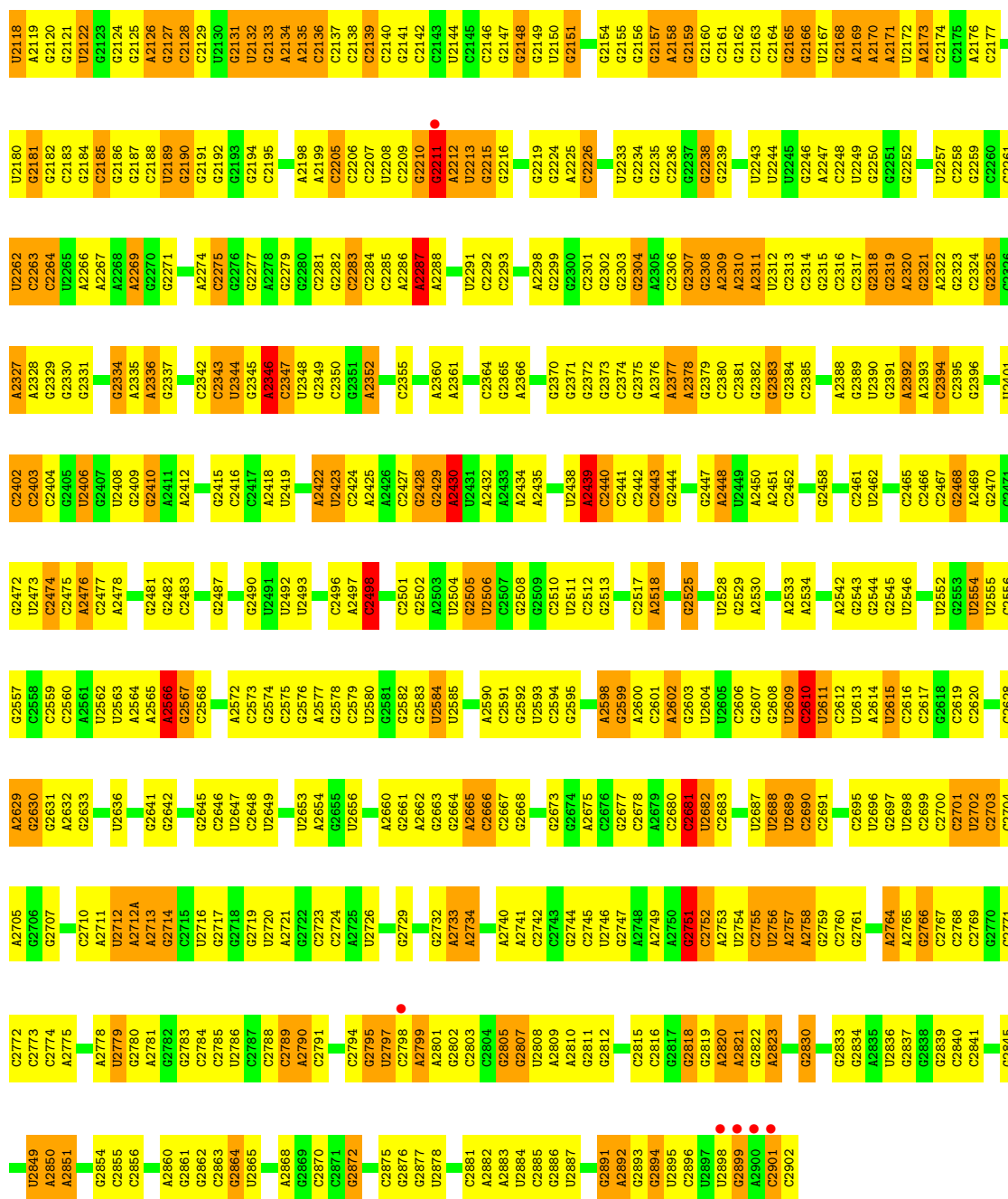
• Molecule 24: MRNA



Chain BA: %

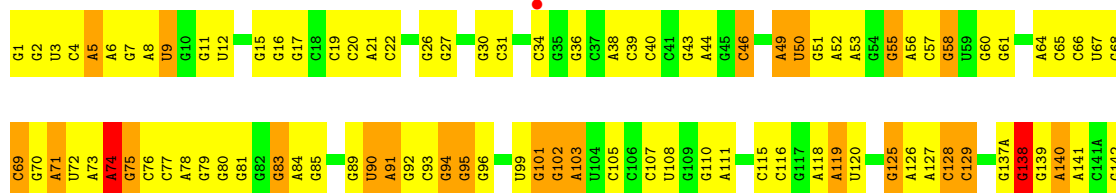


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C2036	G1857	U1778	U1692	C1600	C1467	G1400	A1321	A1242	G1164	A1096	
G2037	G1858	U1779	U1693	A1536	A1468	G1401	G1243	G1244	U1165	U1097	U1033
G2038	U1956	A1780	G1695	C1537	A1469	G1402	A1322		C1166	A1098	
	G1861			G1538	A1470	C1403	U1324	A1247	U1167	G1099	G1037
A2042	U1884	A1783	A1698	G1539	A1471	C1404	G1328	G1250	U1168	C1100	C1038
C2043	G1869	A1784	G1699	G1540	A1472	U1405	G1329	G1251	U1169	U1101	G1039
	A1785	A1785	A1700	U1541	G1473	U1406	U1329		G1170	C1102	
C2050	A1786	A1786	A1701	G1542	C1474	C1407	A1173	A1253	G1171	A1103	G1042
A2051			G1702	A1543	G1475	C1408	G1174	A1254	C1104	C1043	
				C1611	C1476	C1409	A1175	U1255	U1105	G1044	
	G1878	A1789		C1544	A1477	G1409	G1332	U1256	G1106	A1045	
		C1790	G1705	A1545	G1478	G1410		C1257	G1107	A1046	
C2055	G1888	C1791	G1706	G1612	G1479	C1411	A1336			G1047	
G1968	C1882	A1791	U1706	G1613	G1480	A1412	G1337	C1261	G1110		
A1969	G1883	G1792		A1614	U1482	G1413	G1338	U1262	C1111	A1048	
A2057	A1884	C1793	C1710	C1547	G1483	G1414	A1174	U1263	C1112	C1049	
A2058	A1885	U1794	C1711	C1548	G1484		G1175	U1264	U1113	A1050	
A2059	C1886	C1795	C1712	C1549	G1485	G1415	G1339	G1265	G1114		
A2060	C1887	U1796	U1716	C1550		C1417	U1340				
G2061	G1888	C1797	G1717	A1554	A1486		U1341	G1266			
A2062	A1889	U1798	G1718	G1555	G1487	U1420		U1267	G1117	A1054	
C2063		G1799	G1719	G1556	U1489	G1421	G1344	G1268	G1118	G1055	
C2064	C1894	C1800	G1725	C1557	A1490	G1422	C1345	A1268	C1119	G1056	
C2065	C1895	G1801	G1726	C1558		G1423		U1271		G1057	
G2066	A1981	A1802	U1727	A1559	C1493	C1428	G1348	C1270	G1122	U1058	
G2067	C1982	A1803	G1728	G1560	A1494	G1429	A1349	G1272	G1123	G1059	
G2068	G1983	G1804	U1729	G1561	A1495	C1430	U1352	U1273	C1124	U1060	
G2069	A1900	U1805	G1730	G1562	A1496	U1431	A1353	U1274	G1125	U1061	
G2070	C1901	U1806	G1731	C1563	A1497	C1432	A1354		G1126	G1062	
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U2074	G1903	A1811	G1733	A1565	C1502	A1434		G1279	A1128	U1065	
U2075	G1906	G1813	G1734	A1566	G1503	G1435	G1358	G1280	U1129	U1066	
	A1913	G1816	C1735	A1567	U1504	G1436	A1359	G1281	U1130	U1067	
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G2083	U1915	U1818	G1742	A1569	C1505	U1438				A1069	
	G1999	A1819	G1743	A1570	C1506	A1439	G1364	A1287	G1135	A1070	
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		A1821	G1750	C1575	U1509	G1443	G1368	U1291	G1138	C1073	
	C1925	G1824	C1751	U1576	C1509	G1444		U1292	G1139	A1074	
	U1926	A1825	G1754	C1577	A1510	G1445	U1372	C1293	U1140	G1075	
		G1826	A1755	U1578	A1511	C1446	A1373	U1294	U1141	C1076	
G2012	G1929	G1827	G1756	A1579	U1514	G1447		G1295	U1142	A1077	
A2013	G1930	G1828	U1757	A1580	C1515	G1448	G1376	C1296	A1142	U1078	
A2014	U1931	G1829	G1758	G1581	U1516	G1449	G1377	C1297			
	A1932	A1829	G1759	C1582	U1517	A1450	A1378	C1298	A1143	C1079	
A2019	G1933	G1830	A1760	A1583	C1518	G1451	U1300	G1299	G1144	A1080	
A2020	C1934	G1831	C1761	C1584	G1519	G1452	A1379	U1301	C1147	U1081	
G1935	A1936	C1832	C1762	A1586	U1520	C1453	G1380	A1302	A1148	U1082	
		G1835	G1763	A1587	G1521	U1454	G1381	G1303	G1149	A1084	
	A1937		G1764	C1588	G1522	G1455	G1382		C1150	A1085	
	U1938	G1839		C1589	G1525		A1383	G1309	G1151	A1086	
	U1939		G1769	U1590	G1526	C1458	G1384	G1310	C1152	A1087	
		C1843	G1770	G1591	G1527	G1459	G1385	G1311	C1153	A1088	
	C1942	U1943	G1771	G1592	A1528	A1460	G1386	U1313	G1154	G1089	
	U1944	G1845	G1772	G1593		G1461	G1387	G1230	A1155	U1090	
		G1846	A1773	G1594			G1388	G1231	A1156	G1091	
	G1948	G1847	A1774	G1595	C1531	C1464	G1389	C1315		C1092	
	G1949	U1848	U1775	A1596	C1532	G1465	U1391	G1316	C1161	G1093	
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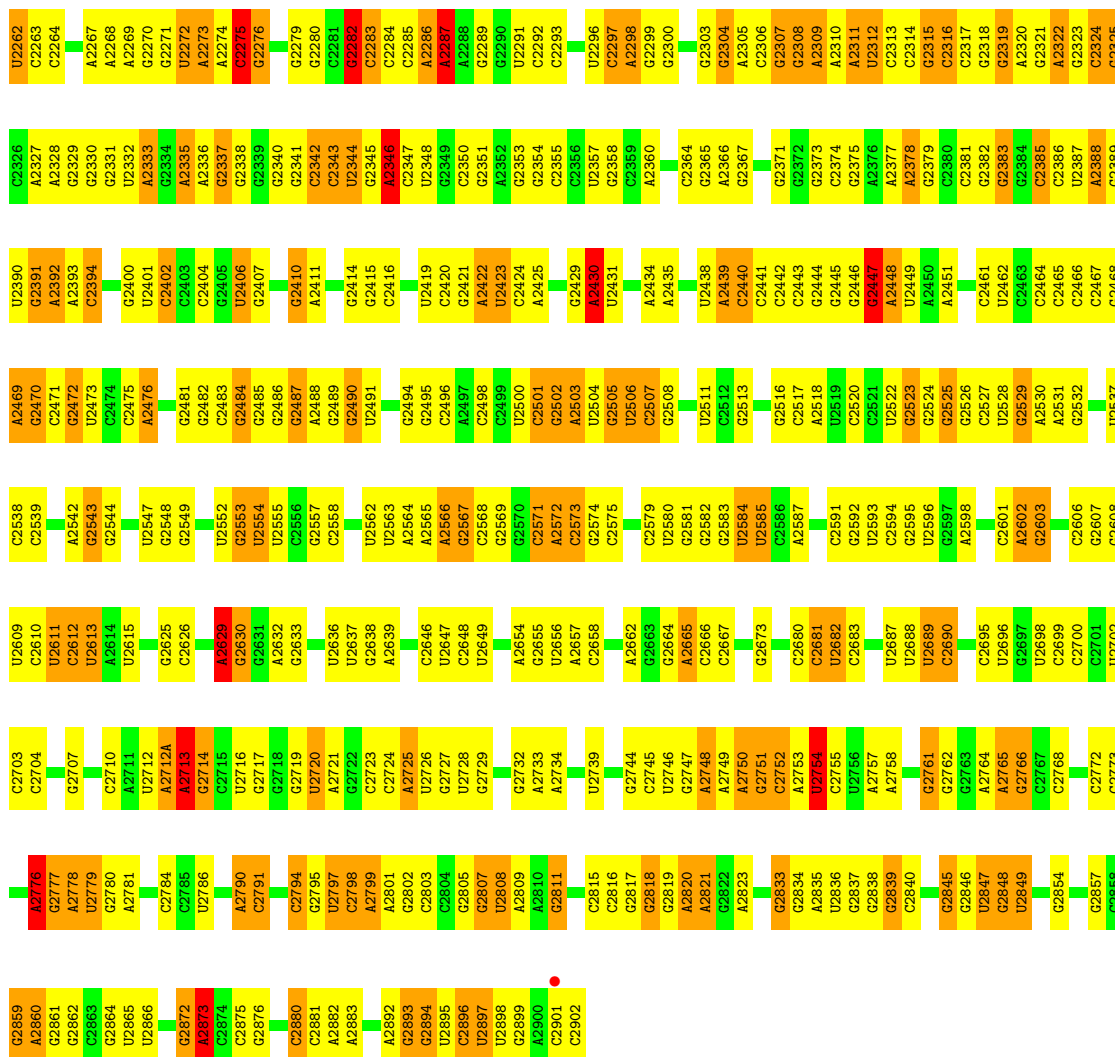
• Molecule 25: RNA (2912-MER)

Chain DA: 36% 45% 18%

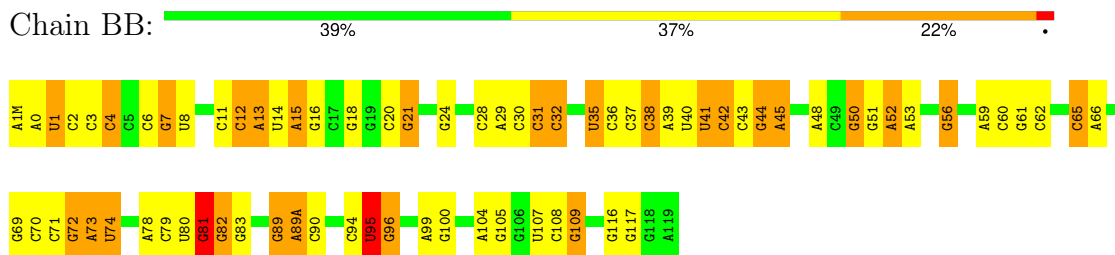


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G977	G978	G979	A980	A981	C982	A983	C986	C987	A988	G989	A990	C991	C992	G993	C994	A996	G997	C998	U999	A1000	G1001	C1002	G1003	C1004	G1005	C1006	A1007	C1008	A1009	C1010	G1011	C1012	C1013	G1016	G1017	U1019	A1020	A1021	G1022	U1023	G1024	G1025	U1026	A1027	A1028	A1029	U1033	G1034	U1035	G1036	G1037	C1038	G1039	C1040											
U839	C840	A841	A842	A843	A844	A845	A846	A847	A848	A849	A850	U851	G854	C855	C856	C857	U858	G859	U860	A861	G862	A863	G864	A865	A866	G867	U868	G869	A870	U871	A872	G873	U877	A878	G879	G880	G881	G882	G883	C884	C885	C886	C887	C888	C889	A890	A891	A892	A893	A894	A895	A896	C897	A898	A899	A900	A901	C902							
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A653	A654	A654A	C654B	C654C	G654D	C654E	C654F	C654G	G654H	C654I	A654J	G654L	G654M	G654N	C654Q	C654R	G654S	A654T	A654U	C654V	A655	G656	U657	G658	C659	G660	G668	G669	A670	A671	A672	A673	A674	A675	A676	A677	A678	A679	A680	A681	A682	A683	A684	A685	C686	G687	G688	U689	C690	A691	A692	A693	A694	A695	A696	A697	A698	A699	A700						
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G775	G776	A777	G778	G779	G780	A781	A782	A783	A784	G785	G786	G787	A788	A789	G792	A793	G794	G795	G796	G797	G798	G801	A802	G803	G804	G805	C806	U807	G808	G809	U810	U811	C812	U813	C814	C817	G818	A819	A820	A821	A824	C825	U826	U827	U828	A829	G830	C831	G832	U833	C834	A835	G836	C837	C838										
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C903	C904	G905	G906	G907	G908	A909	A910	A911	C912	C913	C914	C915	C916	A917	G921	U922	C923	C924	C925	G932	A933	G934	C935	C936	U937	G938	G939	G940	G941	G942	G943	G944	A945	G946	G947	G948	C951	G952	A953	G954	A957	U958	A959	A960	C961	G962	G963	C964	C971	G972	G973	G974	G975	G976	G977	G978	G979	G980							
G977	G978	G979	A980	A981	C982	A983	C986	C987	A988	G989	A990	C991	C992	G993	C994	A996	G997	C998	U999	A1000	G1001	C1002	G1003	C1004	G1005	C1006	A1007	C1008	A1009	C1010	G1011	C1012	C1013	G1016	G1017	U1019	A1020	A1021	G1022	U1023	G1024	G1025	U1026	A1027	A1028	A1029	U1033	G1034	U1035	G1036	G1037	C1038	G1039	C1040											
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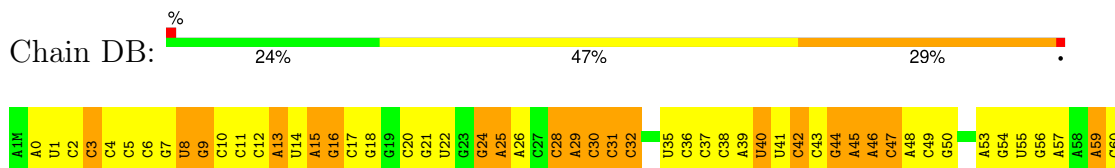
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- Molecule 26: 5S RIBOSOMAL RNA



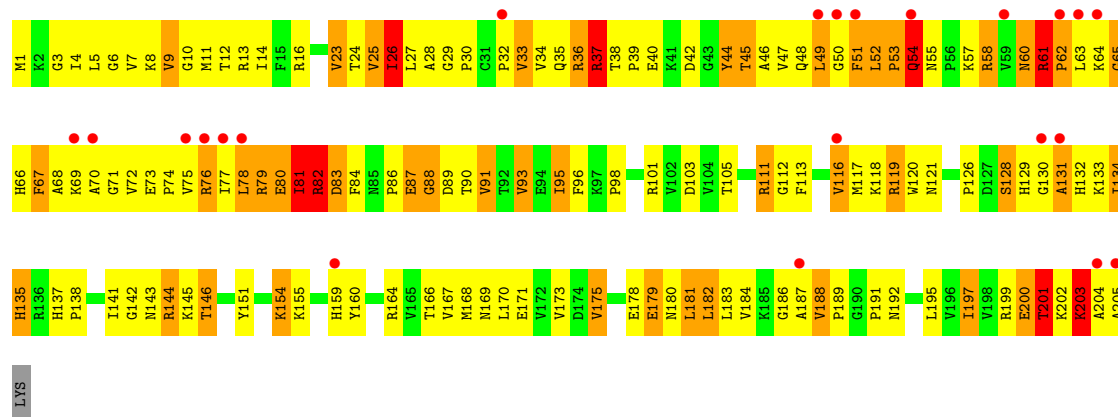
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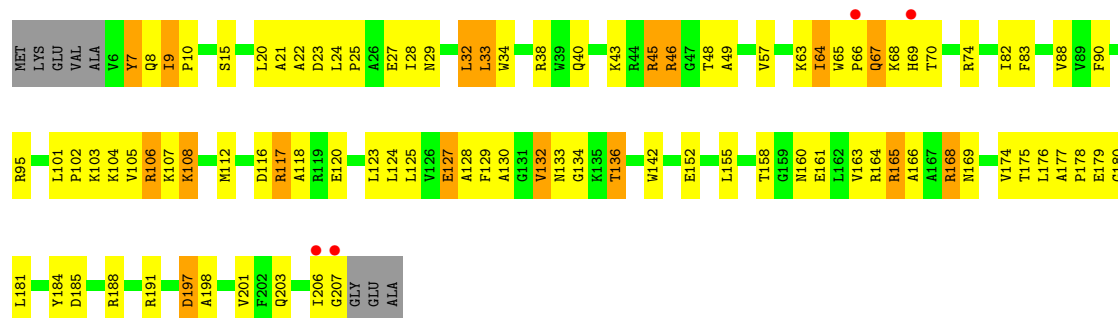




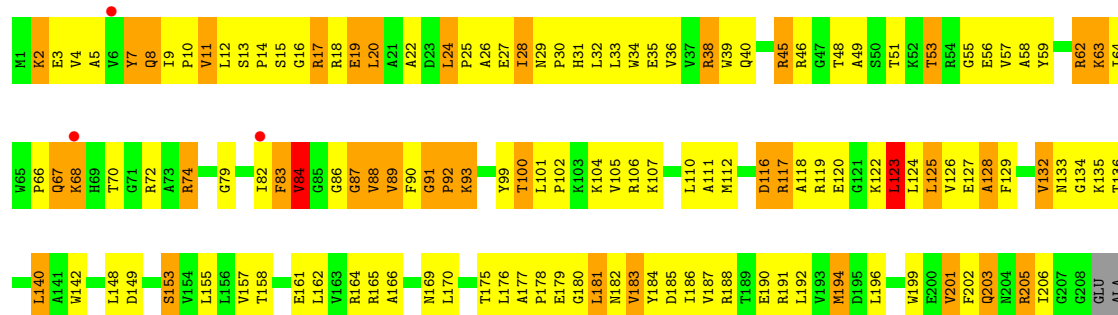
• Molecule 28: 50S ribosomal protein L3



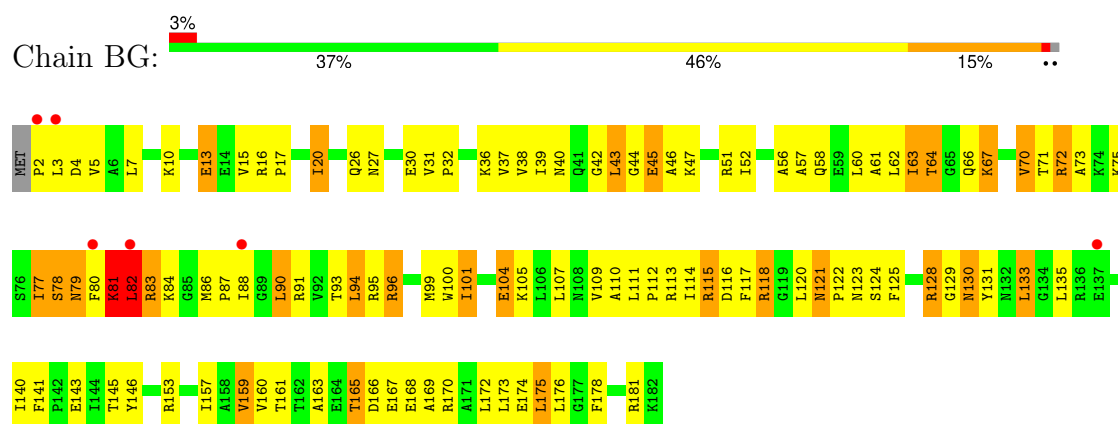
• Molecule 29: 50S ribosomal protein L4



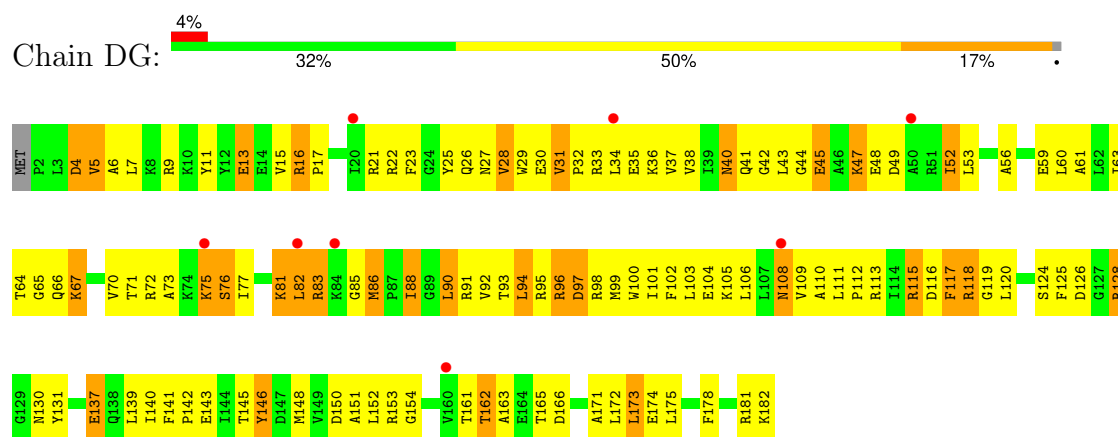
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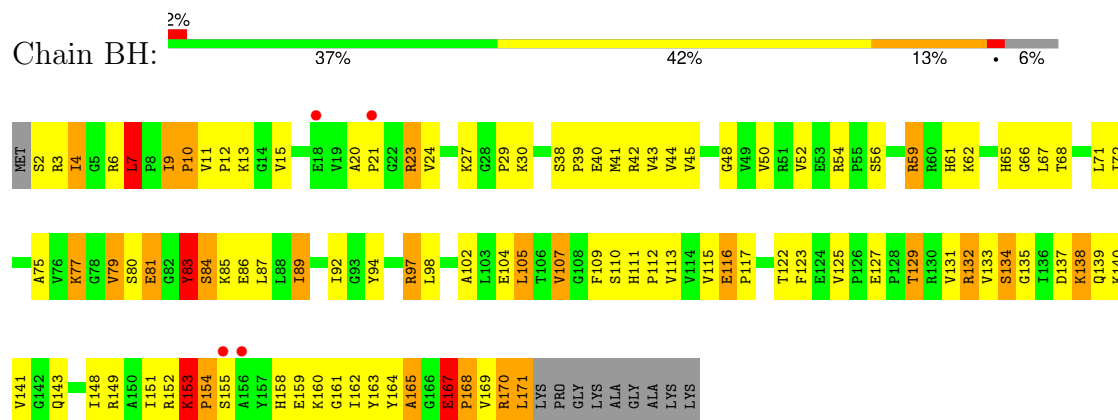
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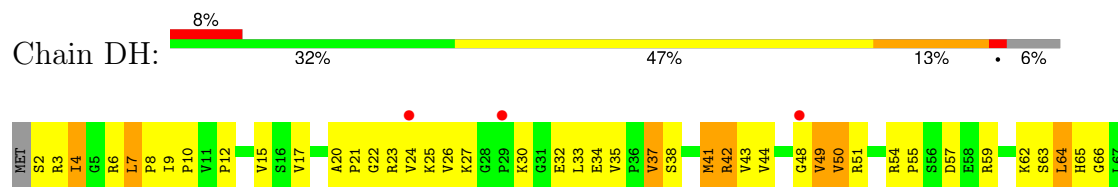
• Molecule 30: 50S ribosomal protein L5

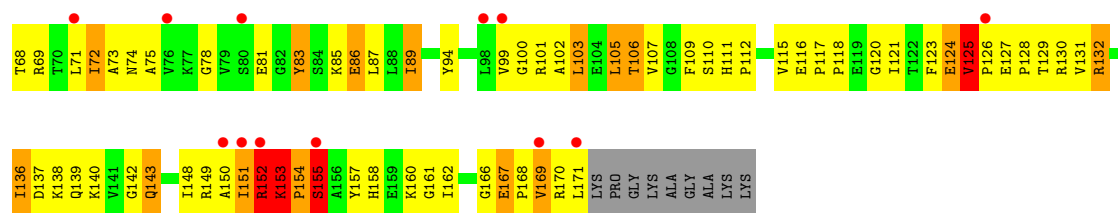


• Molecule 31: 50S ribosomal protein L6



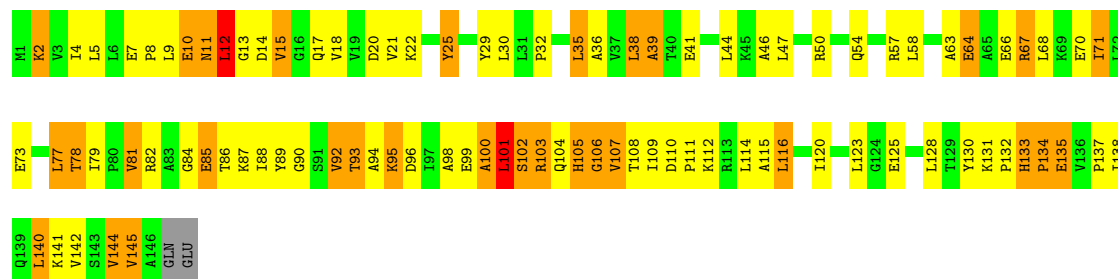
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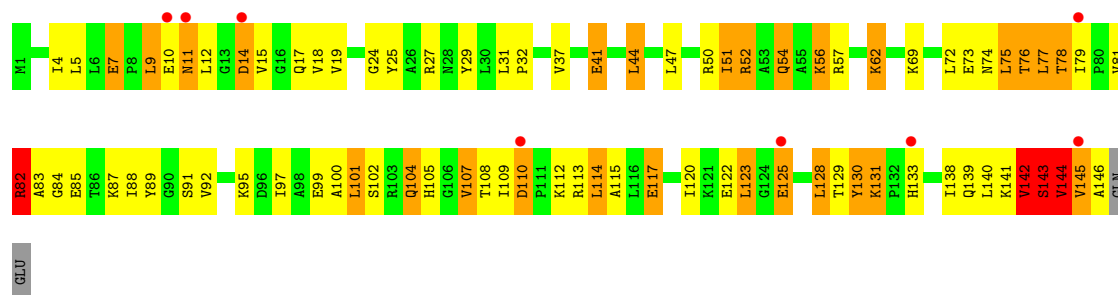
• Molecule 32: 50S ribosomal protein L9

Chain BK: 36% 41% 21% ..



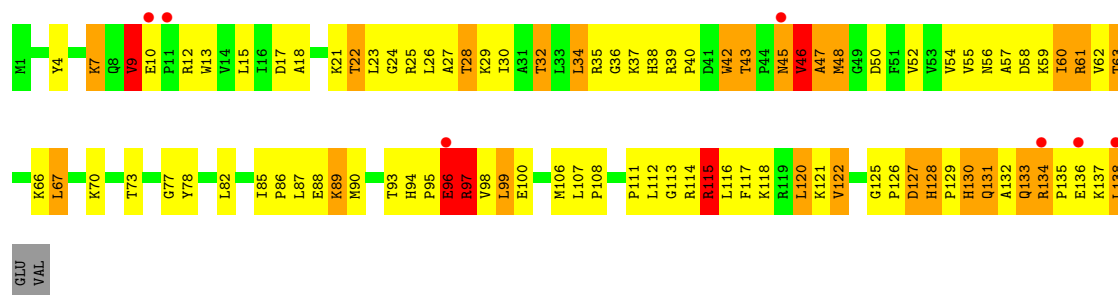
• Molecule 32: 50S ribosomal protein L9

Chain DK: 5% 43% 35% 18% ..



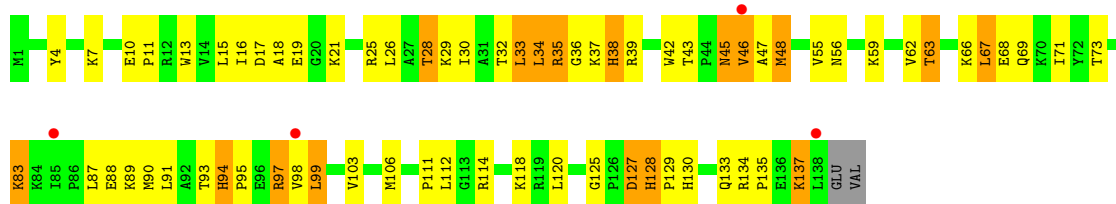
• Molecule 33: 50S ribosomal protein L13

Chain BM: 5% 31% 46% 18% ..



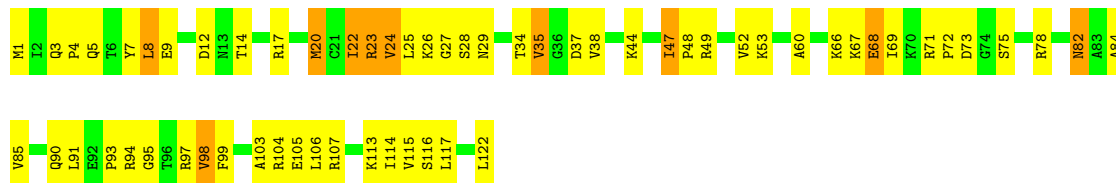
• Molecule 33: 50S ribosomal protein L13

Chain DM: 3% 49% 37% 12% ..



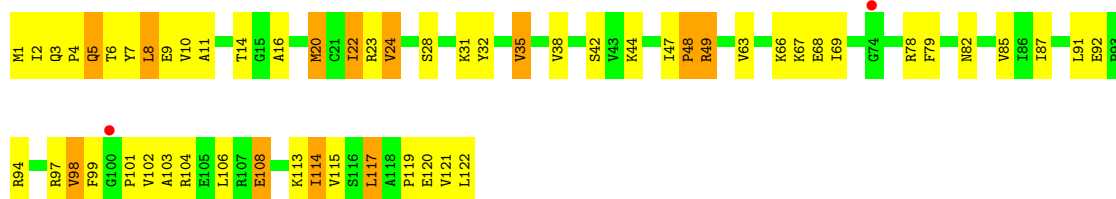
• Molecule 34: 50S ribosomal protein L14

Chain BN: 50% 42% 8%



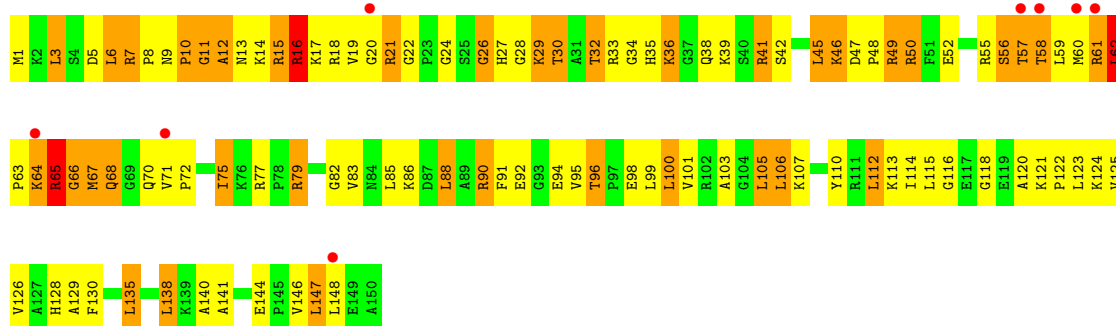
• Molecule 34: 50S ribosomal protein L14

Chain DN: 2% 53% 37% 10%



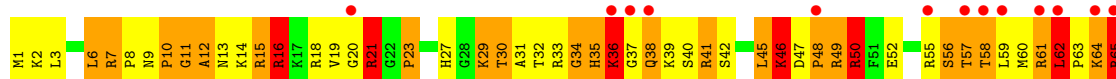
• Molecule 35: 50S ribosomal protein L15

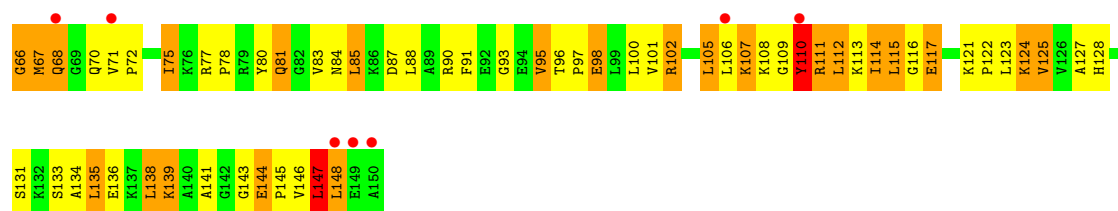
Chain BO: 5% 29% 43% 25%



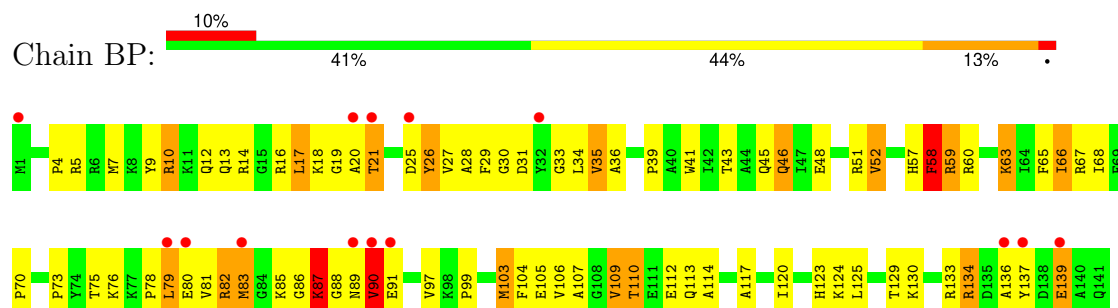
• Molecule 35: 50S ribosomal protein L15

Chain DO: 13% 25% 39% 29% 6%

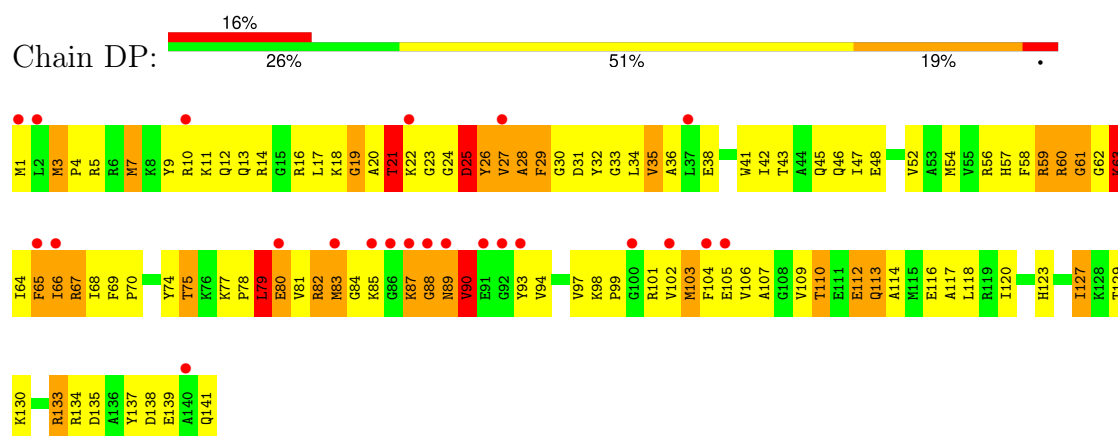




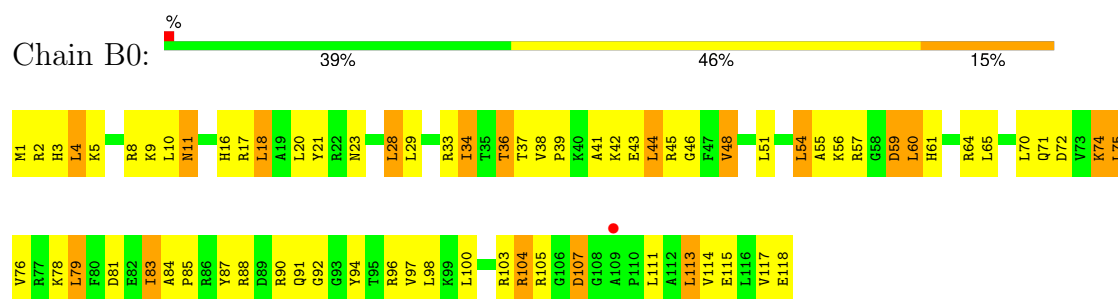
• Molecule 36: 50S ribosomal protein L16



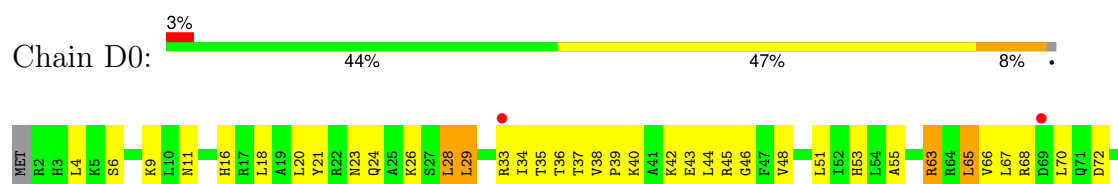
• Molecule 36: 50S ribosomal protein L16

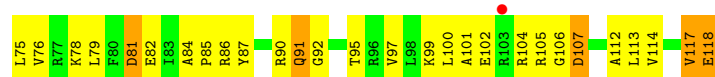


• Molecule 37: 50S ribosomal protein L17

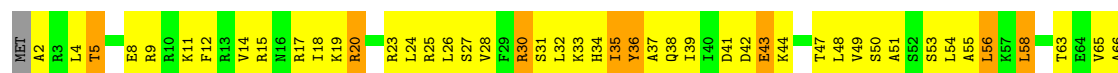


• Molecule 37: 50S ribosomal protein L17

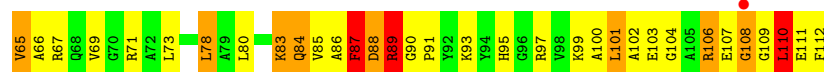
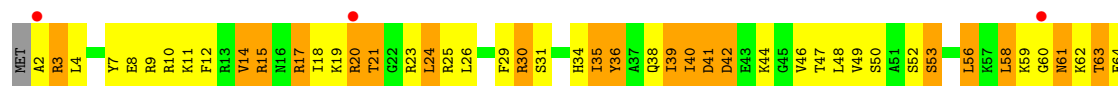




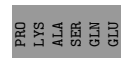
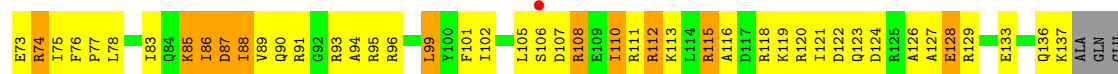
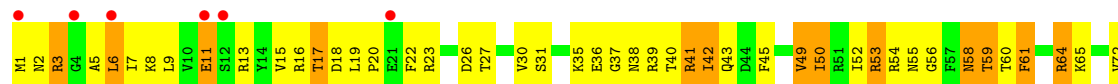
• Molecule 38: 50S ribosomal protein L18



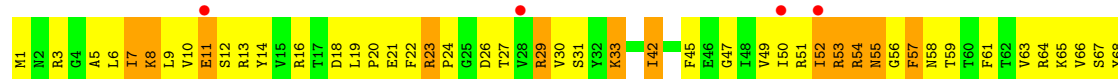
• Molecule 38: 50S ribosomal protein L18

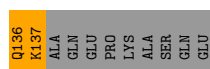


• Molecule 39: 50S ribosomal protein L19

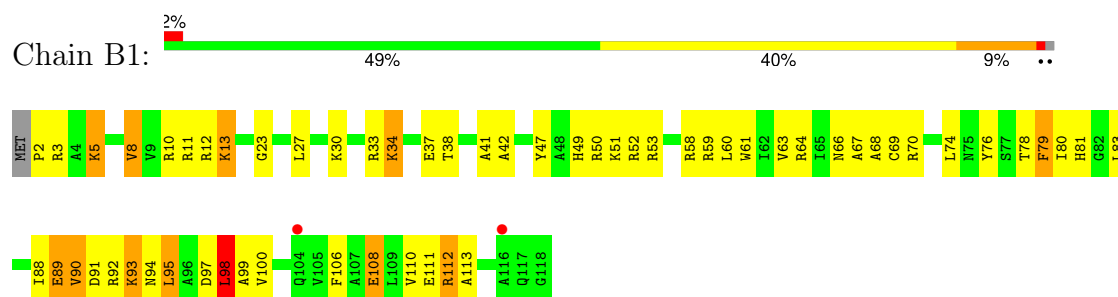


• Molecule 39: 50S ribosomal protein L19

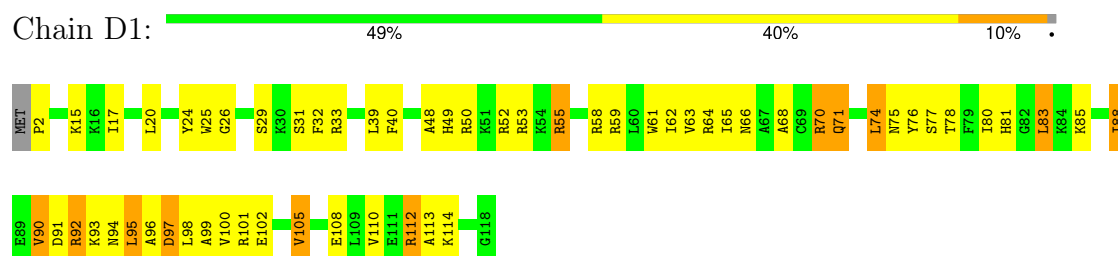




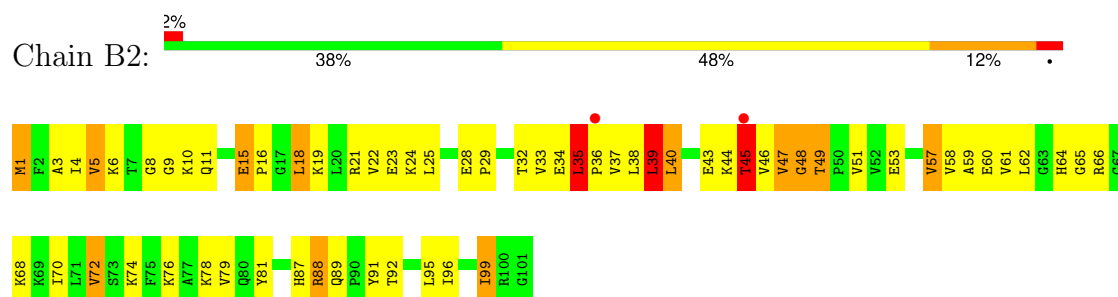
• Molecule 40: 50S ribosomal protein L20



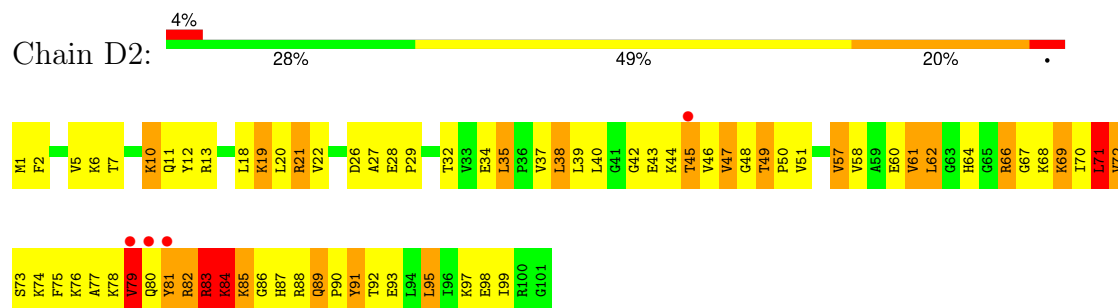
• Molecule 40: 50S ribosomal protein L20



• Molecule 41: 50S ribosomal protein L21

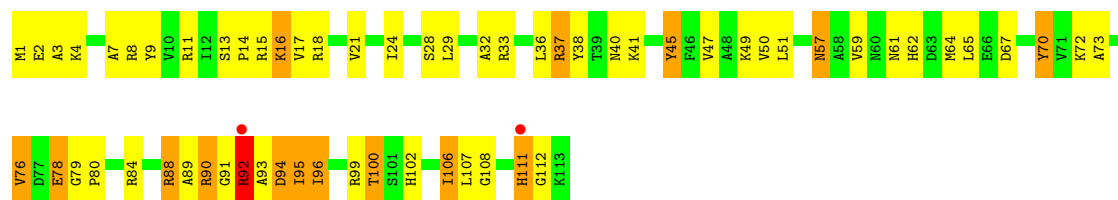


• Molecule 41: 50S ribosomal protein L21

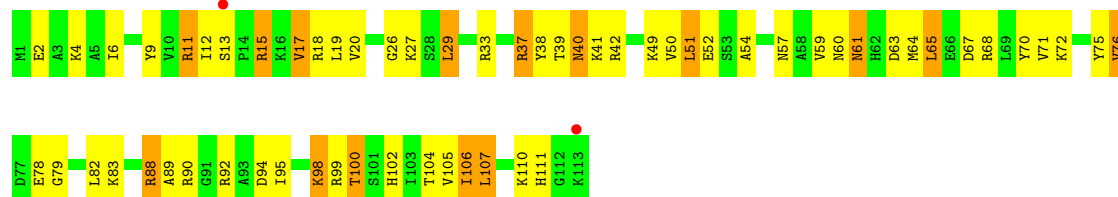


• Molecule 42: 50S ribosomal protein L22

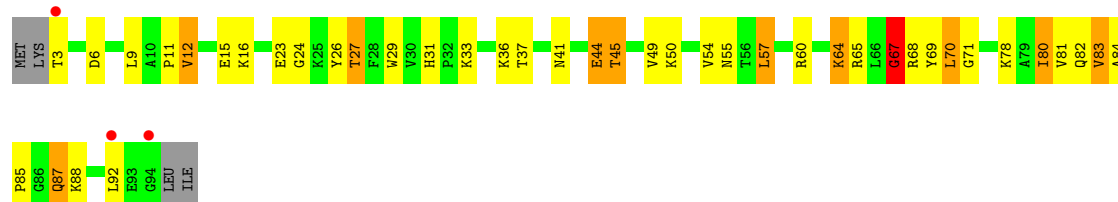




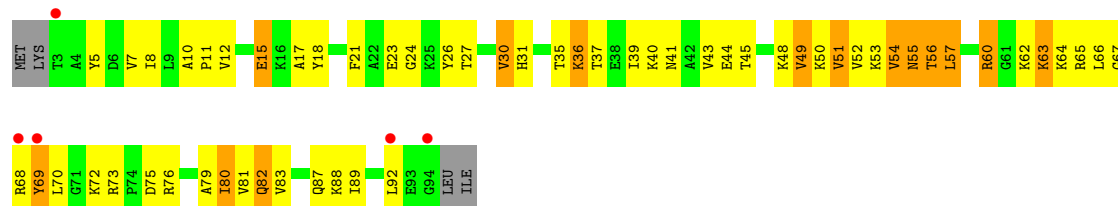
• Molecule 42: 50S ribosomal protein L22



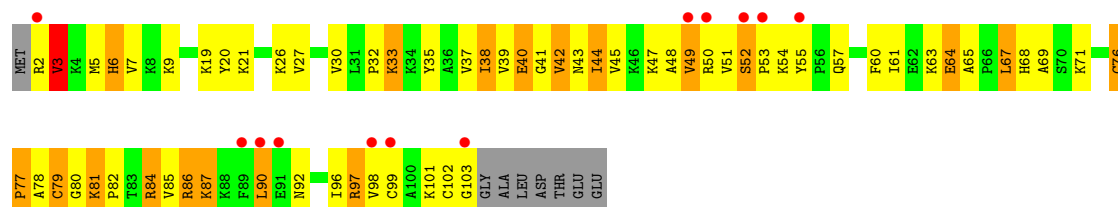
• Molecule 43: 50S ribosomal protein L23



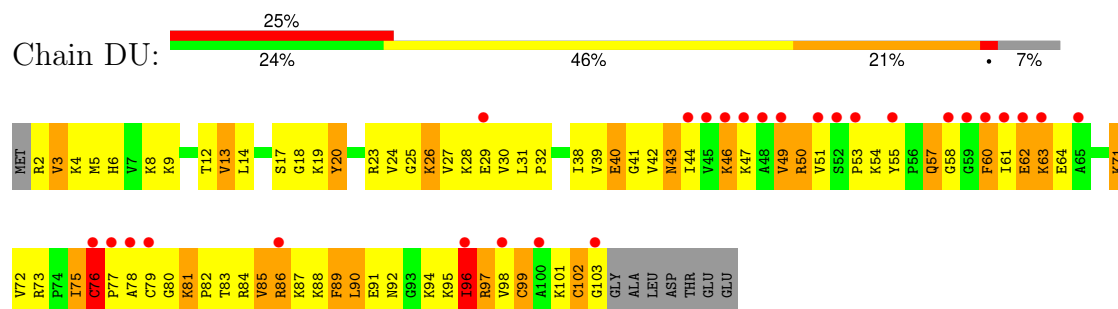
• Molecule 43: 50S ribosomal protein L23



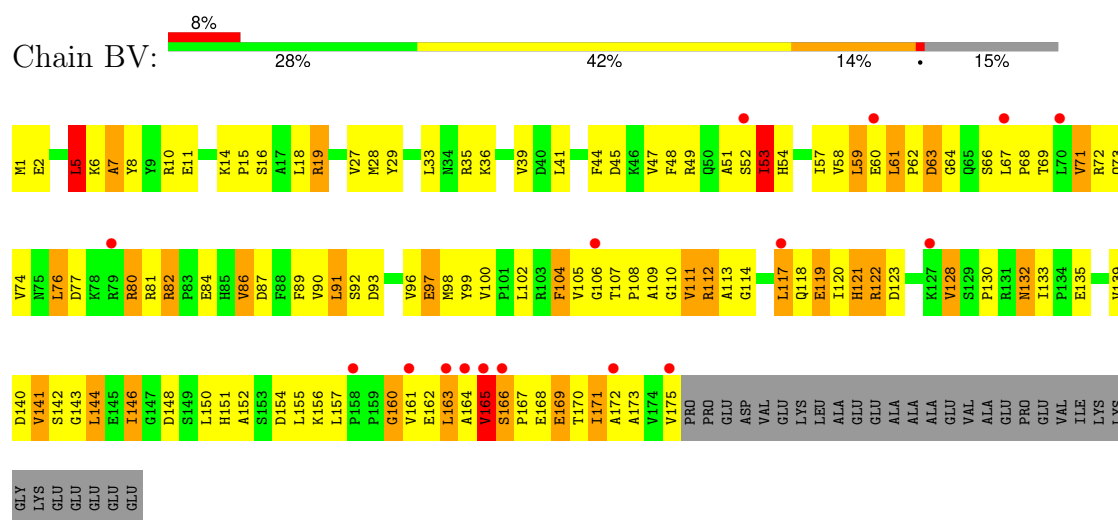
• Molecule 44: 50S ribosomal protein L24

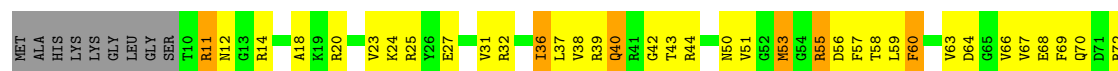


- Molecule 44: 50S ribosomal protein L24

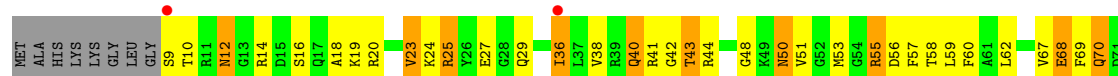
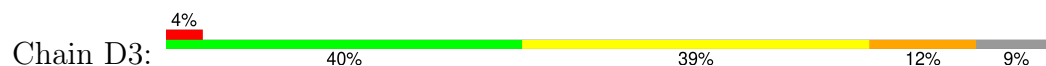


- Molecule 45: 50S ribosomal protein L25

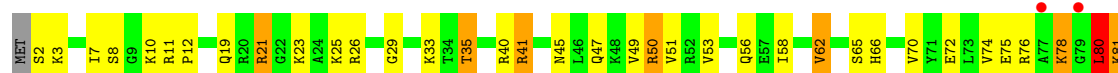




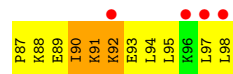
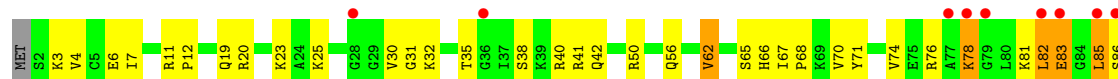
• Molecule 46: 50S ribosomal protein L27



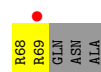
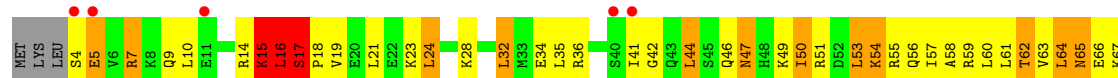
• Molecule 47: 50S ribosomal protein L28




• Molecule 47: 50S ribosomal protein L28



• Molecule 48: 50S ribosomal protein L29



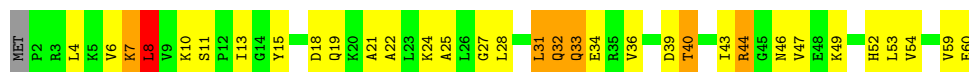
- Molecule 48: 50S ribosomal protein L29

Chain DW: 



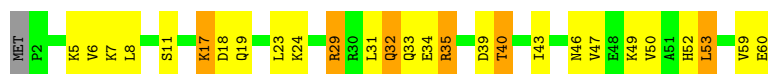
- Molecule 49: 50S ribosomal protein L30

Chain BX: 




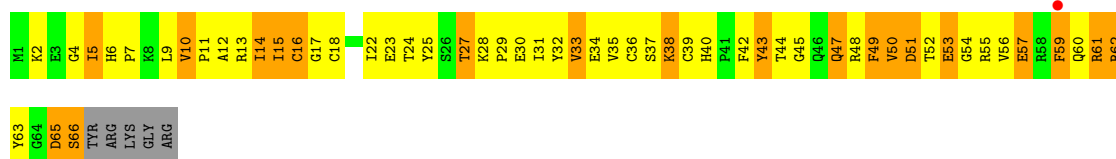
- Molecule 49: 50S ribosomal protein L30

Chain DX: 




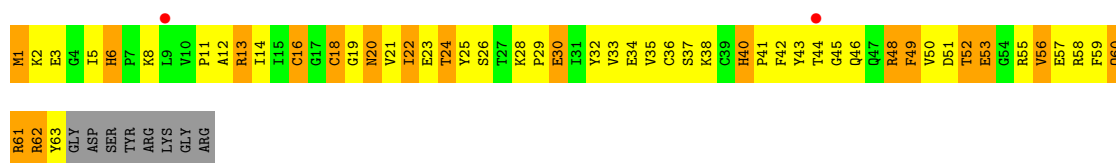
- Molecule 50: 50S ribosomal protein L31

Chain B4: 




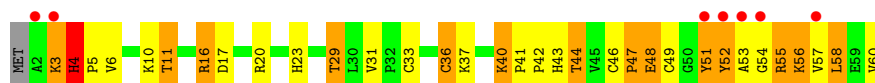
- Molecule 50: 50S ribosomal protein L31

Chain D4: 

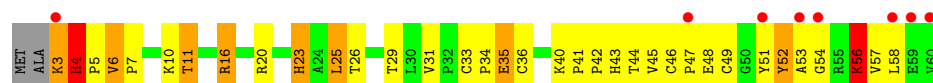
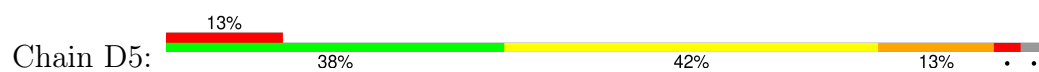


- Molecule 51: 50S ribosomal protein L32

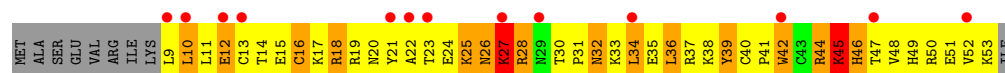
Chain B5: 



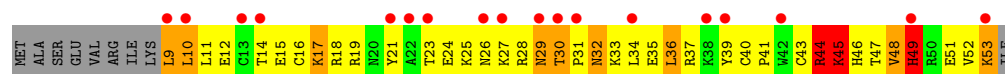
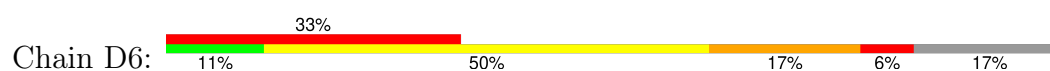
- Molecule 51: 50S ribosomal protein L32



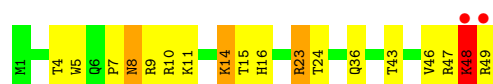
- Molecule 52: 50S ribosomal protein L33



- Molecule 52: 50S ribosomal protein L33



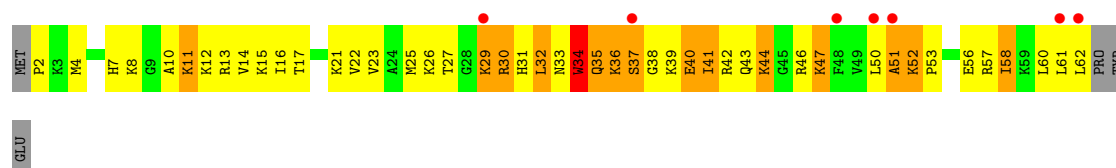
- Molecule 53: 50S ribosomal protein L34



- Molecule 53: 50S ribosomal protein L34

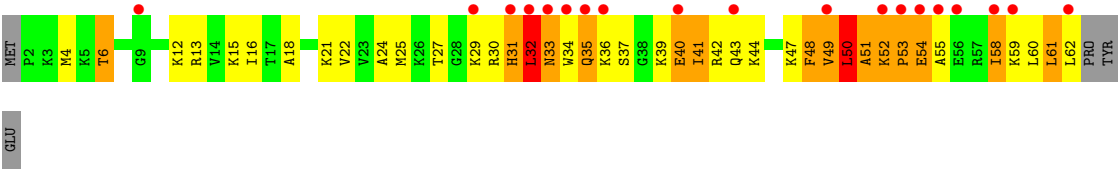


- Molecule 54: 50S ribosomal protein L35



- Molecule 54: 50S ribosomal protein L35





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.00Å 450.05Å 621.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	153.53 – 3.00 153.53 – 3.00	Depositor EDS
% Data completeness (in resolution range)	94.1 (153.53-3.00) 93.7 (153.53-3.00)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.7.1 _743	Depositor
R, R_{free}	0.211 , 0.272 0.209 , 0.247	Depositor DCC
R_{free} test set	2000 reflections (0.17%)	wwPDB-VP
Wilson B-factor (Å ²)	77.4	Xtriage
Anisotropy	0.190	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 50.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	299552	wwPDB-VP
Average B, all atoms (Å ²)	100.0	wwPDB-VP

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

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

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

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

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

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

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

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

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

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

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

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

There are no chirality outliers.

5 of 99 planarity outliers are listed below:

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

5.2 Too-close contacts [i](#)

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

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

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

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

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

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

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

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

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

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

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

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AE	235/256 (92%)	190 (81%)	45 (19%)	0	100	100
2	CE	235/256 (92%)	190 (81%)	41 (17%)	4 (2%)	7	33
3	AF	203/239 (85%)	179 (88%)	24 (12%)	0	100	100
3	CF	204/239 (85%)	179 (88%)	23 (11%)	2 (1%)	13	46
4	AG	206/208 (99%)	179 (87%)	24 (12%)	3 (2%)	8	36
4	CG	206/208 (99%)	179 (87%)	25 (12%)	2 (1%)	13	46
5	AH	149/162 (92%)	137 (92%)	10 (7%)	2 (1%)	10	39
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%)	19	54
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%)	2	13
11	AN	117/129 (91%)	102 (87%)	14 (12%)	1 (1%)	14	49
11	CN	117/129 (91%)	104 (89%)	13 (11%)	0	100	100
12	AO	123/132 (93%)	105 (85%)	16 (13%)	2 (2%)	8	34
12	CO	123/132 (93%)	105 (85%)	15 (12%)	3 (2%)	5	25
13	AP	114/126 (90%)	89 (78%)	23 (20%)	2 (2%)	7	32
13	CP	115/126 (91%)	96 (84%)	17 (15%)	2 (2%)	7	33
14	AQ	58/61 (95%)	49 (84%)	9 (16%)	0	100	100
14	CQ	58/61 (95%)	49 (84%)	8 (14%)	1 (2%)	7	33
15	AR	86/89 (97%)	74 (86%)	11 (13%)	1 (1%)	11	41
15	CR	86/89 (97%)	76 (88%)	10 (12%)	0	100	100
16	AS	82/88 (93%)	71 (87%)	8 (10%)	3 (4%)	2	15
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%)	9	37
18	CU	70/88 (80%)	61 (87%)	9 (13%)	0	100	100
19	AV	76/93 (82%)	68 (90%)	6 (8%)	2 (3%)	4	23
19	CV	76/93 (82%)	60 (79%)	12 (16%)	4 (5%)	1	9
20	AW	97/106 (92%)	84 (87%)	13 (13%)	0	100	100
20	CW	97/106 (92%)	80 (82%)	16 (16%)	1 (1%)	13	46
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%)	6	31
27	DD	270/276 (98%)	248 (92%)	15 (6%)	7 (3%)	4	23
28	BE	203/206 (98%)	149 (73%)	30 (15%)	24 (12%)	0	1
28	DE	203/206 (98%)	144 (71%)	41 (20%)	18 (9%)	0	2
29	BF	200/210 (95%)	179 (90%)	21 (10%)	0	100	100
29	DF	206/210 (98%)	168 (82%)	30 (15%)	8 (4%)	2	14
30	BG	179/182 (98%)	154 (86%)	20 (11%)	5 (3%)	4	21
30	DG	179/182 (98%)	150 (84%)	28 (16%)	1 (1%)	22	57

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	BH	168/180 (93%)	133 (79%)	28 (17%)	7 (4%)	2	13
31	DH	168/180 (93%)	125 (74%)	35 (21%)	8 (5%)	2	11
32	BK	144/148 (97%)	102 (71%)	32 (22%)	10 (7%)	1	5
32	DK	144/148 (97%)	113 (78%)	28 (19%)	3 (2%)	5	28
33	BM	136/140 (97%)	113 (83%)	16 (12%)	7 (5%)	1	10
33	DM	136/140 (97%)	119 (88%)	15 (11%)	2 (2%)	8	36
34	BN	120/122 (98%)	111 (92%)	9 (8%)	0	100	100
34	DN	120/122 (98%)	113 (94%)	6 (5%)	1 (1%)	16	51
35	BO	148/150 (99%)	107 (72%)	27 (18%)	14 (10%)	0	2
35	DO	148/150 (99%)	102 (69%)	24 (16%)	22 (15%)	0	0
36	BP	139/141 (99%)	109 (78%)	27 (19%)	3 (2%)	5	27
36	DP	139/141 (99%)	93 (67%)	30 (22%)	16 (12%)	0	1
37	B0	116/118 (98%)	101 (87%)	13 (11%)	2 (2%)	7	33
37	D0	115/118 (98%)	109 (95%)	6 (5%)	0	100	100
38	BQ	109/112 (97%)	86 (79%)	20 (18%)	3 (3%)	4	21
38	DQ	109/112 (97%)	87 (80%)	19 (17%)	3 (3%)	4	21
39	BR	135/146 (92%)	114 (84%)	21 (16%)	0	100	100
39	DR	135/146 (92%)	119 (88%)	14 (10%)	2 (2%)	8	36
40	B1	115/118 (98%)	103 (90%)	11 (10%)	1 (1%)	14	49
40	D1	115/118 (98%)	101 (88%)	14 (12%)	0	100	100
41	B2	99/101 (98%)	92 (93%)	5 (5%)	2 (2%)	6	29
41	D2	99/101 (98%)	78 (79%)	14 (14%)	7 (7%)	1	4
42	BS	111/113 (98%)	97 (87%)	10 (9%)	4 (4%)	3	16
42	DS	111/113 (98%)	103 (93%)	8 (7%)	0	100	100
43	BT	90/96 (94%)	84 (93%)	4 (4%)	2 (2%)	5	27
43	DT	90/96 (94%)	78 (87%)	10 (11%)	2 (2%)	5	27
44	BU	100/110 (91%)	80 (80%)	15 (15%)	5 (5%)	1	10
44	DU	100/110 (91%)	70 (70%)	24 (24%)	6 (6%)	1	7
45	BV	173/206 (84%)	129 (75%)	37 (21%)	7 (4%)	2	14
45	DV	177/206 (86%)	132 (75%)	35 (20%)	10 (6%)	1	8
46	B3	74/85 (87%)	67 (90%)	5 (7%)	2 (3%)	4	22

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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%)	3	19
47	DZ	95/98 (97%)	84 (88%)	10 (10%)	1 (1%)	12	44
48	BW	64/72 (89%)	58 (91%)	4 (6%)	2 (3%)	3	19
48	DW	67/72 (93%)	60 (90%)	6 (9%)	1 (2%)	8	36
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%)	3	19
50	D4	61/71 (86%)	32 (52%)	28 (46%)	1 (2%)	8	34
51	B5	57/60 (95%)	49 (86%)	7 (12%)	1 (2%)	7	32
51	D5	56/60 (93%)	48 (86%)	7 (12%)	1 (2%)	7	32
52	B6	43/54 (80%)	27 (63%)	14 (33%)	2 (5%)	2	11
52	D6	43/54 (80%)	29 (67%)	10 (23%)	4 (9%)	0	2
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%)	0	3
54	D8	59/65 (91%)	40 (68%)	12 (20%)	7 (12%)	0	1
All	All	11335/12052 (94%)	9588 (85%)	1457 (13%)	290 (3%)	4	23

5 of 290 Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AE	205/220 (93%)	155 (76%)	50 (24%)	0	3
2	CE	205/220 (93%)	159 (78%)	46 (22%)	1	3
3	AF	159/188 (85%)	120 (76%)	39 (24%)	0	2
3	CF	160/188 (85%)	124 (78%)	36 (22%)	1	3
4	AG	180/180 (100%)	144 (80%)	36 (20%)	1	5
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%)	0	3
6	AI	90/90 (100%)	76 (84%)	14 (16%)	2	11
6	CI	90/90 (100%)	74 (82%)	16 (18%)	1	8
7	AJ	126/127 (99%)	104 (82%)	22 (18%)	1	8
7	CJ	126/127 (99%)	89 (71%)	37 (29%)	0	1
8	AK	119/119 (100%)	100 (84%)	19 (16%)	2	10
8	CK	119/119 (100%)	94 (79%)	25 (21%)	1	4
9	AL	98/99 (99%)	70 (71%)	28 (29%)	0	1
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%)	1	8
11	CN	90/99 (91%)	73 (81%)	17 (19%)	1	7
12	AO	104/109 (95%)	88 (85%)	16 (15%)	2	11
12	CO	104/109 (95%)	80 (77%)	24 (23%)	0	3
13	AP	94/101 (93%)	71 (76%)	23 (24%)	0	2
13	CP	94/101 (93%)	75 (80%)	19 (20%)	1	5
14	AQ	49/50 (98%)	33 (67%)	16 (33%)	0	1
14	CQ	49/50 (98%)	39 (80%)	10 (20%)	1	5
15	AR	79/80 (99%)	68 (86%)	11 (14%)	3	14
15	CR	79/80 (99%)	66 (84%)	13 (16%)	2	9
16	AS	72/74 (97%)	53 (74%)	19 (26%)	0	2
16	CS	72/74 (97%)	62 (86%)	10 (14%)	3	14
17	AT	95/97 (98%)	82 (86%)	13 (14%)	3	14
17	CT	95/97 (98%)	89 (94%)	6 (6%)	15	45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	AU	63/77 (82%)	50 (79%)	13 (21%)	1	5
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	4
20	AW	76/82 (93%)	60 (79%)	16 (21%)	1	4
20	CW	76/82 (93%)	55 (72%)	21 (28%)	0	1
21	AX	20/22 (91%)	17 (85%)	3 (15%)	2	12
21	CX	20/22 (91%)	20 (100%)	0	100	100
27	BD	214/218 (98%)	172 (80%)	42 (20%)	1	6
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	6
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	2
31	DH	142/148 (96%)	110 (78%)	32 (22%)	1	3
32	BK	122/124 (98%)	91 (75%)	31 (25%)	0	2
32	DK	122/124 (98%)	84 (69%)	38 (31%)	0	1
33	BM	117/119 (98%)	87 (74%)	30 (26%)	0	2
33	DM	117/119 (98%)	96 (82%)	21 (18%)	1	8
34	BN	100/100 (100%)	83 (83%)	17 (17%)	1	9
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%)	0	3
37	B0	101/101 (100%)	78 (77%)	23 (23%)	0	3
37	D0	100/101 (99%)	80 (80%)	20 (20%)	1	5
38	BQ	87/88 (99%)	65 (75%)	22 (25%)	0	2

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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%)	0	3
39	DR	120/127 (94%)	84 (70%)	36 (30%)	0	1
40	B1	93/94 (99%)	76 (82%)	17 (18%)	1	7
40	D1	93/94 (99%)	80 (86%)	13 (14%)	3	13
41	B2	82/82 (100%)	61 (74%)	21 (26%)	0	2
41	D2	82/82 (100%)	50 (61%)	32 (39%)	0	0
42	BS	92/92 (100%)	72 (78%)	20 (22%)	1	4
42	DS	92/92 (100%)	65 (71%)	27 (29%)	0	1
43	BT	74/78 (95%)	61 (82%)	13 (18%)	1	8
43	DT	74/78 (95%)	57 (77%)	17 (23%)	0	3
44	BU	85/91 (93%)	65 (76%)	20 (24%)	0	3
44	DU	85/91 (93%)	51 (60%)	34 (40%)	0	0
45	BV	154/179 (86%)	116 (75%)	38 (25%)	0	2
45	DV	158/179 (88%)	124 (78%)	34 (22%)	1	4
46	B3	61/67 (91%)	54 (88%)	7 (12%)	4	20
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	4
49	BX	51/52 (98%)	41 (80%)	10 (20%)	1	6
49	DX	51/52 (98%)	42 (82%)	9 (18%)	1	8
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	7
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	4
54	D8	51/55 (93%)	41 (80%)	10 (20%)	1	6
All	All	9579/9996 (96%)	7317 (76%)	2262 (24%)	0	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 ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	1506/1506 (100%)	-0.30	9 (0%) 85 71	50, 98, 179, 234	0
1	CA	1506/1506 (100%)	-0.19	17 (1%) 77 58	62, 109, 181, 235	0
2	AE	237/256 (92%)	0.16	7 (2%) 52 31	103, 136, 174, 185	0
2	CE	237/256 (92%)	0.23	2 (0%) 82 66	114, 151, 185, 201	0
3	AF	205/239 (85%)	0.34	5 (2%) 59 37	84, 111, 144, 153	0
3	CF	206/239 (86%)	0.91	18 (8%) 17 10	118, 138, 166, 174	0
4	AG	208/208 (100%)	0.43	10 (4%) 36 21	80, 105, 129, 142	0
4	CG	208/208 (100%)	0.39	6 (2%) 54 32	77, 102, 123, 136	0
5	AH	151/162 (93%)	0.07	2 (1%) 74 54	74, 97, 118, 152	0
5	CH	151/162 (93%)	0.50	8 (5%) 33 19	91, 112, 134, 153	0
6	AI	101/101 (100%)	0.03	1 (0%) 79 60	76, 99, 115, 137	0
6	CI	101/101 (100%)	-0.43	0 100 100	74, 95, 116, 141	0
7	AJ	155/156 (99%)	0.17	9 (5%) 30 17	99, 114, 145, 155	0
7	CJ	155/156 (99%)	0.25	8 (5%) 34 19	102, 122, 149, 156	0
8	AK	138/138 (100%)	-0.11	0 100 100	84, 103, 117, 122	0
8	CK	138/138 (100%)	-0.02	0 100 100	94, 116, 128, 136	0
9	AL	127/128 (99%)	0.09	5 (3%) 44 26	85, 133, 153, 160	0
9	CL	127/128 (99%)	0.37	10 (7%) 20 11	107, 145, 160, 164	0
10	AM	99/105 (94%)	0.44	7 (7%) 23 13	81, 132, 162, 165	0
10	CM	99/105 (94%)	0.55	8 (8%) 19 11	111, 149, 165, 170	0
11	AN	119/129 (92%)	0.26	6 (5%) 35 20	64, 97, 128, 154	0
11	CN	119/129 (92%)	0.23	7 (5%) 29 16	79, 101, 134, 158	0
12	AO	125/132 (94%)	0.19	4 (3%) 50 30	63, 73, 105, 151	0
12	CO	125/132 (94%)	0.77	11 (8%) 17 9	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%)	0.35	8 (6%) 24 14	86, 117, 136, 145	0
13	CP	117/126 (92%)	0.41	7 (5%) 29 16	106, 146, 161, 164	0
14	AQ	60/61 (98%)	0.59	3 (5%) 35 20	86, 101, 115, 126	0
14	CQ	60/61 (98%)	1.14	12 (20%) 3 2	118, 132, 146, 153	0
15	AR	88/89 (98%)	-0.02	2 (2%) 61 39	72, 93, 114, 117	0
15	CR	88/89 (98%)	-0.00	1 (1%) 77 58	73, 104, 127, 133	0
16	AS	84/88 (95%)	0.22	2 (2%) 59 37	90, 107, 133, 165	0
16	CS	84/88 (95%)	-0.08	0 100 100	81, 96, 120, 153	0
17	AT	100/105 (95%)	0.11	4 (4%) 43 25	82, 100, 118, 130	0
17	CT	100/105 (95%)	0.34	4 (4%) 43 25	82, 102, 125, 137	0
18	AU	72/88 (81%)	0.01	0 100 100	78, 99, 132, 159	0
18	CU	72/88 (81%)	-0.25	0 100 100	85, 106, 144, 157	0
19	AV	78/93 (83%)	-0.10	4 (5%) 34 19	100, 122, 137, 144	0
19	CV	78/93 (83%)	0.25	3 (3%) 44 26	136, 154, 174, 177	0
20	AW	99/106 (93%)	0.39	3 (3%) 52 31	93, 115, 144, 155	0
20	CW	99/106 (93%)	0.26	3 (3%) 52 31	83, 109, 143, 157	0
21	AX	25/27 (92%)	0.33	0 100 100	88, 109, 125, 147	0
21	CX	25/27 (92%)	1.16	1 (4%) 43 25	112, 133, 148, 160	0
22	AB	87/87 (100%)	0.25	6 (6%) 24 14	78, 145, 185, 196	0
22	CB	87/87 (100%)	0.50	10 (11%) 11 6	92, 148, 188, 200	0
23	AC	77/77 (100%)	0.04	2 (2%) 57 35	63, 100, 132, 147	0
23	AD	77/77 (100%)	0.35	3 (3%) 44 26	71, 218, 232, 234	0
23	CC	77/77 (100%)	-0.05	1 (1%) 74 54	73, 107, 141, 153	0
23	CD	77/77 (100%)	0.79	10 (12%) 9 5	77, 219, 231, 234	0
24	A1	10/10 (100%)	0.52	3 (30%) 1 1	67, 81, 112, 112	0
24	C1	10/10 (100%)	1.10	3 (30%) 1 1	81, 98, 118, 124	0
25	BA	2912/2912 (100%)	-0.63	16 (0%) 87 75	36, 66, 200, 234	0
25	DA	2907/2912 (99%)	-0.42	7 (0%) 92 84	45, 80, 220, 235	0
26	BB	122/122 (100%)	-0.53	0 100 100	66, 91, 110, 169	0
26	DB	122/122 (100%)	-0.09	1 (0%) 82 66	84, 120, 141, 189	0
27	BD	272/276 (98%)	-0.07	7 (2%) 57 35	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%)	-0.05	11 (4%) 43 25	42, 67, 88, 119	0
28	BE	205/206 (99%)	0.30	10 (4%) 36 20	42, 77, 123, 132	0
28	DE	205/206 (99%)	0.51	22 (10%) 12 7	52, 88, 137, 159	0
29	BF	202/210 (96%)	-0.20	4 (1%) 64 43	38, 70, 108, 123	0
29	DF	208/210 (99%)	0.16	3 (1%) 73 52	48, 94, 152, 175	0
30	BG	181/182 (99%)	0.14	6 (3%) 49 29	81, 101, 130, 142	0
30	DG	181/182 (99%)	0.53	8 (4%) 39 23	112, 135, 155, 162	0
31	BH	170/180 (94%)	0.12	4 (2%) 59 37	74, 104, 121, 146	0
31	DH	170/180 (94%)	0.58	15 (8%) 17 9	148, 188, 209, 218	0
32	BK	146/148 (98%)	0.14	0 100 100	69, 121, 137, 142	0
32	DK	146/148 (98%)	0.42	8 (5%) 32 18	77, 120, 143, 150	0
33	BM	138/140 (98%)	0.44	7 (5%) 34 19	57, 81, 116, 129	0
33	DM	138/140 (98%)	0.23	4 (2%) 54 32	71, 102, 133, 143	0
34	BN	122/122 (100%)	-0.20	0 100 100	48, 67, 83, 97	0
34	DN	122/122 (100%)	0.21	2 (1%) 70 49	62, 82, 102, 118	0
35	BO	150/150 (100%)	0.37	8 (5%) 33 19	42, 77, 106, 153	0
35	DO	150/150 (100%)	0.71	20 (13%) 8 5	44, 99, 135, 171	0
36	BP	141/141 (100%)	0.47	14 (9%) 14 8	52, 78, 99, 125	0
36	DP	141/141 (100%)	1.05	23 (16%) 5 4	58, 98, 129, 148	0
37	B0	118/118 (100%)	-0.21	1 (0%) 82 66	50, 76, 94, 110	0
37	D0	117/118 (99%)	-0.16	3 (2%) 57 35	50, 74, 97, 113	0
38	BQ	111/112 (99%)	0.02	3 (2%) 56 34	70, 88, 110, 127	0
38	DQ	111/112 (99%)	0.41	4 (3%) 46 27	83, 117, 139, 159	0
39	BR	137/146 (93%)	0.36	7 (5%) 34 19	60, 82, 134, 163	0
39	DR	137/146 (93%)	0.45	7 (5%) 34 19	69, 93, 154, 174	0
40	B1	117/118 (99%)	-0.12	2 (1%) 69 47	44, 70, 101, 132	0
40	D1	117/118 (99%)	-0.16	0 100 100	58, 89, 131, 152	0
41	B2	101/101 (100%)	0.04	2 (1%) 64 43	48, 92, 115, 132	0
41	D2	101/101 (100%)	0.23	4 (3%) 43 25	58, 115, 133, 142	0
42	BS	113/113 (100%)	-0.09	2 (1%) 67 45	41, 65, 97, 147	0
42	DS	113/113 (100%)	0.02	2 (1%) 67 45	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	3 (3%)	49	29	49, 63, 87, 104	0
43	DT	92/96 (95%)	0.19	5 (5%)	32	18	64, 80, 104, 121	0
44	BU	102/110 (92%)	0.59	12 (11%)	10	6	67, 92, 142, 159	0
44	DU	102/110 (92%)	1.37	27 (26%)	2	2	82, 109, 160, 176	0
45	BV	175/206 (84%)	0.75	16 (9%)	16	9	80, 117, 179, 183	0
45	DV	179/206 (86%)	0.52	3 (1%)	69	47	110, 151, 199, 206	0
46	B3	76/85 (89%)	-0.24	1 (1%)	74	54	52, 68, 83, 117	0
46	D3	77/85 (90%)	0.41	3 (3%)	44	26	65, 86, 108, 141	0
47	BZ	97/98 (98%)	0.39	13 (13%)	8	5	46, 64, 122, 151	0
47	DZ	97/98 (98%)	0.79	13 (13%)	8	5	54, 77, 126, 148	0
48	BW	66/72 (91%)	0.12	6 (9%)	16	9	55, 73, 90, 120	0
48	DW	69/72 (95%)	-0.09	2 (2%)	54	32	77, 100, 130, 167	0
49	BX	59/60 (98%)	-0.07	0	100	100	60, 75, 105, 120	0
49	DX	59/60 (98%)	-0.07	0	100	100	73, 98, 130, 153	0
50	B4	66/71 (92%)	0.25	1 (1%)	71	50	111, 146, 164, 173	0
50	D4	63/71 (88%)	0.59	2 (3%)	50	30	140, 176, 185, 191	0
51	B5	59/60 (98%)	0.58	7 (11%)	10	6	43, 80, 163, 168	0
51	D5	58/60 (96%)	0.58	8 (13%)	8	4	52, 78, 167, 178	0
52	B6	45/54 (83%)	1.46	13 (28%)	1	1	105, 134, 156, 160	0
52	D6	45/54 (83%)	2.04	18 (40%)	1	1	121, 156, 173, 176	0
53	B7	49/49 (100%)	-0.40	2 (4%)	42	24	35, 45, 88, 118	0
53	D7	49/49 (100%)	0.14	4 (8%)	19	10	44, 54, 112, 131	0
54	B8	61/65 (93%)	0.62	7 (11%)	11	6	51, 64, 81, 102	0
54	D8	61/65 (93%)	1.46	19 (31%)	1	1	65, 79, 94, 123	0
All	All	21104/21634 (97%)	-0.02	677 (3%)	50	30	35, 96, 177, 235	0

The worst 5 of 677 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
51	B5	2	ALA	12.0
9	CL	115	GLY	11.6
28	BE	79	ARG	8.2
30	BG	80	PHE	6.8
9	CL	127	LYS	6.3

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
55	MG	CA	1644	1/1	0.18	0.33	120,120,120,120	0
55	MG	DA	3441	1/1	0.18	0.17	137,137,137,137	0
55	MG	AA	1761	1/1	0.27	0.41	113,113,113,113	0
55	MG	CA	1753	1/1	0.31	0.26	123,123,123,123	0
55	MG	AA	1729	1/1	0.31	0.34	113,113,113,113	0
55	MG	DB	207	1/1	0.32	0.39	115,115,115,115	0
55	MG	DA	3315	1/1	0.34	0.20	108,108,108,108	0
55	MG	AA	1713	1/1	0.42	0.25	115,115,115,115	0
55	MG	BA	3490	1/1	0.44	0.18	166,166,166,166	0
55	MG	AA	1715	1/1	0.45	0.27	115,115,115,115	0
55	MG	BA	3484	1/1	0.46	0.28	117,117,117,117	0
55	MG	AB	103	1/1	0.47	0.22	111,111,111,111	0
55	MG	CA	1759	1/1	0.47	0.37	103,103,103,103	0
55	MG	DA	3064	1/1	0.47	0.23	101,101,101,101	0
55	MG	BA	3075	1/1	0.48	0.32	110,110,110,110	0
55	MG	CA	1632	1/1	0.49	0.37	95,95,95,95	0
55	MG	DA	3462	1/1	0.49	0.32	107,107,107,107	0
55	MG	CC	107	1/1	0.49	0.18	99,99,99,99	0
55	MG	AA	1769	1/1	0.50	0.32	104,104,104,104	0
55	MG	DA	3273	1/1	0.50	0.25	99,99,99,99	0
55	MG	CA	1622	1/1	0.52	0.47	95,95,95,95	0
55	MG	AA	1731	1/1	0.53	0.28	103,103,103,103	0
55	MG	CA	1719	1/1	0.54	0.26	129,129,129,129	0
55	MG	AA	1710	1/1	0.55	0.31	92,92,92,92	0
55	MG	BA	3379	1/1	0.56	0.40	82,82,82,82	0
55	MG	AA	1828	1/1	0.57	0.31	105,105,105,105	0
55	MG	AA	1638	1/1	0.57	0.31	104,104,104,104	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	DA	3405	1/1	0.57	0.34	79,79,79,79	0
55	MG	CA	1713	1/1	0.58	0.43	102,102,102,102	0
55	MG	DA	3491	1/1	0.58	0.53	103,103,103,103	0
55	MG	DA	3129	1/1	0.58	0.33	82,82,82,82	0
55	MG	AA	1797	1/1	0.59	0.40	99,99,99,99	0
55	MG	BA	3505	1/1	0.59	0.30	96,96,96,96	0
55	MG	BA	3552	1/1	0.59	0.32	102,102,102,102	0
55	MG	DA	3072	1/1	0.59	0.31	112,112,112,112	0
55	MG	DA	3487	1/1	0.59	0.25	95,95,95,95	0
55	MG	BA	3580	1/1	0.59	0.16	71,71,71,71	0
55	MG	DA	3524	1/1	0.59	0.22	105,105,105,105	0
55	MG	AA	1744	1/1	0.59	0.19	117,117,117,117	0
55	MG	BA	3495	1/1	0.60	0.24	123,123,123,123	0
55	MG	BA	3313	1/1	0.60	0.22	88,88,88,88	0
55	MG	DA	3068	1/1	0.60	0.30	91,91,91,91	0
55	MG	BA	3507	1/1	0.60	0.32	89,89,89,89	0
55	MG	DA	3490	1/1	0.60	0.11	126,126,126,126	0
55	MG	AC	106	1/1	0.60	0.36	89,89,89,89	0
55	MG	AA	1737	1/1	0.60	0.38	83,83,83,83	0
55	MG	BA	3134	1/1	0.60	0.18	81,81,81,81	0
55	MG	CA	1659	1/1	0.61	0.22	110,110,110,110	0
55	MG	AA	1782	1/1	0.61	0.10	96,96,96,96	0
55	MG	DA	3508	1/1	0.61	0.36	80,80,80,80	0
55	MG	AA	1833	1/1	0.61	0.35	88,88,88,88	0
55	MG	AA	1689	1/1	0.61	0.27	115,115,115,115	0
55	MG	AA	1728	1/1	0.62	0.18	108,108,108,108	0
55	MG	AA	1708	1/1	0.62	0.36	91,91,91,91	0
55	MG	AA	1711	1/1	0.62	0.26	89,89,89,89	0
55	MG	BA	3519	1/1	0.62	0.34	80,80,80,80	0
55	MG	BA	3300	1/1	0.62	0.28	88,88,88,88	0
55	MG	DA	3026	1/1	0.62	0.45	95,95,95,95	0
55	MG	CA	1704	1/1	0.62	0.29	99,99,99,99	0
55	MG	AA	1618	1/1	0.63	0.29	82,82,82,82	0
55	MG	DA	3481	1/1	0.63	0.41	96,96,96,96	0
55	MG	DA	3020	1/1	0.63	0.20	85,85,85,85	0
55	MG	AA	1621	1/1	0.63	0.24	108,108,108,108	0
55	MG	DA	3059	1/1	0.63	0.37	106,106,106,106	0
55	MG	DA	3503	1/1	0.63	0.45	80,80,80,80	0
55	MG	BB	216	1/1	0.63	0.24	94,94,94,94	0
55	MG	DA	3429	1/1	0.63	0.33	99,99,99,99	0
55	MG	AA	1826	1/1	0.63	0.17	101,101,101,101	0
55	MG	BA	3541	1/1	0.64	0.23	96,96,96,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	AA	1758	1/1	0.64	0.25	85,85,85,85	0
55	MG	AA	1831	1/1	0.64	0.50	90,90,90,90	0
55	MG	CA	1717	1/1	0.64	0.28	106,106,106,106	0
55	MG	AA	1640	1/1	0.64	0.36	90,90,90,90	0
55	MG	CA	1741	1/1	0.64	0.28	106,106,106,106	0
55	MG	DA	3083	1/1	0.64	0.38	85,85,85,85	0
55	MG	AA	1836	1/1	0.64	0.32	79,79,79,79	0
55	MG	AH	201	1/1	0.64	0.31	99,99,99,99	0
55	MG	CA	1774	1/1	0.64	0.25	104,104,104,104	0
55	MG	AA	1692	1/1	0.64	0.29	115,115,115,115	0
55	MG	CA	1660	1/1	0.65	0.26	85,85,85,85	0
55	MG	CA	1757	1/1	0.65	0.28	97,97,97,97	0
55	MG	AA	1700	1/1	0.65	0.26	99,99,99,99	0
55	MG	CA	1699	1/1	0.66	0.14	97,97,97,97	0
55	MG	CA	1626	1/1	0.66	0.23	93,93,93,93	0
55	MG	DA	3086	1/1	0.66	0.24	114,114,114,114	0
55	MG	BA	3591	1/1	0.66	0.33	64,64,64,64	0
55	MG	CA	1638	1/1	0.66	0.48	101,101,101,101	0
55	MG	BA	3438	1/1	0.66	0.26	91,91,91,91	0
55	MG	CA	1601	1/1	0.66	0.57	96,96,96,96	0
55	MG	AA	1647	1/1	0.66	0.29	88,88,88,88	0
55	MG	CA	1689	1/1	0.66	0.28	89,89,89,89	0
55	MG	DB	213	1/1	0.66	0.23	94,94,94,94	0
55	MG	CA	1807	1/1	0.67	0.31	126,126,126,126	0
55	MG	AA	1720	1/1	0.67	0.22	93,93,93,93	0
55	MG	DA	3007	1/1	0.67	0.21	74,74,74,74	0
55	MG	BA	3334	1/1	0.67	0.36	96,96,96,96	0
55	MG	CA	1687	1/1	0.67	0.23	89,89,89,89	0
55	MG	BB	209	1/1	0.67	0.34	102,102,102,102	0
55	MG	BA	3164	1/1	0.67	0.43	86,86,86,86	0
55	MG	AA	1755	1/1	0.67	0.25	104,104,104,104	0
55	MG	CA	1645	1/1	0.67	0.27	86,86,86,86	0
55	MG	CA	1770	1/1	0.68	0.33	102,102,102,102	0
55	MG	DA	3151	1/1	0.68	0.30	85,85,85,85	0
55	MG	AA	1781	1/1	0.68	0.39	94,94,94,94	0
55	MG	AA	1693	1/1	0.68	0.24	87,87,87,87	0
55	MG	DA	3379	1/1	0.68	0.36	85,85,85,85	0
55	MG	CC	104	1/1	0.68	0.29	89,89,89,89	0
55	MG	CA	1714	1/1	0.68	0.21	92,92,92,92	0
55	MG	CA	1657	1/1	0.68	0.34	95,95,95,95	0
55	MG	DA	3010	1/1	0.68	0.28	97,97,97,97	0
55	MG	CA	1609	1/1	0.68	0.21	115,115,115,115	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	CA	1727	1/1	0.68	0.36	94,94,94,94	0
55	MG	BA	3420	1/1	0.68	0.24	94,94,94,94	0
55	MG	CA	1747	1/1	0.68	0.33	94,94,94,94	0
55	MG	AA	1832	1/1	0.68	0.33	94,94,94,94	0
55	MG	BB	201	1/1	0.68	0.37	92,92,92,92	0
55	MG	BA	3115	1/1	0.68	0.27	87,87,87,87	0
55	MG	DA	3085	1/1	0.68	0.27	91,91,91,91	0
55	MG	DB	211	1/1	0.68	0.28	93,93,93,93	0
55	MG	CA	1762	1/1	0.68	0.28	96,96,96,96	0
55	MG	CA	1805	1/1	0.69	0.30	94,94,94,94	0
55	MG	AA	1714	1/1	0.69	0.28	107,107,107,107	0
55	MG	CB	101	1/1	0.69	0.29	101,101,101,101	0
55	MG	BA	3403	1/1	0.69	0.43	93,93,93,93	0
55	MG	CA	1707	1/1	0.69	0.44	98,98,98,98	0
55	MG	BA	3461	1/1	0.69	0.19	91,91,91,91	0
55	MG	CA	1662	1/1	0.69	0.29	90,90,90,90	0
55	MG	CA	1684	1/1	0.69	0.55	85,85,85,85	0
55	MG	BA	3621	1/1	0.69	0.20	63,63,63,63	0
55	MG	DA	3350	1/1	0.69	0.28	91,91,91,91	0
55	MG	BA	3500	1/1	0.69	0.21	97,97,97,97	0
55	MG	DA	3394	1/1	0.69	0.25	90,90,90,90	0
55	MG	CA	1797	1/1	0.69	0.25	87,87,87,87	0
55	MG	DA	3371	1/1	0.70	0.34	82,82,82,82	0
55	MG	AD	101	1/1	0.70	0.22	101,101,101,101	0
55	MG	DA	3381	1/1	0.70	0.45	99,99,99,99	0
55	MG	DA	3047	1/1	0.70	0.32	76,76,76,76	0
55	MG	BA	3594	1/1	0.70	0.37	79,79,79,79	0
55	MG	CA	1685	1/1	0.70	0.31	93,93,93,93	0
55	MG	BA	3303	1/1	0.70	0.26	72,72,72,72	0
55	MG	CS	101	1/1	0.70	0.31	87,87,87,87	0
55	MG	BA	3448	1/1	0.70	0.38	100,100,100,100	0
55	MG	BB	206	1/1	0.70	0.25	86,86,86,86	0
55	MG	CC	106	1/1	0.70	0.30	96,96,96,96	0
55	MG	DA	3120	1/1	0.70	0.31	90,90,90,90	0
55	MG	AA	1754	1/1	0.70	0.28	95,95,95,95	0
55	MG	AC	102	1/1	0.70	0.38	93,93,93,93	0
55	MG	AC	105	1/1	0.70	0.36	93,93,93,93	0
55	MG	DA	3277	1/1	0.70	0.31	89,89,89,89	0
55	MG	AA	1770	1/1	0.70	0.27	102,102,102,102	0
55	MG	DA	3024	1/1	0.70	0.38	108,108,108,108	0
55	MG	CA	1761	1/1	0.71	0.43	92,92,92,92	0
55	MG	DA	3004	1/1	0.71	0.37	99,99,99,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	BA	3272	1/1	0.71	0.21	94,94,94,94	0
55	MG	DA	3088	1/1	0.71	0.24	96,96,96,96	0
55	MG	CA	1718	1/1	0.71	0.18	92,92,92,92	0
55	MG	CA	1694	1/1	0.71	0.41	97,97,97,97	0
55	MG	BA	3588	1/1	0.71	0.33	83,83,83,83	0
55	MG	CA	1730	1/1	0.71	0.22	106,106,106,106	0
55	MG	AB	105	1/1	0.71	0.21	110,110,110,110	0
55	MG	AA	1772	1/1	0.71	0.30	85,85,85,85	0
55	MG	DA	3343	1/1	0.71	0.25	95,95,95,95	0
55	MG	BA	3547	1/1	0.71	0.28	77,77,77,77	0
55	MG	DA	3357	1/1	0.71	0.26	96,96,96,96	0
55	MG	AA	1698	1/1	0.71	0.24	72,72,72,72	0
55	MG	CA	1715	1/1	0.71	0.29	104,104,104,104	0
55	MG	DA	3380	1/1	0.71	0.14	139,139,139,139	0
55	MG	CA	1735	1/1	0.72	0.27	89,89,89,89	0
55	MG	AA	1748	1/1	0.72	0.40	84,84,84,84	0
55	MG	AA	1686	1/1	0.72	0.39	85,85,85,85	0
55	MG	BA	3315	1/1	0.72	0.39	78,78,78,78	0
55	MG	DA	3413	1/1	0.72	0.30	94,94,94,94	0
55	MG	AA	1696	1/1	0.72	0.35	88,88,88,88	0
55	MG	BA	3349	1/1	0.72	0.22	97,97,97,97	0
55	MG	AA	1757	1/1	0.72	0.15	110,110,110,110	0
55	MG	BA	3509	1/1	0.72	0.30	83,83,83,83	0
55	MG	AA	1732	1/1	0.72	0.37	92,92,92,92	0
55	MG	CA	1771	1/1	0.72	0.22	76,76,76,76	0
55	MG	DA	3304	1/1	0.72	0.29	85,85,85,85	0
55	MG	AB	101	1/1	0.72	0.18	90,90,90,90	0
55	MG	DA	3028	1/1	0.72	0.30	101,101,101,101	0
55	MG	CA	1778	1/1	0.72	0.32	96,96,96,96	0
55	MG	AA	1813	1/1	0.72	0.24	107,107,107,107	0
55	MG	DB	208	1/1	0.72	0.30	90,90,90,90	0
55	MG	AA	1643	1/1	0.72	0.42	85,85,85,85	0
55	MG	AA	1678	1/1	0.72	0.39	74,74,74,74	0
55	MG	BA	3086	1/1	0.73	0.20	95,95,95,95	0
55	MG	CA	1783	1/1	0.73	0.35	100,100,100,100	0
55	MG	DA	3366	1/1	0.73	0.31	83,83,83,83	0
55	MG	CA	1785	1/1	0.73	0.36	105,105,105,105	0
55	MG	CA	1796	1/1	0.73	0.24	102,102,102,102	0
55	MG	DA	3061	1/1	0.73	0.27	74,74,74,74	0
55	MG	AA	1738	1/1	0.73	0.29	79,79,79,79	0
55	MG	DA	3393	1/1	0.73	0.32	69,69,69,69	0
55	MG	CA	1803	1/1	0.73	0.31	96,96,96,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	AA	1639	1/1	0.73	0.38	91,91,91,91	0
55	MG	BA	3151	1/1	0.73	0.31	83,83,83,83	0
55	MG	DA	3417	1/1	0.73	0.32	81,81,81,81	0
55	MG	DA	3419	1/1	0.73	0.33	84,84,84,84	0
55	MG	DA	3084	1/1	0.73	0.29	88,88,88,88	0
55	MG	AA	1674	1/1	0.73	0.29	98,98,98,98	0
55	MG	BA	3534	1/1	0.73	0.28	79,79,79,79	0
55	MG	DA	3476	1/1	0.73	0.32	107,107,107,107	0
55	MG	DA	3477	1/1	0.73	0.34	89,89,89,89	0
55	MG	CA	1710	1/1	0.73	0.29	106,106,106,106	0
55	MG	BA	3479	1/1	0.73	0.29	82,82,82,82	0
55	MG	BA	3215	1/1	0.73	0.33	74,74,74,74	0
55	MG	CC	108	1/1	0.73	0.21	106,106,106,106	0
55	MG	DA	3269	1/1	0.73	0.38	84,84,84,84	0
55	MG	BA	3219	1/1	0.73	0.36	76,76,76,76	0
55	MG	DA	3515	1/1	0.73	0.21	82,82,82,82	0
55	MG	CA	1765	1/1	0.73	0.27	101,101,101,101	0
55	MG	DB	202	1/1	0.73	0.20	98,98,98,98	0
55	MG	DA	3279	1/1	0.73	0.33	84,84,84,84	0
55	MG	BA	3222	1/1	0.73	0.37	89,89,89,89	0
55	MG	CA	1612	1/1	0.73	0.16	82,82,82,82	0
55	MG	CA	1614	1/1	0.73	0.31	86,86,86,86	0
55	MG	CA	1633	1/1	0.74	0.32	91,91,91,91	0
55	MG	CA	1635	1/1	0.74	0.38	86,86,86,86	0
55	MG	AA	1834	1/1	0.74	0.32	97,97,97,97	0
55	MG	DA	3458	1/1	0.74	0.41	92,92,92,92	0
55	MG	BA	3053	1/1	0.74	0.26	95,95,95,95	0
55	MG	AA	1630	1/1	0.74	0.25	101,101,101,101	0
55	MG	AA	1752	1/1	0.74	0.23	78,78,78,78	0
55	MG	AA	1768	1/1	0.74	0.34	101,101,101,101	0
55	MG	AA	1753	1/1	0.74	0.21	108,108,108,108	0
55	MG	AA	1637	1/1	0.74	0.24	98,98,98,98	0
55	MG	DA	3377	1/1	0.74	0.20	98,98,98,98	0
55	MG	AA	1702	1/1	0.74	0.27	93,93,93,93	0
55	MG	BA	3354	1/1	0.74	0.17	72,72,72,72	0
55	MG	CA	1773	1/1	0.74	0.36	92,92,92,92	0
55	MG	DA	3516	1/1	0.74	0.29	105,105,105,105	0
55	MG	CA	1725	1/1	0.74	0.28	86,86,86,86	0
55	MG	AA	1777	1/1	0.74	0.33	90,90,90,90	0
55	MG	AA	1716	1/1	0.74	0.33	92,92,92,92	0
55	MG	DA	3412	1/1	0.74	0.33	89,89,89,89	0
55	MG	CA	1732	1/1	0.74	0.27	109,109,109,109	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	CA	1787	1/1	0.74	0.18	87,87,87,87	0
55	MG	CA	1748	1/1	0.75	0.25	87,87,87,87	0
55	MG	DA	3451	1/1	0.75	0.28	75,75,75,75	0
55	MG	BA	3290	1/1	0.75	0.27	97,97,97,97	0
55	MG	CA	1667	1/1	0.75	0.13	102,102,102,102	0
55	MG	AA	1790	1/1	0.75	0.25	98,98,98,98	0
55	MG	BA	3391	1/1	0.75	0.35	86,86,86,86	0
55	MG	DA	3375	1/1	0.75	0.30	88,88,88,88	0
55	MG	BA	3546	1/1	0.75	0.19	87,87,87,87	0
55	MG	AA	1607	1/1	0.75	0.30	89,89,89,89	0
55	MG	DA	3040	1/1	0.75	0.18	81,81,81,81	0
55	MG	DA	3208	1/1	0.75	0.37	74,74,74,74	0
55	MG	AA	1735	1/1	0.75	0.24	79,79,79,79	0
55	MG	BA	3247	1/1	0.75	0.30	70,70,70,70	0
55	MG	CA	1651	1/1	0.75	0.30	90,90,90,90	0
55	MG	BA	3257	1/1	0.75	0.22	64,64,64,64	0
55	MG	DA	3302	1/1	0.75	0.42	95,95,95,95	0
55	MG	BA	3089	1/1	0.75	0.19	88,88,88,88	0
55	MG	BA	3513	1/1	0.75	0.34	90,90,90,90	0
55	MG	DA	3337	1/1	0.75	0.22	89,89,89,89	0
55	MG	DA	3437	1/1	0.75	0.28	87,87,87,87	0
55	MG	DA	3473	1/1	0.76	0.36	96,96,96,96	0
55	MG	CA	1630	1/1	0.76	0.36	91,91,91,91	0
55	MG	DA	3387	1/1	0.76	0.30	92,92,92,92	0
55	MG	DA	3478	1/1	0.76	0.33	80,80,80,80	0
55	MG	BA	3477	1/1	0.76	0.38	95,95,95,95	0
55	MG	DA	3485	1/1	0.76	0.17	81,81,81,81	0
55	MG	DA	3091	1/1	0.76	0.28	92,92,92,92	0
55	MG	DA	3117	1/1	0.76	0.38	78,78,78,78	0
55	MG	DA	3338	1/1	0.76	0.29	86,86,86,86	0
55	MG	DA	3493	1/1	0.76	0.29	82,82,82,82	0
55	MG	AA	1736	1/1	0.76	0.29	90,90,90,90	0
55	MG	BA	3325	1/1	0.76	0.31	76,76,76,76	0
55	MG	DA	3146	1/1	0.76	0.46	92,92,92,92	0
55	MG	CA	1781	1/1	0.76	0.17	117,117,117,117	0
55	MG	BA	3486	1/1	0.76	0.32	80,80,80,80	0
55	MG	DA	3073	1/1	0.76	0.49	80,80,80,80	0
55	MG	DB	206	1/1	0.76	0.27	90,90,90,90	0
55	MG	CA	1723	1/1	0.76	0.16	86,86,86,86	0
55	MG	CA	1769	1/1	0.76	0.31	105,105,105,105	0
55	MG	DA	3461	1/1	0.76	0.21	84,84,84,84	0
55	MG	CA	1639	1/1	0.76	0.45	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	CA	1628	1/1	0.77	0.25	101,101,101,101	0
55	MG	BA	3342	1/1	0.77	0.28	66,66,66,66	0
55	MG	BA	3204	1/1	0.77	0.33	78,78,78,78	0
55	MG	AA	1818	1/1	0.77	0.49	76,76,76,76	0
55	MG	BA	3570	1/1	0.77	0.34	87,87,87,87	0
55	MG	DA	3231	1/1	0.77	0.40	72,72,72,72	0
55	MG	B8	101	1/1	0.77	0.35	97,97,97,97	0
55	MG	DA	3067	1/1	0.77	0.33	94,94,94,94	0
55	MG	CA	1691	1/1	0.77	0.29	78,78,78,78	0
55	MG	DA	3396	1/1	0.77	0.27	82,82,82,82	0
55	MG	DA	3492	1/1	0.77	0.29	88,88,88,88	0
55	MG	AA	1611	1/1	0.77	0.26	92,92,92,92	0
55	MG	DA	3292	1/1	0.77	0.23	89,89,89,89	0
55	MG	BA	3582	1/1	0.77	0.33	86,86,86,86	0
55	MG	AA	1767	1/1	0.77	0.39	96,96,96,96	0
55	MG	DA	3005	1/1	0.77	0.35	77,77,77,77	0
55	MG	AA	1791	1/1	0.77	0.19	109,109,109,109	0
55	MG	DA	3436	1/1	0.77	0.32	98,98,98,98	0
55	MG	CA	1616	1/1	0.77	0.28	88,88,88,88	0
55	MG	AA	1648	1/1	0.77	0.31	78,78,78,78	0
55	MG	DA	3089	1/1	0.77	0.42	82,82,82,82	0
55	MG	AA	1614	1/1	0.77	0.26	91,91,91,91	0
55	MG	CA	1661	1/1	0.77	0.27	87,87,87,87	0
55	MG	DB	214	1/1	0.77	0.16	96,96,96,96	0
55	MG	BA	3496	1/1	0.78	0.28	96,96,96,96	0
55	MG	DA	3025	1/1	0.78	0.51	84,84,84,84	0
55	MG	BA	3584	1/1	0.78	0.19	72,72,72,72	0
55	MG	CA	1663	1/1	0.78	0.34	81,81,81,81	0
55	MG	BA	3432	1/1	0.78	0.28	80,80,80,80	0
55	MG	BA	3059	1/1	0.78	0.29	91,91,91,91	0
55	MG	DA	3057	1/1	0.78	0.27	83,83,83,83	0
55	MG	BA	3441	1/1	0.78	0.10	86,86,86,86	0
55	MG	AA	1747	1/1	0.78	0.44	88,88,88,88	0
55	MG	DA	3312	1/1	0.78	0.30	85,85,85,85	0
55	MG	BA	3449	1/1	0.78	0.28	80,80,80,80	0
55	MG	DA	3333	1/1	0.78	0.34	87,87,87,87	0
55	MG	BB	202	1/1	0.78	0.17	79,79,79,79	0
55	MG	CA	1637	1/1	0.78	0.29	79,79,79,79	0
55	MG	DA	3340	1/1	0.78	0.20	85,85,85,85	0
55	MG	DA	3342	1/1	0.78	0.43	82,82,82,82	0
55	MG	CG	301	1/1	0.78	0.31	83,83,83,83	0
55	MG	BA	3368	1/1	0.78	0.21	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	DA	3080	1/1	0.78	0.41	75,75,75,75	0
55	MG	BA	3472	1/1	0.78	0.33	89,89,89,89	0
55	MG	AA	1615	1/1	0.78	0.30	105,105,105,105	0
55	MG	DA	3501	1/1	0.78	0.41	88,88,88,88	0
55	MG	BA	3385	1/1	0.78	0.16	87,87,87,87	0
55	MG	DA	3507	1/1	0.78	0.46	91,91,91,91	0
55	MG	AA	1804	1/1	0.78	0.21	74,74,74,74	0
55	MG	CA	1654	1/1	0.78	0.30	99,99,99,99	0
55	MG	BA	3397	1/1	0.78	0.23	81,81,81,81	0
55	MG	DA	3517	1/1	0.78	0.23	84,84,84,84	0
55	MG	CA	1658	1/1	0.78	0.39	91,91,91,91	0
55	MG	DA	3093	1/1	0.78	0.19	80,80,80,80	0
55	MG	DA	3094	1/1	0.78	0.10	94,94,94,94	0
55	MG	BA	3292	1/1	0.78	0.39	85,85,85,85	0
55	MG	BA	3223	1/1	0.78	0.27	92,92,92,92	0
55	MG	DA	3015	1/1	0.78	0.29	89,89,89,89	0
55	MG	DA	3019	1/1	0.78	0.63	90,90,90,90	0
55	MG	CA	1777	1/1	0.78	0.30	88,88,88,88	0
55	MG	CA	1696	1/1	0.79	0.35	91,91,91,91	0
55	MG	AA	1807	1/1	0.79	0.54	98,98,98,98	0
55	MG	CC	101	1/1	0.79	0.18	92,92,92,92	0
55	MG	DA	3449	1/1	0.79	0.20	87,87,87,87	0
55	MG	AA	1684	1/1	0.79	0.23	90,90,90,90	0
55	MG	BA	3521	1/1	0.79	0.37	79,79,79,79	0
55	MG	DA	3336	1/1	0.79	0.30	87,87,87,87	0
55	MG	BA	3467	1/1	0.79	0.31	78,78,78,78	0
55	MG	BO	201	1/1	0.79	0.35	62,62,62,62	0
55	MG	BA	3321	1/1	0.79	0.31	77,77,77,77	0
55	MG	BA	3473	1/1	0.79	0.28	76,76,76,76	0
55	MG	AA	1743	1/1	0.79	0.20	107,107,107,107	0
55	MG	BA	3399	1/1	0.79	0.36	90,90,90,90	0
55	MG	DA	3090	1/1	0.79	0.36	86,86,86,86	0
55	MG	DA	3363	1/1	0.79	0.57	79,79,79,79	0
55	MG	DA	3014	1/1	0.79	0.38	74,74,74,74	0
55	MG	BA	3563	1/1	0.79	0.23	82,82,82,82	0
55	MG	BA	3400	1/1	0.79	0.42	80,80,80,80	0
55	MG	BA	3327	1/1	0.79	0.21	70,70,70,70	0
55	MG	DA	3498	1/1	0.79	0.26	85,85,85,85	0
55	MG	DA	3500	1/1	0.79	0.22	92,92,92,92	0
55	MG	AA	1822	1/1	0.79	0.18	107,107,107,107	0
55	MG	DA	3502	1/1	0.79	0.36	97,97,97,97	0
55	MG	CA	1627	1/1	0.79	0.23	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	DA	3139	1/1	0.79	0.27	80,80,80,80	0
55	MG	AA	1616	1/1	0.79	0.22	94,94,94,94	0
55	MG	AA	1746	1/1	0.79	0.30	84,84,84,84	0
55	MG	AA	1803	1/1	0.79	0.22	91,91,91,91	0
55	MG	DA	3043	1/1	0.79	0.19	82,82,82,82	0
55	MG	DA	3399	1/1	0.79	0.39	76,76,76,76	0
55	MG	BA	3444	1/1	0.79	0.28	78,78,78,78	0
55	MG	DA	3410	1/1	0.79	0.31	78,78,78,78	0
55	MG	BA	3445	1/1	0.79	0.25	79,79,79,79	0
55	MG	DA	3275	1/1	0.79	0.30	76,76,76,76	0
55	MG	DB	209	1/1	0.79	0.17	92,92,92,92	0
55	MG	AA	1656	1/1	0.79	0.35	87,87,87,87	0
55	MG	CA	1755	1/1	0.79	0.47	92,92,92,92	0
55	MG	CG	302	1/1	0.79	0.20	101,101,101,101	0
55	MG	BB	217	1/1	0.80	0.20	98,98,98,98	0
55	MG	DA	3475	1/1	0.80	0.30	88,88,88,88	0
55	MG	CA	1756	1/1	0.80	0.28	81,81,81,81	0
55	MG	CA	1703	1/1	0.80	0.28	94,94,94,94	0
55	MG	BA	3573	1/1	0.80	0.26	83,83,83,83	0
55	MG	DA	3376	1/1	0.80	0.42	82,82,82,82	0
55	MG	DA	3185	1/1	0.80	0.27	74,74,74,74	0
55	MG	AA	1787	1/1	0.80	0.35	96,96,96,96	0
55	MG	AA	1612	1/1	0.80	0.14	91,91,91,91	0
55	MG	DA	3268	1/1	0.80	0.32	69,69,69,69	0
55	MG	CA	1606	1/1	0.80	0.30	87,87,87,87	0
55	MG	CC	105	1/1	0.80	0.37	82,82,82,82	0
55	MG	AA	1679	1/1	0.80	0.29	86,86,86,86	0
55	MG	BA	3527	1/1	0.80	0.28	93,93,93,93	0
55	MG	BA	3530	1/1	0.80	0.25	81,81,81,81	0
55	MG	BA	3116	1/1	0.80	0.24	73,73,73,73	0
55	MG	BA	3606	1/1	0.80	0.28	77,77,77,77	0
55	MG	CA	1624	1/1	0.80	0.27	88,88,88,88	0
55	MG	BA	3454	1/1	0.80	0.25	92,92,92,92	0
55	MG	DA	3415	1/1	0.80	0.42	96,96,96,96	0
55	MG	BA	3623	1/1	0.80	0.30	60,60,60,60	0
55	MG	BA	3408	1/1	0.80	0.28	87,87,87,87	0
55	MG	DA	3335	1/1	0.80	0.23	61,61,61,61	0
55	MG	AA	1749	1/1	0.80	0.19	81,81,81,81	0
55	MG	AA	1668	1/1	0.80	0.43	76,76,76,76	0
55	MG	BB	208	1/1	0.80	0.25	74,74,74,74	0
55	MG	AA	1609	1/1	0.80	0.38	78,78,78,78	0
55	MG	BB	211	1/1	0.80	0.22	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	AA	1677	1/1	0.80	0.31	87,87,87,87	0
55	MG	DA	3119	1/1	0.80	0.37	98,98,98,98	0
55	MG	DA	3036	1/1	0.80	0.26	99,99,99,99	0
55	MG	DA	3435	1/1	0.81	0.17	72,72,72,72	0
55	MG	BA	3278	1/1	0.81	0.33	81,81,81,81	0
55	MG	BA	3524	1/1	0.81	0.23	66,66,66,66	0
55	MG	DA	3330	1/1	0.81	0.23	81,81,81,81	0
55	MG	BA	3414	1/1	0.81	0.14	72,72,72,72	0
55	MG	CA	1611	1/1	0.81	0.38	93,93,93,93	0
55	MG	BA	3203	1/1	0.81	0.27	85,85,85,85	0
55	MG	BA	3084	1/1	0.81	0.42	82,82,82,82	0
55	MG	BA	3537	1/1	0.81	0.31	89,89,89,89	0
55	MG	BA	3210	1/1	0.81	0.19	74,74,74,74	0
55	MG	AA	1683	1/1	0.81	0.21	87,87,87,87	0
55	MG	CA	1782	1/1	0.81	0.38	93,93,93,93	0
55	MG	CA	1625	1/1	0.81	0.29	90,90,90,90	0
55	MG	DA	3353	1/1	0.81	0.36	93,93,93,93	0
55	MG	DA	3354	1/1	0.81	0.35	73,73,73,73	0
55	MG	CA	1729	1/1	0.81	0.30	77,77,77,77	0
55	MG	DA	3358	1/1	0.81	0.37	88,88,88,88	0
55	MG	DA	3128	1/1	0.81	0.30	77,77,77,77	0
55	MG	AA	1695	1/1	0.81	0.30	90,90,90,90	0
55	MG	DA	3136	1/1	0.81	0.31	76,76,76,76	0
55	MG	AA	1730	1/1	0.81	0.14	78,78,78,78	0
55	MG	BA	3396	1/1	0.81	0.18	82,82,82,82	0
55	MG	AA	1827	1/1	0.81	0.35	87,87,87,87	0
55	MG	BB	214	1/1	0.81	0.16	86,86,86,86	0
55	MG	DA	3056	1/1	0.81	0.43	81,81,81,81	0
55	MG	BB	215	1/1	0.81	0.26	82,82,82,82	0
55	MG	DA	3259	1/1	0.81	0.18	72,72,72,72	0
55	MG	AA	1760	1/1	0.81	0.28	78,78,78,78	0
55	MG	AA	1794	1/1	0.81	0.31	84,84,84,84	0
55	MG	BF	303	1/1	0.81	0.34	66,66,66,66	0
55	MG	AA	1817	1/1	0.81	0.29	85,85,85,85	0
55	MG	DA	3518	1/1	0.81	0.36	83,83,83,83	0
55	MG	DA	3519	1/1	0.81	0.30	85,85,85,85	0
55	MG	CA	1758	1/1	0.81	0.37	78,78,78,78	0
55	MG	DA	3406	1/1	0.81	0.26	86,86,86,86	0
55	MG	CA	1640	1/1	0.81	0.30	81,81,81,81	0
55	MG	DA	3283	1/1	0.81	0.18	61,61,61,61	0
55	MG	BA	3406	1/1	0.81	0.30	82,82,82,82	0
55	MG	CA	1708	1/1	0.81	0.20	97,97,97,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	CA	1763	1/1	0.81	0.26	91,91,91,91	0
55	MG	DA	3308	1/1	0.81	0.29	97,97,97,97	0
55	MG	DA	3309	1/1	0.81	0.23	94,94,94,94	0
55	MG	CA	1617	1/1	0.82	0.26	93,93,93,93	0
55	MG	AA	1625	1/1	0.82	0.20	57,57,57,57	0
55	MG	BA	3068	1/1	0.82	0.28	75,75,75,75	0
55	MG	BA	3330	1/1	0.82	0.30	79,79,79,79	0
55	MG	AA	1740	1/1	0.82	0.12	75,75,75,75	0
55	MG	BA	3340	1/1	0.82	0.23	77,77,77,77	0
55	MG	AA	1819	1/1	0.82	0.42	87,87,87,87	0
55	MG	CA	1629	1/1	0.82	0.19	98,98,98,98	0
55	MG	BA	3568	1/1	0.82	0.34	83,83,83,83	0
55	MG	BA	3345	1/1	0.82	0.54	73,73,73,73	0
55	MG	BA	3455	1/1	0.82	0.18	76,76,76,76	0
55	MG	DA	3237	1/1	0.82	0.25	83,83,83,83	0
55	MG	BA	3458	1/1	0.82	0.18	82,82,82,82	0
55	MG	AQ	101	1/1	0.82	0.18	88,88,88,88	0
55	MG	CA	1737	1/1	0.82	0.28	99,99,99,99	0
55	MG	BA	3087	1/1	0.82	0.34	77,77,77,77	0
55	MG	CA	1743	1/1	0.82	0.39	80,80,80,80	0
55	MG	DA	3445	1/1	0.82	0.28	78,78,78,78	0
55	MG	BA	3470	1/1	0.82	0.26	88,88,88,88	0
55	MG	BA	3358	1/1	0.82	0.28	74,74,74,74	0
55	MG	AA	1685	1/1	0.82	0.28	88,88,88,88	0
55	MG	DA	3459	1/1	0.82	0.23	86,86,86,86	0
55	MG	DA	3289	1/1	0.82	0.29	90,90,90,90	0
55	MG	BA	3475	1/1	0.82	0.25	83,83,83,83	0
55	MG	BA	3613	1/1	0.82	0.46	93,93,93,93	0
55	MG	BA	3371	1/1	0.82	0.32	70,70,70,70	0
55	MG	BA	3265	1/1	0.82	0.36	60,60,60,60	0
55	MG	BA	3481	1/1	0.82	0.33	69,69,69,69	0
55	MG	AA	1824	1/1	0.82	0.34	86,86,86,86	0
55	MG	DA	3041	1/1	0.82	0.35	86,86,86,86	0
55	MG	BA	3485	1/1	0.82	0.25	80,80,80,80	0
55	MG	AA	1706	1/1	0.82	0.36	74,74,74,74	0
55	MG	BA	3489	1/1	0.82	0.18	70,70,70,70	0
55	MG	CA	1767	1/1	0.82	0.34	77,77,77,77	0
55	MG	BA	3394	1/1	0.82	0.20	81,81,81,81	0
55	MG	BA	3127	1/1	0.82	0.36	53,53,53,53	0
55	MG	DA	3063	1/1	0.82	0.49	75,75,75,75	0
55	MG	DA	3341	1/1	0.82	0.34	84,84,84,84	0
55	MG	BA	3291	1/1	0.82	0.25	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	AA	1682	1/1	0.82	0.23	91,91,91,91	0
55	MG	BA	3145	1/1	0.82	0.36	74,74,74,74	0
55	MG	AA	1620	1/1	0.82	0.23	66,66,66,66	0
55	MG	BA	3404	1/1	0.82	0.12	60,60,60,60	0
55	MG	DA	3509	1/1	0.82	0.23	64,64,64,64	0
55	MG	CA	1780	1/1	0.82	0.37	88,88,88,88	0
55	MG	CA	1693	1/1	0.82	0.43	76,76,76,76	0
55	MG	AA	1725	1/1	0.82	0.23	82,82,82,82	0
55	MG	AA	1690	1/1	0.82	0.31	96,96,96,96	0
55	MG	DA	3369	1/1	0.82	0.23	74,74,74,74	0
55	MG	BA	3317	1/1	0.82	0.45	89,89,89,89	0
55	MG	CA	1786	1/1	0.82	0.28	73,73,73,73	0
55	MG	BA	3417	1/1	0.82	0.23	99,99,99,99	0
55	MG	BA	3525	1/1	0.82	0.27	77,77,77,77	0
55	MG	AA	1786	1/1	0.82	0.19	86,86,86,86	0
55	MG	BA	3431	1/1	0.82	0.35	88,88,88,88	0
55	MG	BA	3324	1/1	0.82	0.33	73,73,73,73	0
55	MG	DA	3383	1/1	0.82	0.39	87,87,87,87	0
55	MG	CA	1806	1/1	0.82	0.38	96,96,96,96	0
55	MG	DA	3038	1/1	0.83	0.40	97,97,97,97	0
55	MG	BA	3511	1/1	0.83	0.19	89,89,89,89	0
55	MG	BA	3295	1/1	0.83	0.32	81,81,81,81	0
55	MG	BA	3514	1/1	0.83	0.23	71,71,71,71	0
55	MG	DA	3045	1/1	0.83	0.36	94,94,94,94	0
55	MG	BA	3060	1/1	0.83	0.23	64,64,64,64	0
55	MG	DA	3282	1/1	0.83	0.18	69,69,69,69	0
55	MG	DA	3049	1/1	0.83	0.28	74,74,74,74	0
55	MG	DA	3430	1/1	0.83	0.26	62,62,62,62	0
55	MG	CA	1664	1/1	0.83	0.36	99,99,99,99	0
55	MG	CA	1788	1/1	0.83	0.29	84,84,84,84	0
55	MG	DA	3297	1/1	0.83	0.20	83,83,83,83	0
55	MG	BA	3065	1/1	0.83	0.27	91,91,91,91	0
55	MG	DA	3303	1/1	0.83	0.32	70,70,70,70	0
55	MG	CA	1677	1/1	0.83	0.34	73,73,73,73	0
55	MG	CA	1798	1/1	0.83	0.23	85,85,85,85	0
55	MG	CA	1801	1/1	0.83	0.20	89,89,89,89	0
55	MG	AA	1681	1/1	0.83	0.37	80,80,80,80	0
55	MG	CA	1742	1/1	0.83	0.22	97,97,97,97	0
55	MG	DA	3319	1/1	0.83	0.34	74,74,74,74	0
55	MG	DA	3468	1/1	0.83	0.23	92,92,92,92	0
55	MG	DA	3471	1/1	0.83	0.26	80,80,80,80	0
55	MG	BA	3239	1/1	0.83	0.21	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	CA	1744	1/1	0.83	0.34	79,79,79,79	0
55	MG	CA	1686	1/1	0.83	0.42	73,73,73,73	0
55	MG	BA	3366	1/1	0.83	0.45	94,94,94,94	0
55	MG	CA	1749	1/1	0.83	0.24	89,89,89,89	0
55	MG	DA	3479	1/1	0.83	0.17	99,99,99,99	0
55	MG	BA	3529	1/1	0.83	0.29	68,68,68,68	0
55	MG	DA	3484	1/1	0.83	0.36	83,83,83,83	0
55	MG	CB	103	1/1	0.83	0.20	103,103,103,103	0
55	MG	BB	203	1/1	0.83	0.36	65,65,65,65	0
55	MG	BA	3367	1/1	0.83	0.23	82,82,82,82	0
55	MG	BA	3143	1/1	0.83	0.59	72,72,72,72	0
55	MG	DA	3349	1/1	0.83	0.23	63,63,63,63	0
55	MG	AA	1756	1/1	0.83	0.16	69,69,69,69	0
55	MG	DA	3494	1/1	0.83	0.16	75,75,75,75	0
55	MG	DA	3497	1/1	0.83	0.20	74,74,74,74	0
55	MG	DA	3092	1/1	0.83	0.20	68,68,68,68	0
55	MG	AA	1727	1/1	0.83	0.37	87,87,87,87	0
55	MG	CA	1702	1/1	0.83	0.32	78,78,78,78	0
55	MG	DA	3002	1/1	0.83	0.53	93,93,93,93	0
55	MG	AA	1724	1/1	0.83	0.29	84,84,84,84	0
55	MG	AA	1823	1/1	0.83	0.32	77,77,77,77	0
55	MG	BA	3328	1/1	0.83	0.41	69,69,69,69	0
55	MG	AB	102	1/1	0.83	0.23	86,86,86,86	0
55	MG	DA	3511	1/1	0.83	0.32	76,76,76,76	0
55	MG	BE	305	1/1	0.83	0.30	71,71,71,71	0
55	MG	BA	3565	1/1	0.83	0.30	77,77,77,77	0
55	MG	BA	3110	1/1	0.83	0.29	59,59,59,59	0
55	MG	BA	3337	1/1	0.83	0.24	72,72,72,72	0
55	MG	DA	3153	1/1	0.83	0.22	70,70,70,70	0
55	MG	BA	3457	1/1	0.83	0.47	88,88,88,88	0
55	MG	DA	3207	1/1	0.83	0.33	66,66,66,66	0
55	MG	BA	3506	1/1	0.83	0.29	78,78,78,78	0
55	MG	BA	3339	1/1	0.83	0.33	88,88,88,88	0
55	MG	DA	3236	1/1	0.83	0.13	55,55,55,55	0
55	MG	AA	1814	1/1	0.83	0.33	83,83,83,83	0
55	MG	CA	1724	1/1	0.83	0.29	84,84,84,84	0
55	MG	DA	3401	1/1	0.83	0.21	71,71,71,71	0
55	MG	DA	3266	1/1	0.83	0.32	55,55,55,55	0
55	MG	BA	3388	1/1	0.84	0.32	88,88,88,88	0
55	MG	BA	3072	1/1	0.84	0.23	77,77,77,77	0
55	MG	DA	3070	1/1	0.84	0.23	78,78,78,78	0
55	MG	CA	1760	1/1	0.84	0.24	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	DA	3434	1/1	0.84	0.10	74,74,74,74	0
55	MG	BA	3577	1/1	0.84	0.22	73,73,73,73	0
55	MG	DA	3075	1/1	0.84	0.35	79,79,79,79	0
55	MG	BA	3393	1/1	0.84	0.30	81,81,81,81	0
55	MG	DA	3440	1/1	0.84	0.16	86,86,86,86	0
55	MG	BA	3073	1/1	0.84	0.28	82,82,82,82	0
55	MG	DA	3442	1/1	0.84	0.23	91,91,91,91	0
55	MG	BA	3133	1/1	0.84	0.24	66,66,66,66	0
55	MG	CA	1608	1/1	0.84	0.34	81,81,81,81	0
55	MG	CA	1768	1/1	0.84	0.20	84,84,84,84	0
55	MG	AA	1636	1/1	0.84	0.33	87,87,87,87	0
55	MG	CA	1610	1/1	0.84	0.27	97,97,97,97	0
55	MG	BA	3104	1/1	0.84	0.16	57,57,57,57	0
55	MG	BA	3446	1/1	0.84	0.20	92,92,92,92	0
55	MG	DA	3464	1/1	0.84	0.28	98,98,98,98	0
55	MG	BA	3447	1/1	0.84	0.30	71,71,71,71	0
55	MG	BA	3364	1/1	0.84	0.23	82,82,82,82	0
55	MG	BA	3618	1/1	0.84	0.36	73,73,73,73	0
55	MG	DA	3112	1/1	0.84	0.11	81,81,81,81	0
55	MG	BA	3619	1/1	0.84	0.42	69,69,69,69	0
55	MG	DA	3018	1/1	0.84	0.30	77,77,77,77	0
55	MG	BA	3533	1/1	0.84	0.34	72,72,72,72	0
55	MG	BA	3301	1/1	0.84	0.28	76,76,76,76	0
55	MG	DA	3345	1/1	0.84	0.29	64,64,64,64	0
55	MG	DA	3483	1/1	0.84	0.19	90,90,90,90	0
55	MG	AA	1739	1/1	0.84	0.08	93,93,93,93	0
55	MG	CA	1784	1/1	0.84	0.23	81,81,81,81	0
55	MG	DA	3138	1/1	0.84	0.25	70,70,70,70	0
55	MG	BA	3276	1/1	0.84	0.24	74,74,74,74	0
55	MG	DA	3140	1/1	0.84	0.22	78,78,78,78	0
55	MG	DA	3143	1/1	0.84	0.25	58,58,58,58	0
55	MG	BA	3085	1/1	0.84	0.15	73,73,73,73	0
55	MG	DA	3150	1/1	0.84	0.30	68,68,68,68	0
55	MG	DA	3367	1/1	0.84	0.32	82,82,82,82	0
55	MG	BA	3282	1/1	0.84	0.10	83,83,83,83	0
55	MG	BA	3548	1/1	0.84	0.46	76,76,76,76	0
55	MG	DA	3183	1/1	0.84	0.30	57,57,57,57	0
55	MG	DA	3039	1/1	0.84	0.21	85,85,85,85	0
55	MG	CA	1790	1/1	0.84	0.20	110,110,110,110	0
55	MG	DA	3505	1/1	0.84	0.34	81,81,81,81	0
55	MG	CA	1791	1/1	0.84	0.25	79,79,79,79	0
55	MG	DA	3209	1/1	0.84	0.32	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	DA	3228	1/1	0.84	0.30	44,44,44,44	0
55	MG	BA	3415	1/1	0.84	0.30	84,84,84,84	0
55	MG	BA	3562	1/1	0.84	0.30	79,79,79,79	0
55	MG	BA	3341	1/1	0.84	0.23	81,81,81,81	0
55	MG	CA	1800	1/1	0.84	0.19	78,78,78,78	0
55	MG	CA	1751	1/1	0.84	0.32	94,94,94,94	0
55	MG	DA	3397	1/1	0.84	0.20	60,60,60,60	0
55	MG	DA	3522	1/1	0.84	0.18	78,78,78,78	0
55	MG	CA	1752	1/1	0.84	0.20	70,70,70,70	0
55	MG	BA	3419	1/1	0.84	0.32	85,85,85,85	0
55	MG	DA	3403	1/1	0.84	0.28	76,76,76,76	0
55	MG	BA	3566	1/1	0.84	0.28	88,88,88,88	0
55	MG	DA	3062	1/1	0.84	0.17	72,72,72,72	0
55	MG	DA	3276	1/1	0.84	0.41	68,68,68,68	0
55	MG	BA	3510	1/1	0.84	0.22	108,108,108,108	0
55	MG	CA	1706	1/1	0.84	0.30	87,87,87,87	0
55	MG	DA	3281	1/1	0.84	0.53	76,76,76,76	0
55	MG	BA	3146	1/1	0.85	0.29	59,59,59,59	0
55	MG	BA	3402	1/1	0.85	0.27	91,91,91,91	0
55	MG	DA	3427	1/1	0.85	0.27	76,76,76,76	0
55	MG	BA	3266	1/1	0.85	0.34	77,77,77,77	0
55	MG	BA	3360	1/1	0.85	0.16	84,84,84,84	0
55	MG	DA	3432	1/1	0.85	0.27	69,69,69,69	0
55	MG	BA	3363	1/1	0.85	0.38	67,67,67,67	0
55	MG	BA	3585	1/1	0.85	0.26	60,60,60,60	0
55	MG	BA	3094	1/1	0.85	0.34	78,78,78,78	0
55	MG	CA	1698	1/1	0.85	0.11	107,107,107,107	0
55	MG	BA	3463	1/1	0.85	0.14	72,72,72,72	0
55	MG	DA	3322	1/1	0.85	0.32	70,70,70,70	0
55	MG	DA	3327	1/1	0.85	0.19	61,61,61,61	0
55	MG	CA	1764	1/1	0.85	0.44	72,72,72,72	0
55	MG	DA	3448	1/1	0.85	0.40	79,79,79,79	0
55	MG	DA	3332	1/1	0.85	0.21	76,76,76,76	0
55	MG	BA	3592	1/1	0.85	0.31	89,89,89,89	0
55	MG	DA	3453	1/1	0.85	0.18	66,66,66,66	0
55	MG	DA	3456	1/1	0.85	0.55	83,83,83,83	0
55	MG	CA	1766	1/1	0.85	0.34	85,85,85,85	0
55	MG	BA	3593	1/1	0.85	0.22	80,80,80,80	0
55	MG	BA	3518	1/1	0.85	0.23	70,70,70,70	0
55	MG	BA	3411	1/1	0.85	0.29	68,68,68,68	0
55	MG	DA	3127	1/1	0.85	0.40	74,74,74,74	0
55	MG	DA	3466	1/1	0.85	0.39	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	BA	3412	1/1	0.85	0.25	78,78,78,78	0
55	MG	DA	3469	1/1	0.85	0.38	80,80,80,80	0
55	MG	BA	3615	1/1	0.85	0.34	81,81,81,81	0
55	MG	CA	1772	1/1	0.85	0.34	72,72,72,72	0
55	MG	DA	3344	1/1	0.85	0.27	95,95,95,95	0
55	MG	CA	1709	1/1	0.85	0.39	108,108,108,108	0
55	MG	BA	3071	1/1	0.85	0.24	70,70,70,70	0
55	MG	BA	3106	1/1	0.85	0.25	75,75,75,75	0
55	MG	AA	1776	1/1	0.85	0.25	82,82,82,82	0
55	MG	BA	3476	1/1	0.85	0.23	81,81,81,81	0
55	MG	BA	3369	1/1	0.85	0.30	73,73,73,73	0
55	MG	BA	3532	1/1	0.85	0.34	85,85,85,85	0
55	MG	DA	3362	1/1	0.85	0.25	53,53,53,53	0
55	MG	DA	3486	1/1	0.85	0.14	68,68,68,68	0
55	MG	AA	1809	1/1	0.85	0.30	63,63,63,63	0
55	MG	DA	3364	1/1	0.85	0.20	71,71,71,71	0
55	MG	AA	1635	1/1	0.85	0.31	86,86,86,86	0
55	MG	DA	3042	1/1	0.85	0.26	81,81,81,81	0
55	MG	DA	3193	1/1	0.85	0.31	63,63,63,63	0
55	MG	DA	3197	1/1	0.85	0.32	70,70,70,70	0
55	MG	AA	1703	1/1	0.85	0.34	92,92,92,92	0
55	MG	BA	3437	1/1	0.85	0.28	67,67,67,67	0
55	MG	DA	3499	1/1	0.85	0.23	61,61,61,61	0
55	MG	BA	3293	1/1	0.85	0.23	65,65,65,65	0
55	MG	DA	3048	1/1	0.85	0.53	75,75,75,75	0
55	MG	BA	3487	1/1	0.85	0.16	94,94,94,94	0
55	MG	CA	1655	1/1	0.85	0.36	87,87,87,87	0
55	MG	BA	3132	1/1	0.85	0.28	71,71,71,71	0
55	MG	DA	3058	1/1	0.85	0.21	76,76,76,76	0
55	MG	BA	3551	1/1	0.85	0.27	87,87,87,87	0
55	MG	AA	1825	1/1	0.85	0.13	93,93,93,93	0
55	MG	BA	3493	1/1	0.85	0.33	63,63,63,63	0
55	MG	DA	3513	1/1	0.85	0.27	67,67,67,67	0
55	MG	AA	1694	1/1	0.85	0.25	91,91,91,91	0
55	MG	DA	3398	1/1	0.85	0.28	74,74,74,74	0
55	MG	AA	1805	1/1	0.85	0.34	65,65,65,65	0
55	MG	DA	3400	1/1	0.85	0.30	89,89,89,89	0
55	MG	BA	3498	1/1	0.85	0.23	85,85,85,85	0
55	MG	DA	3402	1/1	0.85	0.29	101,101,101,101	0
55	MG	BA	3309	1/1	0.85	0.24	68,68,68,68	0
55	MG	CA	1604	1/1	0.85	0.25	81,81,81,81	0
55	MG	CA	1668	1/1	0.85	0.24	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	DA	3409	1/1	0.85	0.25	76,76,76,76	0
55	MG	BA	3069	1/1	0.85	0.31	77,77,77,77	0
55	MG	CA	1607	1/1	0.85	0.45	85,85,85,85	0
55	MG	BA	3571	1/1	0.85	0.26	92,92,92,92	0
55	MG	DA	3414	1/1	0.85	0.38	85,85,85,85	0
55	MG	DA	3082	1/1	0.85	0.23	91,91,91,91	0
55	MG	D1	201	1/1	0.85	0.41	71,71,71,71	0
55	MG	DU	201	1/1	0.85	0.16	72,72,72,72	0
55	MG	BA	3226	1/1	0.86	0.21	50,50,50,50	0
55	MG	DA	3290	1/1	0.86	0.27	79,79,79,79	0
55	MG	DA	3428	1/1	0.86	0.32	84,84,84,84	0
55	MG	BA	3238	1/1	0.86	0.33	41,41,41,41	0
55	MG	BA	3535	1/1	0.86	0.29	80,80,80,80	0
55	MG	CA	1648	1/1	0.86	0.24	65,65,65,65	0
55	MG	AA	1624	1/1	0.86	0.23	79,79,79,79	0
55	MG	DA	3081	1/1	0.86	0.34	64,64,64,64	0
55	MG	BA	3032	1/1	0.86	0.52	49,49,49,49	0
55	MG	AA	1789	1/1	0.86	0.31	74,74,74,74	0
55	MG	CA	1736	1/1	0.86	0.37	79,79,79,79	0
55	MG	DA	3313	1/1	0.86	0.26	85,85,85,85	0
55	MG	CA	1656	1/1	0.86	0.25	92,92,92,92	0
55	MG	DA	3443	1/1	0.86	0.28	80,80,80,80	0
55	MG	CA	1740	1/1	0.86	0.21	68,68,68,68	0
55	MG	DA	3320	1/1	0.86	0.15	76,76,76,76	0
55	MG	BA	3054	1/1	0.86	0.26	80,80,80,80	0
55	MG	BA	3055	1/1	0.86	0.36	57,57,57,57	0
55	MG	BA	3550	1/1	0.86	0.18	93,93,93,93	0
55	MG	DA	3454	1/1	0.86	0.29	92,92,92,92	0
55	MG	AA	1742	1/1	0.86	0.25	78,78,78,78	0
55	MG	BD	301	1/1	0.86	0.31	85,85,85,85	0
55	MG	BA	3275	1/1	0.86	0.23	73,73,73,73	0
55	MG	AA	1718	1/1	0.86	0.27	82,82,82,82	0
55	MG	AA	1840	1/1	0.86	0.45	87,87,87,87	0
55	MG	CA	1665	1/1	0.86	0.21	83,83,83,83	0
55	MG	BU	202	1/1	0.86	0.11	55,55,55,55	0
55	MG	AA	1793	1/1	0.86	0.24	73,73,73,73	0
55	MG	DA	3125	1/1	0.86	0.31	45,45,45,45	0
55	MG	BA	3422	1/1	0.86	0.26	78,78,78,78	0
55	MG	CA	1681	1/1	0.86	0.27	72,72,72,72	0
55	MG	CA	1682	1/1	0.86	0.23	86,86,86,86	0
55	MG	CA	1603	1/1	0.86	0.40	77,77,77,77	0
55	MG	BA	3425	1/1	0.86	0.39	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	BA	3569	1/1	0.86	0.34	85,85,85,85	0
55	MG	BA	3137	1/1	0.86	0.28	47,47,47,47	0
55	MG	DA	3356	1/1	0.86	0.24	67,67,67,67	0
55	MG	BA	3362	1/1	0.86	0.10	48,48,48,48	0
55	MG	BA	3140	1/1	0.86	0.17	58,58,58,58	0
55	MG	AA	1649	1/1	0.86	0.22	79,79,79,79	0
55	MG	AA	1775	1/1	0.86	0.11	79,79,79,79	0
55	MG	AA	1801	1/1	0.86	0.45	84,84,84,84	0
55	MG	DA	3179	1/1	0.86	0.26	70,70,70,70	0
55	MG	BA	3583	1/1	0.86	0.11	86,86,86,86	0
55	MG	DA	3368	1/1	0.86	0.44	73,73,73,73	0
55	MG	AA	1655	1/1	0.86	0.40	88,88,88,88	0
55	MG	AB	104	1/1	0.86	0.24	82,82,82,82	0
55	MG	BA	3586	1/1	0.86	0.34	63,63,63,63	0
55	MG	BA	3167	1/1	0.86	0.33	73,73,73,73	0
55	MG	BA	3304	1/1	0.86	0.22	56,56,56,56	0
55	MG	DA	3378	1/1	0.86	0.33	63,63,63,63	0
55	MG	BA	3191	1/1	0.86	0.20	81,81,81,81	0
55	MG	DA	3044	1/1	0.86	0.24	73,73,73,73	0
55	MG	DA	3230	1/1	0.86	0.16	59,59,59,59	0
55	MG	BA	3080	1/1	0.86	0.14	91,91,91,91	0
55	MG	BA	3314	1/1	0.86	0.32	64,64,64,64	0
55	MG	AA	1613	1/1	0.86	0.14	85,85,85,85	0
55	MG	DA	3242	1/1	0.86	0.35	63,63,63,63	0
55	MG	DA	3395	1/1	0.86	0.38	69,69,69,69	0
55	MG	DA	3249	1/1	0.86	0.29	72,72,72,72	0
55	MG	DA	3251	1/1	0.86	0.26	74,74,74,74	0
55	MG	DA	3253	1/1	0.86	0.18	87,87,87,87	0
55	MG	DA	3254	1/1	0.86	0.34	50,50,50,50	0
55	MG	CA	1711	1/1	0.86	0.40	90,90,90,90	0
55	MG	CA	1712	1/1	0.86	0.39	86,86,86,86	0
55	MG	AA	1661	1/1	0.86	0.23	48,48,48,48	0
55	MG	BA	3460	1/1	0.86	0.16	83,83,83,83	0
55	MG	DA	3525	1/1	0.86	0.26	79,79,79,79	0
55	MG	DA	3270	1/1	0.86	0.21	83,83,83,83	0
55	MG	AA	1666	1/1	0.86	0.39	62,62,62,62	0
55	MG	CA	1716	1/1	0.86	0.21	79,79,79,79	0
55	MG	AA	1626	1/1	0.86	0.22	69,69,69,69	0
55	MG	AC	107	1/1	0.86	0.24	94,94,94,94	0
55	MG	DB	210	1/1	0.86	0.36	71,71,71,71	0
55	MG	BA	3468	1/1	0.86	0.27	77,77,77,77	0
55	MG	DA	3065	1/1	0.86	0.27	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	CA	1720	1/1	0.86	0.43	102,102,102,102	0
55	MG	DE	302	1/1	0.86	0.30	65,65,65,65	0
55	MG	DA	3416	1/1	0.86	0.28	59,59,59,59	0
55	MG	AC	109	1/1	0.86	0.28	82,82,82,82	0
55	MG	DA	3439	1/1	0.87	0.16	62,62,62,62	0
55	MG	BA	3232	1/1	0.87	0.19	72,72,72,72	0
55	MG	DA	3031	1/1	0.87	0.27	72,72,72,72	0
55	MG	BA	3343	1/1	0.87	0.25	60,60,60,60	0
55	MG	DA	3037	1/1	0.87	0.32	98,98,98,98	0
55	MG	DA	3148	1/1	0.87	0.34	75,75,75,75	0
55	MG	CA	1775	1/1	0.87	0.29	72,72,72,72	0
55	MG	AA	1802	1/1	0.87	0.32	85,85,85,85	0
55	MG	BA	3348	1/1	0.87	0.22	61,61,61,61	0
55	MG	DA	3162	1/1	0.87	0.29	66,66,66,66	0
55	MG	DA	3167	1/1	0.87	0.33	70,70,70,70	0
55	MG	DA	3455	1/1	0.87	0.23	69,69,69,69	0
55	MG	AA	1751	1/1	0.87	0.26	98,98,98,98	0
55	MG	CA	1722	1/1	0.87	0.37	75,75,75,75	0
55	MG	BE	301	1/1	0.87	0.28	59,59,59,59	0
55	MG	AA	1721	1/1	0.87	0.26	77,77,77,77	0
55	MG	DA	3355	1/1	0.87	0.40	77,77,77,77	0
55	MG	BA	3462	1/1	0.87	0.27	87,87,87,87	0
55	MG	BA	3248	1/1	0.87	0.23	53,53,53,53	0
55	MG	DA	3467	1/1	0.87	0.27	61,61,61,61	0
55	MG	BO	202	1/1	0.87	0.20	37,37,37,37	0
55	MG	DA	3361	1/1	0.87	0.42	79,79,79,79	0
55	MG	BA	3466	1/1	0.87	0.31	97,97,97,97	0
55	MG	DA	3212	1/1	0.87	0.35	48,48,48,48	0
55	MG	DA	3222	1/1	0.87	0.32	60,60,60,60	0
55	MG	DA	3224	1/1	0.87	0.35	66,66,66,66	0
55	MG	BA	3311	1/1	0.87	0.24	83,83,83,83	0
55	MG	CA	1789	1/1	0.87	0.36	71,71,71,71	0
55	MG	CA	1734	1/1	0.87	0.28	93,93,93,93	0
55	MG	BA	3361	1/1	0.87	0.26	64,64,64,64	0
55	MG	BA	3312	1/1	0.87	0.30	57,57,57,57	0
55	MG	BA	3523	1/1	0.87	0.51	70,70,70,70	0
55	MG	BA	3254	1/1	0.87	0.20	43,43,43,43	0
55	MG	BA	3005	1/1	0.87	0.31	43,43,43,43	0
55	MG	BA	3166	1/1	0.87	0.35	72,72,72,72	0
55	MG	DA	3066	1/1	0.87	0.27	65,65,65,65	0
55	MG	AA	1820	1/1	0.87	0.34	75,75,75,75	0
55	MG	CA	1804	1/1	0.87	0.25	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	BA	3038	1/1	0.87	0.22	56,56,56,56	0
55	MG	CA	1745	1/1	0.87	0.21	91,91,91,91	0
55	MG	BA	3273	1/1	0.87	0.34	94,94,94,94	0
55	MG	DA	3272	1/1	0.87	0.15	64,64,64,64	0
55	MG	BA	3122	1/1	0.87	0.19	37,37,37,37	0
55	MG	DA	3078	1/1	0.87	0.30	89,89,89,89	0
55	MG	BA	3595	1/1	0.87	0.18	65,65,65,65	0
55	MG	BA	3598	1/1	0.87	0.11	77,77,77,77	0
55	MG	BA	3600	1/1	0.87	0.25	66,66,66,66	0
55	MG	CB	102	1/1	0.87	0.16	87,87,87,87	0
55	MG	CA	1618	1/1	0.87	0.27	93,93,93,93	0
55	MG	CA	1754	1/1	0.87	0.28	86,86,86,86	0
55	MG	BA	3076	1/1	0.87	0.37	68,68,68,68	0
55	MG	BA	3607	1/1	0.87	0.24	96,96,96,96	0
55	MG	DA	3407	1/1	0.87	0.33	73,73,73,73	0
55	MG	BA	3384	1/1	0.87	0.26	73,73,73,73	0
55	MG	AA	1778	1/1	0.87	0.19	106,106,106,106	0
55	MG	DA	3298	1/1	0.87	0.30	77,77,77,77	0
55	MG	BA	3540	1/1	0.87	0.20	61,61,61,61	0
55	MG	BA	3387	1/1	0.87	0.33	73,73,73,73	0
55	MG	AA	1733	1/1	0.87	0.39	71,71,71,71	0
55	MG	CA	1705	1/1	0.87	0.32	80,80,80,80	0
55	MG	BA	3622	1/1	0.87	0.24	59,59,59,59	0
55	MG	AA	1734	1/1	0.87	0.14	96,96,96,96	0
55	MG	DA	3422	1/1	0.87	0.32	84,84,84,84	0
55	MG	DA	3425	1/1	0.87	0.24	81,81,81,81	0
55	MG	DA	3118	1/1	0.87	0.30	71,71,71,71	0
55	MG	AC	103	1/1	0.87	0.29	66,66,66,66	0
55	MG	BA	3549	1/1	0.87	0.26	68,68,68,68	0
55	MG	AA	1672	1/1	0.87	0.27	87,87,87,87	0
55	MG	DB	212	1/1	0.87	0.14	88,88,88,88	0
55	MG	BB	204	1/1	0.87	0.29	78,78,78,78	0
55	MG	BA	3225	1/1	0.87	0.19	65,65,65,65	0
55	MG	AA	1765	1/1	0.87	0.24	84,84,84,84	0
55	MG	BA	3555	1/1	0.87	0.14	38,38,38,38	0
55	MG	D1	202	1/1	0.87	0.20	89,89,89,89	0
55	MG	BA	3499	1/1	0.87	0.27	68,68,68,68	0
55	MG	DA	3034	1/1	0.88	0.26	62,62,62,62	0
55	MG	BA	3286	1/1	0.88	0.26	66,66,66,66	0
55	MG	BA	3287	1/1	0.88	0.31	62,62,62,62	0
55	MG	BA	3289	1/1	0.88	0.39	60,60,60,60	0
55	MG	BA	3474	1/1	0.88	0.30	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	DA	3156	1/1	0.88	0.36	48,48,48,48	0
55	MG	BA	3108	1/1	0.88	0.30	86,86,86,86	0
55	MG	BA	3109	1/1	0.88	0.22	70,70,70,70	0
55	MG	DA	3450	1/1	0.88	0.24	88,88,88,88	0
55	MG	AA	1812	1/1	0.88	0.28	73,73,73,73	0
55	MG	BA	3478	1/1	0.88	0.30	63,63,63,63	0
55	MG	DA	3347	1/1	0.88	0.09	75,75,75,75	0
55	MG	AA	1605	1/1	0.88	0.30	82,82,82,82	0
55	MG	BA	3480	1/1	0.88	0.35	50,50,50,50	0
55	MG	DA	3351	1/1	0.88	0.20	79,79,79,79	0
55	MG	BA	3016	1/1	0.88	0.36	39,39,39,39	0
55	MG	BA	3418	1/1	0.88	0.29	78,78,78,78	0
55	MG	CA	1646	1/1	0.88	0.31	76,76,76,76	0
55	MG	BB	207	1/1	0.88	0.20	83,83,83,83	0
55	MG	BA	3019	1/1	0.88	0.33	66,66,66,66	0
55	MG	DA	3218	1/1	0.88	0.29	62,62,62,62	0
55	MG	BA	3031	1/1	0.88	0.19	33,33,33,33	0
55	MG	AA	1835	1/1	0.88	0.26	87,87,87,87	0
55	MG	BA	3560	1/1	0.88	0.36	78,78,78,78	0
55	MG	BA	3227	1/1	0.88	0.35	91,91,91,91	0
55	MG	BA	3426	1/1	0.88	0.46	85,85,85,85	0
55	MG	BA	3078	1/1	0.88	0.33	65,65,65,65	0
55	MG	AC	101	1/1	0.88	0.23	53,53,53,53	0
55	MG	BA	3044	1/1	0.88	0.27	62,62,62,62	0
55	MG	DA	3248	1/1	0.88	0.36	75,75,75,75	0
55	MG	CA	1802	1/1	0.88	0.35	74,74,74,74	0
55	MG	BA	3246	1/1	0.88	0.33	68,68,68,68	0
55	MG	AA	1617	1/1	0.88	0.32	69,69,69,69	0
55	MG	AA	1726	1/1	0.88	0.28	81,81,81,81	0
55	MG	BA	3375	1/1	0.88	0.20	50,50,50,50	0
55	MG	DA	3263	1/1	0.88	0.71	82,82,82,82	0
55	MG	DA	3264	1/1	0.88	0.46	59,59,59,59	0
55	MG	DA	3074	1/1	0.88	0.20	70,70,70,70	0
55	MG	B2	201	1/1	0.88	0.31	85,85,85,85	0
55	MG	DA	3390	1/1	0.88	0.30	75,75,75,75	0
55	MG	BA	3575	1/1	0.88	0.24	71,71,71,71	0
55	MG	DA	3496	1/1	0.88	0.25	83,83,83,83	0
55	MG	B3	101	1/1	0.88	0.46	71,71,71,71	0
55	MG	DA	3271	1/1	0.88	0.36	58,58,58,58	0
55	MG	CA	1678	1/1	0.88	0.16	70,70,70,70	0
55	MG	CA	1680	1/1	0.88	0.37	68,68,68,68	0
55	MG	BA	3316	1/1	0.88	0.41	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	CA	1750	1/1	0.88	0.33	79,79,79,79	0
55	MG	BA	3579	1/1	0.88	0.19	92,92,92,92	0
55	MG	BA	3381	1/1	0.88	0.49	90,90,90,90	0
55	MG	DA	3506	1/1	0.88	0.23	78,78,78,78	0
55	MG	AA	1795	1/1	0.88	0.21	73,73,73,73	0
55	MG	BA	3256	1/1	0.88	0.33	61,61,61,61	0
55	MG	BA	3088	1/1	0.88	0.12	77,77,77,77	0
55	MG	DA	3510	1/1	0.88	0.28	85,85,85,85	0
55	MG	CA	1688	1/1	0.88	0.31	71,71,71,71	0
55	MG	AA	1601	1/1	0.88	0.27	56,56,56,56	0
55	MG	BA	3160	1/1	0.88	0.31	42,42,42,42	0
55	MG	CA	1692	1/1	0.88	0.34	82,82,82,82	0
55	MG	DA	3096	1/1	0.88	0.37	53,53,53,53	0
55	MG	DA	3300	1/1	0.88	0.21	81,81,81,81	0
55	MG	BA	3090	1/1	0.88	0.38	49,49,49,49	0
55	MG	DA	3008	1/1	0.88	0.27	70,70,70,70	0
55	MG	AA	1633	1/1	0.88	0.31	74,74,74,74	0
55	MG	AC	108	1/1	0.88	0.30	85,85,85,85	0
55	MG	BA	3522	1/1	0.88	0.37	82,82,82,82	0
55	MG	DB	205	1/1	0.88	0.24	69,69,69,69	0
55	MG	DA	3124	1/1	0.88	0.34	54,54,54,54	0
55	MG	BA	3335	1/1	0.88	0.25	58,58,58,58	0
55	MG	DA	3426	1/1	0.88	0.25	58,58,58,58	0
55	MG	BA	3336	1/1	0.88	0.34	66,66,66,66	0
55	MG	BA	3465	1/1	0.88	0.24	93,93,93,93	0
55	MG	DA	3022	1/1	0.88	0.33	60,60,60,60	0
55	MG	BA	3185	1/1	0.88	0.32	76,76,76,76	0
55	MG	DA	3326	1/1	0.88	0.28	70,70,70,70	0
55	MG	BA	3604	1/1	0.88	0.16	61,61,61,61	0
55	MG	BA	3105	1/1	0.88	0.23	75,75,75,75	0
55	MG	AA	1810	1/1	0.88	0.33	67,67,67,67	0
55	MG	BA	3609	1/1	0.88	0.37	70,70,70,70	0
55	MG	DA	3438	1/1	0.88	0.20	87,87,87,87	0
55	MG	AA	1764	1/1	0.89	0.16	79,79,79,79	0
55	MG	CA	1697	1/1	0.89	0.31	65,65,65,65	0
55	MG	DA	3029	1/1	0.89	0.33	79,79,79,79	0
55	MG	AA	1606	1/1	0.89	0.13	91,91,91,91	0
55	MG	DA	3032	1/1	0.89	0.15	76,76,76,76	0
55	MG	AA	1785	1/1	0.89	0.30	96,96,96,96	0
55	MG	DA	3447	1/1	0.89	0.20	82,82,82,82	0
55	MG	BA	3378	1/1	0.89	0.46	76,76,76,76	0
55	MG	BA	3512	1/1	0.89	0.25	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	AA	1766	1/1	0.89	0.14	79,79,79,79	0
55	MG	DA	3164	1/1	0.89	0.36	47,47,47,47	0
55	MG	DA	3452	1/1	0.89	0.20	83,83,83,83	0
55	MG	CA	1621	1/1	0.89	0.30	66,66,66,66	0
55	MG	DA	3168	1/1	0.89	0.23	49,49,49,49	0
55	MG	BA	3380	1/1	0.89	0.17	65,65,65,65	0
55	MG	BA	3517	1/1	0.89	0.41	70,70,70,70	0
55	MG	BA	3252	1/1	0.89	0.26	67,67,67,67	0
55	MG	BA	3318	1/1	0.89	0.41	75,75,75,75	0
55	MG	BA	3156	1/1	0.89	0.21	40,40,40,40	0
55	MG	DA	3198	1/1	0.89	0.22	47,47,47,47	0
55	MG	BA	3603	1/1	0.89	0.23	63,63,63,63	0
55	MG	BA	3323	1/1	0.89	0.28	66,66,66,66	0
55	MG	BA	3459	1/1	0.89	0.38	70,70,70,70	0
55	MG	AA	1808	1/1	0.89	0.35	76,76,76,76	0
55	MG	DA	3051	1/1	0.89	0.29	85,85,85,85	0
55	MG	DA	3470	1/1	0.89	0.18	80,80,80,80	0
55	MG	BA	3097	1/1	0.89	0.28	59,59,59,59	0
55	MG	BA	3526	1/1	0.89	0.29	86,86,86,86	0
55	MG	DA	3227	1/1	0.89	0.47	50,50,50,50	0
55	MG	DA	3365	1/1	0.89	0.37	58,58,58,58	0
55	MG	BA	3392	1/1	0.89	0.33	70,70,70,70	0
55	MG	BA	3528	1/1	0.89	0.31	76,76,76,76	0
55	MG	BA	3101	1/1	0.89	0.37	63,63,63,63	0
55	MG	BA	3464	1/1	0.89	0.31	77,77,77,77	0
55	MG	DA	3482	1/1	0.89	0.24	81,81,81,81	0
55	MG	CA	1642	1/1	0.89	0.22	91,91,91,91	0
55	MG	DA	3373	1/1	0.89	0.29	79,79,79,79	0
55	MG	AA	1610	1/1	0.89	0.32	51,51,51,51	0
55	MG	BA	3062	1/1	0.89	0.26	56,56,56,56	0
55	MG	BA	3187	1/1	0.89	0.45	73,73,73,73	0
55	MG	CA	1799	1/1	0.89	0.22	96,96,96,96	0
55	MG	AA	1657	1/1	0.89	0.26	50,50,50,50	0
55	MG	BA	3195	1/1	0.89	0.40	47,47,47,47	0
55	MG	AA	1604	1/1	0.89	0.26	67,67,67,67	0
55	MG	AA	1662	1/1	0.89	0.43	81,81,81,81	0
55	MG	BA	3285	1/1	0.89	0.29	72,72,72,72	0
55	MG	BA	3205	1/1	0.89	0.17	80,80,80,80	0
55	MG	BA	3206	1/1	0.89	0.32	75,75,75,75	0
55	MG	AA	1687	1/1	0.89	0.34	72,72,72,72	0
55	MG	CA	1739	1/1	0.89	0.47	75,75,75,75	0
55	MG	BA	3211	1/1	0.89	0.29	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	BA	3413	1/1	0.89	0.33	78,78,78,78	0
55	MG	AA	1815	1/1	0.89	0.48	84,84,84,84	0
55	MG	BA	3553	1/1	0.89	0.20	78,78,78,78	0
55	MG	AA	1816	1/1	0.89	0.24	81,81,81,81	0
55	MG	BA	3482	1/1	0.89	0.21	57,57,57,57	0
55	MG	BA	3561	1/1	0.89	0.20	74,74,74,74	0
55	MG	BA	3351	1/1	0.89	0.50	78,78,78,78	0
55	MG	CA	1675	1/1	0.89	0.29	62,62,62,62	0
55	MG	BA	3221	1/1	0.89	0.31	60,60,60,60	0
55	MG	BA	3357	1/1	0.89	0.36	81,81,81,81	0
55	MG	AA	1688	1/1	0.89	0.26	72,72,72,72	0
55	MG	DA	3003	1/1	0.89	0.20	64,64,64,64	0
55	MG	DA	3293	1/1	0.89	0.31	75,75,75,75	0
55	MG	DA	3295	1/1	0.89	0.33	50,50,50,50	0
55	MG	DA	3103	1/1	0.89	0.29	50,50,50,50	0
55	MG	DA	3521	1/1	0.89	0.27	69,69,69,69	0
55	MG	AA	1665	1/1	0.89	0.50	70,70,70,70	0
55	MG	DA	3523	1/1	0.89	0.34	81,81,81,81	0
55	MG	DA	3113	1/1	0.89	0.29	43,43,43,43	0
55	MG	DA	3116	1/1	0.89	0.27	74,74,74,74	0
55	MG	DA	3418	1/1	0.89	0.35	78,78,78,78	0
55	MG	AN	202	1/1	0.89	0.20	82,82,82,82	0
55	MG	BA	3026	1/1	0.89	0.20	47,47,47,47	0
55	MG	AA	1650	1/1	0.89	0.33	71,71,71,71	0
55	MG	CA	1602	1/1	0.89	0.28	80,80,80,80	0
55	MG	DA	3310	1/1	0.89	0.35	71,71,71,71	0
55	MG	BA	3229	1/1	0.89	0.11	50,50,50,50	0
55	MG	BA	3433	1/1	0.89	0.19	70,70,70,70	0
55	MG	BA	3435	1/1	0.89	0.22	65,65,65,65	0
55	MG	CA	1690	1/1	0.89	0.27	68,68,68,68	0
55	MG	BA	3310	1/1	0.89	0.23	57,57,57,57	0
55	MG	DA	3134	1/1	0.89	0.24	72,72,72,72	0
55	MG	BA	3501	1/1	0.89	0.18	55,55,55,55	0
55	MG	AA	1762	1/1	0.89	0.23	80,80,80,80	0
55	MG	AA	1779	1/1	0.89	0.36	72,72,72,72	0
55	MG	DA	3123	1/1	0.90	0.28	83,83,83,83	0
55	MG	BA	3118	1/1	0.90	0.27	61,61,61,61	0
55	MG	DA	3433	1/1	0.90	0.38	57,57,57,57	0
55	MG	BA	3558	1/1	0.90	0.12	63,63,63,63	0
55	MG	BA	3559	1/1	0.90	0.20	81,81,81,81	0
55	MG	CA	1670	1/1	0.90	0.37	56,56,56,56	0
55	MG	CA	1673	1/1	0.90	0.21	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	DA	3316	1/1	0.90	0.25	61,61,61,61	0
55	MG	DA	3131	1/1	0.90	0.31	79,79,79,79	0
55	MG	BE	304	1/1	0.90	0.19	80,80,80,80	0
55	MG	BA	3048	1/1	0.90	0.35	77,77,77,77	0
55	MG	DA	3137	1/1	0.90	0.25	82,82,82,82	0
55	MG	BA	3049	1/1	0.90	0.37	68,68,68,68	0
55	MG	DA	3023	1/1	0.90	0.23	57,57,57,57	0
55	MG	BA	3359	1/1	0.90	0.33	79,79,79,79	0
55	MG	BA	3423	1/1	0.90	0.29	61,61,61,61	0
55	MG	BA	3492	1/1	0.90	0.36	77,77,77,77	0
55	MG	DA	3027	1/1	0.90	0.16	77,77,77,77	0
55	MG	BA	3424	1/1	0.90	0.39	72,72,72,72	0
55	MG	BA	3131	1/1	0.90	0.24	59,59,59,59	0
55	MG	DA	3339	1/1	0.90	0.35	66,66,66,66	0
55	MG	AA	1675	1/1	0.90	0.24	80,80,80,80	0
55	MG	DA	3154	1/1	0.90	0.27	69,69,69,69	0
55	MG	AA	1653	1/1	0.90	0.41	81,81,81,81	0
55	MG	AA	1723	1/1	0.90	0.35	84,84,84,84	0
55	MG	BA	3136	1/1	0.90	0.12	74,74,74,74	0
55	MG	DA	3165	1/1	0.90	0.51	65,65,65,65	0
55	MG	BA	3574	1/1	0.90	0.36	78,78,78,78	0
55	MG	DA	3348	1/1	0.90	0.37	73,73,73,73	0
55	MG	CA	1605	1/1	0.90	0.43	76,76,76,76	0
55	MG	DA	3172	1/1	0.90	0.27	88,88,88,88	0
55	MG	BA	3057	1/1	0.90	0.11	70,70,70,70	0
55	MG	DA	3352	1/1	0.90	0.29	64,64,64,64	0
55	MG	AA	1654	1/1	0.90	0.32	75,75,75,75	0
55	MG	BA	3142	1/1	0.90	0.24	51,51,51,51	0
55	MG	DA	3192	1/1	0.90	0.32	62,62,62,62	0
55	MG	CA	1695	1/1	0.90	0.45	87,87,87,87	0
55	MG	DA	3196	1/1	0.90	0.29	50,50,50,50	0
55	MG	BA	3439	1/1	0.90	0.32	71,71,71,71	0
55	MG	BA	3581	1/1	0.90	0.33	69,69,69,69	0
55	MG	AA	1841	1/1	0.90	0.29	59,59,59,59	0
55	MG	DA	3480	1/1	0.90	0.20	63,63,63,63	0
55	MG	BA	3370	1/1	0.90	0.27	56,56,56,56	0
55	MG	AA	1628	1/1	0.90	0.44	69,69,69,69	0
55	MG	AA	1680	1/1	0.90	0.25	80,80,80,80	0
55	MG	BA	3376	1/1	0.90	0.29	73,73,73,73	0
55	MG	BA	3587	1/1	0.90	0.18	64,64,64,64	0
55	MG	BA	3149	1/1	0.90	0.27	80,80,80,80	0
55	MG	BA	3242	1/1	0.90	0.25	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	BA	3244	1/1	0.90	0.21	58,58,58,58	0
55	MG	BA	3067	1/1	0.90	0.15	48,48,48,48	0
55	MG	BA	3102	1/1	0.90	0.25	66,66,66,66	0
55	MG	AA	1667	1/1	0.90	0.27	68,68,68,68	0
55	MG	BA	3251	1/1	0.90	0.34	68,68,68,68	0
55	MG	AA	1646	1/1	0.90	0.25	67,67,67,67	0
55	MG	BA	3253	1/1	0.90	0.17	51,51,51,51	0
55	MG	CA	1795	1/1	0.90	0.21	76,76,76,76	0
55	MG	AA	1669	1/1	0.90	0.34	68,68,68,68	0
55	MG	DA	3382	1/1	0.90	0.33	78,78,78,78	0
55	MG	AA	1670	1/1	0.90	0.32	63,63,63,63	0
55	MG	DA	3386	1/1	0.90	0.32	61,61,61,61	0
55	MG	BA	3169	1/1	0.90	0.39	63,63,63,63	0
55	MG	DA	3389	1/1	0.90	0.34	64,64,64,64	0
55	MG	BA	3258	1/1	0.90	0.23	45,45,45,45	0
55	MG	BA	3170	1/1	0.90	0.36	55,55,55,55	0
55	MG	BA	3531	1/1	0.90	0.15	53,53,53,53	0
55	MG	BA	3182	1/1	0.90	0.17	43,43,43,43	0
55	MG	CA	1641	1/1	0.90	0.30	66,66,66,66	0
55	MG	BA	3269	1/1	0.90	0.30	61,61,61,61	0
55	MG	BA	3620	1/1	0.90	0.29	68,68,68,68	0
55	MG	AA	1774	1/1	0.90	0.16	91,91,91,91	0
55	MG	AA	1642	1/1	0.90	0.48	72,72,72,72	0
55	MG	CA	1647	1/1	0.90	0.35	61,61,61,61	0
55	MG	DA	3274	1/1	0.90	0.27	87,87,87,87	0
55	MG	CA	1731	1/1	0.90	0.51	72,72,72,72	0
55	MG	BA	3536	1/1	0.90	0.26	73,73,73,73	0
55	MG	CA	1649	1/1	0.90	0.21	64,64,64,64	0
55	MG	BA	3112	1/1	0.90	0.21	77,77,77,77	0
55	MG	CA	1653	1/1	0.90	0.15	77,77,77,77	0
55	MG	BA	3194	1/1	0.90	0.30	68,68,68,68	0
55	MG	DA	3411	1/1	0.90	0.12	70,70,70,70	0
55	MG	BA	3407	1/1	0.90	0.09	59,59,59,59	0
55	MG	BA	3543	1/1	0.90	0.29	80,80,80,80	0
55	MG	BA	3277	1/1	0.90	0.40	86,86,86,86	0
55	MG	BA	3113	1/1	0.90	0.33	57,57,57,57	0
55	MG	DA	3104	1/1	0.90	0.28	43,43,43,43	0
55	MG	BA	3197	1/1	0.90	0.39	46,46,46,46	0
55	MG	DA	3001	1/1	0.90	0.27	67,67,67,67	0
55	MG	BA	3114	1/1	0.90	0.18	74,74,74,74	0
55	MG	AA	1759	1/1	0.90	0.21	77,77,77,77	0
55	MG	DA	3301	1/1	0.90	0.25	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	BA	3350	1/1	0.90	0.28	55,55,55,55	0
55	MG	DR	201	1/1	0.90	0.14	71,71,71,71	0
55	MG	BA	3416	1/1	0.90	0.20	87,87,87,87	0
55	MG	AA	1651	1/1	0.90	0.45	71,71,71,71	0
55	MG	DA	3307	1/1	0.90	0.27	77,77,77,77	0
55	MG	BA	3267	1/1	0.91	0.17	61,61,61,61	0
55	MG	BA	3268	1/1	0.91	0.41	67,67,67,67	0
55	MG	AA	1705	1/1	0.91	0.28	83,83,83,83	0
55	MG	BA	3070	1/1	0.91	0.13	63,63,63,63	0
55	MG	DA	3194	1/1	0.91	0.34	73,73,73,73	0
55	MG	BA	3168	1/1	0.91	0.25	49,49,49,49	0
55	MG	CC	102	1/1	0.91	0.27	73,73,73,73	0
55	MG	BA	3098	1/1	0.91	0.14	48,48,48,48	0
55	MG	BA	3516	1/1	0.91	0.34	78,78,78,78	0
55	MG	BA	3319	1/1	0.91	0.27	65,65,65,65	0
55	MG	BA	3320	1/1	0.91	0.24	62,62,62,62	0
55	MG	DA	3346	1/1	0.91	0.33	75,75,75,75	0
55	MG	AA	1660	1/1	0.91	0.33	53,53,53,53	0
55	MG	DA	3214	1/1	0.91	0.18	40,40,40,40	0
55	MG	DA	3216	1/1	0.91	0.16	49,49,49,49	0
55	MG	CA	1634	1/1	0.91	0.35	77,77,77,77	0
55	MG	BA	3176	1/1	0.91	0.31	48,48,48,48	0
55	MG	CA	1636	1/1	0.91	0.29	78,78,78,78	0
55	MG	BA	3471	1/1	0.91	0.24	72,72,72,72	0
55	MG	AA	1773	1/1	0.91	0.25	87,87,87,87	0
55	MG	BB	212	1/1	0.91	0.31	81,81,81,81	0
55	MG	DA	3087	1/1	0.91	0.30	63,63,63,63	0
55	MG	BA	3236	1/1	0.91	0.30	52,52,52,52	0
55	MG	BA	3372	1/1	0.91	0.16	73,73,73,73	0
55	MG	DA	3239	1/1	0.91	0.23	45,45,45,45	0
55	MG	DA	3011	1/1	0.91	0.13	65,65,65,65	0
55	MG	DA	3246	1/1	0.91	0.34	53,53,53,53	0
55	MG	BA	3051	1/1	0.91	0.21	74,74,74,74	0
55	MG	BA	3135	1/1	0.91	0.37	72,72,72,72	0
55	MG	DA	3016	1/1	0.91	0.33	78,78,78,78	0
55	MG	DA	3017	1/1	0.91	0.31	75,75,75,75	0
55	MG	BA	3240	1/1	0.91	0.43	88,88,88,88	0
55	MG	BA	3333	1/1	0.91	0.34	80,80,80,80	0
55	MG	DA	3370	1/1	0.91	0.14	67,67,67,67	0
55	MG	BE	302	1/1	0.91	0.21	56,56,56,56	0
55	MG	DA	3106	1/1	0.91	0.28	48,48,48,48	0
55	MG	DA	3265	1/1	0.91	0.23	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	DA	3107	1/1	0.91	0.25	53,53,53,53	0
55	MG	DA	3267	1/1	0.91	0.25	64,64,64,64	0
55	MG	DA	3110	1/1	0.91	0.29	58,58,58,58	0
55	MG	BA	3430	1/1	0.91	0.18	57,57,57,57	0
55	MG	BA	3288	1/1	0.91	0.34	76,76,76,76	0
55	MG	BF	302	1/1	0.91	0.11	72,72,72,72	0
55	MG	AA	1783	1/1	0.91	0.42	67,67,67,67	0
55	MG	BA	3193	1/1	0.91	0.32	85,85,85,85	0
55	MG	DA	3384	1/1	0.91	0.31	65,65,65,65	0
55	MG	CA	1779	1/1	0.91	0.22	72,72,72,72	0
55	MG	BA	3001	1/1	0.91	0.34	47,47,47,47	0
55	MG	BA	3338	1/1	0.91	0.16	71,71,71,71	0
55	MG	BA	3590	1/1	0.91	0.30	63,63,63,63	0
55	MG	AA	1629	1/1	0.91	0.17	86,86,86,86	0
55	MG	B7	101	1/1	0.91	0.33	67,67,67,67	0
55	MG	AA	1634	1/1	0.91	0.29	62,62,62,62	0
55	MG	BA	3058	1/1	0.91	0.18	62,62,62,62	0
55	MG	DA	3286	1/1	0.91	0.08	47,47,47,47	0
55	MG	DA	3504	1/1	0.91	0.23	65,65,65,65	0
55	MG	DA	3287	1/1	0.91	0.36	65,65,65,65	0
55	MG	BA	3299	1/1	0.91	0.40	89,89,89,89	0
55	MG	BA	3111	1/1	0.91	0.27	59,59,59,59	0
55	MG	DA	3291	1/1	0.91	0.36	65,65,65,65	0
55	MG	AA	1839	1/1	0.91	0.32	74,74,74,74	0
55	MG	AA	1631	1/1	0.91	0.18	66,66,66,66	0
55	MG	CA	1666	1/1	0.91	0.29	71,71,71,71	0
55	MG	AA	1788	1/1	0.91	0.42	77,77,77,77	0
55	MG	DA	3514	1/1	0.91	0.29	59,59,59,59	0
55	MG	BA	3305	1/1	0.91	0.38	70,70,70,70	0
55	MG	BA	3152	1/1	0.91	0.32	40,40,40,40	0
55	MG	AA	1712	1/1	0.91	0.28	78,78,78,78	0
55	MG	BA	3456	1/1	0.91	0.33	78,78,78,78	0
55	MG	BA	3611	1/1	0.91	0.30	87,87,87,87	0
55	MG	BA	3035	1/1	0.91	0.17	37,37,37,37	0
55	MG	DA	3305	1/1	0.91	0.28	77,77,77,77	0
55	MG	DA	3052	1/1	0.91	0.40	71,71,71,71	0
55	MG	DA	3053	1/1	0.91	0.36	62,62,62,62	0
55	MG	DA	3155	1/1	0.91	0.24	46,46,46,46	0
55	MG	CA	1679	1/1	0.91	0.38	85,85,85,85	0
55	MG	DA	3157	1/1	0.91	0.31	47,47,47,47	0
55	MG	DA	3421	1/1	0.91	0.21	62,62,62,62	0
55	MG	DA	3160	1/1	0.91	0.19	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	BA	3614	1/1	0.91	0.12	69,69,69,69	0
55	MG	BA	3405	1/1	0.91	0.32	56,56,56,56	0
55	MG	BA	3617	1/1	0.91	0.42	71,71,71,71	0
55	MG	CA	1683	1/1	0.91	0.35	87,87,87,87	0
55	MG	BA	3557	1/1	0.91	0.28	77,77,77,77	0
55	MG	CA	1619	1/1	0.91	0.26	61,61,61,61	0
55	MG	DA	3173	1/1	0.91	0.19	60,60,60,60	0
55	MG	DE	301	1/1	0.91	0.23	41,41,41,41	0
55	MG	DA	3175	1/1	0.91	0.38	83,83,83,83	0
55	MG	DA	3331	1/1	0.91	0.34	50,50,50,50	0
55	MG	AA	1658	1/1	0.91	0.32	49,49,49,49	0
55	MG	DA	3181	1/1	0.91	0.32	50,50,50,50	0
55	MG	DA	3334	1/1	0.91	0.16	68,68,68,68	0
55	MG	BA	3129	1/1	0.92	0.34	52,52,52,52	0
55	MG	BA	3331	1/1	0.92	0.21	65,65,65,65	0
55	MG	BA	3332	1/1	0.92	0.19	61,61,61,61	0
55	MG	DA	3311	1/1	0.92	0.30	73,73,73,73	0
55	MG	BA	3130	1/1	0.92	0.29	44,44,44,44	0
55	MG	BA	3616	1/1	0.92	0.19	58,58,58,58	0
55	MG	DA	3314	1/1	0.92	0.33	76,76,76,76	0
55	MG	BA	3056	1/1	0.92	0.18	54,54,54,54	0
55	MG	DA	3166	1/1	0.92	0.32	58,58,58,58	0
55	MG	DA	3318	1/1	0.92	0.18	63,63,63,63	0
55	MG	BA	3002	1/1	0.92	0.27	43,43,43,43	0
55	MG	AA	1701	1/1	0.92	0.18	70,70,70,70	0
55	MG	BA	3006	1/1	0.92	0.25	38,38,38,38	0
55	MG	BA	3095	1/1	0.92	0.25	37,37,37,37	0
55	MG	DA	3174	1/1	0.92	0.28	44,44,44,44	0
55	MG	CA	1793	1/1	0.92	0.30	91,91,91,91	0
55	MG	BA	3096	1/1	0.92	0.34	56,56,56,56	0
55	MG	BA	3008	1/1	0.92	0.31	37,37,37,37	0
55	MG	DA	3446	1/1	0.92	0.36	75,75,75,75	0
55	MG	BA	3281	1/1	0.92	0.34	72,72,72,72	0
55	MG	DA	3184	1/1	0.92	0.44	61,61,61,61	0
55	MG	BA	3209	1/1	0.92	0.25	39,39,39,39	0
55	MG	DA	3186	1/1	0.92	0.24	60,60,60,60	0
55	MG	DA	3189	1/1	0.92	0.26	41,41,41,41	0
55	MG	BA	3284	1/1	0.92	0.34	56,56,56,56	0
55	MG	CA	1721	1/1	0.92	0.24	80,80,80,80	0
55	MG	BA	3015	1/1	0.92	0.21	38,38,38,38	0
55	MG	AA	1829	1/1	0.92	0.35	77,77,77,77	0
55	MG	BA	3066	1/1	0.92	0.30	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	DA	3457	1/1	0.92	0.33	65,65,65,65	0
55	MG	BA	3483	1/1	0.92	0.25	68,68,68,68	0
55	MG	BA	3556	1/1	0.92	0.33	58,58,58,58	0
55	MG	DA	3460	1/1	0.92	0.37	72,72,72,72	0
55	MG	CA	1652	1/1	0.92	0.27	71,71,71,71	0
55	MG	BA	3144	1/1	0.92	0.24	48,48,48,48	0
55	MG	AA	1619	1/1	0.92	0.25	63,63,63,63	0
55	MG	DA	3465	1/1	0.92	0.24	74,74,74,74	0
55	MG	AA	1741	1/1	0.92	0.27	67,67,67,67	0
55	MG	DA	3215	1/1	0.92	0.26	42,42,42,42	0
55	MG	DA	3079	1/1	0.92	0.29	54,54,54,54	0
55	MG	CA	1733	1/1	0.92	0.36	69,69,69,69	0
55	MG	DA	3220	1/1	0.92	0.31	66,66,66,66	0
55	MG	BA	3421	1/1	0.92	0.24	62,62,62,62	0
55	MG	DA	3472	1/1	0.92	0.38	71,71,71,71	0
55	MG	BA	3147	1/1	0.92	0.13	55,55,55,55	0
55	MG	DA	3225	1/1	0.92	0.41	73,73,73,73	0
55	MG	DA	3226	1/1	0.92	0.30	62,62,62,62	0
55	MG	BA	3148	1/1	0.92	0.17	32,32,32,32	0
55	MG	AA	1602	1/1	0.92	0.21	79,79,79,79	0
55	MG	DA	3359	1/1	0.92	0.31	76,76,76,76	0
55	MG	AA	1704	1/1	0.92	0.11	83,83,83,83	0
55	MG	BA	3494	1/1	0.92	0.45	76,76,76,76	0
55	MG	DA	3234	1/1	0.92	0.28	52,52,52,52	0
55	MG	DA	3235	1/1	0.92	0.27	48,48,48,48	0
55	MG	BA	3297	1/1	0.92	0.22	58,58,58,58	0
55	MG	BA	3429	1/1	0.92	0.09	75,75,75,75	0
55	MG	AA	1697	1/1	0.92	0.23	84,84,84,84	0
55	MG	BA	3153	1/1	0.92	0.28	52,52,52,52	0
55	MG	DA	3488	1/1	0.92	0.25	86,86,86,86	0
55	MG	BA	3572	1/1	0.92	0.26	87,87,87,87	0
55	MG	DA	3247	1/1	0.92	0.17	87,87,87,87	0
55	MG	BA	3234	1/1	0.92	0.36	86,86,86,86	0
55	MG	DA	3372	1/1	0.92	0.28	65,65,65,65	0
55	MG	BA	3235	1/1	0.92	0.29	54,54,54,54	0
55	MG	BA	3503	1/1	0.92	0.18	65,65,65,65	0
55	MG	BA	3155	1/1	0.92	0.08	45,45,45,45	0
55	MG	DA	3100	1/1	0.92	0.28	44,44,44,44	0
55	MG	BA	3578	1/1	0.92	0.34	81,81,81,81	0
55	MG	DA	3262	1/1	0.92	0.42	48,48,48,48	0
55	MG	AA	1821	1/1	0.92	0.31	75,75,75,75	0
55	MG	BA	3308	1/1	0.92	0.23	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	AA	1837	1/1	0.92	0.28	73,73,73,73	0
55	MG	DA	3108	1/1	0.92	0.22	54,54,54,54	0
55	MG	DA	3109	1/1	0.92	0.22	65,65,65,65	0
55	MG	DA	3012	1/1	0.92	0.39	66,66,66,66	0
55	MG	DA	3013	1/1	0.92	0.37	56,56,56,56	0
55	MG	DA	3388	1/1	0.92	0.19	74,74,74,74	0
55	MG	BA	3440	1/1	0.92	0.36	74,74,74,74	0
55	MG	BA	3045	1/1	0.92	0.25	45,45,45,45	0
55	MG	DA	3391	1/1	0.92	0.16	78,78,78,78	0
55	MG	DA	3512	1/1	0.92	0.34	75,75,75,75	0
55	MG	BA	3442	1/1	0.92	0.25	76,76,76,76	0
55	MG	AA	1644	1/1	0.92	0.14	62,62,62,62	0
55	MG	AA	1780	1/1	0.92	0.17	86,86,86,86	0
55	MG	BA	3245	1/1	0.92	0.44	49,49,49,49	0
55	MG	DA	3121	1/1	0.92	0.20	64,64,64,64	0
55	MG	AA	1603	1/1	0.92	0.26	63,63,63,63	0
55	MG	BA	3052	1/1	0.92	0.17	64,64,64,64	0
55	MG	BA	3117	1/1	0.92	0.39	60,60,60,60	0
55	MG	BA	3249	1/1	0.92	0.13	30,30,30,30	0
55	MG	BA	3173	1/1	0.92	0.33	52,52,52,52	0
55	MG	DA	3285	1/1	0.92	0.19	50,50,50,50	0
55	MG	CA	1615	1/1	0.92	0.23	81,81,81,81	0
55	MG	DA	3526	1/1	0.92	0.32	68,68,68,68	0
55	MG	BA	3174	1/1	0.92	0.51	71,71,71,71	0
55	MG	AA	1717	1/1	0.92	0.33	74,74,74,74	0
55	MG	BA	3179	1/1	0.92	0.38	64,64,64,64	0
55	MG	DA	3030	1/1	0.92	0.24	74,74,74,74	0
55	MG	BA	3181	1/1	0.92	0.24	39,39,39,39	0
55	MG	CA	1620	1/1	0.92	0.36	64,64,64,64	0
55	MG	BA	3601	1/1	0.92	0.25	85,85,85,85	0
55	MG	BA	3602	1/1	0.92	0.27	67,67,67,67	0
55	MG	DA	3145	1/1	0.92	0.36	60,60,60,60	0
55	MG	AA	1796	1/1	0.92	0.23	75,75,75,75	0
55	MG	CA	1700	1/1	0.92	0.33	77,77,77,77	0
55	MG	CA	1701	1/1	0.92	0.43	88,88,88,88	0
55	MG	BA	3184	1/1	0.92	0.12	39,39,39,39	0
55	MG	DE	303	1/1	0.92	0.33	56,56,56,56	0
55	MG	AA	1709	1/1	0.92	0.24	70,70,70,70	0
55	MG	BA	3395	1/1	0.92	0.15	72,72,72,72	0
55	MG	DA	3424	1/1	0.92	0.34	70,70,70,70	0
55	MG	BA	3128	1/1	0.92	0.36	46,46,46,46	0
55	MG	D3	101	1/1	0.92	0.30	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	ZN	AQ	102	1/1	0.92	0.15	122,122,122,122	0
55	MG	BA	3329	1/1	0.93	0.31	65,65,65,65	0
55	MG	DA	3076	1/1	0.93	0.25	86,86,86,86	0
55	MG	BA	3033	1/1	0.93	0.25	38,38,38,38	0
55	MG	BA	3003	1/1	0.93	0.28	47,47,47,47	0
55	MG	BA	3188	1/1	0.93	0.29	60,60,60,60	0
55	MG	BA	3189	1/1	0.93	0.33	49,49,49,49	0
55	MG	BA	3589	1/1	0.93	0.18	41,41,41,41	0
55	MG	DA	3169	1/1	0.93	0.23	69,69,69,69	0
55	MG	DA	3280	1/1	0.93	0.31	46,46,46,46	0
55	MG	BA	3190	1/1	0.93	0.25	63,63,63,63	0
55	MG	BA	3063	1/1	0.93	0.07	43,43,43,43	0
55	MG	BA	3294	1/1	0.93	0.27	72,72,72,72	0
55	MG	DA	3284	1/1	0.93	0.25	56,56,56,56	0
55	MG	BA	3434	1/1	0.93	0.34	75,75,75,75	0
55	MG	DA	3176	1/1	0.93	0.35	65,65,65,65	0
55	MG	BA	3386	1/1	0.93	0.28	59,59,59,59	0
55	MG	AA	1771	1/1	0.93	0.07	70,70,70,70	0
55	MG	BA	3296	1/1	0.93	0.26	53,53,53,53	0
55	MG	BA	3120	1/1	0.93	0.26	56,56,56,56	0
55	MG	DA	3385	1/1	0.93	0.40	62,62,62,62	0
55	MG	BA	3040	1/1	0.93	0.31	54,54,54,54	0
55	MG	BA	3545	1/1	0.93	0.20	69,69,69,69	0
55	MG	DA	3187	1/1	0.93	0.22	42,42,42,42	0
55	MG	BA	3126	1/1	0.93	0.33	46,46,46,46	0
55	MG	DA	3191	1/1	0.93	0.27	46,46,46,46	0
55	MG	BA	3154	1/1	0.93	0.21	55,55,55,55	0
55	MG	DA	3095	1/1	0.93	0.25	49,49,49,49	0
55	MG	BA	3043	1/1	0.93	0.14	32,32,32,32	0
55	MG	AA	1784	1/1	0.93	0.40	66,66,66,66	0
55	MG	CA	1728	1/1	0.93	0.33	69,69,69,69	0
55	MG	BA	3159	1/1	0.93	0.31	58,58,58,58	0
55	MG	DA	3202	1/1	0.93	0.31	47,47,47,47	0
55	MG	DA	3205	1/1	0.93	0.26	67,67,67,67	0
55	MG	BA	3398	1/1	0.93	0.30	70,70,70,70	0
55	MG	CA	1672	1/1	0.93	0.30	75,75,75,75	0
55	MG	BA	3497	1/1	0.93	0.28	71,71,71,71	0
55	MG	DA	3210	1/1	0.93	0.29	63,63,63,63	0
55	MG	DA	3404	1/1	0.93	0.14	61,61,61,61	0
55	MG	AA	1645	1/1	0.93	0.34	50,50,50,50	0
55	MG	CA	1794	1/1	0.93	0.29	74,74,74,74	0
55	MG	BA	3163	1/1	0.93	0.39	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	BA	3453	1/1	0.93	0.36	60,60,60,60	0
55	MG	DA	3317	1/1	0.93	0.16	81,81,81,81	0
55	MG	BA	3010	1/1	0.93	0.30	46,46,46,46	0
55	MG	BA	3502	1/1	0.93	0.22	67,67,67,67	0
55	MG	DA	3221	1/1	0.93	0.47	63,63,63,63	0
55	MG	BA	3014	1/1	0.93	0.33	53,53,53,53	0
55	MG	DA	3324	1/1	0.93	0.29	78,78,78,78	0
55	MG	BA	3356	1/1	0.93	0.35	70,70,70,70	0
55	MG	AA	1664	1/1	0.93	0.10	45,45,45,45	0
55	MG	DA	3328	1/1	0.93	0.22	47,47,47,47	0
55	MG	CA	1623	1/1	0.93	0.15	90,90,90,90	0
55	MG	AA	1632	1/1	0.93	0.22	67,67,67,67	0
55	MG	DA	3046	1/1	0.93	0.20	65,65,65,65	0
55	MG	DA	3229	1/1	0.93	0.42	62,62,62,62	0
55	MG	AA	1622	1/1	0.93	0.23	76,76,76,76	0
55	MG	BA	3024	1/1	0.93	0.22	27,27,27,27	0
55	MG	DA	3232	1/1	0.93	0.30	44,44,44,44	0
55	MG	A1	101	1/1	0.93	0.15	66,66,66,66	0
55	MG	BA	3567	1/1	0.93	0.33	80,80,80,80	0
55	MG	BA	3028	1/1	0.93	0.34	46,46,46,46	0
55	MG	BA	3081	1/1	0.93	0.31	75,75,75,75	0
55	MG	BA	3177	1/1	0.93	0.31	57,57,57,57	0
55	MG	BA	3515	1/1	0.93	0.22	72,72,72,72	0
55	MG	DA	3244	1/1	0.93	0.39	71,71,71,71	0
55	MG	DB	201	1/1	0.93	0.33	81,81,81,81	0
55	MG	BA	3365	1/1	0.93	0.16	50,50,50,50	0
55	MG	BB	210	1/1	0.93	0.35	64,64,64,64	0
55	MG	BA	3082	1/1	0.93	0.33	64,64,64,64	0
55	MG	BA	3180	1/1	0.93	0.24	37,37,37,37	0
55	MG	CC	103	1/1	0.93	0.38	72,72,72,72	0
55	MG	BA	3283	1/1	0.93	0.26	49,49,49,49	0
55	MG	DA	3147	1/1	0.93	0.27	53,53,53,53	0
55	MG	DA	3255	1/1	0.93	0.21	75,75,75,75	0
55	MG	DA	3256	1/1	0.93	0.24	49,49,49,49	0
55	MG	BA	3520	1/1	0.93	0.31	44,44,44,44	0
55	MG	DA	3261	1/1	0.93	0.29	58,58,58,58	0
55	MG	DA	3149	1/1	0.93	0.36	57,57,57,57	0
55	MG	BA	3469	1/1	0.93	0.24	60,60,60,60	0
55	MG	BA	3030	1/1	0.93	0.33	44,44,44,44	0
55	MG	AA	1699	1/1	0.93	0.20	64,64,64,64	0
55	MG	CA	1643	1/1	0.93	0.29	82,82,82,82	0
55	MG	BA	3183	1/1	0.93	0.13	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	AA	1799	1/1	0.93	0.36	78,78,78,78	0
55	MG	BA	3373	1/1	0.93	0.32	64,64,64,64	0
55	MG	DA	3158	1/1	0.93	0.36	44,44,44,44	0
55	MG	BA	3326	1/1	0.94	0.24	52,52,52,52	0
55	MG	BA	3100	1/1	0.94	0.27	42,42,42,42	0
55	MG	BA	3039	1/1	0.94	0.21	42,42,42,42	0
55	MG	AA	1806	1/1	0.94	0.23	81,81,81,81	0
55	MG	DA	3360	1/1	0.94	0.21	65,65,65,65	0
55	MG	BA	3279	1/1	0.94	0.13	70,70,70,70	0
55	MG	BA	3041	1/1	0.94	0.23	46,46,46,46	0
55	MG	BA	3175	1/1	0.94	0.12	69,69,69,69	0
55	MG	DA	3069	1/1	0.94	0.31	60,60,60,60	0
55	MG	AA	1745	1/1	0.94	0.41	67,67,67,67	0
55	MG	DA	3071	1/1	0.94	0.19	81,81,81,81	0
55	MG	DA	3463	1/1	0.94	0.16	73,73,73,73	0
55	MG	AA	1800	1/1	0.94	0.39	82,82,82,82	0
55	MG	BA	3139	1/1	0.94	0.25	35,35,35,35	0
55	MG	BA	3107	1/1	0.94	0.27	36,36,36,36	0
55	MG	CA	1631	1/1	0.94	0.13	81,81,81,81	0
55	MG	BA	3564	1/1	0.94	0.28	84,84,84,84	0
55	MG	DA	3170	1/1	0.94	0.41	68,68,68,68	0
55	MG	BA	3233	1/1	0.94	0.22	48,48,48,48	0
55	MG	BA	3141	1/1	0.94	0.27	35,35,35,35	0
55	MG	AA	1652	1/1	0.94	0.35	81,81,81,81	0
55	MG	BA	3018	1/1	0.94	0.26	54,54,54,54	0
55	MG	DA	3006	1/1	0.94	0.25	71,71,71,71	0
55	MG	DA	3178	1/1	0.94	0.32	59,59,59,59	0
55	MG	AA	1763	1/1	0.94	0.32	53,53,53,53	0
55	MG	BA	3050	1/1	0.94	0.26	39,39,39,39	0
55	MG	BA	3020	1/1	0.94	0.35	41,41,41,41	0
55	MG	BA	3344	1/1	0.94	0.26	55,55,55,55	0
55	MG	BA	3021	1/1	0.94	0.32	41,41,41,41	0
55	MG	DA	3288	1/1	0.94	0.22	47,47,47,47	0
55	MG	BA	3346	1/1	0.94	0.16	51,51,51,51	0
55	MG	BA	3022	1/1	0.94	0.27	30,30,30,30	0
55	MG	A1	102	1/1	0.94	0.31	86,86,86,86	0
55	MG	BA	3025	1/1	0.94	0.23	42,42,42,42	0
55	MG	AA	1811	1/1	0.94	0.34	67,67,67,67	0
55	MG	BA	3409	1/1	0.94	0.14	68,68,68,68	0
55	MG	DA	3489	1/1	0.94	0.10	71,71,71,71	0
55	MG	DA	3296	1/1	0.94	0.41	51,51,51,51	0
55	MG	BA	3352	1/1	0.94	0.29	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	DA	3195	1/1	0.94	0.32	70,70,70,70	0
55	MG	AA	1722	1/1	0.94	0.36	68,68,68,68	0
55	MG	DA	3021	1/1	0.94	0.25	51,51,51,51	0
55	MG	DA	3098	1/1	0.94	0.16	68,68,68,68	0
55	MG	DA	3099	1/1	0.94	0.14	40,40,40,40	0
55	MG	DA	3203	1/1	0.94	0.14	48,48,48,48	0
55	MG	DA	3204	1/1	0.94	0.23	51,51,51,51	0
55	MG	CA	1776	1/1	0.94	0.34	71,71,71,71	0
55	MG	DA	3102	1/1	0.94	0.23	51,51,51,51	0
55	MG	CA	1650	1/1	0.94	0.21	102,102,102,102	0
55	MG	BA	3029	1/1	0.94	0.30	35,35,35,35	0
55	MG	BA	3250	1/1	0.94	0.19	60,60,60,60	0
55	MG	BA	3121	1/1	0.94	0.26	57,57,57,57	0
55	MG	DA	3408	1/1	0.94	0.09	73,73,73,73	0
55	MG	DA	3213	1/1	0.94	0.24	41,41,41,41	0
55	MG	BA	3199	1/1	0.94	0.23	49,49,49,49	0
55	MG	BA	3201	1/1	0.94	0.47	66,66,66,66	0
55	MG	BU	201	1/1	0.94	0.22	81,81,81,81	0
55	MG	BA	3202	1/1	0.94	0.22	51,51,51,51	0
55	MG	BA	3255	1/1	0.94	0.22	46,46,46,46	0
55	MG	AG	301	1/1	0.94	0.39	81,81,81,81	0
55	MG	DA	3033	1/1	0.94	0.18	62,62,62,62	0
55	MG	DA	3223	1/1	0.94	0.25	52,52,52,52	0
55	MG	BA	3125	1/1	0.94	0.45	52,52,52,52	0
55	MG	BA	3004	1/1	0.94	0.28	35,35,35,35	0
55	MG	BA	3259	1/1	0.94	0.14	40,40,40,40	0
55	MG	CA	1726	1/1	0.94	0.50	75,75,75,75	0
55	MG	DA	3520	1/1	0.94	0.35	76,76,76,76	0
55	MG	BA	3260	1/1	0.94	0.25	47,47,47,47	0
55	MG	CA	1792	1/1	0.94	0.31	70,70,70,70	0
55	MG	AA	1627	1/1	0.94	0.27	53,53,53,53	0
55	MG	BA	3597	1/1	0.94	0.26	79,79,79,79	0
55	MG	BA	3207	1/1	0.94	0.31	41,41,41,41	0
55	MG	BA	3599	1/1	0.94	0.34	69,69,69,69	0
55	MG	DA	3130	1/1	0.94	0.13	60,60,60,60	0
55	MG	DA	3431	1/1	0.94	0.39	91,91,91,91	0
55	MG	DB	203	1/1	0.94	0.26	66,66,66,66	0
55	MG	BA	3428	1/1	0.94	0.33	68,68,68,68	0
55	MG	BA	3208	1/1	0.94	0.07	45,45,45,45	0
55	MG	AN	201	1/1	0.94	0.16	68,68,68,68	0
55	MG	DA	3240	1/1	0.94	0.31	42,42,42,42	0
55	MG	BA	3544	1/1	0.94	0.24	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	BA	3007	1/1	0.94	0.41	53,53,53,53	0
55	MG	DA	3245	1/1	0.94	0.36	60,60,60,60	0
55	MG	CA	1676	1/1	0.94	0.39	55,55,55,55	0
55	MG	CA	1738	1/1	0.94	0.34	63,63,63,63	0
55	MG	BA	3270	1/1	0.94	0.09	76,76,76,76	0
55	MG	BA	3488	1/1	0.94	0.25	80,80,80,80	0
55	MG	DA	3250	1/1	0.94	0.29	63,63,63,63	0
55	MG	BA	3037	1/1	0.94	0.21	44,44,44,44	0
55	MG	AA	1663	1/1	0.94	0.12	47,47,47,47	0
55	MG	BA	3218	1/1	0.94	0.27	48,48,48,48	0
55	MG	DA	3060	1/1	0.94	0.41	73,73,73,73	0
55	MG	BA	3436	1/1	0.94	0.19	59,59,59,59	0
55	MG	DA	3257	1/1	0.94	0.20	49,49,49,49	0
55	MG	DA	3258	1/1	0.94	0.14	37,37,37,37	0
56	ZN	CG	303	1/1	0.94	0.22	118,118,118,118	0
55	MG	BA	3610	1/1	0.95	0.34	61,61,61,61	0
55	MG	BA	3401	1/1	0.95	0.25	62,62,62,62	0
55	MG	DA	3474	1/1	0.95	0.32	83,83,83,83	0
55	MG	DA	3321	1/1	0.95	0.44	66,66,66,66	0
55	MG	DA	3097	1/1	0.95	0.19	52,52,52,52	0
55	MG	BA	3263	1/1	0.95	0.43	54,54,54,54	0
55	MG	DA	3325	1/1	0.95	0.34	73,73,73,73	0
55	MG	DA	3171	1/1	0.95	0.31	63,63,63,63	0
55	MG	CN	201	1/1	0.95	0.14	74,74,74,74	0
55	MG	BA	3103	1/1	0.95	0.30	52,52,52,52	0
55	MG	AA	1830	1/1	0.95	0.32	73,73,73,73	0
55	MG	BA	3443	1/1	0.95	0.23	77,77,77,77	0
55	MG	BA	3124	1/1	0.95	0.39	45,45,45,45	0
55	MG	DA	3177	1/1	0.95	0.32	74,74,74,74	0
55	MG	DA	3105	1/1	0.95	0.20	45,45,45,45	0
55	MG	BA	3200	1/1	0.95	0.28	62,62,62,62	0
55	MG	DA	3180	1/1	0.95	0.30	52,52,52,52	0
55	MG	AA	1676	1/1	0.95	0.24	70,70,70,70	0
55	MG	CA	1613	1/1	0.95	0.20	68,68,68,68	0
55	MG	DA	3050	1/1	0.95	0.35	66,66,66,66	0
55	MG	BA	3302	1/1	0.95	0.25	26,26,26,26	0
55	MG	BA	3237	1/1	0.95	0.37	57,57,57,57	0
55	MG	BA	3017	1/1	0.95	0.24	25,25,25,25	0
55	MG	DA	3188	1/1	0.95	0.50	56,56,56,56	0
55	MG	DA	3114	1/1	0.95	0.41	54,54,54,54	0
55	MG	DA	3420	1/1	0.95	0.18	67,67,67,67	0
55	MG	DA	3190	1/1	0.95	0.34	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	DA	3115	1/1	0.95	0.26	49,49,49,49	0
55	MG	DA	3423	1/1	0.95	0.40	75,75,75,75	0
55	MG	BA	3451	1/1	0.95	0.32	65,65,65,65	0
55	MG	AA	1641	1/1	0.95	0.19	57,57,57,57	0
55	MG	BA	3576	1/1	0.95	0.26	74,74,74,74	0
55	MG	CA	1669	1/1	0.95	0.10	60,60,60,60	0
55	MG	BA	3307	1/1	0.95	0.32	39,39,39,39	0
55	MG	AA	1719	1/1	0.95	0.21	79,79,79,79	0
55	MG	BA	3374	1/1	0.95	0.35	71,71,71,71	0
55	MG	BA	3091	1/1	0.95	0.26	35,35,35,35	0
55	MG	BA	3150	1/1	0.95	0.28	36,36,36,36	0
55	MG	BA	3538	1/1	0.95	0.38	66,66,66,66	0
55	MG	BA	3539	1/1	0.95	0.13	74,74,74,74	0
55	MG	BA	3092	1/1	0.95	0.25	32,32,32,32	0
55	MG	BA	3093	1/1	0.95	0.19	57,57,57,57	0
55	MG	BA	3542	1/1	0.95	0.29	72,72,72,72	0
55	MG	AA	1659	1/1	0.95	0.34	69,69,69,69	0
55	MG	DA	3211	1/1	0.95	0.26	42,42,42,42	0
55	MG	DA	3135	1/1	0.95	0.20	49,49,49,49	0
55	MG	BA	3061	1/1	0.95	0.45	61,61,61,61	0
55	MG	BA	3383	1/1	0.95	0.20	71,71,71,71	0
55	MG	AA	1798	1/1	0.95	0.16	58,58,58,58	0
55	MG	DA	3444	1/1	0.95	0.11	73,73,73,73	0
55	MG	BA	3504	1/1	0.95	0.22	45,45,45,45	0
55	MG	DA	3217	1/1	0.95	0.27	55,55,55,55	0
55	MG	BA	3347	1/1	0.95	0.30	68,68,68,68	0
55	MG	DA	3294	1/1	0.95	0.19	64,64,64,64	0
55	MG	DA	3142	1/1	0.95	0.27	40,40,40,40	0
55	MG	BA	3034	1/1	0.95	0.23	41,41,41,41	0
55	MG	DA	3077	1/1	0.95	0.10	64,64,64,64	0
55	MG	DB	204	1/1	0.95	0.26	82,82,82,82	0
55	MG	BA	3217	1/1	0.95	0.18	52,52,52,52	0
55	MG	BA	3012	1/1	0.95	0.20	45,45,45,45	0
55	MG	BA	3023	1/1	0.95	0.24	45,45,45,45	0
55	MG	BA	3161	1/1	0.95	0.11	56,56,56,56	0
55	MG	BA	3554	1/1	0.95	0.28	45,45,45,45	0
55	MG	B0	201	1/1	0.95	0.21	51,51,51,51	0
55	MG	BA	3353	1/1	0.95	0.29	52,52,52,52	0
55	MG	DA	3306	1/1	0.95	0.33	65,65,65,65	0
55	MG	CA	1746	1/1	0.95	0.38	57,57,57,57	0
55	MG	BA	3162	1/1	0.95	0.30	45,45,45,45	0
55	MG	BA	3322	1/1	0.95	0.40	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	DA	3233	1/1	0.95	0.36	52,52,52,52	0
55	MG	BA	3013	1/1	0.95	0.29	34,34,34,34	0
55	MG	B5	101	1/1	0.95	0.17	45,45,45,45	0
55	MG	BA	3119	1/1	0.95	0.26	62,62,62,62	0
55	MG	BA	3605	1/1	0.95	0.34	47,47,47,47	0
55	MG	DA	3238	1/1	0.95	0.31	60,60,60,60	0
55	MG	BA	3192	1/1	0.95	0.16	34,34,34,34	0
55	MG	BA	3165	1/1	0.95	0.36	61,61,61,61	0
55	MG	AA	1691	1/1	0.95	0.34	50,50,50,50	0
55	MG	BA	3213	1/1	0.96	0.40	49,49,49,49	0
55	MG	DA	3495	1/1	0.96	0.14	63,63,63,63	0
55	MG	DA	3163	1/1	0.96	0.43	62,62,62,62	0
55	MG	BA	3241	1/1	0.96	0.28	60,60,60,60	0
55	MG	BA	3064	1/1	0.96	0.11	49,49,49,49	0
55	MG	BA	3009	1/1	0.96	0.18	36,36,36,36	0
55	MG	DA	3219	1/1	0.96	0.14	70,70,70,70	0
55	MG	DA	3035	1/1	0.96	0.17	62,62,62,62	0
55	MG	CA	1671	1/1	0.96	0.32	49,49,49,49	0
55	MG	AA	1750	1/1	0.96	0.37	62,62,62,62	0
55	MG	BA	3158	1/1	0.96	0.15	41,41,41,41	0
55	MG	DA	3392	1/1	0.96	0.36	68,68,68,68	0
55	MG	DA	3278	1/1	0.96	0.30	42,42,42,42	0
55	MG	CA	1674	1/1	0.96	0.11	70,70,70,70	0
55	MG	DA	3122	1/1	0.96	0.32	46,46,46,46	0
55	MG	BA	3271	1/1	0.96	0.07	35,35,35,35	0
55	MG	BA	3083	1/1	0.96	0.10	62,62,62,62	0
55	MG	BB	205	1/1	0.96	0.26	74,74,74,74	0
55	MG	DA	3126	1/1	0.96	0.12	41,41,41,41	0
55	MG	BA	3198	1/1	0.96	0.09	45,45,45,45	0
55	MG	BA	3274	1/1	0.96	0.15	46,46,46,46	0
55	MG	BA	3410	1/1	0.96	0.31	62,62,62,62	0
55	MG	BA	3011	1/1	0.96	0.20	42,42,42,42	0
55	MG	AA	1673	1/1	0.96	0.29	78,78,78,78	0
55	MG	DA	3132	1/1	0.96	0.15	53,53,53,53	0
55	MG	DA	3009	1/1	0.96	0.26	68,68,68,68	0
55	MG	AA	1792	1/1	0.96	0.11	55,55,55,55	0
55	MG	AA	1608	1/1	0.96	0.18	64,64,64,64	0
55	MG	BB	213	1/1	0.96	0.30	66,66,66,66	0
55	MG	BA	3508	1/1	0.96	0.32	59,59,59,59	0
55	MG	DA	3241	1/1	0.96	0.25	46,46,46,46	0
55	MG	BA	3046	1/1	0.96	0.22	39,39,39,39	0
55	MG	DA	3243	1/1	0.96	0.32	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	BA	3306	1/1	0.96	0.21	67,67,67,67	0
55	MG	DA	3141	1/1	0.96	0.31	38,38,38,38	0
55	MG	BA	3280	1/1	0.96	0.32	50,50,50,50	0
55	MG	BA	3389	1/1	0.96	0.17	59,59,59,59	0
55	MG	DA	3144	1/1	0.96	0.24	60,60,60,60	0
55	MG	BA	3390	1/1	0.96	0.31	60,60,60,60	0
55	MG	BA	3047	1/1	0.96	0.35	74,74,74,74	0
55	MG	AC	104	1/1	0.96	0.26	56,56,56,56	0
55	MG	DA	3252	1/1	0.96	0.26	64,64,64,64	0
55	MG	BA	3186	1/1	0.96	0.21	36,36,36,36	0
55	MG	DA	3200	1/1	0.96	0.29	44,44,44,44	0
55	MG	DA	3201	1/1	0.96	0.12	47,47,47,47	0
55	MG	BF	301	1/1	0.96	0.08	73,73,73,73	0
55	MG	BA	3612	1/1	0.96	0.37	66,66,66,66	0
55	MG	AA	1671	1/1	0.96	0.15	67,67,67,67	0
55	MG	DA	3152	1/1	0.96	0.12	67,67,67,67	0
55	MG	DA	3260	1/1	0.96	0.36	41,41,41,41	0
55	MG	AA	1623	1/1	0.96	0.37	65,65,65,65	0
55	MG	BA	3027	1/1	0.96	0.31	36,36,36,36	0
55	MG	BA	3138	1/1	0.96	0.42	46,46,46,46	0
55	MG	BA	3427	1/1	0.96	0.28	65,65,65,65	0
55	MG	BA	3262	1/1	0.96	0.36	33,33,33,33	0
55	MG	D5	2001	1/1	0.96	0.23	46,46,46,46	0
56	ZN	AG	302	1/1	0.96	0.23	95,95,95,95	0
55	MG	DA	3111	1/1	0.96	0.17	52,52,52,52	0
55	MG	BA	3172	1/1	0.96	0.17	34,34,34,34	0
55	MG	BA	3450	1/1	0.97	0.09	54,54,54,54	0
55	MG	DA	3329	1/1	0.97	0.17	44,44,44,44	0
55	MG	DA	3182	1/1	0.97	0.38	44,44,44,44	0
55	MG	DA	3299	1/1	0.97	0.15	38,38,38,38	0
55	MG	BA	3355	1/1	0.97	0.32	46,46,46,46	0
55	MG	DA	3054	1/1	0.97	0.23	58,58,58,58	0
55	MG	DA	3055	1/1	0.97	0.47	68,68,68,68	0
55	MG	BA	3099	1/1	0.97	0.39	67,67,67,67	0
55	MG	DA	3159	1/1	0.97	0.12	37,37,37,37	0
55	MG	BA	3074	1/1	0.97	0.30	49,49,49,49	0
55	MG	BA	3224	1/1	0.97	0.11	55,55,55,55	0
55	MG	BA	3377	1/1	0.97	0.41	62,62,62,62	0
55	MG	BA	3042	1/1	0.97	0.17	41,41,41,41	0
55	MG	BA	3123	1/1	0.97	0.11	51,51,51,51	0
55	MG	AA	1842	1/1	0.97	0.28	59,59,59,59	0
55	MG	BE	303	1/1	0.97	0.29	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	AA	1838	1/1	0.97	0.22	61,61,61,61	0
55	MG	BA	3261	1/1	0.97	0.38	52,52,52,52	0
55	MG	BA	3230	1/1	0.97	0.45	56,56,56,56	0
55	MG	BA	3231	1/1	0.97	0.36	73,73,73,73	0
55	MG	DA	3199	1/1	0.97	0.26	61,61,61,61	0
55	MG	BA	3216	1/1	0.97	0.17	33,33,33,33	0
55	MG	BA	3298	1/1	0.97	0.27	65,65,65,65	0
55	MG	BA	3608	1/1	0.97	0.23	39,39,39,39	0
55	MG	BA	3079	1/1	0.97	0.32	55,55,55,55	0
55	MG	B1	201	1/1	0.97	0.23	47,47,47,47	0
55	MG	AA	1707	1/1	0.97	0.33	50,50,50,50	0
55	MG	DA	3323	1/1	0.97	0.10	42,42,42,42	0
55	MG	DA	3206	1/1	0.97	0.45	65,65,65,65	0
55	MG	BA	3196	1/1	0.97	0.15	33,33,33,33	0
55	MG	BA	3220	1/1	0.97	0.23	44,44,44,44	0
55	MG	BA	3178	1/1	0.97	0.20	36,36,36,36	0
55	MG	BA	3264	1/1	0.98	0.08	30,30,30,30	0
55	MG	DA	3101	1/1	0.98	0.20	43,43,43,43	0
55	MG	BA	3452	1/1	0.98	0.25	41,41,41,41	0
55	MG	DA	3161	1/1	0.98	0.20	45,45,45,45	0
55	MG	BA	3382	1/1	0.98	0.26	43,43,43,43	0
55	MG	BA	3214	1/1	0.98	0.29	67,67,67,67	0
55	MG	DA	3133	1/1	0.98	0.24	42,42,42,42	0
55	MG	BA	3596	1/1	0.98	0.30	55,55,55,55	0
55	MG	DP	201	1/1	0.98	0.26	65,65,65,65	0
55	MG	DA	3374	1/1	0.98	0.33	62,62,62,62	0
55	MG	BA	3157	1/1	0.98	0.39	45,45,45,45	0
55	MG	BA	3228	1/1	0.98	0.53	72,72,72,72	0
55	MG	BA	3243	1/1	0.98	0.32	48,48,48,48	0
55	MG	BA	3491	1/1	0.98	0.34	42,42,42,42	0
55	MG	BA	3077	1/1	0.98	0.21	54,54,54,54	0
55	MG	BA	3171	1/1	0.98	0.33	61,61,61,61	0
55	MG	BA	3212	1/1	0.98	0.33	43,43,43,43	0
55	MG	BA	3036	1/1	0.98	0.29	44,44,44,44	0
56	ZN	CQ	101	1/1	0.98	0.05	120,120,120,120	0

6.5 Other polymers

There are no such residues in this entry.