



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 08:07 AM UTC

PDB ID : 4V5K / pdb_00004v5k
Title : Structure of cytotoxic domain of colicin E3 bound to the 70S ribosome
Authors : Ng, C.L.; Lang, K.; Meenan, N.A.G.; Sharma, A.; Kelley, A.C.; Kleanthous, C.; Ramakrishnan, V.
Deposited on : 2010-05-29
Resolution : 3.20 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

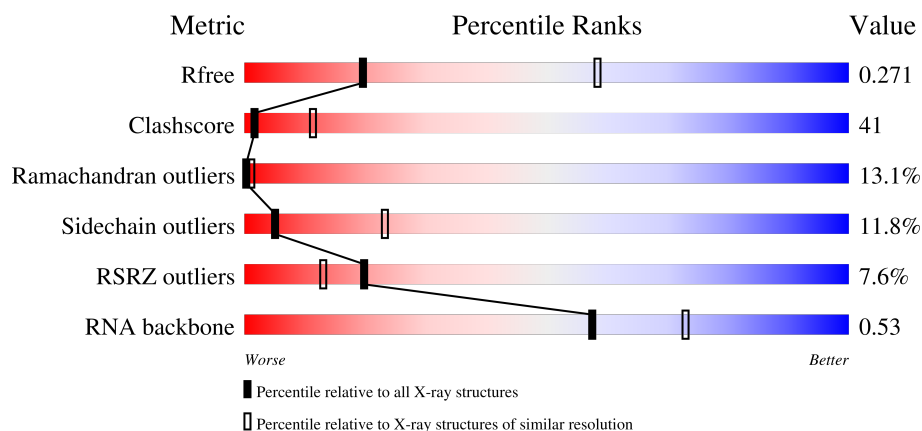
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)
RNA backbone	3983	1222 (3.50-2.90)

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	1522	3% 28% 60% 9% ..
1	CA	1522	24% 23% 62% 12% ..
2	AB	256	6% 15% 61% 14% 8%
2	CB	256	9% 16% 61% 13% 8%

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Mol	Chain	Length	Quality of chain
3	AC	239	
3	CC	239	
4	AD	209	
4	CD	209	
5	AE	162	
5	CE	162	
6	AF	101	
6	CF	101	
7	AG	156	
7	CG	156	
8	AH	138	
8	CH	138	
9	AI	128	
9	CI	128	
10	AJ	105	
10	CJ	105	
11	AK	129	
11	CK	129	
12	AL	135	
12	CL	135	
13	AM	126	
13	CM	126	
14	AN	61	
14	CN	61	
15	AO	89	

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Mol	Chain	Length	Quality of chain
15	CO	89	
16	AP	88	
16	CP	88	
17	AQ	105	
17	CQ	105	
18	AR	88	
18	CR	88	
19	AS	93	
19	CS	93	
20	AT	106	
20	CT	106	
21	AU	27	
21	CU	27	
22	AV	77	
22	AW	77	
22	CV	77	
22	CW	77	
23	AX	25	
24	AY	97	
24	CY	97	
25	B0	85	
25	D0	85	
26	B1	98	
26	D1	98	
27	B2	72	

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Mol	Chain	Length	Quality of chain
27	D2	72	
28	B3	60	
28	D3	60	
29	B4	71	
29	D4	71	
30	B5	60	
30	D5	60	
31	B6	54	
31	D6	54	
32	B7	49	
32	D7	49	
33	B8	65	
33	D8	65	
34	B9	37	
34	D9	37	
35	BA	2848	
35	DA	2848	
36	BB	122	
36	DB	122	
37	BC	229	
37	DC	229	
38	BD	276	
38	DD	276	
39	BE	206	
39	DE	206	

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Mol	Chain	Length	Quality of chain
40	BF	210	
40	DF	210	
41	BG	182	
41	DG	182	
42	BH	180	
42	DH	180	
43	BI	148	
43	DI	148	
44	BJ	131	
44	DJ	131	
45	BN	140	
45	DN	140	
46	BO	122	
46	DO	122	
47	BP	150	
47	DP	150	
48	BQ	141	
48	DQ	141	
49	BR	118	
49	DR	118	
50	BS	112	
50	DS	112	
51	BT	146	
51	DT	146	
52	BU	118	

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Mol	Chain	Length	Quality of chain
52	DU	118	
53	BV	101	
53	DV	101	
54	BW	113	
54	DW	113	
55	BX	96	
55	DX	96	
56	BY	110	
56	DY	110	
57	BZ	206	
57	DZ	206	
58	CX	25	

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
1	A3P	AA	1493	-	-	X	-
59	MG	AA	1625	-	-	-	X
59	MG	AA	1640	-	-	-	X
59	MG	AA	1666	-	-	-	X
59	MG	AA	1698	-	-	-	X
59	MG	AA	1757	-	-	-	X
59	MG	AA	1776	-	-	-	X
59	MG	AA	1790	-	-	-	X
59	MG	AA	1831	-	-	-	X
59	MG	AA	1850	-	-	-	X
59	MG	AA	1886	-	-	-	X
59	MG	AA	1905	-	-	-	X
59	MG	AA	1924	-	-	-	X
59	MG	AA	1938	-	-	-	X
59	MG	AA	1952	-	-	-	X
59	MG	AA	1959	-	-	-	X
59	MG	AA	1964	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
59	MG	AA	1972	-	-	-	X
59	MG	AV	102	-	-	-	X
59	MG	BA	2914	-	-	-	X
59	MG	BA	2922	-	-	-	X
59	MG	BA	2963	-	-	-	X
59	MG	BA	2967	-	-	-	X
59	MG	BA	2977	-	-	-	X
59	MG	BA	2993	-	-	-	X
59	MG	BA	3005	-	-	-	X
59	MG	BA	3039	-	-	-	X
59	MG	BA	3043	-	-	-	X
59	MG	BA	3044	-	-	-	X
59	MG	BA	3071	-	-	-	X
59	MG	BA	3115	-	-	-	X
59	MG	BA	3117	-	-	-	X
59	MG	BA	3150	-	-	-	X
59	MG	BA	3190	-	-	-	X
59	MG	BA	3192	-	-	-	X
59	MG	BA	3193	-	-	-	X
59	MG	BA	3199	-	-	-	X
59	MG	BA	3210	-	-	-	X
59	MG	BA	3213	-	-	-	X
59	MG	BA	3215	-	-	-	X
59	MG	BA	3234	-	-	-	X
59	MG	BA	3272	-	-	-	X
59	MG	BA	3284	-	-	-	X
59	MG	BA	3316	-	-	-	X
59	MG	BA	3331	-	-	-	X
59	MG	BA	3335	-	-	-	X
59	MG	BA	3339	-	-	-	X
59	MG	BA	3342	-	-	-	X
59	MG	BA	3350	-	-	-	X
59	MG	BA	3361	-	-	-	X
59	MG	BA	3364	-	-	-	X
59	MG	BA	3379	-	-	-	X
59	MG	BA	3391	-	-	-	X
59	MG	BA	3477	-	-	-	X
59	MG	BA	3498	-	-	-	X
59	MG	BA	3502	-	-	-	X
59	MG	BA	3540	-	-	-	X
59	MG	BA	3564	-	-	-	X
59	MG	BA	3583	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
59	MG	BA	3585	-	-	-	X
59	MG	BA	3598	-	-	-	X
59	MG	BA	3602	-	-	-	X
59	MG	BP	202	-	-	X	-
59	MG	BP	203	-	-	X	-
59	MG	CA	1622	-	-	-	X
59	MG	CA	1626	-	-	-	X
59	MG	CA	1695	-	-	-	X
59	MG	CA	1721	-	-	-	X
59	MG	CA	1741	-	-	-	X
59	MG	CA	1759	-	-	-	X
59	MG	CV	101	-	-	-	X
59	MG	D3	101	-	-	-	X
59	MG	D7	104	-	-	-	X
59	MG	DA	2906	-	-	-	X
59	MG	DA	2920	-	-	-	X
59	MG	DA	2921	-	-	-	X
59	MG	DA	2925	-	-	-	X
59	MG	DA	2927	-	-	-	X
59	MG	DA	2930	-	-	-	X
59	MG	DA	2931	-	-	-	X
59	MG	DA	2939	-	-	-	X
59	MG	DA	2942	-	-	-	X
59	MG	DA	2944	-	-	-	X
59	MG	DA	2950	-	-	-	X
59	MG	DA	2954	-	-	-	X
59	MG	DA	2958	-	-	-	X
59	MG	DA	2961	-	-	-	X
59	MG	DA	2976	-	-	-	X
59	MG	DA	2982	-	-	-	X
59	MG	DA	2988	-	-	-	X
59	MG	DA	3021	-	-	-	X
59	MG	DA	3025	-	-	-	X
59	MG	DA	3049	-	-	-	X
59	MG	DA	3079	-	-	-	X
59	MG	DA	3113	-	-	-	X
59	MG	DA	3123	-	-	-	X
59	MG	DA	3131	-	-	-	X
59	MG	DA	3138	-	-	-	X
59	MG	DA	3143	-	-	-	X
59	MG	DA	3145	-	-	-	X
59	MG	DA	3148	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
59	MG	DA	3172	-	-	-	X
59	MG	DA	3241	-	-	-	X
59	MG	DA	3322	-	-	-	X
59	MG	DA	3329	-	-	-	X
59	MG	DA	3330	-	-	-	X
59	MG	DA	3345	-	-	-	X
59	MG	DA	3349	-	-	-	X
59	MG	DA	3366	-	-	-	X
59	MG	DA	3374	-	-	-	X
59	MG	DA	3376	-	-	-	X
59	MG	DA	3390	-	-	-	X
59	MG	DA	3419	-	-	-	X
59	MG	DA	3443	-	-	-	X
59	MG	DA	3459	-	-	-	X
59	MG	DA	3467	-	-	-	X
59	MG	DA	3468	-	-	-	X
59	MG	DA	3506	-	-	-	X
59	MG	DA	3515	-	-	-	X
59	MG	DA	3516	-	-	-	X
59	MG	DA	3534	-	-	-	X
59	MG	DA	3556	-	-	-	X
59	MG	DA	3569	-	-	-	X
59	MG	DA	3577	-	-	-	X
59	MG	DA	3591	-	-	-	X
59	MG	DA	3617	-	-	-	X
59	MG	DA	3628	-	-	-	X
59	MG	DA	3640	-	-	-	X
59	MG	DA	3651	-	-	-	X
59	MG	DA	3665	-	-	-	X
59	MG	DA	3682	-	-	-	X
59	MG	DA	3696	-	-	-	X
59	MG	DA	3712	-	-	-	X
59	MG	DA	3717	-	-	-	X
59	MG	DA	3728	-	-	-	X
59	MG	DA	3748	-	-	-	X
59	MG	DA	3784	-	-	-	X

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 296762 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	1508	Total	C	N	O	P	0	0	0
			32412	14427	6003	10475	1507			
1	CA	1508	Total	C	N	O	P	0	0	0
			32413	14427	6004	10475	1507			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AB	235	Total	C	N	O	S	0	0	1
			1901	1213	342	341	5			
2	CB	235	Total	C	N	O	S	0	0	1
			1901	1213	342	341	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AC	207	Total	C	N	O	S	0	0	1
			1613	1016	315	281	1			
3	CC	207	Total	C	N	O	S	0	0	1
			1613	1016	315	281	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AD	208	Total	C	N	O	S	0	0	1
			1692	1060	336	289	7			
4	CD	208	Total	C	N	O	S	0	0	1
			1692	1060	336	289	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AE	151	Total	C	N	O	S	0	0	1
			1147	724	218	201	4			
5	CE	151	Total	C	N	O	S	0	0	1
			1147	724	218	201	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AF	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			
6	CF	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	AG	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			
7	CG	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	AH	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			
8	CH	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	AI	127	Total	C	N	O		0	0	0
			1011	639	198	174				
9	CI	127	Total	C	N	O		0	0	0
			1011	639	198	174				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AJ	99	Total	C	N	O	S	0	0	1
			795	499	157	138	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	CJ	99	Total	C	N	O	S	0	0	1
			795	499	157	138	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	AK	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			
11	CK	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	AL	125	Total	C	N	O	S	0	0	1
			971	611	196	163	1			
12	CL	125	Total	C	N	O	S	0	0	1
			971	611	196	163	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AM	118	Total	C	N	O	S	0	0	1
			934	577	193	162	2			
13	CM	118	Total	C	N	O	S	0	0	1
			934	577	193	162	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AN	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			
14	CN	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	AO	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			
15	CO	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	AP	84	Total	C	N	O	S	0	0	1
			701	443	140	117	1			
16	CP	84	Total	C	N	O	S	0	0	1
			701	443	140	117	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AQ	100	Total	C	N	O	S	0	0	1
			824	528	152	142	2			
17	CQ	100	Total	C	N	O	S	0	0	1
			824	528	152	142	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	AR	70	Total	C	N	O	0	0	0
			574	367	112	95			
18	CR	70	Total	C	N	O	0	0	0
			574	367	112	95			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AS	85	Total	C	N	O	S	0	0	1
			671	427	124	118	2			
19	CS	85	Total	C	N	O	S	0	0	1
			671	427	124	118	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AT	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			
20	CT	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	AU	25	Total	C	N	O	0	0	1
			209	128	51	30			
21	CU	25	Total	C	N	O	0	0	1
			209	128	51	30			

- Molecule 22 is a RNA chain called E-SITE TRNA PHE OR P-SITE TRNA PHE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AV	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			
22	AW	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			
22	CV	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			
22	CW	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			

- Molecule 23 is a RNA chain called MRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AX	16	Total	C	N	O	P	0	0	0
			341	155	66	105	15			

- Molecule 24 is a protein called COLICIN-E3.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
24	AY	97	Total	C	N	O	0	0	0
			769	483	144	142			
24	CY	16	Total	C	N	O	0	0	1
			126	82	23	21			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AY	58	ALA	HIS	engineered mutation	UNP P06646
CY	58	ALA	HIS	engineered mutation	UNP P06646

- Molecule 25 is a protein called 50S RIBOSOMAL PROTEIN L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	B0	84	Total	C	N	O	S	0	0	0
			662	410	140	111	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	D0	84	Total	C	N	O	S	0	0	0
			662	410	140	111	1			

- Molecule 26 is a protein called 50S RIBOSOMAL PROTEIN L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	B1	94	Total	C	N	O	S	0	0	1
			734	460	148	125	1			
26	D1	94	Total	C	N	O	S	0	0	1
			734	460	148	125	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B1	81	ARG	LYS	conflict	UNP P60494
D1	81	ARG	LYS	conflict	UNP P60494

- Molecule 27 is a protein called 50S RIBOSOMAL PROTEIN L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	B2	71	Total	C	N	O	S	0	0	0
			598	370	121	106	1			
27	D2	71	Total	C	N	O	S	0	0	0
			598	370	121	106	1			

- Molecule 28 is a protein called 50S RIBOSOMAL PROTEIN L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	B3	60	Total	C	N	O	S	0	0	1
			468	298	91	78	1			
28	D3	60	Total	C	N	O	S	0	0	1
			468	298	91	78	1			

- Molecule 29 is a protein called 50S RIBOSOMAL PROTEIN L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	B4	56	Total	C	N	O	S	0	0	1
			434	274	75	81	4			
29	D4	56	Total	C	N	O	S	0	0	1
			434	274	75	81	4			

- Molecule 30 is a protein called 50S RIBOSOMAL PROTEIN L32.

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

- Molecule 31 is a protein called 50S RIBOSOMAL PROTEIN L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	B6	45	Total	C	N	O	S	0	0	1
			381	235	78	64	4			
31	D6	45	Total	C	N	O	S	0	0	1
			381	235	78	64	4			

- Molecule 32 is a protein called 50S RIBOSOMAL PROTEIN L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	B7	49	Total	C	N	O	S	0	0	1
			419	257	105	55	2			
32	D7	49	Total	C	N	O	S	0	0	1
			419	257	105	55	2			

- Molecule 33 is a protein called 50S RIBOSOMAL PROTEIN L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	B8	64	Total	C	N	O	S	0	0	1
			508	326	102	78	2			
33	D8	64	Total	C	N	O	S	0	0	1
			508	326	102	78	2			

- Molecule 34 is a protein called 50S RIBOSOMAL PROTEIN L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	B9	36	Total	C	N	O	S	0	0	0
			299	183	67	46	3			
34	D9	36	Total	C	N	O	S	0	0	0
			299	183	67	46	3			

- Molecule 35 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BA	2807	Total	C	N	O	P	0	0	0
			60459	26907	11311	19435	2806			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	DA	2807	Total	C	N	O	P	0	0	0
			60459	26907	11311	19435	2806			

- Molecule 36 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	BB	119	Total	C	N	O	P	0	0	0
			2551	1136	471	826	118			
36	DB	119	Total	C	N	O	P	0	0	0
			2551	1136	471	826	118			

- Molecule 37 is a protein called 50S RIBOSOMAL PROTEIN L1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
37	BC	191	Total	C	N	O	0	0	1
			1142	691	221	230			
37	DC	191	Total	C	N	O	0	0	1
			1142	691	221	230			

- Molecule 38 is a protein called 50S RIBOSOMAL PROTEIN L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	BD	272	Total	C	N	O	S	0	0	1
			2105	1329	417	356	3			
38	DD	272	Total	C	N	O	S	0	0	1
			2105	1329	417	356	3			

- Molecule 39 is a protein called 50S RIBOSOMAL PROTEIN L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BE	205	Total	C	N	O	S	0	0	1
			1564	988	300	270	6			
39	DE	205	Total	C	N	O	S	0	0	1
			1564	988	300	270	6			

- Molecule 40 is a protein called 50S RIBOSOMAL PROTEIN L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	BF	208	Total	C	N	O	S	0	0	1
			1624	1035	304	282	3			
40	DF	208	Total	C	N	O	S	0	0	1
			1624	1035	304	282	3			

- Molecule 41 is a protein called 50S RIBOSOMAL PROTEIN L5.

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

- Molecule 42 is a protein called 50S RIBOSOMAL PROTEIN L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BH	165	Total	C	N	O	S	0	0	1
			1260	800	234	225	1			
42	DH	165	Total	C	N	O	S	0	0	1
			1260	800	234	225	1			

- Molecule 43 is a protein called 50S RIBOSOMAL PROTEIN L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BI	145	Total	C	N	O	S	0	0	1
			1125	718	200	206	1			
43	DI	145	Total	C	N	O	S	0	0	1
			1125	718	200	206	1			

- Molecule 44 is a protein called 50S RIBOSOMAL PROTEIN L10.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
44	BJ	130	Total	C	N	O	0	0	0
			651	390	130	131			
44	DJ	131	Total	C	N	O	0	0	1
			651	390	131	130			

- Molecule 45 is a protein called 50S RIBOSOMAL PROTEIN L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	BN	139	Total	C	N	O	S	0	0	1
			1105	712	207	182	4			
45	DN	139	Total	C	N	O	S	0	0	1
			1105	712	207	182	4			

- Molecule 46 is a protein called 50S RIBOSOMAL PROTEIN L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	BO	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			
46	DO	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

- Molecule 47 is a protein called 50S RIBOSOMAL PROTEIN L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	BP	146	Total	C	N	O	S	0	0	0
			1114	692	227	193	2			
47	DP	146	Total	C	N	O	S	0	0	0
			1114	692	227	193	2			

- Molecule 48 is a protein called 50S RIBOSOMAL PROTEIN L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	BQ	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			
48	DQ	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			

- Molecule 49 is a protein called 50S RIBOSOMAL PROTEIN L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	BR	117	Total	C	N	O		0	0	0
			960	599	202	159				
49	DR	117	Total	C	N	O		0	0	0
			960	599	202	159				

- Molecule 50 is a protein called 50S RIBOSOMAL PROTEIN L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	BS	99	Total	C	N	O		0	0	1
			771	486	155	130				
50	DS	99	Total	C	N	O		0	0	1
			771	486	155	130				

- Molecule 51 is a protein called 50S RIBOSOMAL PROTEIN L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	BT	138	Total	C	N	O	S	0	0	1
			1142	710	235	196	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	DT	138	Total	C	N	O	S	0	0	1
			1142	710	235	196	1			

- Molecule 52 is a protein called 50S RIBOSOMAL PROTEIN L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	BU	117	Total	C	N	O	S	0	0	0
			958	604	202	151	1			
52	DU	117	Total	C	N	O	S	0	0	0
			958	604	202	151	1			

- Molecule 53 is a protein called 50S RIBOSOMAL PROTEIN L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	BV	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			
53	DV	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			

- Molecule 54 is a protein called 50S RIBOSOMAL PROTEIN L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	BW	113	Total	C	N	O	S	0	0	0
			896	563	176	155	2			
54	DW	113	Total	C	N	O	S	0	0	0
			896	563	176	155	2			

- Molecule 55 is a protein called 50S RIBOSOMAL PROTEIN L23.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
55	BX	93	Total	C	N	O	0	0	1
			726	471	132	123			
55	DX	93	Total	C	N	O	0	0	1
			726	471	132	123			

- Molecule 56 is a protein called 50S RIBOSOMAL PROTEIN L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	BY	101	Total	C	N	O	S	0	0	1
			776	500	149	123	4			
56	DY	101	Total	C	N	O	S	0	0	1
			776	500	149	123	4			

- Molecule 57 is a protein called 50S RIBOSOMAL PROTEIN L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
57	BZ	187	Total	C	N	O	S	0	0	1
			1482	944	264	272	2			
57	DZ	187	Total	C	N	O	S	0	0	1
			1482	944	264	272	2			

- Molecule 58 is a RNA chain called MRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
58	CX	8	Total	C	N	O	P	0	0	0
			173	79	37	50	7			

- Molecule 59 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	AA	373	Total	Mg	0	0
			373	373		
59	AC	2	Total	Mg	0	0
			2	2		
59	AD	3	Total	Mg	0	0
			3	3		
59	AH	1	Total	Mg	0	0
			1	1		
59	AI	3	Total	Mg	0	0
			3	3		
59	AL	6	Total	Mg	0	0
			6	6		
59	AN	2	Total	Mg	0	0
			2	2		
59	AO	2	Total	Mg	0	0
			2	2		
59	AP	1	Total	Mg	0	0
			1	1		
59	AQ	3	Total	Mg	0	0
			3	3		
59	AT	1	Total	Mg	0	0
			1	1		
59	AV	7	Total	Mg	0	0
			7	7		
59	AX	4	Total	Mg	0	0
			4	4		
59	AY	3	Total	Mg	0	0
			3	3		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	B0	2	Total 2	Mg 2	0	0
59	B1	1	Total 1	Mg 1	0	0
59	B5	3	Total 3	Mg 3	0	0
59	B6	1	Total 1	Mg 1	0	0
59	B7	1	Total 1	Mg 1	0	0
59	BA	709	Total 709	Mg 709	0	0
59	BB	6	Total 6	Mg 6	0	0
59	BD	5	Total 5	Mg 5	0	0
59	BE	4	Total 4	Mg 4	0	0
59	BF	1	Total 1	Mg 1	0	0
59	BH	4	Total 4	Mg 4	0	0
59	BN	1	Total 1	Mg 1	0	0
59	BO	1	Total 1	Mg 1	0	0
59	BP	4	Total 4	Mg 4	0	0
59	BQ	1	Total 1	Mg 1	0	0
59	BR	5	Total 5	Mg 5	0	0
59	BT	1	Total 1	Mg 1	0	0
59	BU	2	Total 2	Mg 2	0	0
59	BY	1	Total 1	Mg 1	0	0
59	CA	184	Total 184	Mg 184	0	0
59	CC	3	Total 3	Mg 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	CD	1	Total 1	Mg 1	0	0
59	CH	1	Total 1	Mg 1	0	0
59	CJ	2	Total 2	Mg 2	0	0
59	CM	3	Total 3	Mg 3	0	0
59	CP	1	Total 1	Mg 1	0	0
59	CQ	1	Total 1	Mg 1	0	0
59	CS	2	Total 2	Mg 2	0	0
59	CV	12	Total 12	Mg 12	0	0
59	CY	1	Total 1	Mg 1	0	0
59	D0	4	Total 4	Mg 4	0	0
59	D1	2	Total 2	Mg 2	0	0
59	D2	1	Total 1	Mg 1	0	0
59	D3	1	Total 1	Mg 1	0	0
59	D5	3	Total 3	Mg 3	0	0
59	D6	2	Total 2	Mg 2	0	0
59	D7	4	Total 4	Mg 4	0	0
59	D8	1	Total 1	Mg 1	0	0
59	D9	1	Total 1	Mg 1	0	0
59	DA	897	Total 897	Mg 897	0	0
59	DB	11	Total 11	Mg 11	0	0
59	DD	6	Total 6	Mg 6	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	DE	4	Total	Mg	0	0
			4	4		
59	DF	3	Total	Mg	0	0
			3	3		
59	DN	3	Total	Mg	0	0
			3	3		
59	DO	1	Total	Mg	0	0
			1	1		
59	DP	6	Total	Mg	0	0
			6	6		
59	DR	2	Total	Mg	0	0
			2	2		
59	DT	1	Total	Mg	0	0
			1	1		
59	DU	4	Total	Mg	0	0
			4	4		
59	DW	1	Total	Mg	0	0
			1	1		
59	DY	1	Total	Mg	0	0
			1	1		

- Molecule 60 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	AD	2	Total	Zn	0	0
			2	2		
60	AN	1	Total	Zn	0	0
			1	1		
60	CD	1	Total	Zn	0	0
			1	1		

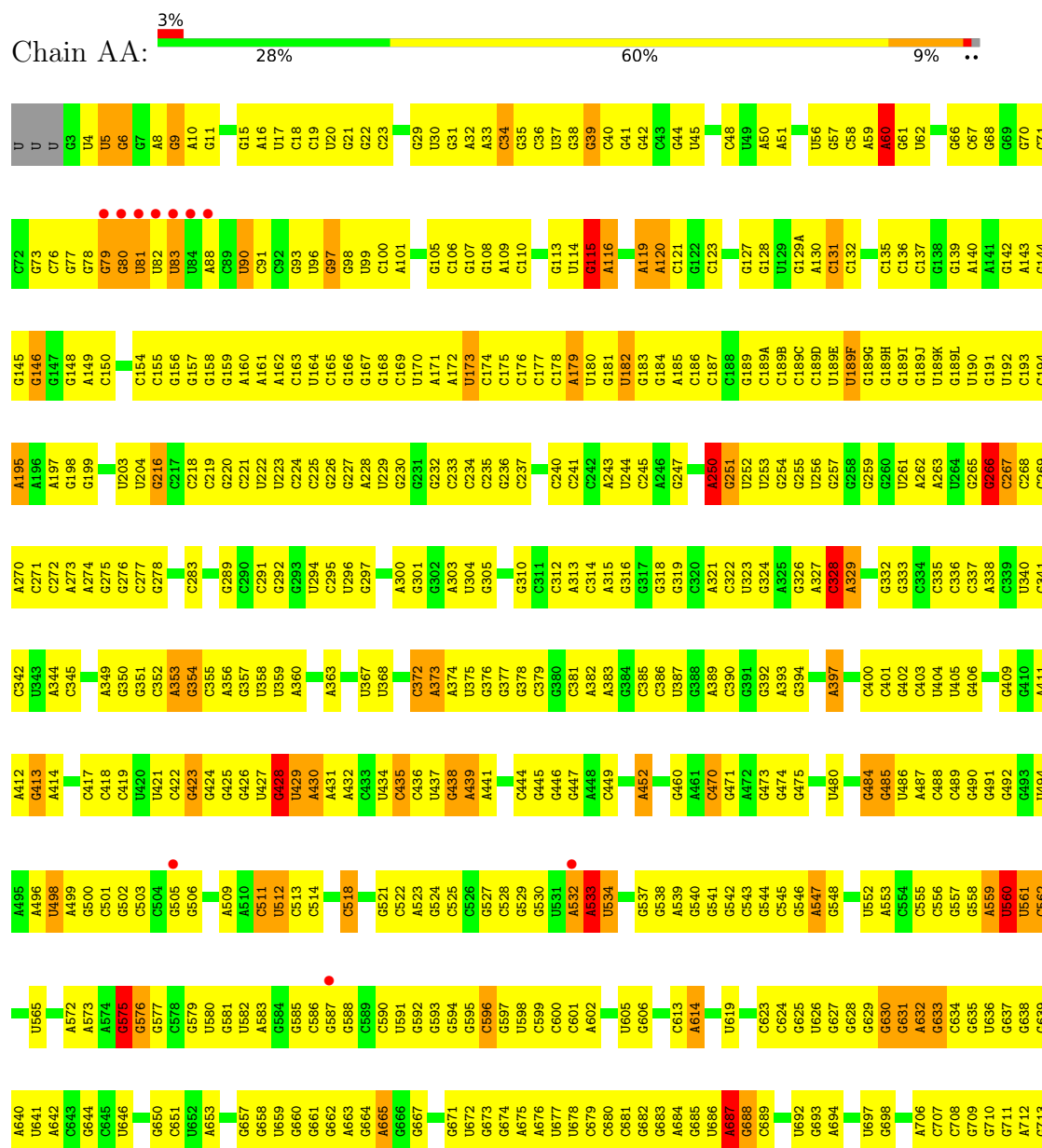
- Molecule 61 is water.

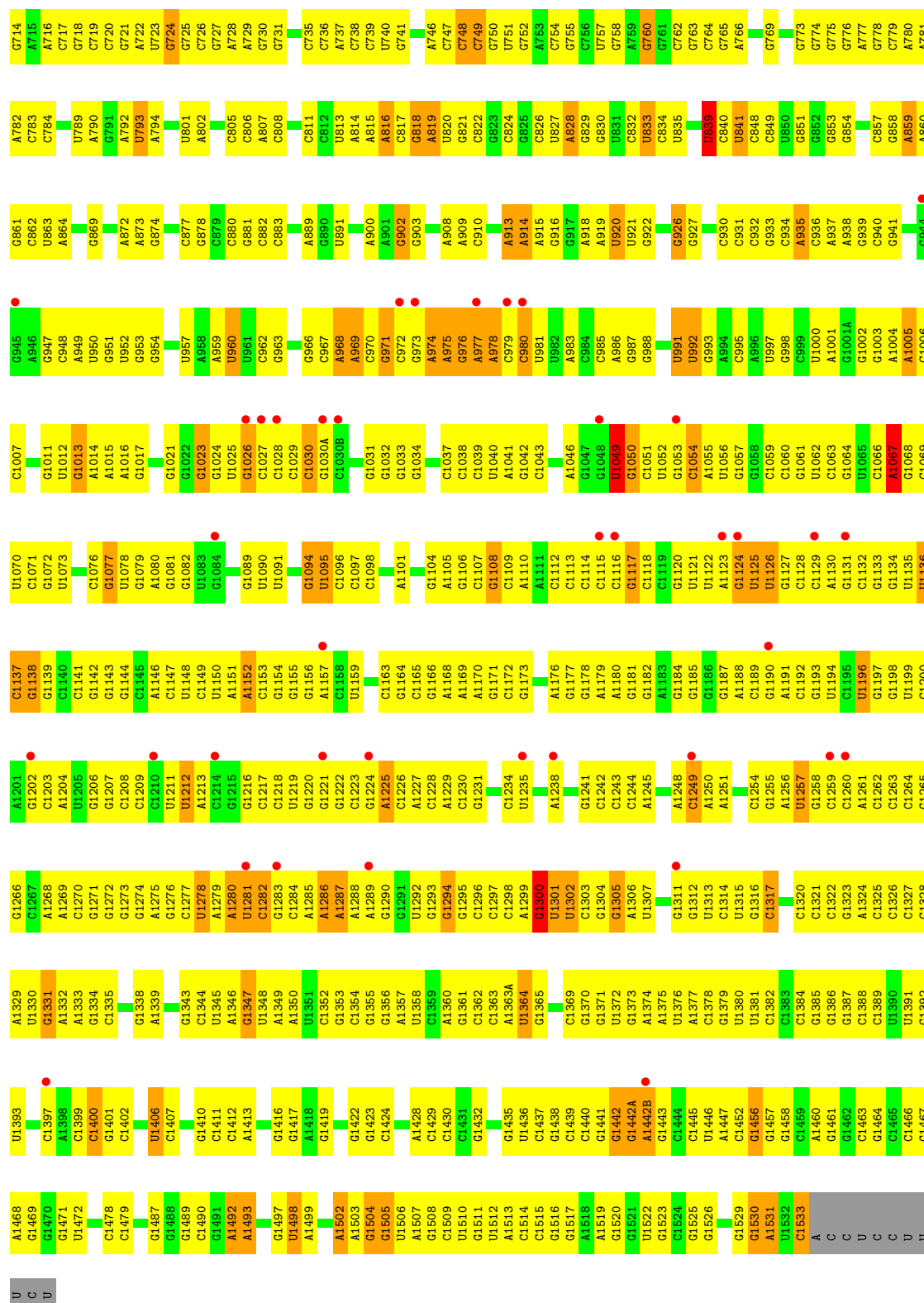
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	AA	2	Total	O	0	0
			2	2		

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.

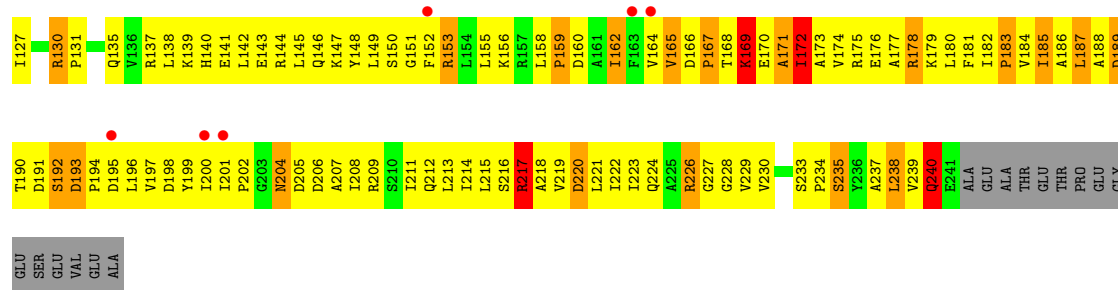
• Molecule 1: 16S ribosomal RNA



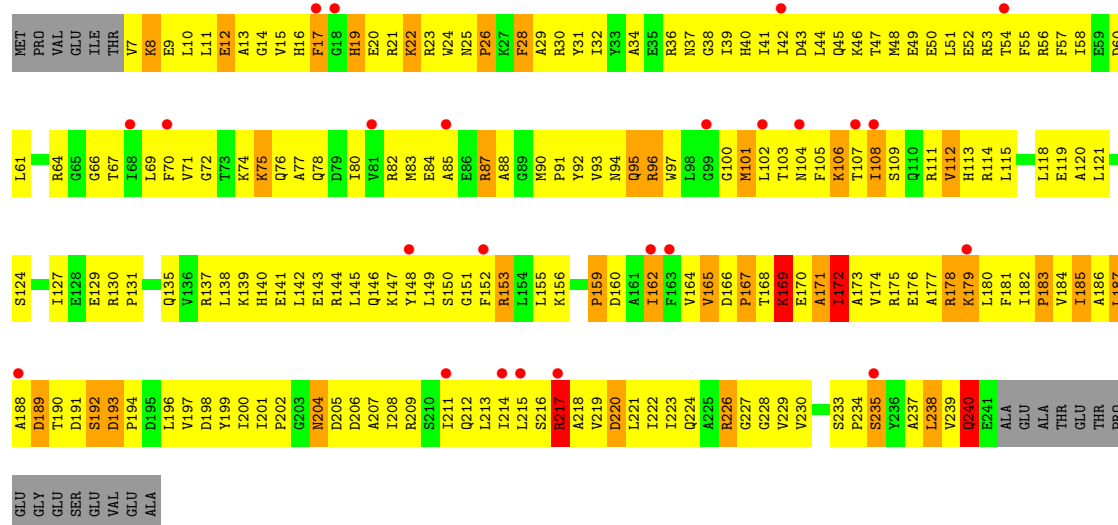




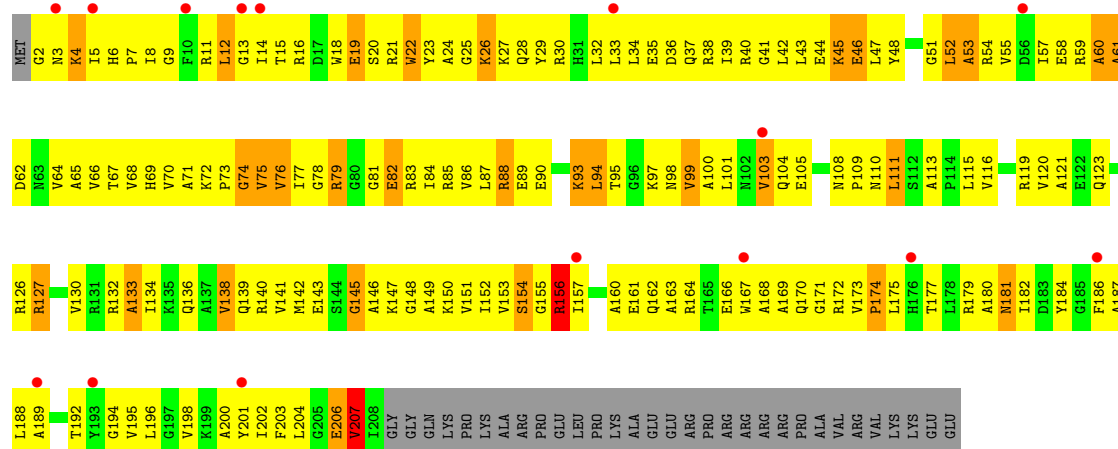
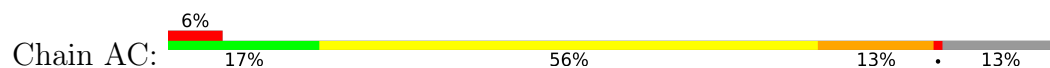




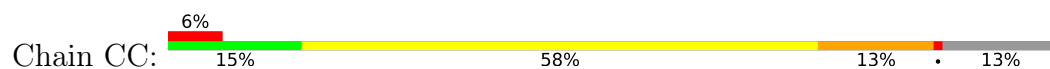
• Molecule 2: 30S RIBOSOMAL PROTEIN S2

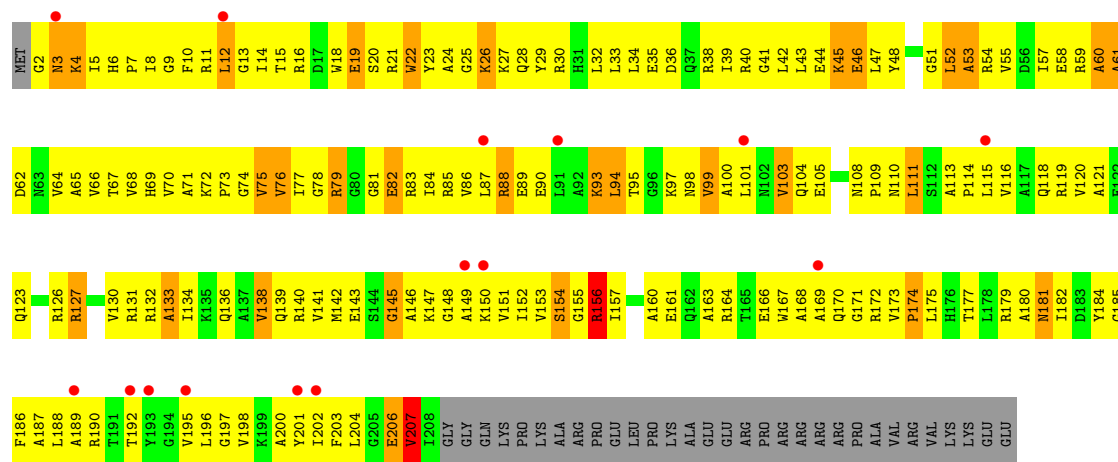


• Molecule 3: 30S RIBOSOMAL PROTEIN S3



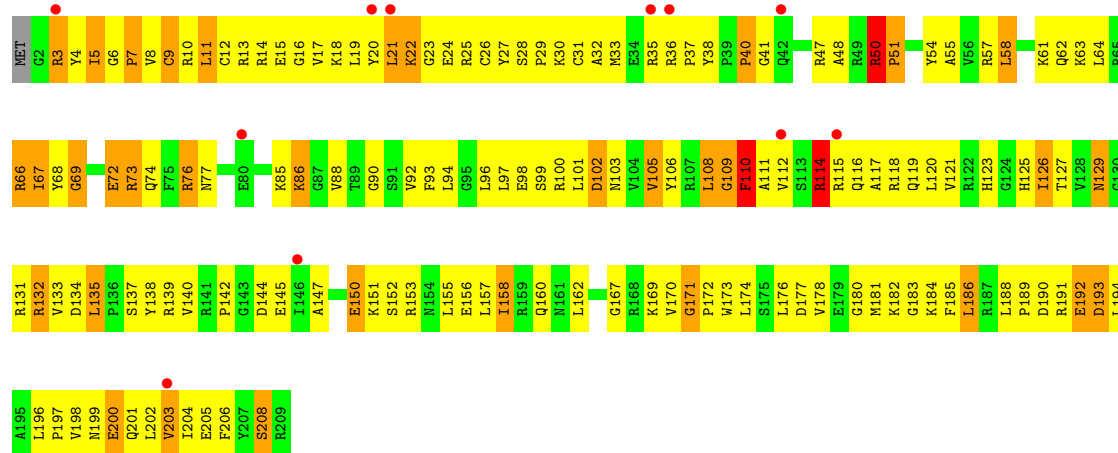
• Molecule 3: 30S RIBOSOMAL PROTEIN S3





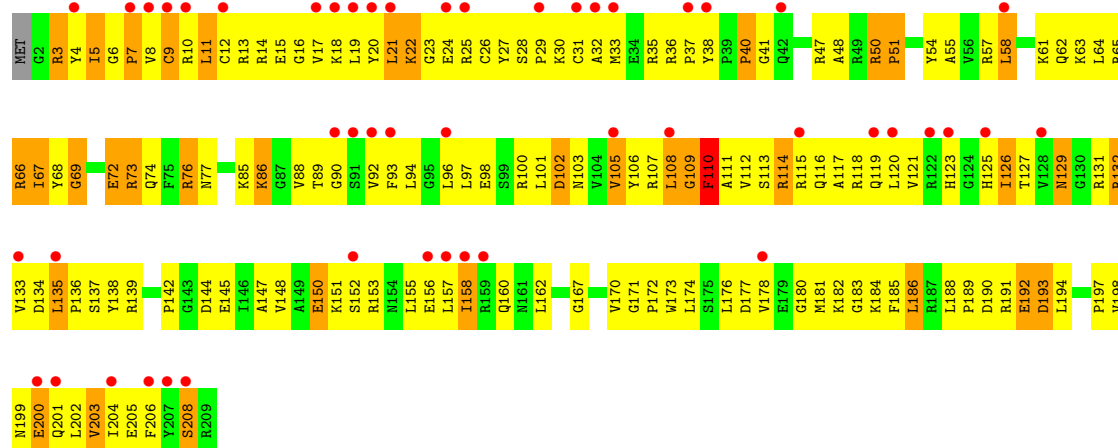
• Molecule 4: 30S RIBOSOMAL PROTEIN S4

Chain AD: 5% 27% 55% 16%

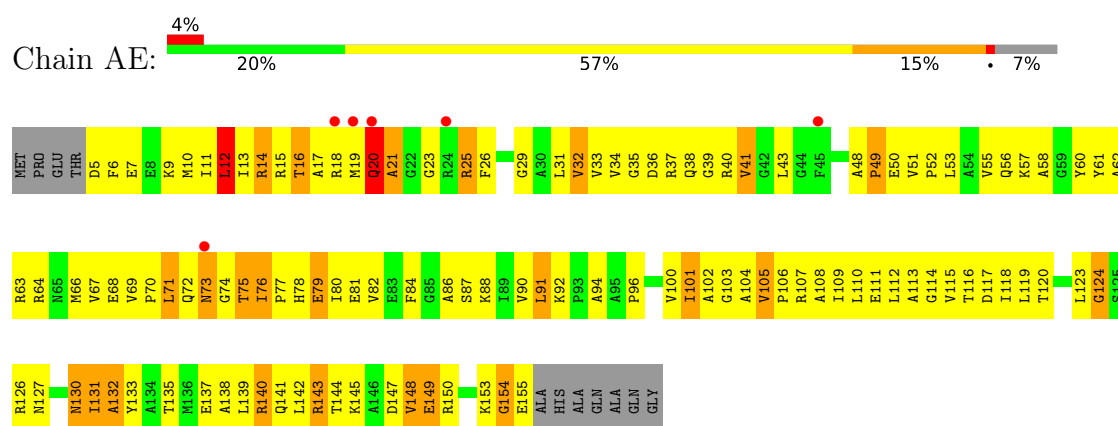


• Molecule 4: 30S RIBOSOMAL PROTEIN S4

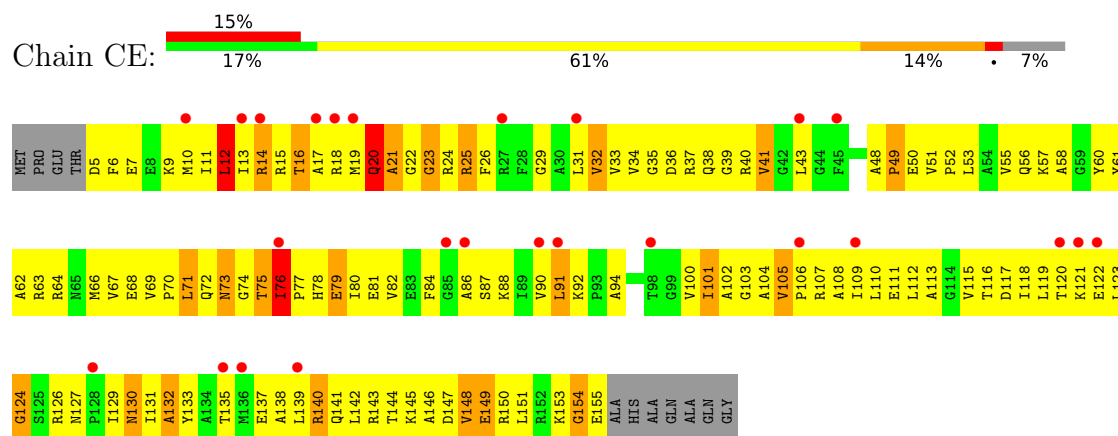
Chain CD: 23% 26% 56% 17%



• Molecule 5: 30S RIBOSOMAL PROTEIN S5



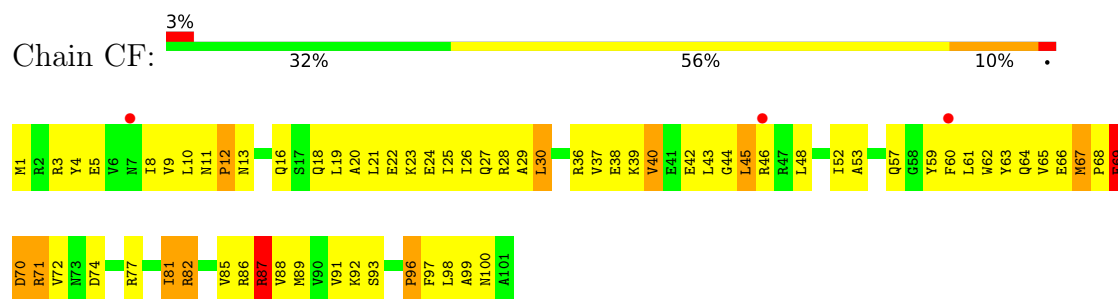
• Molecule 5: 30S RIBOSOMAL PROTEIN S5



• Molecule 6: 30S RIBOSOMAL PROTEIN S6

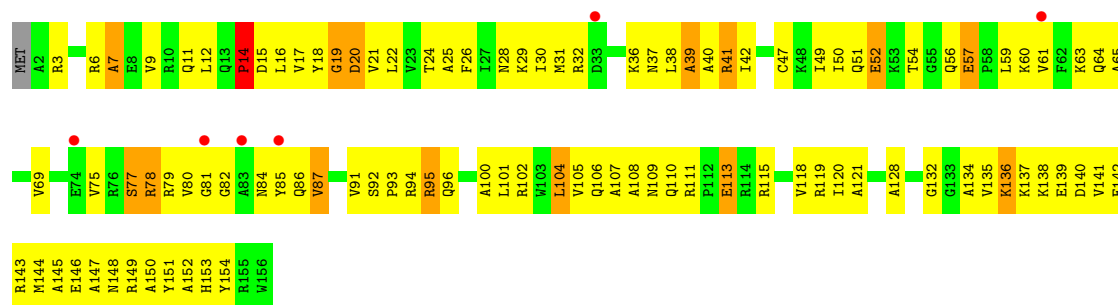


• Molecule 6: 30S RIBOSOMAL PROTEIN S6

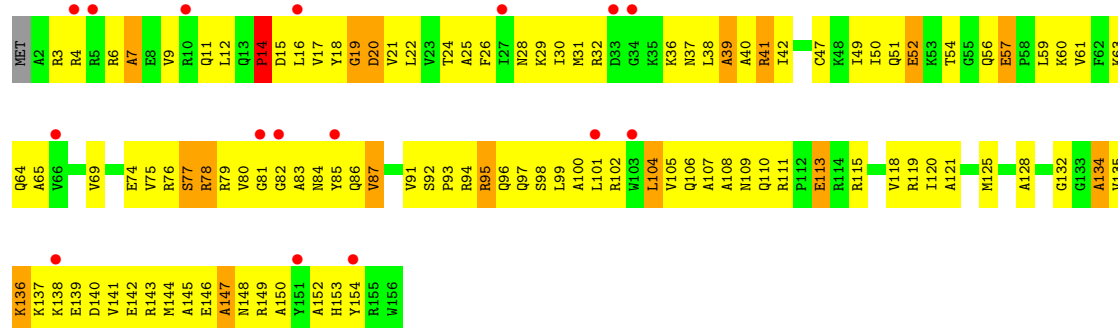


• Molecule 7: 30S RIBOSOMAL PROTEIN S7

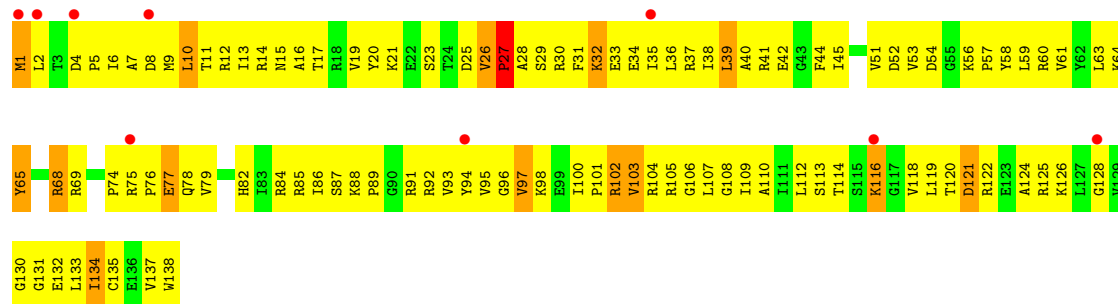




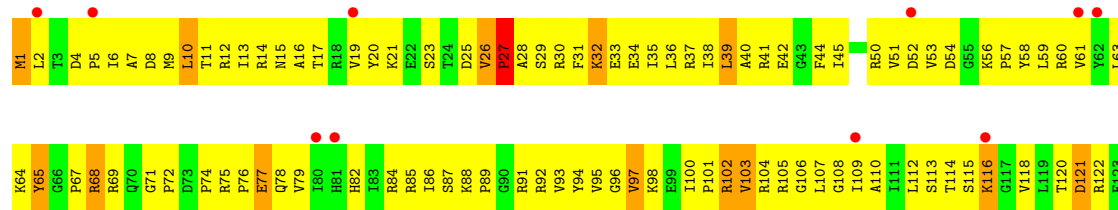
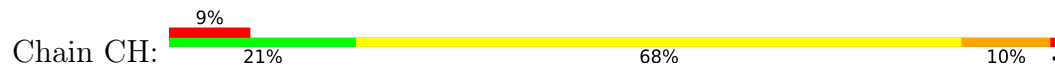
• Molecule 7: 30S RIBOSOMAL PROTEIN S7

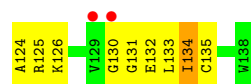


• Molecule 8: 30S RIBOSOMAL PROTEIN S8

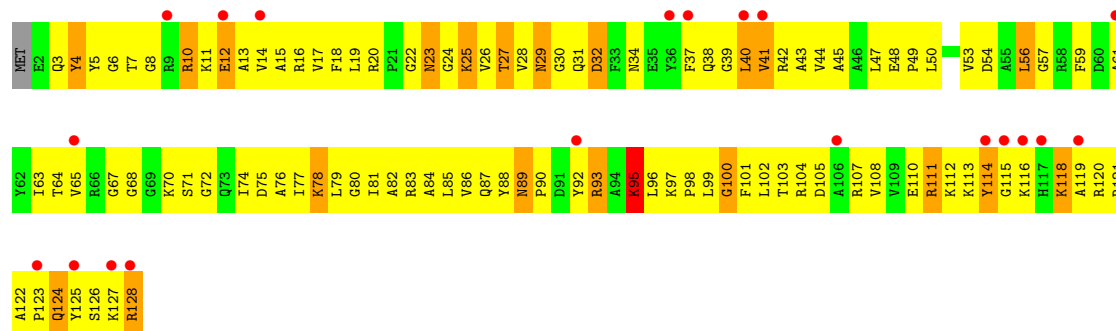


• Molecule 8: 30S RIBOSOMAL PROTEIN S8

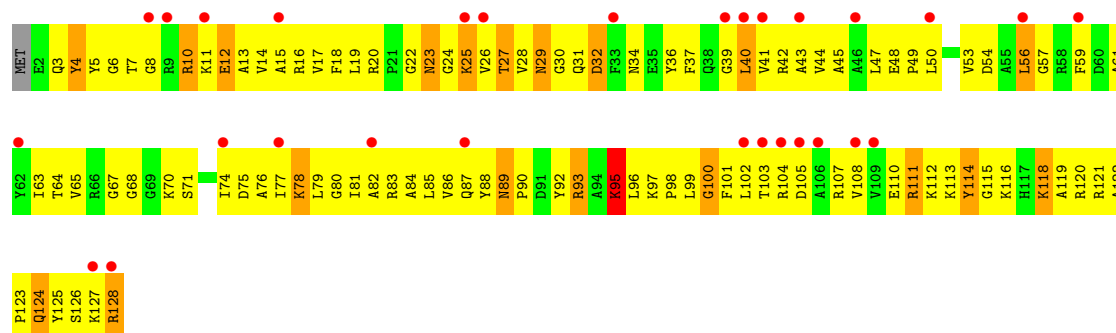




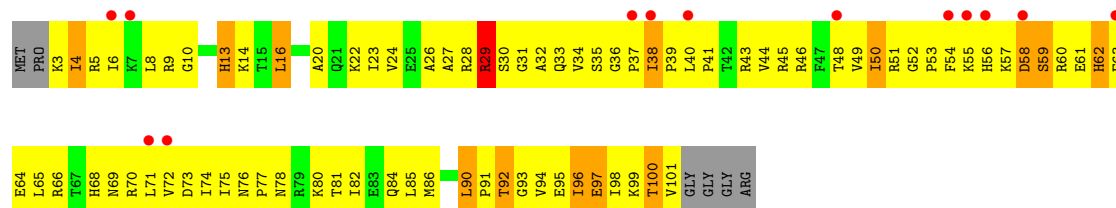
• Molecule 9: 30S RIBOSOMAL PROTEIN S9



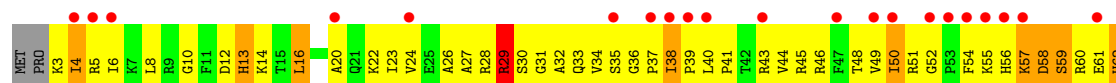
• Molecule 9: 30S RIBOSOMAL PROTEIN S9

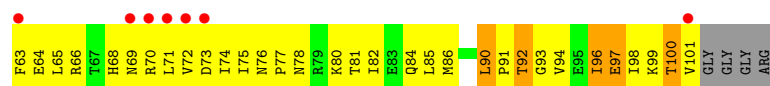


• Molecule 10: 30S RIBOSOMAL PROTEIN S10

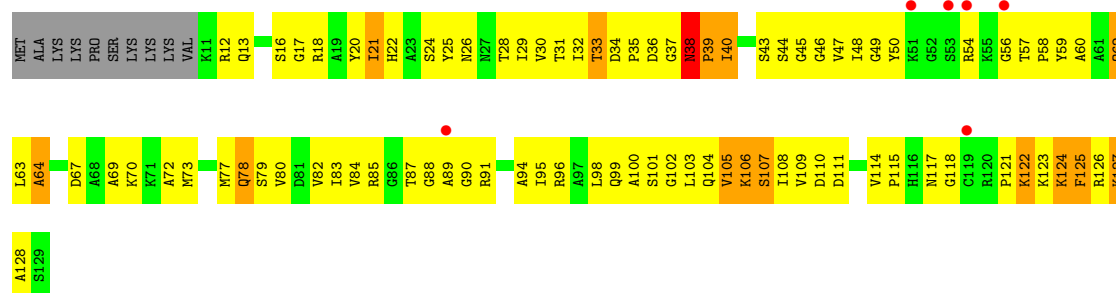


• Molecule 10: 30S RIBOSOMAL PROTEIN S10





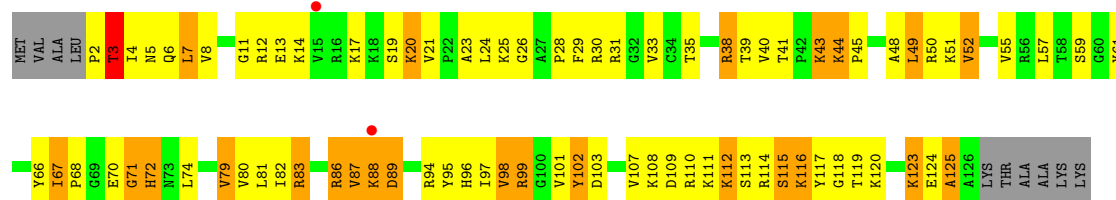
• Molecule 11: 30S RIBOSOMAL PROTEIN S11



• Molecule 11: 30S RIBOSOMAL PROTEIN S11

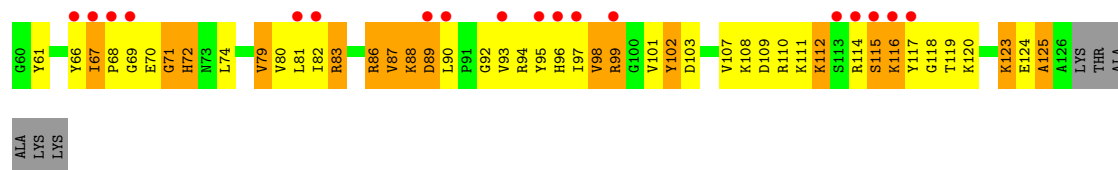


• Molecule 12: 30S RIBOSOMAL PROTEIN S12

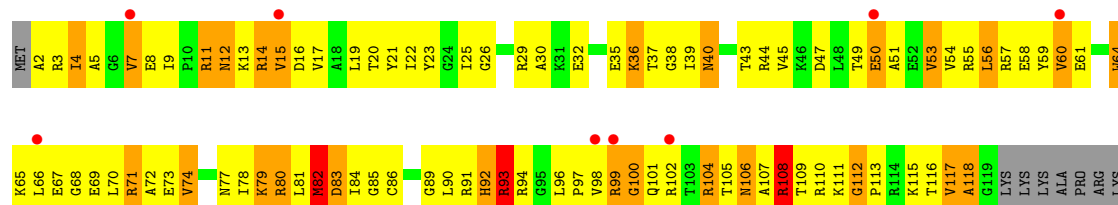


• Molecule 12: 30S RIBOSOMAL PROTEIN S12

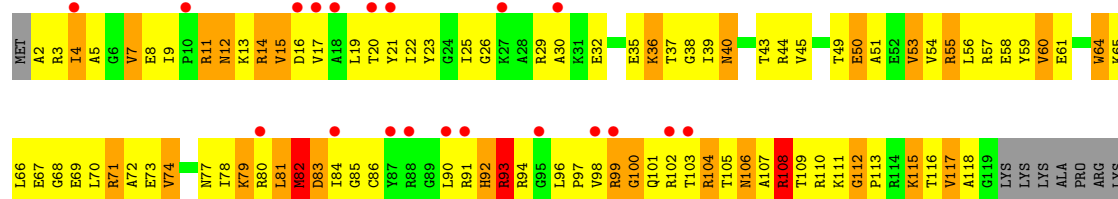




• Molecule 13: 30S RIBOSOMAL PROTEIN S13



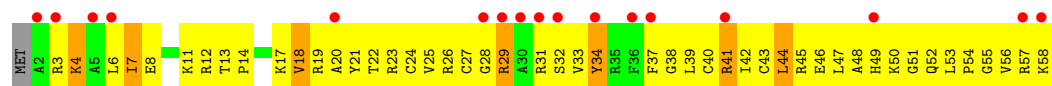
• Molecule 13: 30S RIBOSOMAL PROTEIN S13



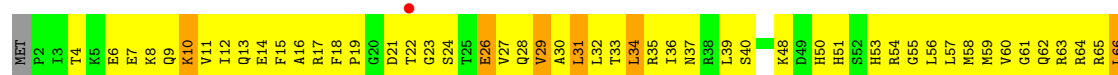
• Molecule 14: 30S RIBOSOMAL PROTEIN S14 TYPE Z

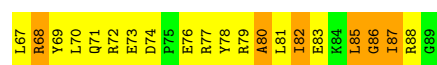


• Molecule 14: 30S RIBOSOMAL PROTEIN S14 TYPE Z



• Molecule 15: 30S RIBOSOMAL PROTEIN S15

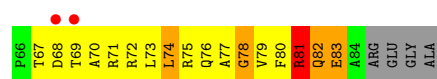
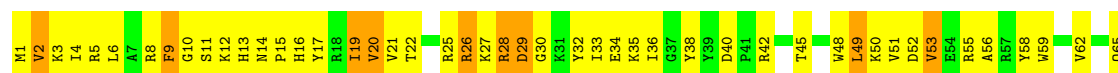




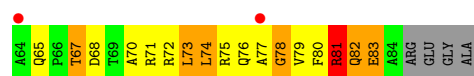
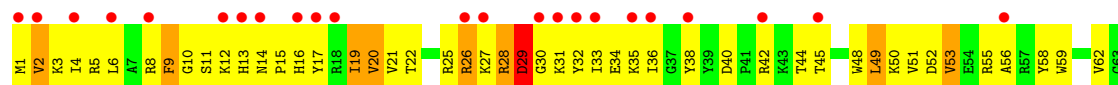
• Molecule 15: 30S RIBOSOMAL PROTEIN S15



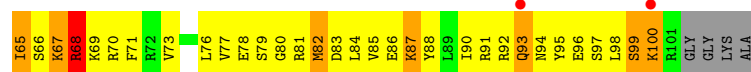
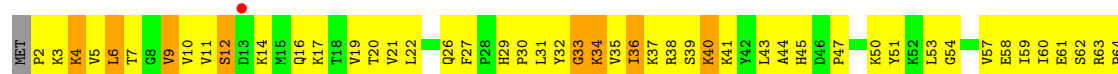
• Molecule 16: 30S RIBOSOMAL PROTEIN S16



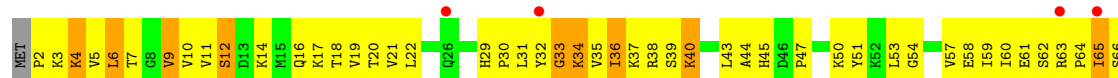
• Molecule 16: 30S RIBOSOMAL PROTEIN S16

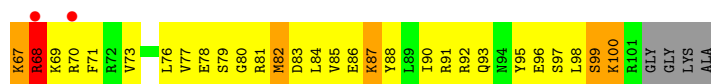


• Molecule 17: 30S RIBOSOMAL PROTEIN S17

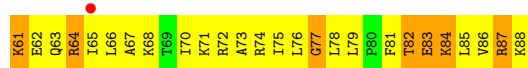
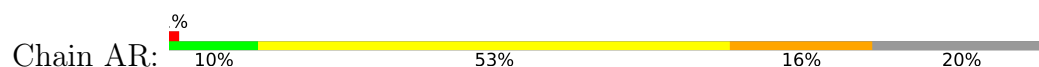


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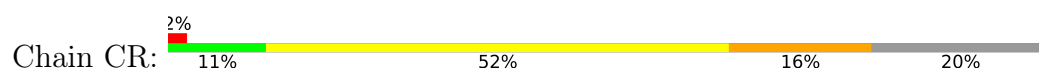




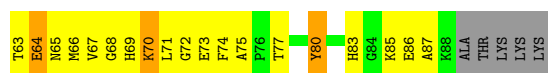
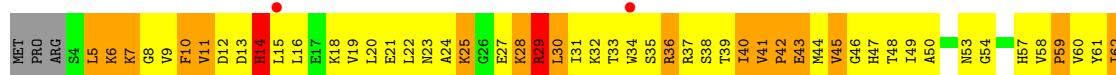
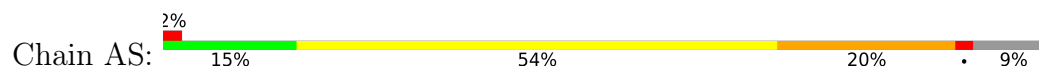
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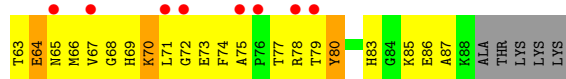
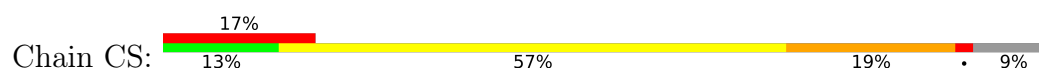
• Molecule 18: 30S RIBOSOMAL PROTEIN S18



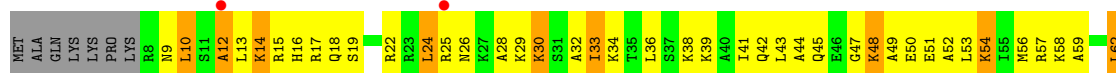
• Molecule 19: 30S RIBOSOMAL PROTEIN S19

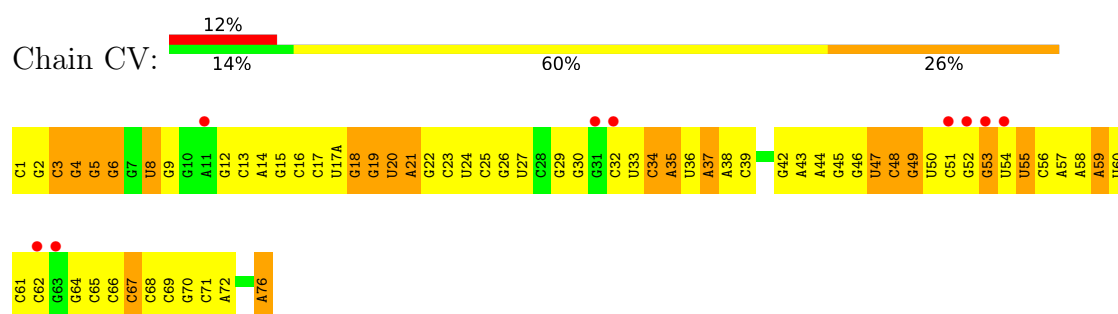


• Molecule 19: 30S RIBOSOMAL PROTEIN S19

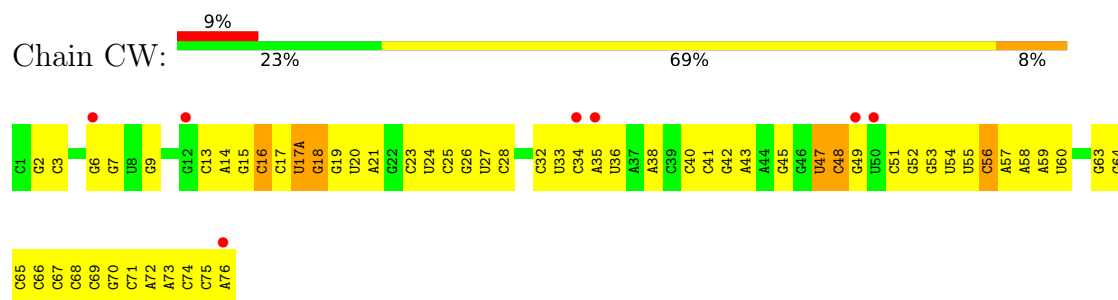


• Molecule 20: 30S RIBOSOMAL PROTEIN S20

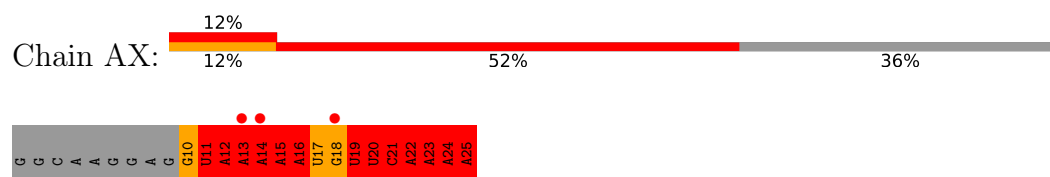




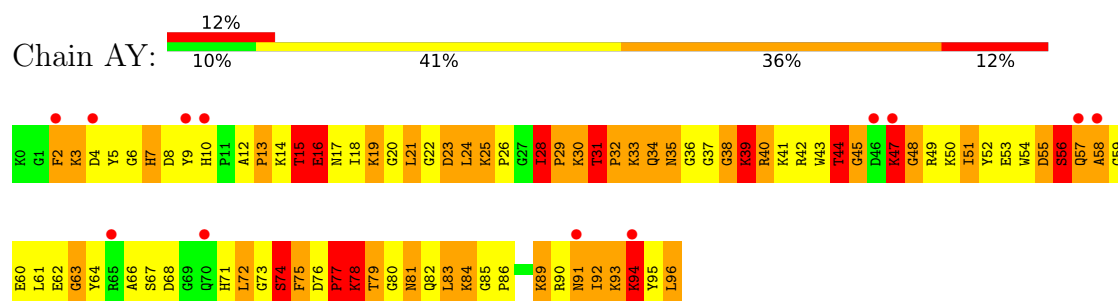
• Molecule 22: E-SITE TRNA PHE OR P-SITE TRNA PHE



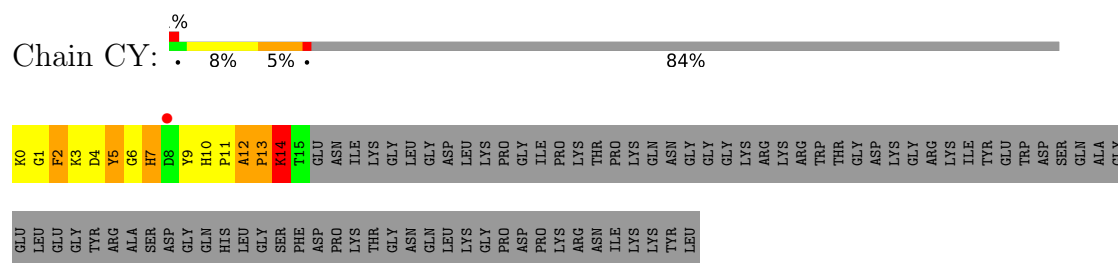
• Molecule 23: MRNA



• Molecule 24: COLICIN-E3

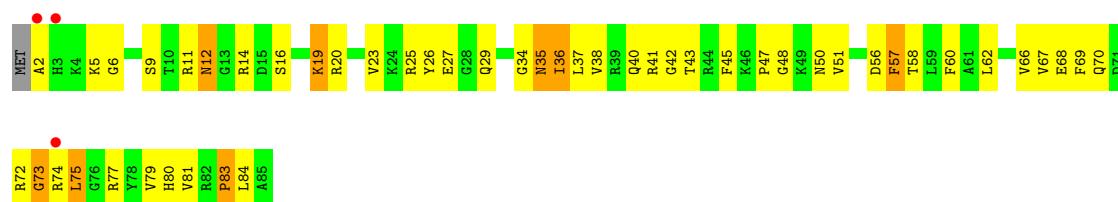


• Molecule 24: COLICIN-E3

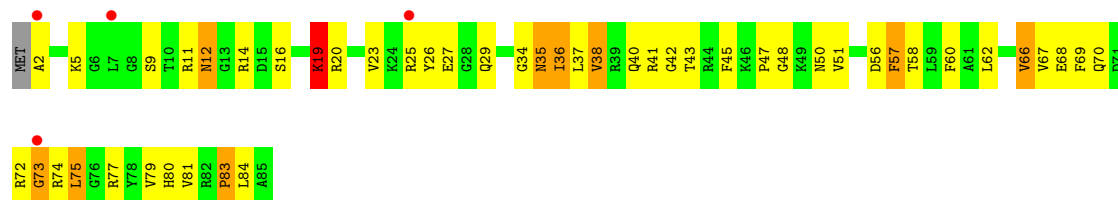
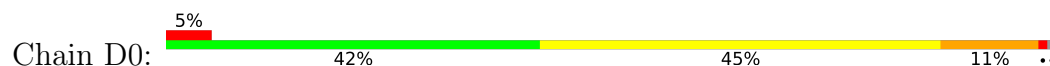


• Molecule 25: 50S RIBOSOMAL PROTEIN L27

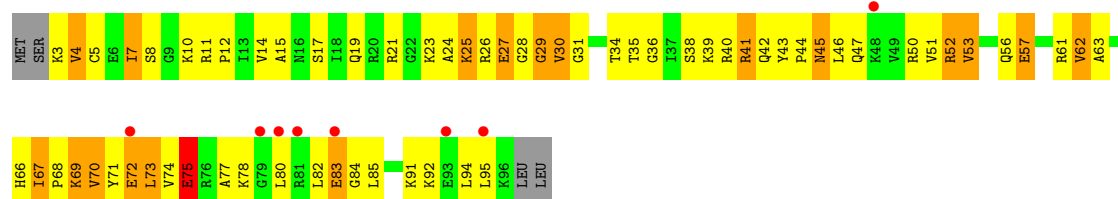




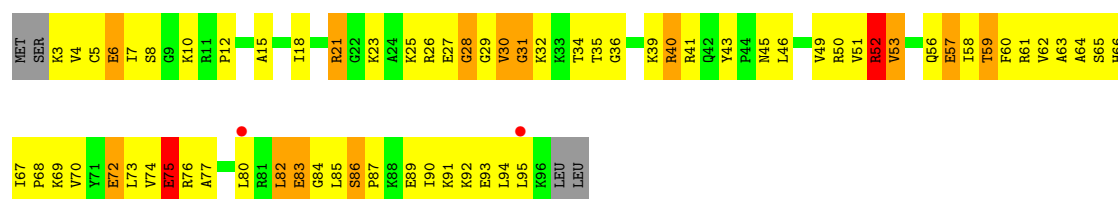
• Molecule 25: 50S RIBOSOMAL PROTEIN L27



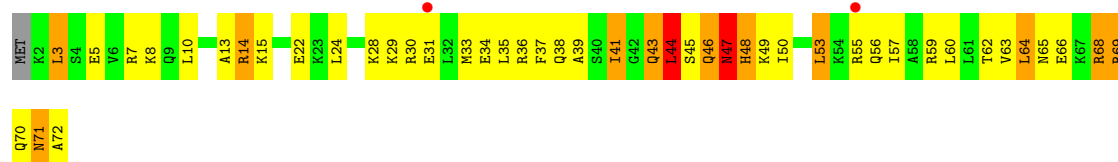
• Molecule 26: 50S RIBOSOMAL PROTEIN L28



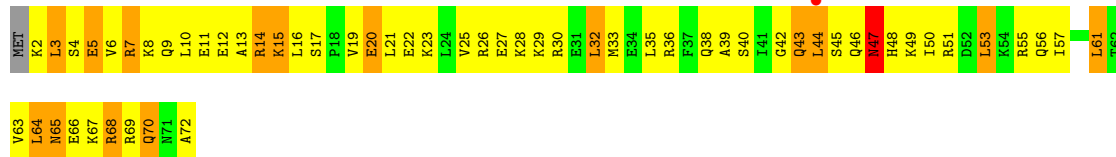
• Molecule 26: 50S RIBOSOMAL PROTEIN L28



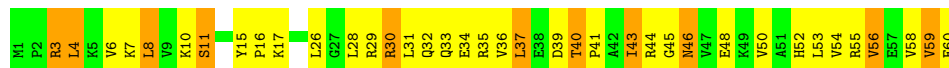
• Molecule 27: 50S RIBOSOMAL PROTEIN L29



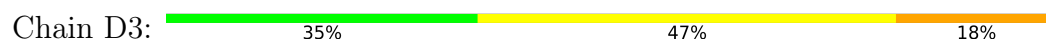
• Molecule 27: 50S RIBOSOMAL PROTEIN L29



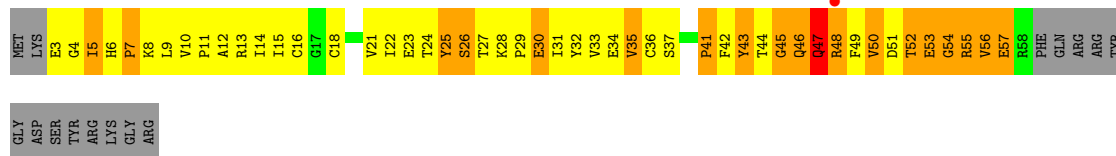
• Molecule 28: 50S RIBOSOMAL PROTEIN L30



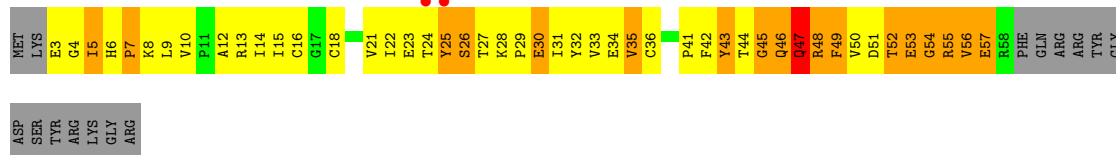
• Molecule 28: 50S RIBOSOMAL PROTEIN L30



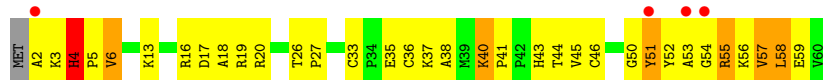
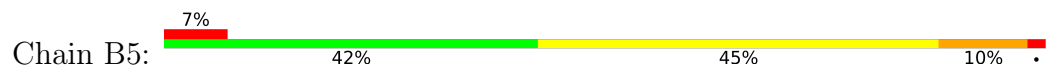
• Molecule 29: 50S RIBOSOMAL PROTEIN L31



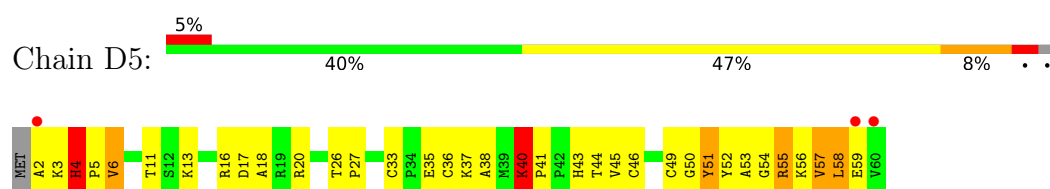
• Molecule 29: 50S RIBOSOMAL PROTEIN L31



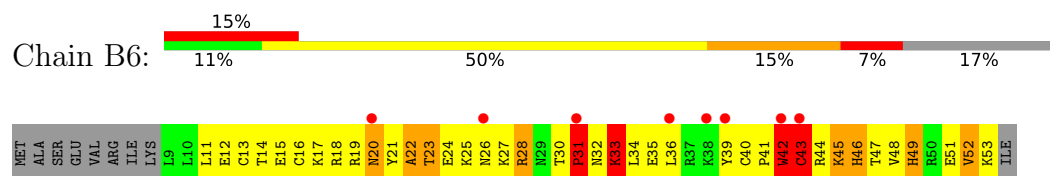
• Molecule 30: 50S RIBOSOMAL PROTEIN L32



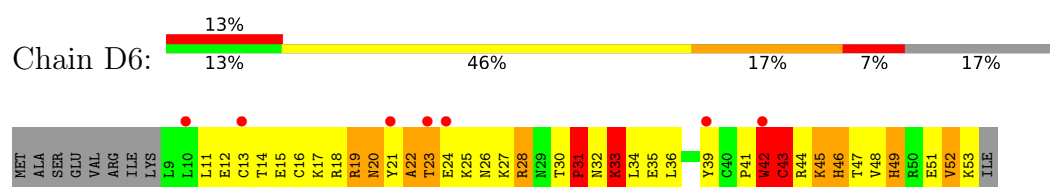
• Molecule 30: 50S RIBOSOMAL PROTEIN L32



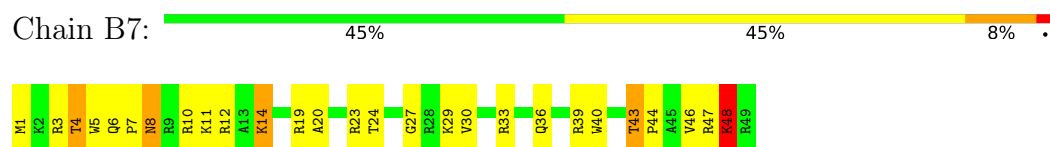
• Molecule 31: 50S RIBOSOMAL PROTEIN L33



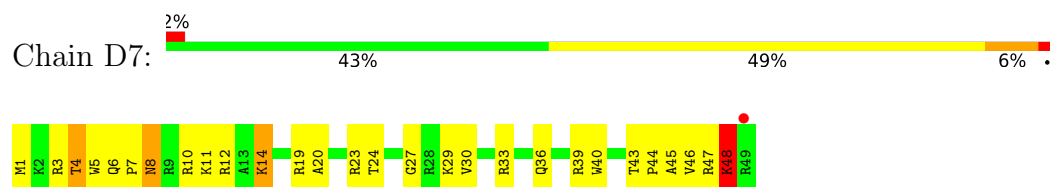
• Molecule 31: 50S RIBOSOMAL PROTEIN L33



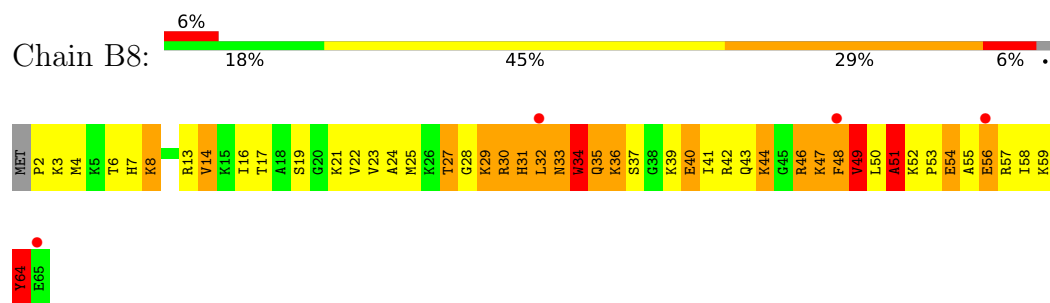
• Molecule 32: 50S RIBOSOMAL PROTEIN L34



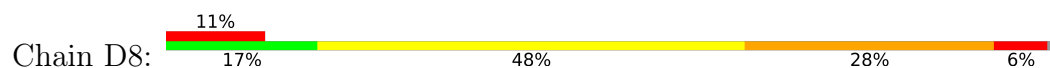
• Molecule 32: 50S RIBOSOMAL PROTEIN L34

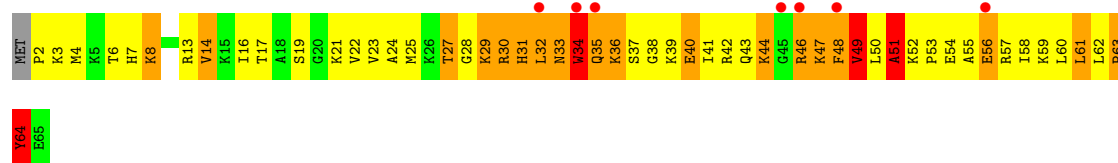


• Molecule 33: 50S RIBOSOMAL PROTEIN L35



• Molecule 33: 50S RIBOSOMAL PROTEIN L35





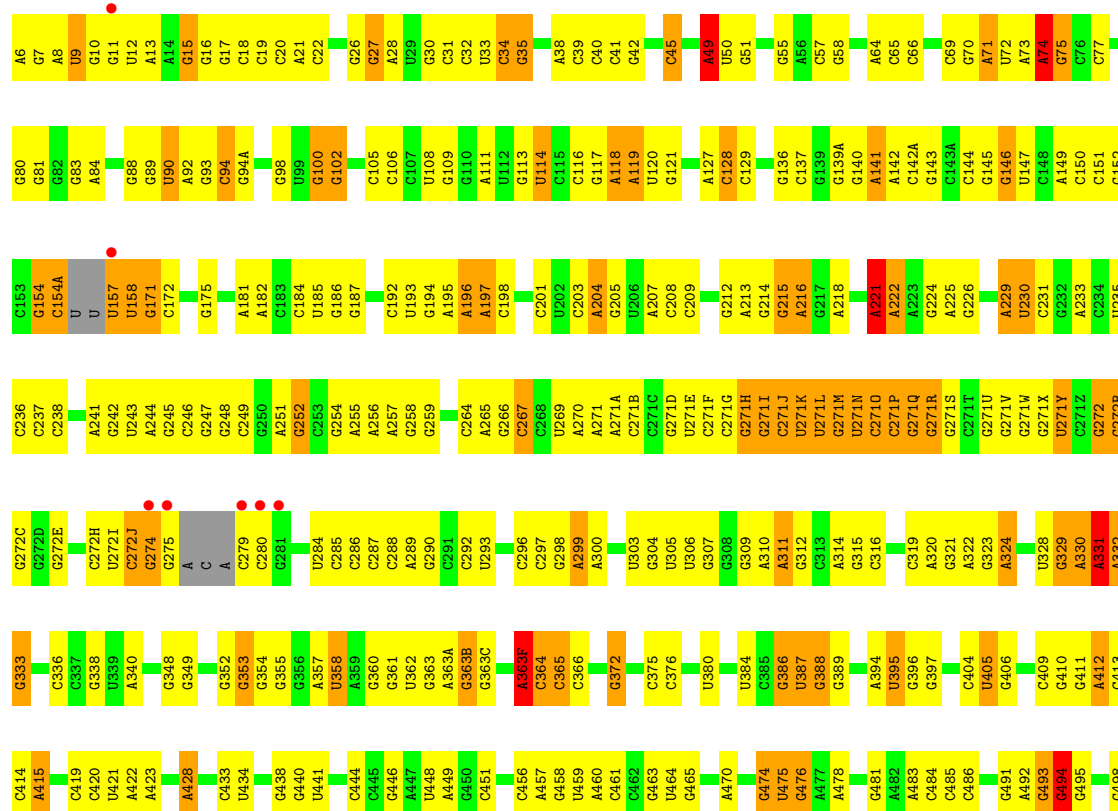
• Molecule 34: 50S RIBOSOMAL PROTEIN L36



• Molecule 34: 50S RIBOSOMAL PROTEIN L36

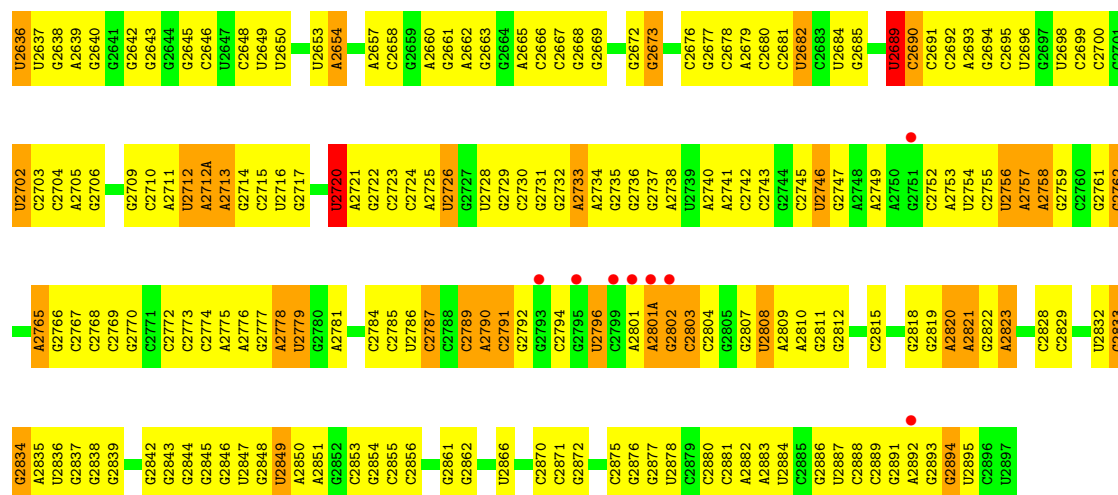


• Molecule 35: 23S ribosomal RNA

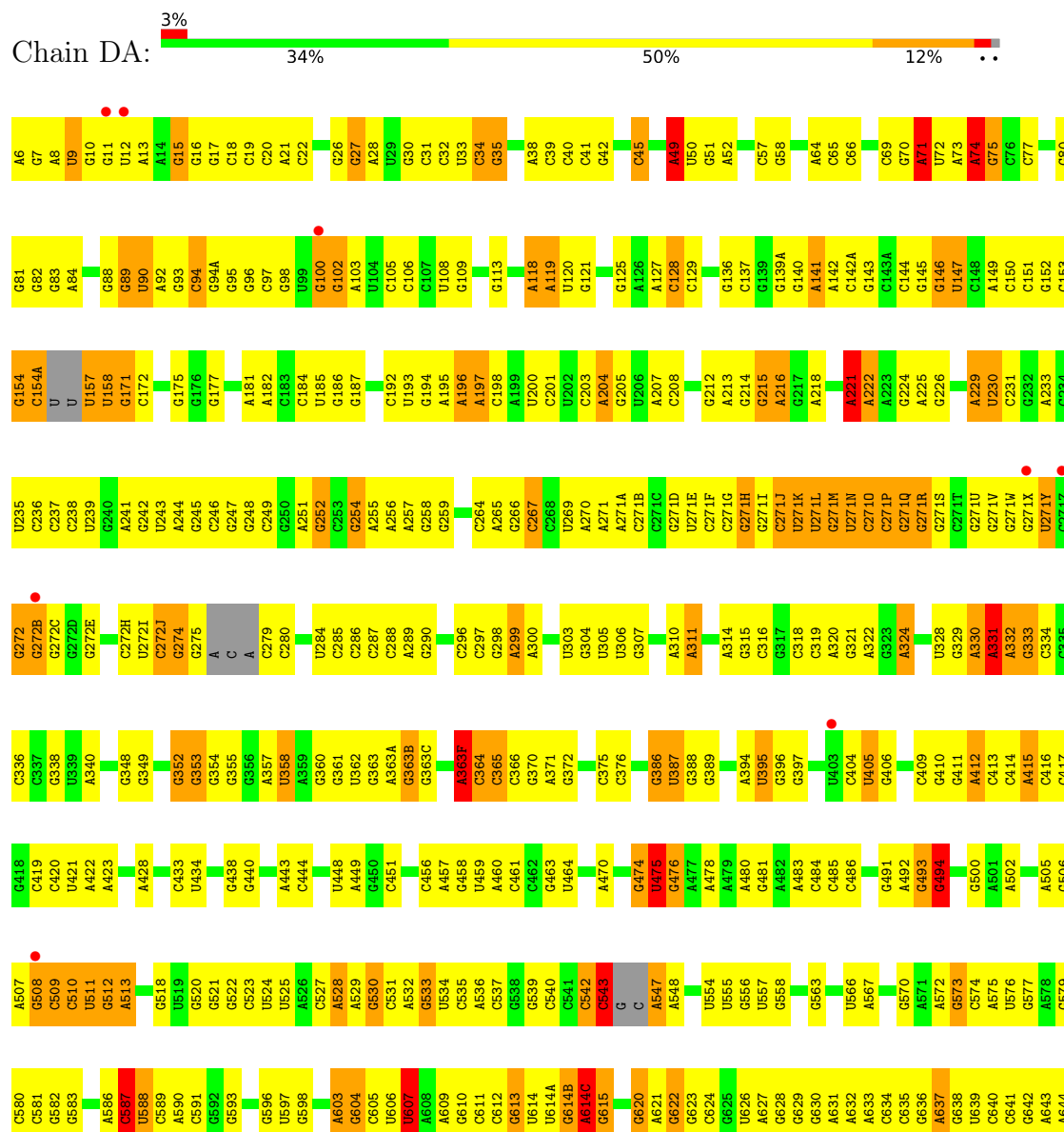


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A502	C580	C580	C646	A788	A788	A861	G927	U999	C1117	A1189	U1287	A1349	A1427	G1491
A505	C581	C581	G647	C708	A789	A863	G932	A1001	C1119	G1191	A1269	U1352	G1429	C1492
G508	C582	C582	G648	U709	G864	A864	G933	G1002	C1120	G1192	C1270	A1353	C1430	A1494
C509	C583	C583	G649	G710	C791	C865	G938	G1003	C1121	G1193	G1271	G1355	U1431	A1495
C510	C584	C584	C652	G712	A793	A866	A941	C1004	A1126	A1194	U1272	G1356	C1432	A1496
C511	C585	C585	A	G715	C796	G869	G942	C1005	U1129	C1196	U1273	G1357	U1433	C1497
C512	C586	C586	A	G716	C797	A870	U943	C1006	A1129	C1197	A1276	U1358	A1434	C1498
C513	C587	C587	C	A717	C797	G873	G944	G1011	U1130	U1198	G1277	A1359	G1435	C1499
C517	C588	C588	C	A718	A802	G874	G946	G1012	C1135	G1203	A1278	A1360	G1436	C1501
C518	C589	C589	G	C719	C805	G875		U1013	G1136	U1204	G1279	G1361	U1437	C1502
C519	C591	C591	G	C720	C806	C876	G950	G1014	G1137	A1205	G1280	C1362	A1439	U1503
C520	C592	C592	C	C721	C807	U877	G951	G1015	C1138	U1206	G1281	C1363	G1440	C1504
C521	C593	C593	C	A722	U807	A878	C952	G1016	G1139	G1207	G1282	G1364	G1441	C1505
C522	C594	C594	C	G723	G808	G879	A953	U1019	C1140	U1211	A1284	A1365	G1442	C1506
C523	C596	C596	C	G729	C812	G880	C954	A1020	U1141	U1212	G1285	G1368	G1443	A1507
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C541	G615	G615	C859	C756	G832	A899	C971	U1039	G1160	C1234	U1314	U1397	G1465	G1527
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C	G622	G622	C664	A764	C837	G906	G977	A1045	U1165	A1242	C1318	U1405	A1469	C1531
A547	G623	G623	A547			U907	G978	A1046	U1166	A1246	G1324	U1406	G1470	C1532
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U556	A627	A627	A670		G845	A910	A990	A1050	G1170	C1251	G1328	G1410	C1476	C
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U573	C635	C635	A676	C777	U851	C915	A990	U1107	G1176	C1258	G1337	C1417	U1481	C
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C573	G637	G637	C679	U779	G853	G920	C992	C1054	C1178	C1260	G1339	A1419	G1483	C
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A2411	A2411	A2274	A2274	G2187	G2117	C2039	U1964	A1885	U1739	U1739	A1641	C1559
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G2415	G2415	G2278	G2278	G2192	G2123	G2043	A1970	C1894	A1815	C1743	C1648	G1563
G2416	G2416	G2279	G2279	G2193	G2124	G2062	A1971	C1895	G1816	C1744	C1648	G1564
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A2450	A2450	G2381	G2381	U2237	G2159	C2093	C2015	C1929	G1857	C1788	A1700	C1607
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A2468	A2468	U2399	U2399	U2255	U2177	C2111	C2033	C1946	C1873	C1804	C1722	C1627
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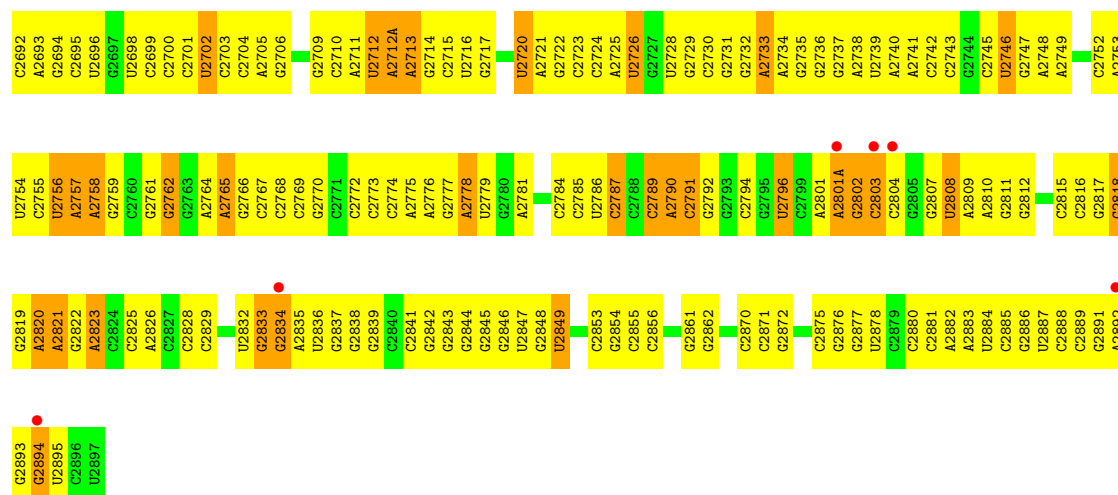


• Molecule 35: 23S ribosomal RNA

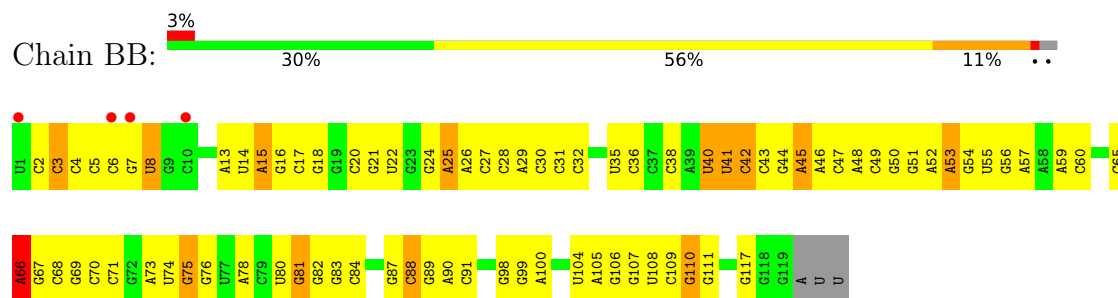




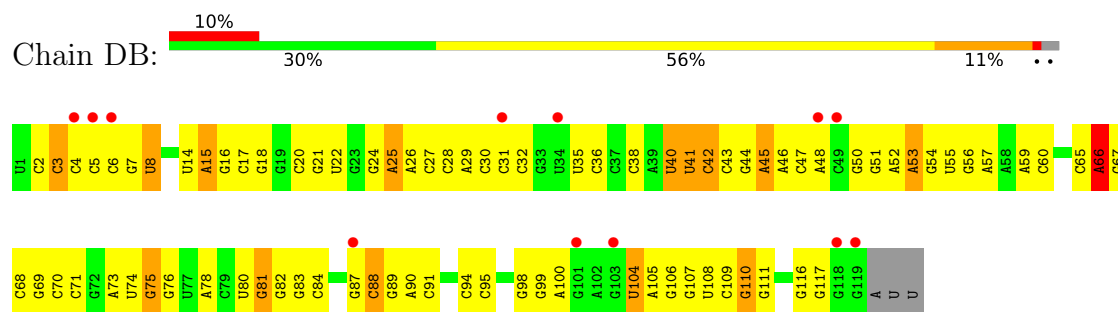
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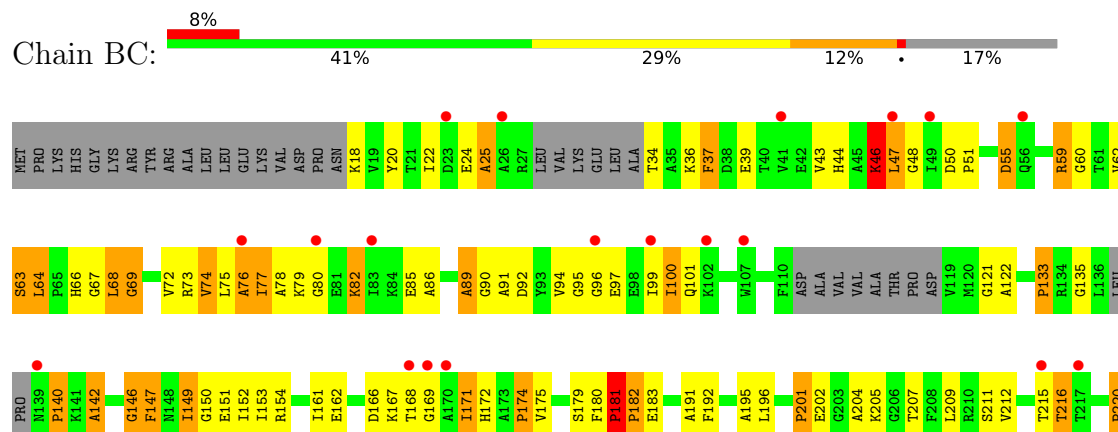
• Molecule 36: 5S ribosomal RNA



• Molecule 36: 5S ribosomal RNA

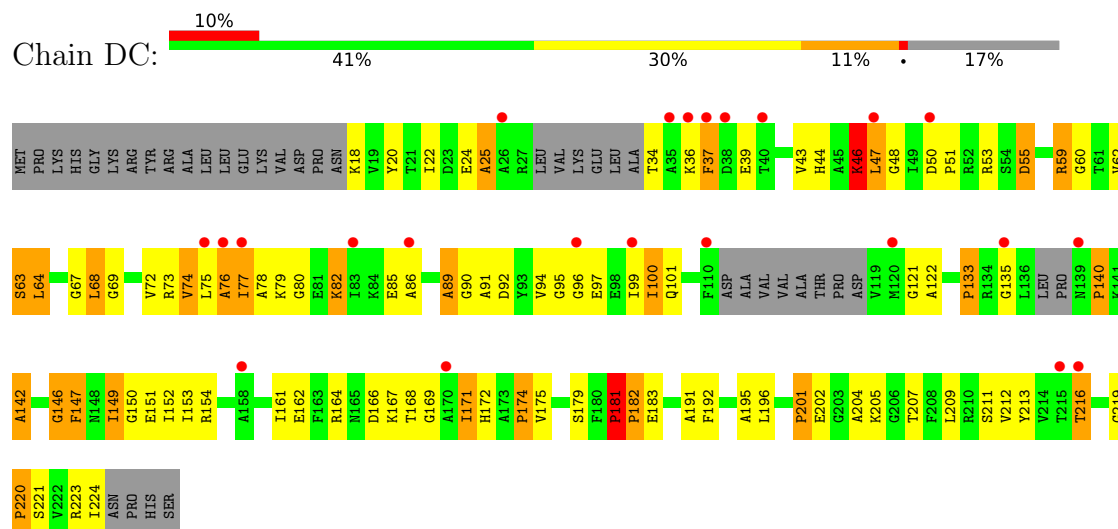


• Molecule 37: 50S RIBOSOMAL PROTEIN L1

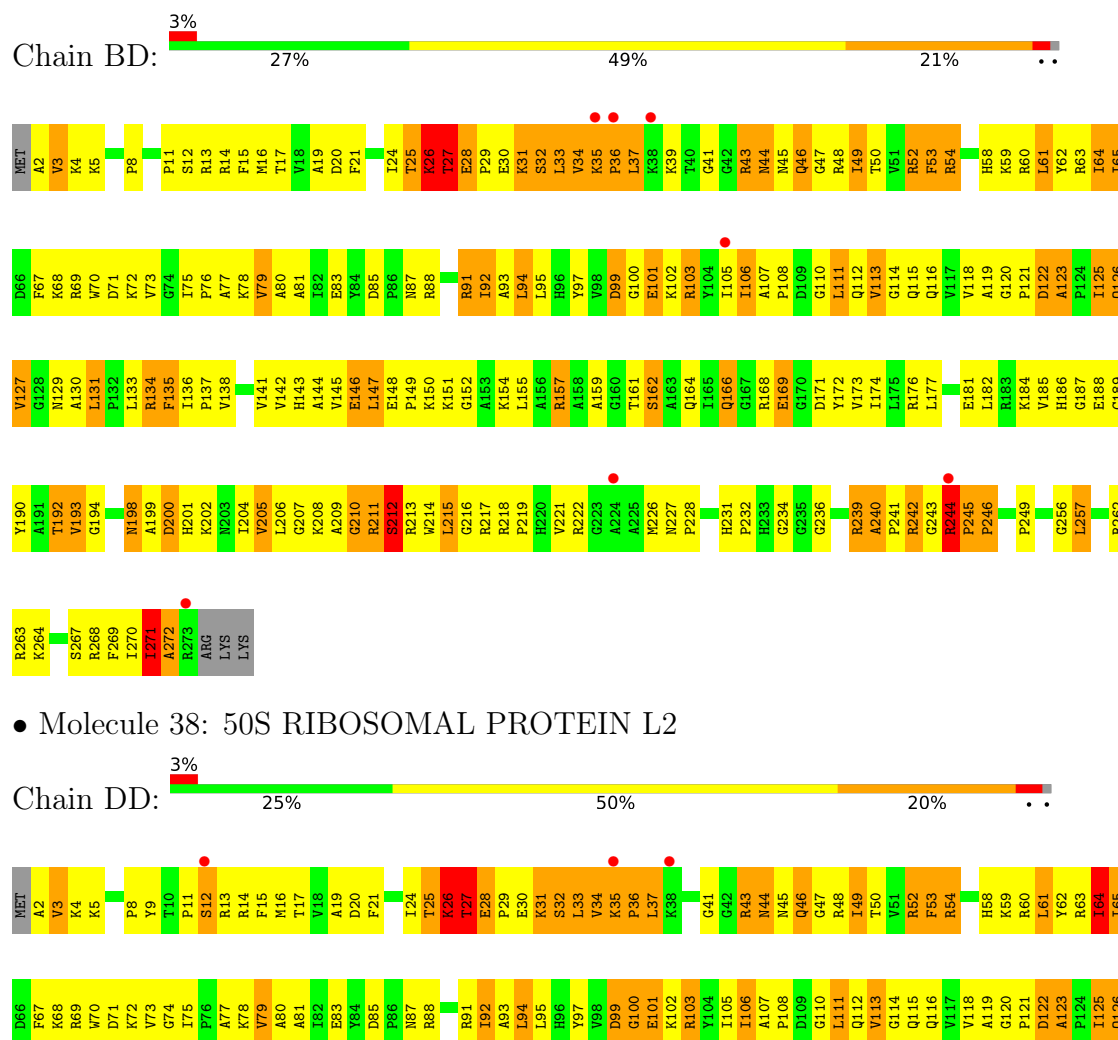




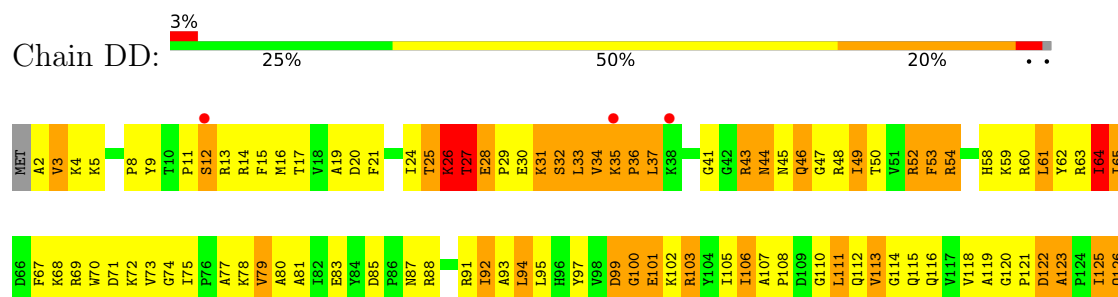
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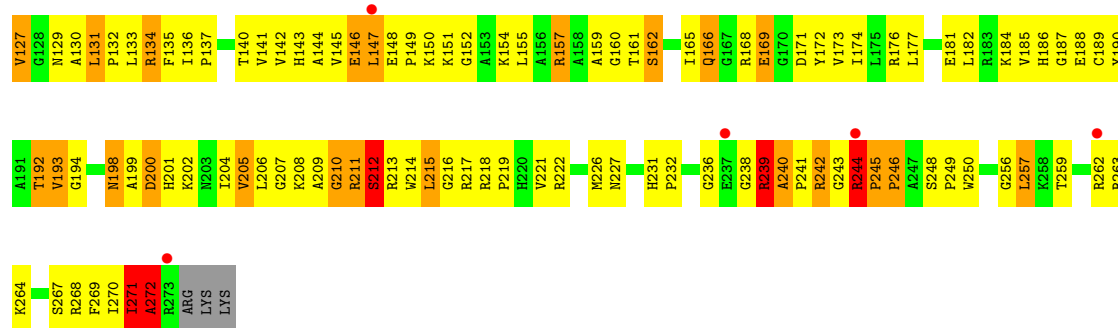


• Molecule 38: 50S RIBOSOMAL PROTEIN L2

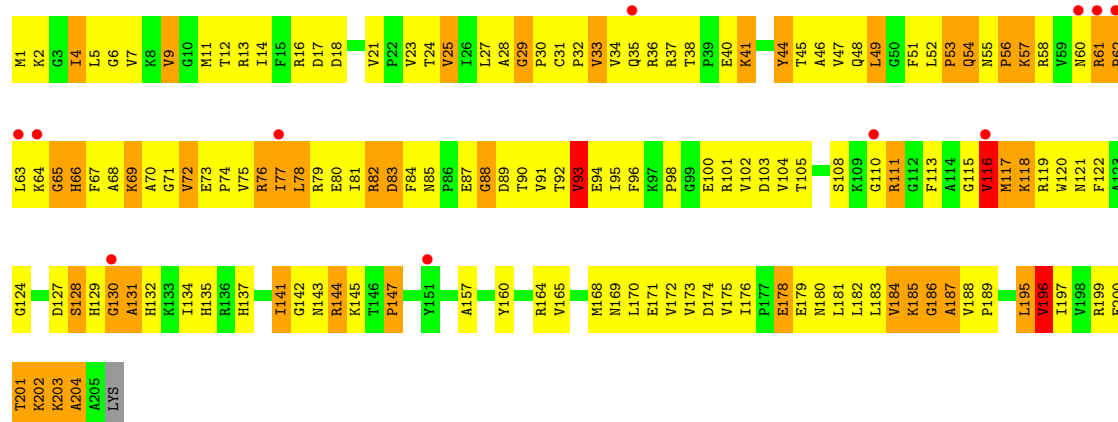


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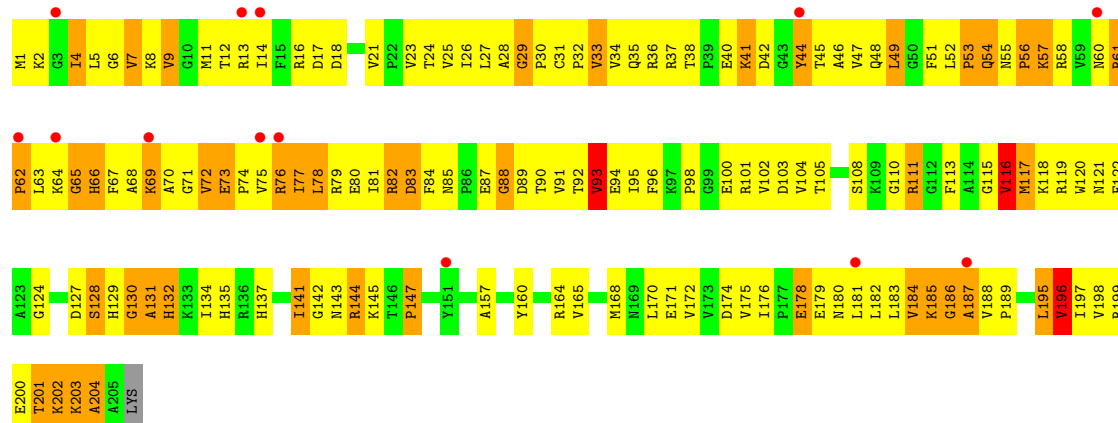




• Molecule 39: 50S RIBOSOMAL PROTEIN L3

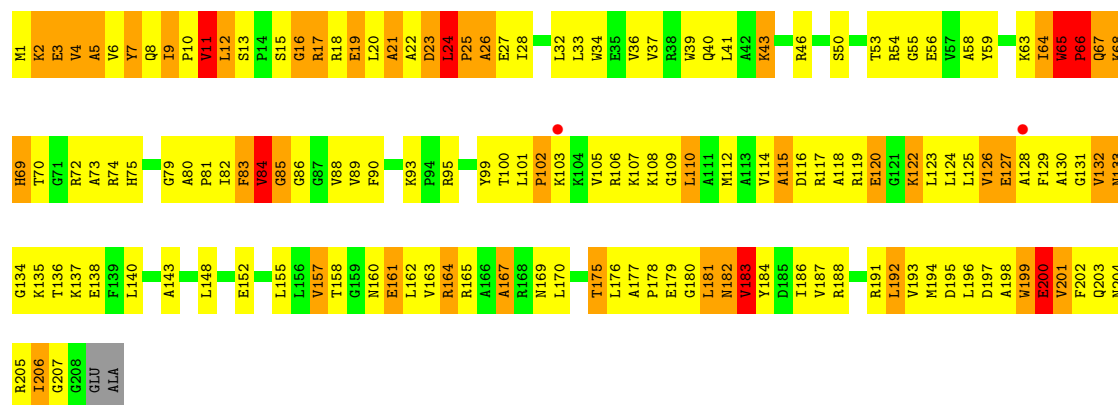


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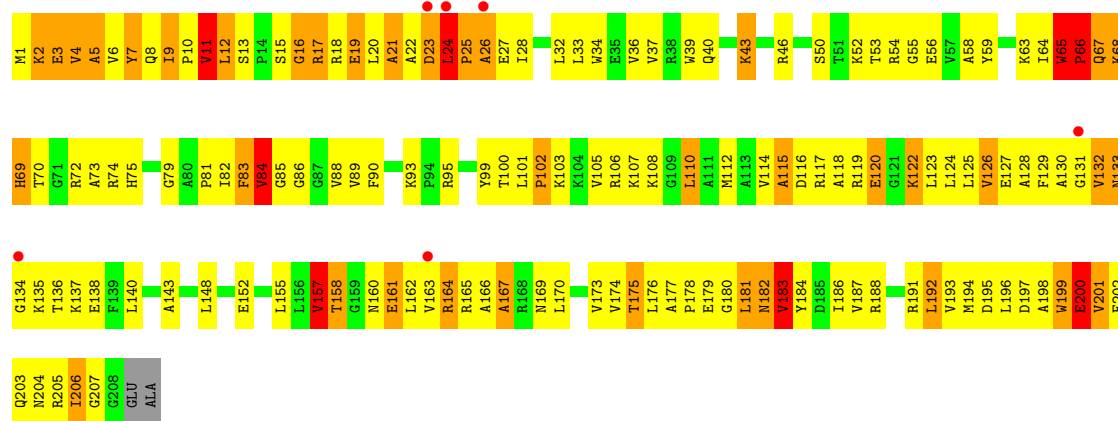


• Molecule 40: 50S RIBOSOMAL PROTEIN L4

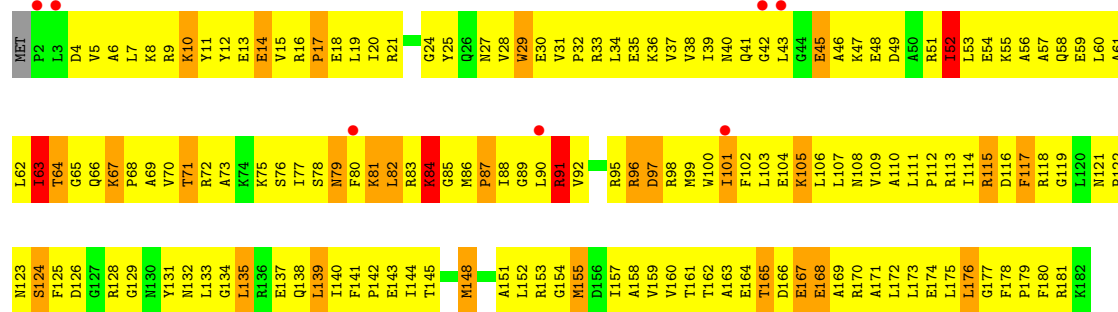




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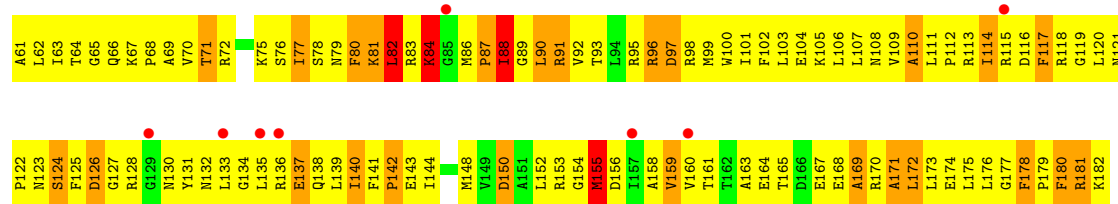


• Molecule 41: 50S RIBOSOMAL PROTEIN L5

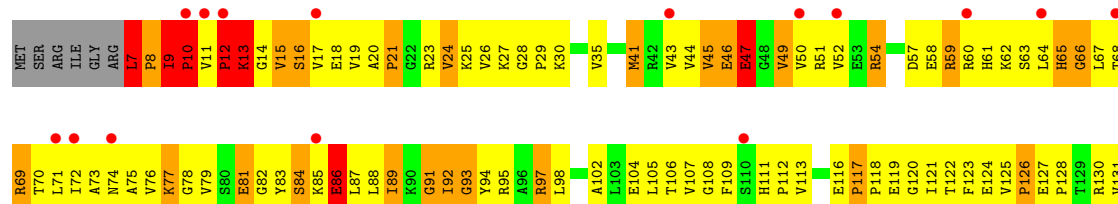
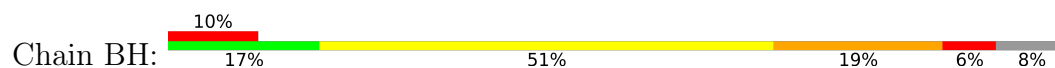


• Molecule 41: 50S RIBOSOMAL PROTEIN L5

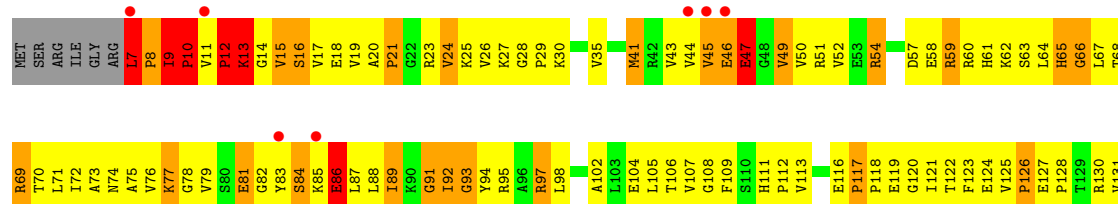
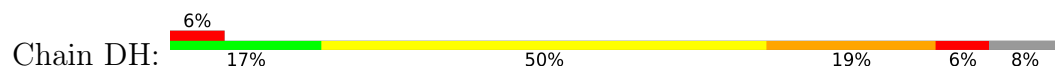




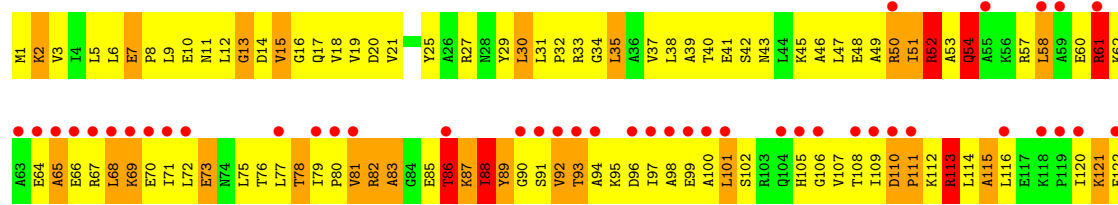
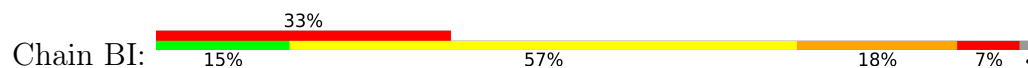
• Molecule 42: 50S RIBOSOMAL PROTEIN L6



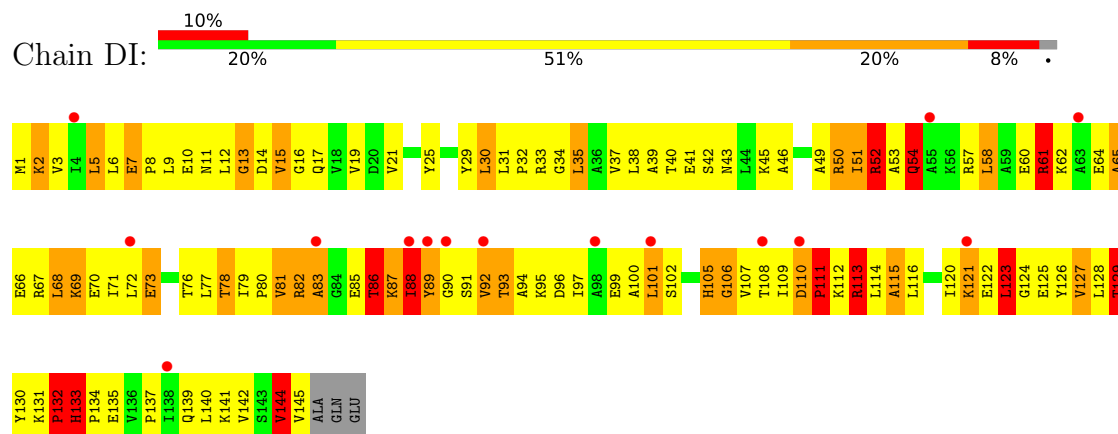
• Molecule 42: 50S RIBOSOMAL PROTEIN L6



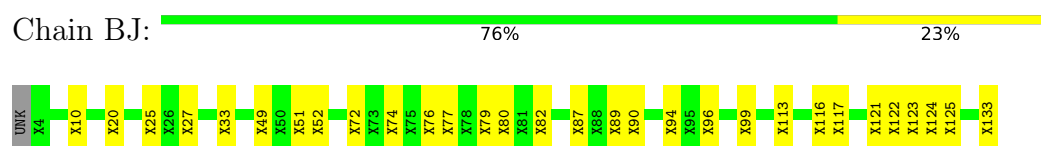
• Molecule 43: 50S RIBOSOMAL PROTEIN L9



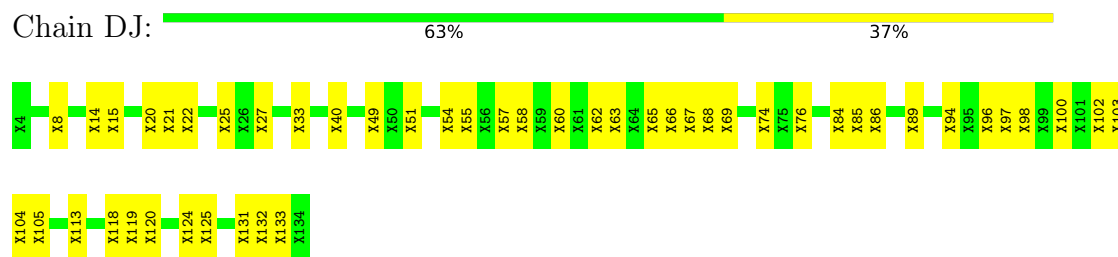
- Molecule 43: 50S RIBOSOMAL PROTEIN L9



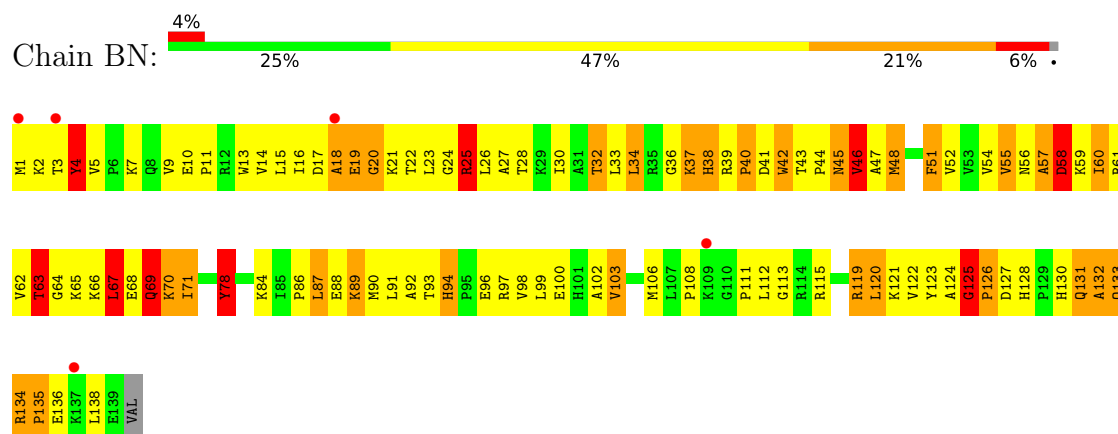
- Molecule 44: 50S RIBOSOMAL PROTEIN L10



- Molecule 44: 50S RIBOSOMAL PROTEIN L10

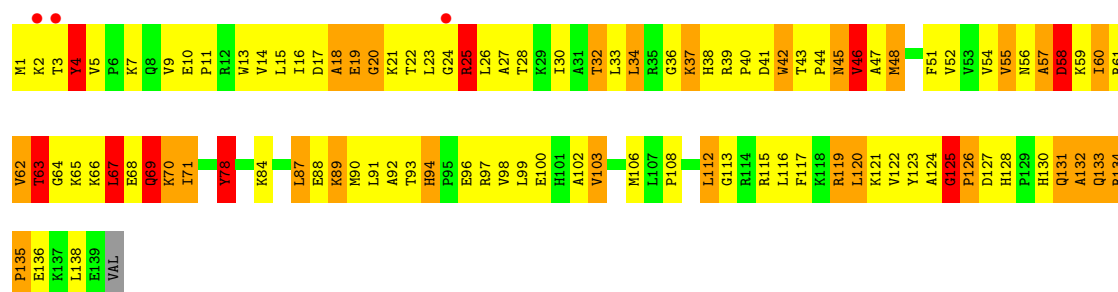


- Molecule 45: 50S RIBOSOMAL PROTEIN L13

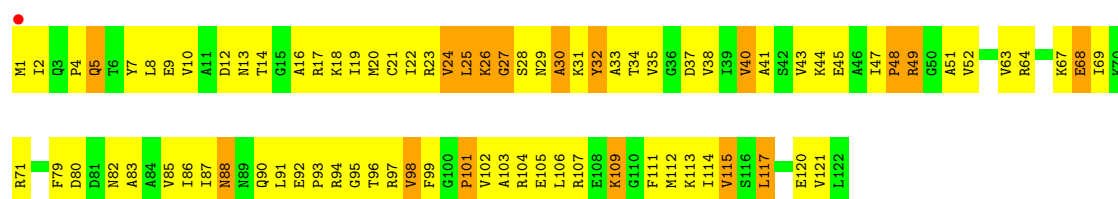


- Molecule 45: 50S RIBOSOMAL PROTEIN L13

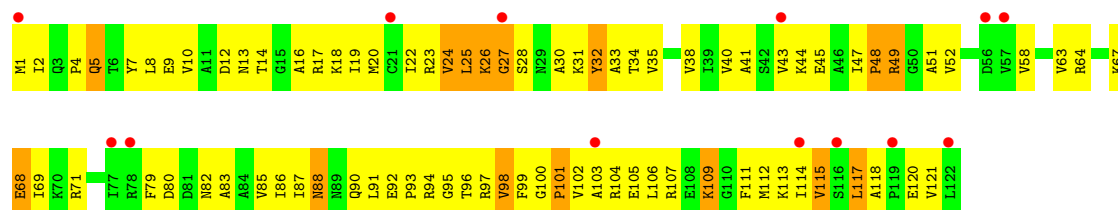




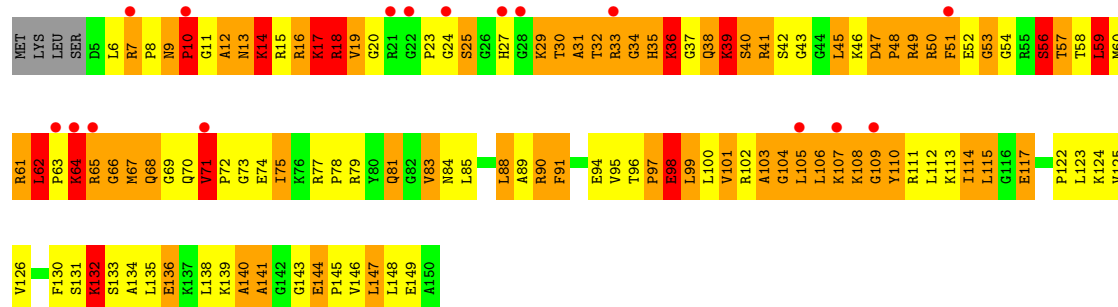
• Molecule 46: 50S RIBOSOMAL PROTEIN L14



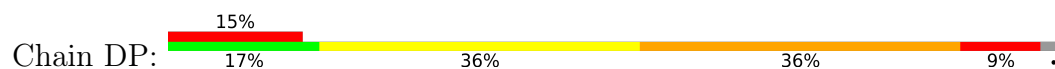
• Molecule 46: 50S RIBOSOMAL PROTEIN L14

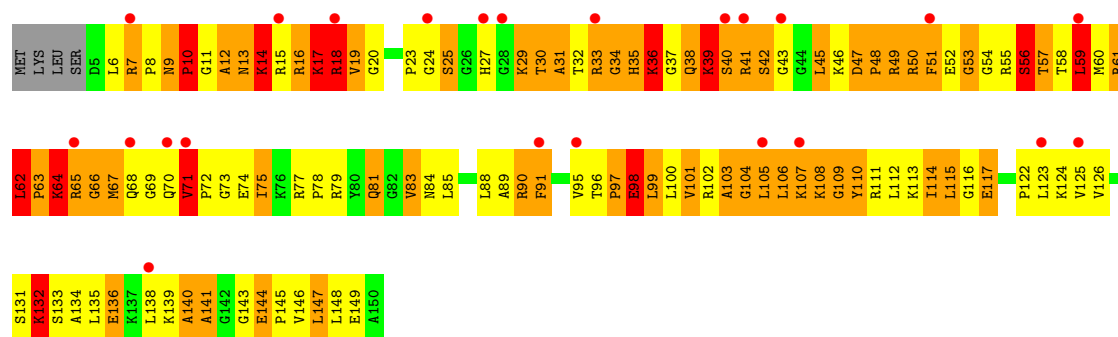


• Molecule 47: 50S RIBOSOMAL PROTEIN L15

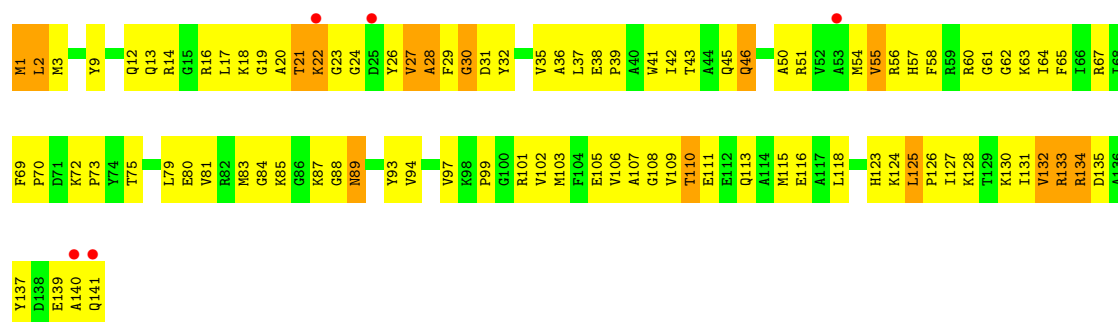


• Molecule 47: 50S RIBOSOMAL PROTEIN L15

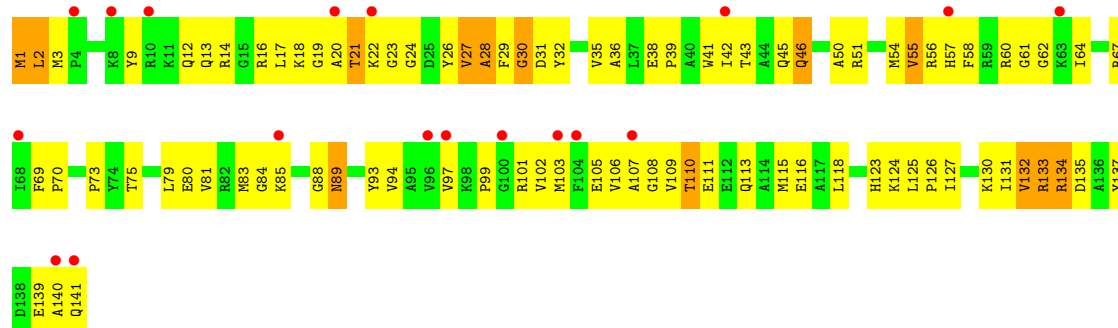




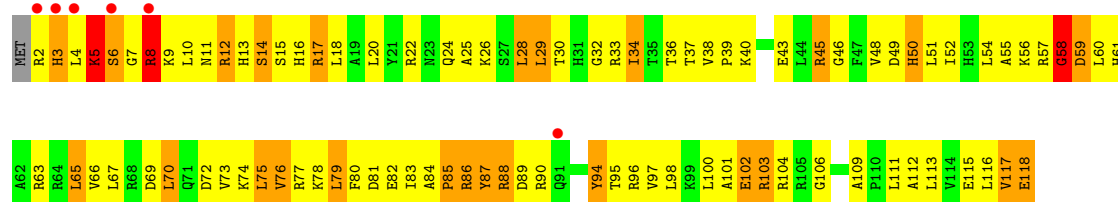
• Molecule 48: 50S RIBOSOMAL PROTEIN L16



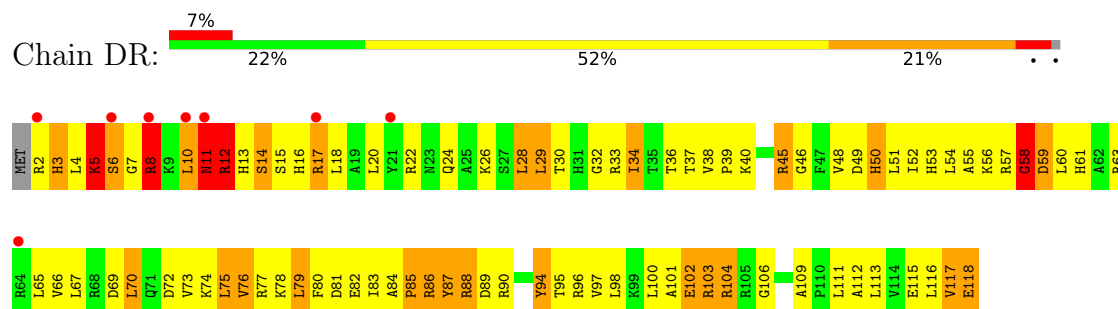
• Molecule 48: 50S RIBOSOMAL PROTEIN L16



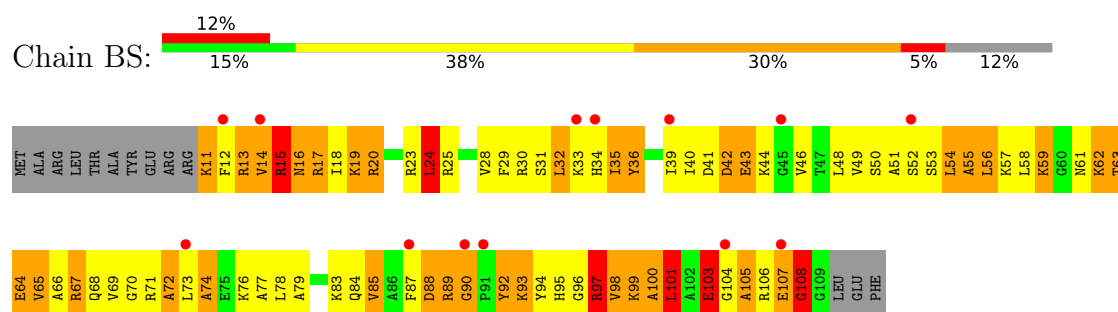
• Molecule 49: 50S RIBOSOMAL PROTEIN L17



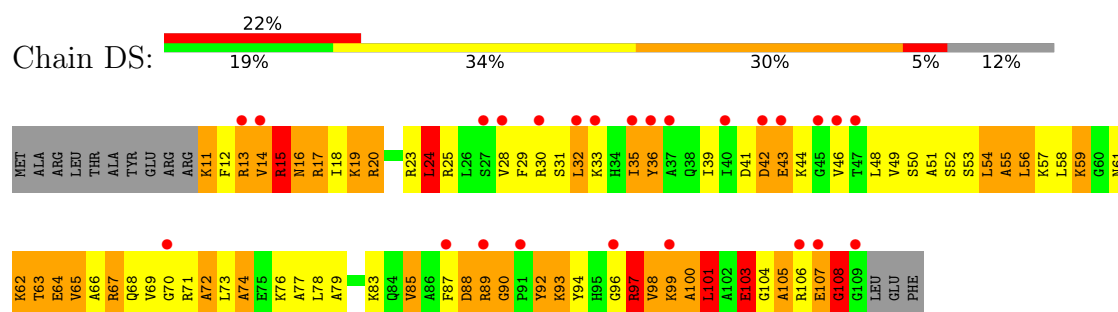
● Molecule 49: 50S RIBOSOMAL PROTEIN L17



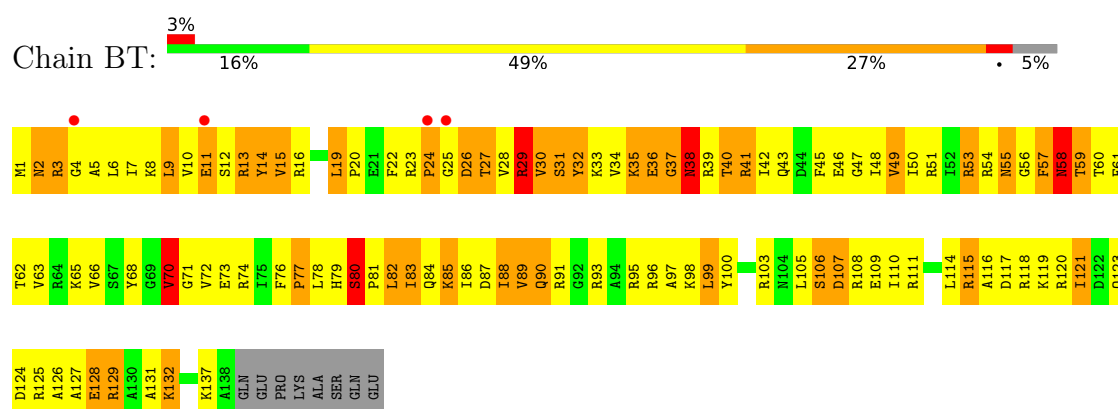
● Molecule 50: 50S RIBOSOMAL PROTEIN L18



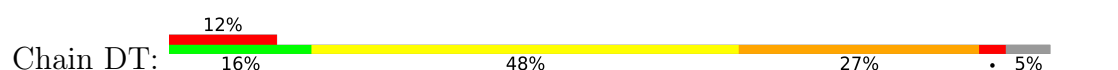
● Molecule 50: 50S RIBOSOMAL PROTEIN L18

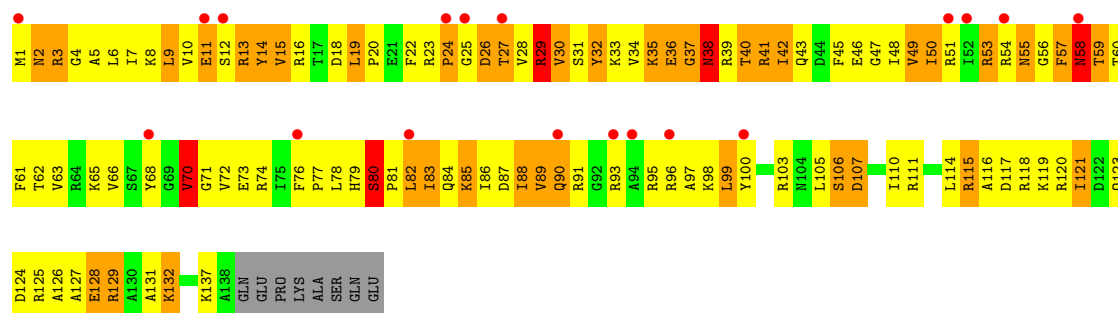


● Molecule 51: 50S RIBOSOMAL PROTEIN L19

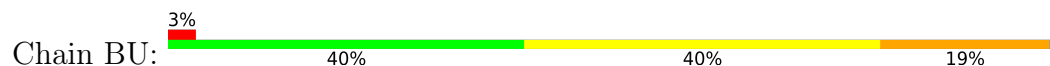


● Molecule 51: 50S RIBOSOMAL PROTEIN L19

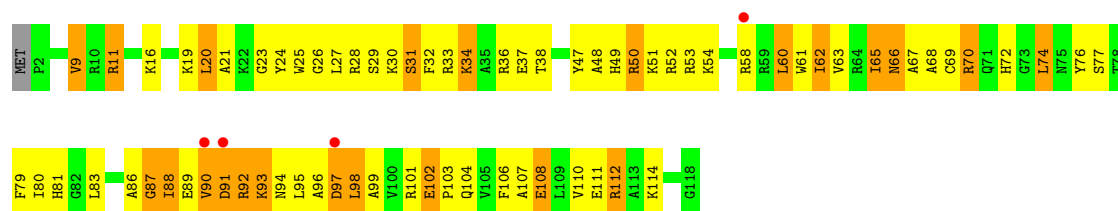




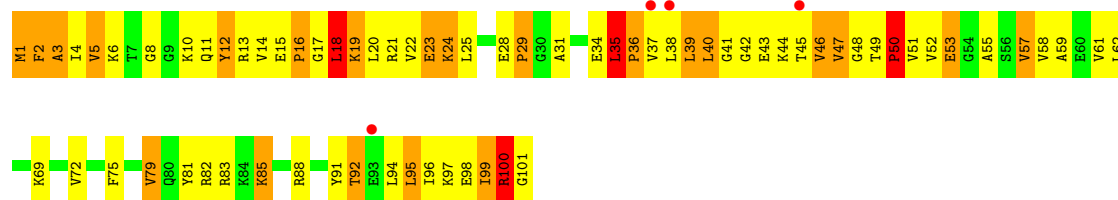
• Molecule 52: 50S RIBOSOMAL PROTEIN L20



• Molecule 52: 50S RIBOSOMAL PROTEIN L20

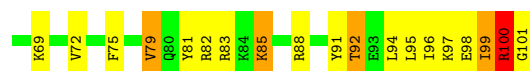


• Molecule 53: 50S RIBOSOMAL PROTEIN L21

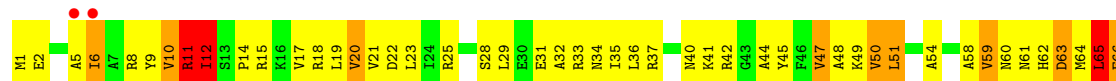


• Molecule 53: 50S RIBOSOMAL PROTEIN L21

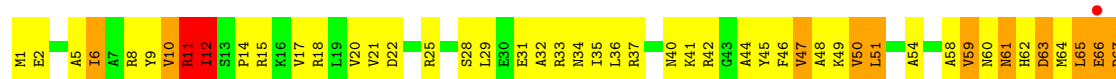




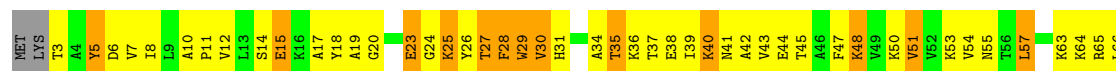
• Molecule 54: 50S RIBOSOMAL PROTEIN L22



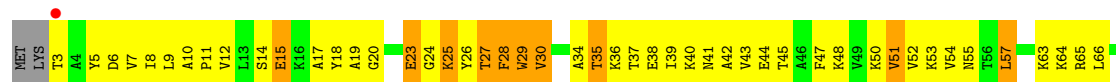
• Molecule 54: 50S RIBOSOMAL PROTEIN L22



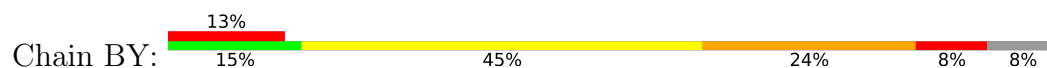
• Molecule 55: 50S RIBOSOMAL PROTEIN L23

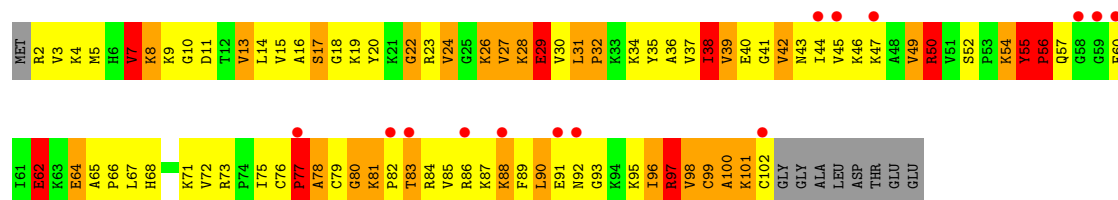


• Molecule 55: 50S RIBOSOMAL PROTEIN L23

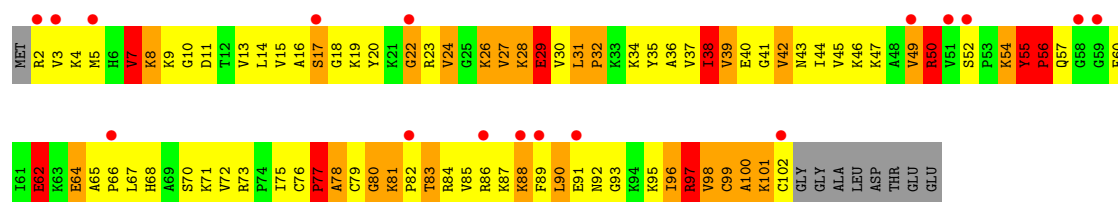
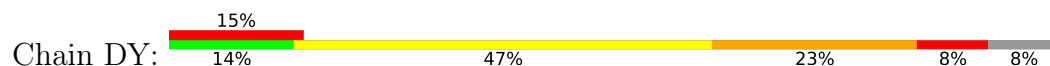


• Molecule 56: 50S RIBOSOMAL PROTEIN L24

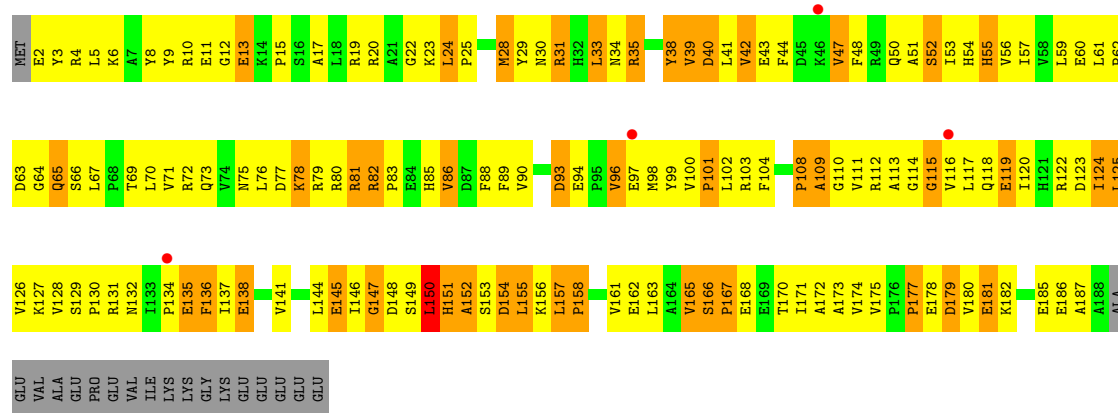
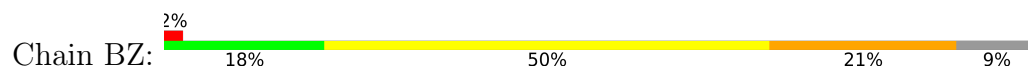




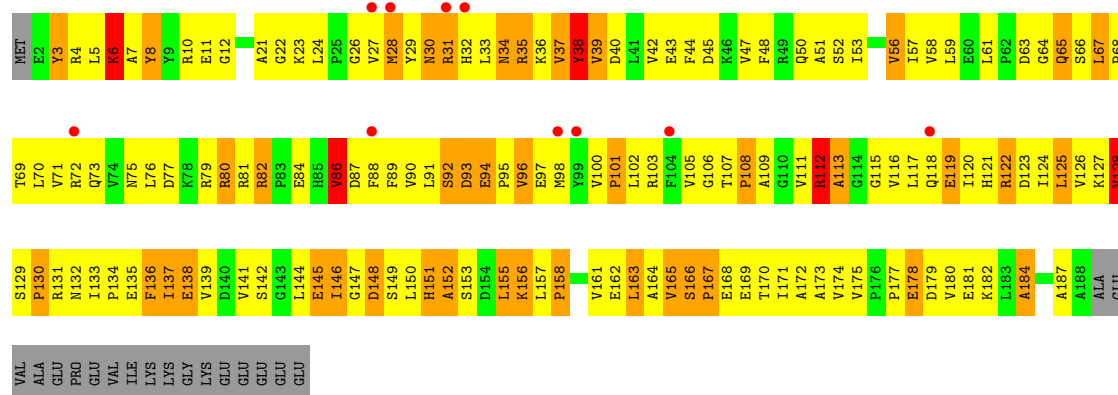
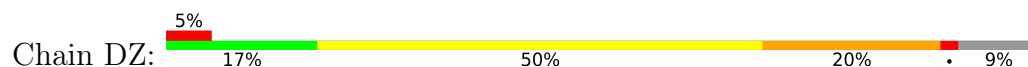
• Molecule 56: 50S RIBOSOMAL PROTEIN L24



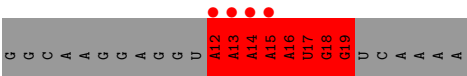
• Molecule 57: 50S RIBOSOMAL PROTEIN L25



• Molecule 57: 50S RIBOSOMAL PROTEIN L25



● Molecule 58: MRNA



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	212.04Å 453.51Å 616.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.53 – 3.20 44.53 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.4 (44.53-3.20) 99.4 (44.53-3.20)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.81 (at 3.19Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.228 , 0.270 0.230 , 0.271	Depositor DCC
R_{free} test set	44837 reflections (4.67%)	wwPDB-VP
Wilson B-factor (Å ²)	87.1	Xtriage
Anisotropy	0.142	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 105.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	296762	wwPDB-VP
Average B, all atoms (Å ²)	113.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.58% 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: MG, ZN, A3P

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	0.41	0/36252	0.60	23/56580 (0.0%)
1	CA	0.41	0/36253	0.61	29/56582 (0.1%)
2	AB	0.38	1/1936 (0.1%)	0.96	13/2611 (0.5%)
2	CB	0.38	1/1936 (0.1%)	0.96	10/2611 (0.4%)
3	AC	0.38	1/1637 (0.1%)	0.88	6/2207 (0.3%)
3	CC	0.38	1/1637 (0.1%)	0.87	6/2207 (0.3%)
4	AD	0.44	1/1722 (0.1%)	1.01	13/2306 (0.6%)
4	CD	0.41	1/1722 (0.1%)	0.97	10/2306 (0.4%)
5	AE	0.44	1/1163 (0.1%)	0.96	3/1566 (0.2%)
5	CE	0.43	1/1163 (0.1%)	0.95	5/1566 (0.3%)
6	AF	0.38	0/856	0.96	1/1154 (0.1%)
6	CF	0.40	0/856	0.96	2/1154 (0.2%)
7	AG	0.34	0/1276	0.93	4/1709 (0.2%)
7	CG	0.34	0/1276	0.92	6/1709 (0.4%)
8	AH	0.38	0/1136	0.94	2/1527 (0.1%)
8	CH	0.36	0/1136	0.94	2/1527 (0.1%)
9	AI	0.34	0/1027	0.90	2/1372 (0.1%)
9	CI	0.34	0/1027	0.90	2/1372 (0.1%)
10	AJ	0.44	1/808 (0.1%)	0.91	1/1087 (0.1%)
10	CJ	0.45	1/808 (0.1%)	0.90	1/1087 (0.1%)
11	AK	0.40	0/900	0.99	6/1213 (0.5%)
11	CK	0.37	0/900	0.94	5/1213 (0.4%)
12	AL	0.49	1/987 (0.1%)	1.15	12/1322 (0.9%)
12	CL	0.45	1/987 (0.1%)	1.16	12/1322 (0.9%)
13	AM	0.39	1/941 (0.1%)	1.01	9/1258 (0.7%)
13	CM	0.40	1/941 (0.1%)	0.99	9/1258 (0.7%)
14	AN	0.35	0/501	0.91	1/664 (0.2%)
14	CN	0.36	0/501	0.92	1/664 (0.2%)
15	AO	0.42	0/745	0.95	1/992 (0.1%)
15	CO	0.41	0/745	0.95	1/992 (0.1%)
16	AP	0.46	1/717 (0.1%)	0.96	4/965 (0.4%)
16	CP	0.43	1/717 (0.1%)	0.93	5/965 (0.5%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AQ	0.44	1/837 (0.1%)	0.93	3/1119 (0.3%)
17	CQ	0.39	1/837 (0.1%)	0.93	3/1119 (0.3%)
18	AR	0.38	0/579	0.98	4/768 (0.5%)
18	CR	0.38	0/579	0.99	4/768 (0.5%)
19	AS	0.42	1/685 (0.1%)	0.79	1/922 (0.1%)
19	CS	0.44	1/685 (0.1%)	0.79	1/922 (0.1%)
20	AT	0.39	0/765	0.98	3/1007 (0.3%)
20	CT	0.33	0/765	0.97	3/1007 (0.3%)
21	AU	0.55	1/213 (0.5%)	0.76	0/279
21	CU	0.56	1/213 (0.5%)	0.77	0/279
22	AV	1.11	20/1832 (1.1%)	1.31	26/2855 (0.9%)
22	AW	0.49	0/1832	0.59	1/2855 (0.0%)
22	CV	0.44	1/1832 (0.1%)	0.67	1/2855 (0.0%)
22	CW	0.47	0/1832	0.58	0/2855
23	AX	1.81	11/383 (2.9%)	3.39	69/595 (11.6%)
24	AY	1.64	12/790 (1.5%)	2.07	47/1055 (4.5%)
24	CY	1.27	1/132 (0.8%)	1.62	2/177 (1.1%)
25	B0	0.45	0/671	0.98	1/892 (0.1%)
25	D0	0.44	0/671	0.97	3/892 (0.3%)
26	B1	0.63	1/741 (0.1%)	1.15	6/986 (0.6%)
26	D1	0.62	1/741 (0.1%)	1.15	5/986 (0.5%)
27	B2	0.45	0/600	1.09	5/793 (0.6%)
27	D2	0.61	0/600	1.06	4/793 (0.5%)
28	B3	0.57	1/473 (0.2%)	1.03	2/636 (0.3%)
28	D3	0.54	1/473 (0.2%)	1.05	3/636 (0.5%)
29	B4	0.52	1/444 (0.2%)	0.95	1/602 (0.2%)
29	D4	0.54	1/444 (0.2%)	0.96	1/602 (0.2%)
30	B5	0.59	0/473	1.09	2/639 (0.3%)
30	D5	0.62	0/473	1.12	3/639 (0.5%)
31	B6	0.53	1/387 (0.3%)	0.90	2/517 (0.4%)
31	D6	0.51	1/387 (0.3%)	0.90	2/517 (0.4%)
32	B7	0.66	1/427 (0.2%)	1.06	3/563 (0.5%)
32	D7	0.76	1/427 (0.2%)	1.06	3/563 (0.5%)
33	B8	0.72	1/516 (0.2%)	1.34	11/681 (1.6%)
33	D8	0.68	1/516 (0.2%)	1.33	10/681 (1.5%)
34	B9	0.38	0/302	1.03	1/397 (0.3%)
34	D9	0.42	0/302	1.03	1/397 (0.3%)
35	BA	0.48	28/67715 (0.0%)	0.73	120/105714 (0.1%)
35	DA	0.48	11/67714 (0.0%)	0.73	102/105710 (0.1%)
36	BB	0.39	0/2853	0.61	0/4451
36	DB	0.39	0/2853	0.61	0/4451
37	BC	0.49	1/1145 (0.1%)	0.97	7/1556 (0.4%)
37	DC	0.49	1/1145 (0.1%)	0.98	7/1556 (0.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	BD	0.62	0/2155	1.20	18/2907 (0.6%)
38	DD	0.65	2/2155 (0.1%)	1.20	15/2907 (0.5%)
39	BE	0.58	1/1597 (0.1%)	1.14	12/2155 (0.6%)
39	DE	0.56	1/1597 (0.1%)	1.16	13/2155 (0.6%)
40	BF	0.60	1/1659 (0.1%)	1.17	15/2246 (0.7%)
40	DF	0.62	1/1659 (0.1%)	1.17	14/2246 (0.6%)
41	BG	0.38	0/1498	0.94	4/2013 (0.2%)
41	DG	0.39	0/1498	0.96	7/2013 (0.3%)
42	BH	0.88	9/1285 (0.7%)	1.20	16/1741 (0.9%)
42	DH	0.89	9/1285 (0.7%)	1.20	16/1741 (0.9%)
43	BI	0.51	1/1140 (0.1%)	1.13	19/1543 (1.2%)
43	DI	0.51	1/1140 (0.1%)	1.14	20/1543 (1.3%)
45	BN	0.55	1/1132 (0.1%)	1.16	12/1527 (0.8%)
45	DN	0.58	1/1132 (0.1%)	1.18	12/1527 (0.8%)
46	BO	0.55	0/943	1.04	6/1269 (0.5%)
46	DO	0.49	0/943	1.03	5/1269 (0.4%)
47	BP	0.72	0/1131	1.47	23/1504 (1.5%)
47	DP	0.67	0/1131	1.46	24/1504 (1.6%)
48	BQ	0.49	0/1143	1.03	7/1527 (0.5%)
48	DQ	0.46	0/1143	1.02	5/1527 (0.3%)
49	BR	0.52	0/974	0.98	4/1302 (0.3%)
49	DR	0.99	6/974 (0.6%)	1.22	14/1302 (1.1%)
50	BS	0.45	1/779 (0.1%)	0.98	4/1038 (0.4%)
50	DS	0.45	1/779 (0.1%)	0.97	4/1038 (0.4%)
51	BT	0.56	2/1156 (0.2%)	1.16	12/1544 (0.8%)
51	DT	0.49	1/1156 (0.1%)	1.13	13/1544 (0.8%)
52	BU	0.53	0/975	1.05	6/1297 (0.5%)
52	DU	0.62	0/975	1.08	6/1297 (0.5%)
53	BV	0.48	0/790	1.05	3/1057 (0.3%)
53	DV	0.56	0/790	1.07	3/1057 (0.3%)
54	BW	0.60	0/907	1.10	6/1216 (0.5%)
54	DW	0.62	0/907	1.11	6/1216 (0.5%)
55	BX	0.60	1/740 (0.1%)	1.07	6/995 (0.6%)
55	DX	0.68	1/740 (0.1%)	1.09	4/995 (0.4%)
56	BY	0.59	1/789 (0.1%)	1.21	9/1053 (0.9%)
56	DY	0.63	1/789 (0.1%)	1.22	8/1053 (0.8%)
57	BZ	0.46	1/1514 (0.1%)	1.03	9/2056 (0.4%)
57	DZ	0.43	1/1514 (0.1%)	0.96	8/2056 (0.4%)
58	CX	2.33	8/195 (4.1%)	3.69	46/303 (15.2%)
All	All	0.49	173/318302 (0.1%)	0.83	1114/475638 (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
1	AA	1	10
1	CA	1	9
22	AV	0	1
22	CV	0	1
24	AY	0	1
35	BA	20	57
35	DA	20	70
36	BB	0	1
36	DB	0	2
42	BH	0	1
42	DH	0	1
49	BR	0	1
49	DR	0	2
All	All	42	157

The worst 5 of 173 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	AV	53	G	O5'-C5'	-17.43	1.16	1.42
22	AV	53	G	P-O5'	-12.83	1.40	1.59
49	DR	12	ARG	C-O	-12.80	1.14	1.24
22	AV	52	G	O5'-C5'	-11.89	1.24	1.42
42	DH	9	ILE	CA-C	-11.49	1.40	1.52

The worst 5 of 1114 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	AV	51	C	O3'-P-O5'	-28.00	61.99	104.00
22	AV	53	G	C5'-C4'-O4'	-21.37	77.74	109.80
35	DA	2319	G	C1'-C2'-O2'	-21.00	80.30	111.80
23	AX	11	U	O4'-C4'-C3'	-20.67	83.33	104.00
23	AX	19	U	O4'-C4'-C3'	-16.99	89.11	106.10

5 of 42 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	AA	575	G	C3'
35	BA	100	G	C1'
35	BA	474	G	C3'
35	BA	587	C	C3'

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Mol	Chain	Res	Type	Atom
35	BA	669	G	C3',C4',C1'

5 of 157 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	115	G	Sidechain
1	AA	120	A	Sidechain
1	AA	575	G	Sidechain
1	AA	587	G	Sidechain
1	AA	731	G	Sidechain

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	32412	0	16354	1308	0
1	CA	32413	0	16353	1704	0
2	AB	1901	0	1951	316	0
2	CB	1901	0	1951	323	0
3	AC	1613	0	1676	258	0
3	CC	1613	0	1677	247	0
4	AD	1692	0	1751	212	0
4	CD	1692	0	1753	230	0
5	AE	1147	0	1206	175	0
5	CE	1147	0	1207	196	0
6	AF	843	0	857	100	0
6	CF	843	0	857	103	0
7	AG	1257	0	1296	136	0
7	CG	1257	0	1296	150	0
8	AH	1116	0	1177	165	0
8	CH	1116	0	1177	175	0
9	AI	1011	0	1041	166	0
9	CI	1011	0	1041	170	0
10	AJ	795	0	840	157	0
10	CJ	795	0	840	159	0
11	AK	885	0	904	106	0
11	CK	885	0	904	103	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	AL	971	0	1055	123	0
12	CL	971	0	1056	122	0
13	AM	934	0	989	132	0
13	CM	934	0	987	145	0
14	AN	492	0	530	77	0
14	CN	492	0	533	81	0
15	AO	734	0	771	90	0
15	CO	734	0	771	81	0
16	AP	701	0	719	97	0
16	CP	701	0	720	108	0
17	AQ	824	0	890	95	0
17	CQ	824	0	891	95	0
18	AR	574	0	644	97	0
18	CR	574	0	644	96	0
19	AS	671	0	689	128	0
19	CS	671	0	689	122	0
20	AT	763	0	861	81	0
20	CT	763	0	861	81	0
21	AU	209	0	221	42	0
21	CU	209	0	221	40	0
22	AV	1640	0	832	85	0
22	AW	1640	0	837	60	0
22	CV	1640	0	833	134	0
22	CW	1640	0	837	71	0
23	AX	341	0	174	126	0
24	AY	769	0	763	238	0
24	CY	126	0	115	33	0
25	B0	662	0	688	61	0
25	D0	662	0	688	59	0
26	B1	734	0	808	88	0
26	D1	734	0	808	89	0
27	B2	598	0	653	66	0
27	D2	598	0	653	84	0
28	B3	468	0	523	44	0
28	D3	468	0	523	45	0
29	B4	434	0	424	96	0
29	D4	434	0	424	72	0
30	B5	459	0	480	46	0
30	D5	459	0	479	46	0
31	B6	381	0	390	62	0
31	D6	381	0	390	64	0
32	B7	419	0	467	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	D7	419	0	467	35	0
33	B8	508	0	576	128	0
33	D8	508	0	576	129	0
34	B9	299	0	326	27	0
34	D9	299	0	326	30	0
35	BA	60459	0	30475	1962	0
35	DA	60459	0	30466	2127	1
36	BB	2551	0	1295	102	0
36	DB	2551	0	1294	87	1
37	BC	1142	0	865	72	0
37	DC	1142	0	865	72	0
38	BD	2105	0	2182	308	0
38	DD	2105	0	2182	320	0
39	BE	1564	0	1628	235	0
39	DE	1564	0	1628	248	0
40	BF	1624	0	1677	232	0
40	DF	1624	0	1676	236	0
41	BG	1474	0	1534	297	0
41	DG	1474	0	1534	314	0
42	BH	1260	0	1326	258	0
42	DH	1260	0	1326	252	0
43	BI	1125	0	1209	184	0
43	DI	1125	0	1209	175	0
44	BJ	651	0	165	21	0
44	DJ	651	0	166	35	0
45	BN	1105	0	1180	149	0
45	DN	1105	0	1180	146	0
46	BO	933	0	996	109	0
46	DO	933	0	996	117	0
47	BP	1114	0	1187	326	0
47	DP	1114	0	1187	322	0
48	BQ	1122	0	1179	124	0
48	DQ	1122	0	1179	119	0
49	BR	960	0	1021	140	0
49	DR	960	0	1019	134	0
50	BS	771	0	832	151	0
50	DS	771	0	832	139	0
51	BT	1142	0	1202	233	0
51	DT	1142	0	1201	235	0
52	BU	958	0	1015	128	0
52	DU	958	0	1015	127	0
53	BV	779	0	852	166	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
53	DV	779	0	852	164	0
54	BW	896	0	953	84	0
54	DW	896	0	952	85	0
55	BX	726	0	778	72	0
55	DX	726	0	778	74	0
56	BY	776	0	870	198	0
56	DY	776	0	870	198	0
57	BZ	1482	0	1503	217	0
57	DZ	1482	0	1503	249	0
58	CX	173	0	89	52	0
59	AA	373	0	0	0	0
59	AC	2	0	0	0	0
59	AD	3	0	0	0	0
59	AH	1	0	0	0	0
59	AI	3	0	0	0	0
59	AL	6	0	0	0	0
59	AN	2	0	0	0	0
59	AO	2	0	0	0	0
59	AP	1	0	0	0	0
59	AQ	3	0	0	0	0
59	AT	1	0	0	0	0
59	AV	7	0	0	0	0
59	AX	4	0	0	0	0
59	AY	3	0	0	0	0
59	B0	2	0	0	0	0
59	B1	1	0	0	0	0
59	B5	3	0	0	0	0
59	B6	1	0	0	0	0
59	B7	1	0	0	0	0
59	BA	709	0	0	0	0
59	BB	6	0	0	0	0
59	BD	5	0	0	0	0
59	BE	4	0	0	0	0
59	BF	1	0	0	0	0
59	BH	4	0	0	0	0
59	BN	1	0	0	0	0
59	BO	1	0	0	0	0
59	BP	4	0	0	5	0
59	BQ	1	0	0	0	0
59	BR	5	0	0	0	0
59	BT	1	0	0	0	0
59	BU	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	BY	1	0	0	0	0
59	CA	184	0	0	0	0
59	CC	3	0	0	0	0
59	CD	1	0	0	0	0
59	CH	1	0	0	0	0
59	CJ	2	0	0	0	0
59	CM	3	0	0	0	0
59	CP	1	0	0	0	0
59	CQ	1	0	0	0	0
59	CS	2	0	0	0	0
59	CV	12	0	0	0	0
59	CY	1	0	0	0	0
59	D0	4	0	0	0	0
59	D1	2	0	0	0	0
59	D2	1	0	0	0	0
59	D3	1	0	0	0	0
59	D5	3	0	0	0	0
59	D6	2	0	0	0	0
59	D7	4	0	0	0	0
59	D8	1	0	0	0	0
59	D9	1	0	0	0	0
59	DA	897	0	0	0	0
59	DB	11	0	0	0	0
59	DD	6	0	0	0	0
59	DE	4	0	0	0	0
59	DF	3	0	0	0	0
59	DN	3	0	0	0	0
59	DO	1	0	0	0	0
59	DP	6	0	0	0	0
59	DR	2	0	0	0	0
59	DT	1	0	0	0	0
59	DU	4	0	0	0	0
59	DW	1	0	0	0	0
59	DY	1	0	0	0	0
60	AD	2	0	0	0	0
60	AN	1	0	0	0	0
60	CD	1	0	0	0	0
61	AA	2	0	0	0	0
All	All	296762	0	199834	20465	1

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 41.

The worst 5 of 20465 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)
3:AC:162:GLN:HB2	23:AX:23:A:C5	1.34	1.59
42:BH:11:VAL:HG22	42:BH:49:VAL:CG1	1.08	1.56
42:DH:11:VAL:HG22	42:DH:49:VAL:CG1	1.08	1.55
1:CA:644:G:C2'	1:CA:645:C:H5''	1.39	1.53
24:AY:57:GLN:HG3	35:BA:1913:A:C2	1.45	1.47

All (1) 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)
35:DA:1411:C:O3'	36:DB:53:A:O2'[1_655]	2.19	0.01

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	233/256 (91%)	133 (57%)	67 (29%)	33 (14%)	0	1
2	CB	233/256 (91%)	133 (57%)	68 (29%)	32 (14%)	0	1
3	AC	205/239 (86%)	130 (63%)	50 (24%)	25 (12%)	0	1
3	CC	205/239 (86%)	128 (62%)	52 (25%)	25 (12%)	0	1
4	AD	206/209 (99%)	139 (68%)	45 (22%)	22 (11%)	0	2
4	CD	206/209 (99%)	138 (67%)	46 (22%)	22 (11%)	0	2
5	AE	149/162 (92%)	101 (68%)	33 (22%)	15 (10%)	0	2
5	CE	149/162 (92%)	101 (68%)	33 (22%)	15 (10%)	0	2
6	AF	99/101 (98%)	74 (75%)	13 (13%)	12 (12%)	0	1
6	CF	99/101 (98%)	74 (75%)	13 (13%)	12 (12%)	0	1
7	AG	153/156 (98%)	107 (70%)	35 (23%)	11 (7%)	1	6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	CG	153/156 (98%)	107 (70%)	35 (23%)	11 (7%)	1	6
8	AH	136/138 (99%)	99 (73%)	31 (23%)	6 (4%)	2	15
8	CH	136/138 (99%)	99 (73%)	30 (22%)	7 (5%)	1	13
9	AI	121/128 (94%)	75 (62%)	31 (26%)	15 (12%)	0	1
9	CI	121/128 (94%)	74 (61%)	33 (27%)	14 (12%)	0	1
10	AJ	97/105 (92%)	64 (66%)	28 (29%)	5 (5%)	1	12
10	CJ	97/105 (92%)	64 (66%)	28 (29%)	5 (5%)	1	12
11	AK	117/129 (91%)	76 (65%)	28 (24%)	13 (11%)	0	2
11	CK	117/129 (91%)	76 (65%)	28 (24%)	13 (11%)	0	2
12	AL	123/135 (91%)	89 (72%)	21 (17%)	13 (11%)	0	2
12	CL	123/135 (91%)	87 (71%)	22 (18%)	14 (11%)	0	2
13	AM	110/126 (87%)	62 (56%)	27 (24%)	21 (19%)	0	0
13	CM	110/126 (87%)	63 (57%)	26 (24%)	21 (19%)	0	0
14	AN	58/61 (95%)	37 (64%)	14 (24%)	7 (12%)	0	1
14	CN	58/61 (95%)	36 (62%)	16 (28%)	6 (10%)	0	2
15	AO	86/89 (97%)	54 (63%)	25 (29%)	7 (8%)	1	4
15	CO	86/89 (97%)	55 (64%)	24 (28%)	7 (8%)	1	4
16	AP	82/88 (93%)	55 (67%)	18 (22%)	9 (11%)	0	2
16	CP	82/88 (93%)	55 (67%)	18 (22%)	9 (11%)	0	2
17	AQ	98/105 (93%)	65 (66%)	21 (21%)	12 (12%)	0	1
17	CQ	98/105 (93%)	66 (67%)	20 (20%)	12 (12%)	0	1
18	AR	68/88 (77%)	36 (53%)	22 (32%)	10 (15%)	0	1
18	CR	68/88 (77%)	35 (52%)	23 (34%)	10 (15%)	0	1
19	AS	83/93 (89%)	48 (58%)	18 (22%)	17 (20%)	0	0
19	CS	83/93 (89%)	48 (58%)	18 (22%)	17 (20%)	0	0
20	AT	97/106 (92%)	62 (64%)	25 (26%)	10 (10%)	0	2
20	CT	97/106 (92%)	62 (64%)	25 (26%)	10 (10%)	0	2
21	AU	23/27 (85%)	11 (48%)	10 (44%)	2 (9%)	0	3
21	CU	23/27 (85%)	11 (48%)	10 (44%)	2 (9%)	0	3
24	AY	95/97 (98%)	81 (85%)	10 (10%)	4 (4%)	2	16
24	CY	14/97 (14%)	8 (57%)	4 (29%)	2 (14%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	B0	82/85 (96%)	67 (82%)	10 (12%)	5 (6%)	1	9
25	D0	82/85 (96%)	66 (80%)	10 (12%)	6 (7%)	1	6
26	B1	92/98 (94%)	70 (76%)	16 (17%)	6 (6%)	1	8
26	D1	92/98 (94%)	74 (80%)	9 (10%)	9 (10%)	0	2
27	B2	69/72 (96%)	51 (74%)	13 (19%)	5 (7%)	1	6
27	D2	69/72 (96%)	47 (68%)	18 (26%)	4 (6%)	1	10
28	B3	58/60 (97%)	49 (84%)	8 (14%)	1 (2%)	7	35
28	D3	58/60 (97%)	50 (86%)	7 (12%)	1 (2%)	7	35
29	B4	54/71 (76%)	28 (52%)	12 (22%)	14 (26%)	0	0
29	D4	54/71 (76%)	28 (52%)	12 (22%)	14 (26%)	0	0
30	B5	57/60 (95%)	42 (74%)	9 (16%)	6 (10%)	0	2
30	D5	57/60 (95%)	41 (72%)	10 (18%)	6 (10%)	0	2
31	B6	41/54 (76%)	17 (42%)	15 (37%)	9 (22%)	0	0
31	D6	41/54 (76%)	16 (39%)	16 (39%)	9 (22%)	0	0
32	B7	47/49 (96%)	45 (96%)	1 (2%)	1 (2%)	5	31
32	D7	47/49 (96%)	45 (96%)	1 (2%)	1 (2%)	5	31
33	B8	62/65 (95%)	35 (56%)	15 (24%)	12 (19%)	0	0
33	D8	62/65 (95%)	34 (55%)	15 (24%)	13 (21%)	0	0
34	B9	34/37 (92%)	24 (71%)	8 (24%)	2 (6%)	1	10
34	D9	34/37 (92%)	24 (71%)	8 (24%)	2 (6%)	1	10
37	BC	183/229 (80%)	75 (41%)	67 (37%)	41 (22%)	0	0
37	DC	183/229 (80%)	76 (42%)	65 (36%)	42 (23%)	0	0
38	BD	270/276 (98%)	199 (74%)	48 (18%)	23 (8%)	0	3
38	DD	270/276 (98%)	198 (73%)	47 (17%)	25 (9%)	0	3
39	BE	203/206 (98%)	142 (70%)	37 (18%)	24 (12%)	0	1
39	DE	203/206 (98%)	143 (70%)	36 (18%)	24 (12%)	0	1
40	BF	206/210 (98%)	137 (66%)	40 (19%)	29 (14%)	0	1
40	DF	206/210 (98%)	137 (66%)	41 (20%)	28 (14%)	0	1
41	BG	177/182 (97%)	109 (62%)	44 (25%)	24 (14%)	0	1
41	DG	177/182 (97%)	107 (60%)	43 (24%)	27 (15%)	0	0
42	BH	163/180 (91%)	90 (55%)	42 (26%)	31 (19%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	DH	163/180 (91%)	90 (55%)	42 (26%)	31 (19%)	0	0
43	BI	143/148 (97%)	80 (56%)	36 (25%)	27 (19%)	0	0
43	DI	143/148 (97%)	80 (56%)	36 (25%)	27 (19%)	0	0
45	BN	137/140 (98%)	97 (71%)	20 (15%)	20 (15%)	0	1
45	DN	137/140 (98%)	96 (70%)	21 (15%)	20 (15%)	0	1
46	BO	120/122 (98%)	99 (82%)	15 (12%)	6 (5%)	1	13
46	DO	120/122 (98%)	99 (82%)	15 (12%)	6 (5%)	1	13
47	BP	144/150 (96%)	70 (49%)	34 (24%)	40 (28%)	0	0
47	DP	144/150 (96%)	70 (49%)	34 (24%)	40 (28%)	0	0
48	BQ	139/141 (99%)	108 (78%)	18 (13%)	13 (9%)	0	3
48	DQ	139/141 (99%)	108 (78%)	18 (13%)	13 (9%)	0	3
49	BR	115/118 (98%)	80 (70%)	20 (17%)	15 (13%)	0	1
49	DR	115/118 (98%)	82 (71%)	20 (17%)	13 (11%)	0	2
50	BS	97/112 (87%)	46 (47%)	20 (21%)	31 (32%)	0	0
50	DS	97/112 (87%)	46 (47%)	20 (21%)	31 (32%)	0	0
51	BT	136/146 (93%)	79 (58%)	33 (24%)	24 (18%)	0	0
51	DT	136/146 (93%)	80 (59%)	31 (23%)	25 (18%)	0	0
52	BU	115/118 (98%)	87 (76%)	18 (16%)	10 (9%)	0	3
52	DU	115/118 (98%)	88 (76%)	17 (15%)	10 (9%)	0	3
53	BV	99/101 (98%)	72 (73%)	12 (12%)	15 (15%)	0	0
53	DV	99/101 (98%)	72 (73%)	12 (12%)	15 (15%)	0	0
54	BW	111/113 (98%)	84 (76%)	17 (15%)	10 (9%)	0	3
54	DW	111/113 (98%)	85 (77%)	16 (14%)	10 (9%)	0	3
55	BX	91/96 (95%)	73 (80%)	15 (16%)	3 (3%)	3	21
55	DX	91/96 (95%)	72 (79%)	16 (18%)	3 (3%)	3	21
56	BY	99/110 (90%)	50 (50%)	23 (23%)	26 (26%)	0	0
56	DY	99/110 (90%)	50 (50%)	23 (23%)	26 (26%)	0	0
57	BZ	185/206 (90%)	123 (66%)	38 (20%)	24 (13%)	0	1
57	DZ	185/206 (90%)	101 (55%)	49 (26%)	35 (19%)	0	0
All	All	11855/12786 (93%)	7751 (65%)	2556 (22%)	1548 (13%)	0	1

5 of 1548 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	75	LYS
2	AB	83	MET
2	AB	101	MET
2	AB	150	SER
2	AB	238	LEU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AB	202/220 (92%)	190 (94%)	12 (6%)	18	50
2	CB	202/220 (92%)	190 (94%)	12 (6%)	18	50
3	AC	160/188 (85%)	150 (94%)	10 (6%)	16	48
3	CC	160/188 (85%)	150 (94%)	10 (6%)	16	48
4	AD	179/181 (99%)	162 (90%)	17 (10%)	8	32
4	CD	179/181 (99%)	162 (90%)	17 (10%)	8	32
5	AE	115/123 (94%)	103 (90%)	12 (10%)	7	28
5	CE	115/123 (94%)	104 (90%)	11 (10%)	8	32
6	AF	90/90 (100%)	85 (94%)	5 (6%)	19	52
6	CF	90/90 (100%)	86 (96%)	4 (4%)	25	59
7	AG	126/127 (99%)	121 (96%)	5 (4%)	28	61
7	CG	126/127 (99%)	121 (96%)	5 (4%)	28	61
8	AH	119/119 (100%)	109 (92%)	10 (8%)	10	38
8	CH	119/119 (100%)	109 (92%)	10 (8%)	10	38
9	AI	98/99 (99%)	88 (90%)	10 (10%)	7	29
9	CI	98/99 (99%)	88 (90%)	10 (10%)	7	29
10	AJ	88/92 (96%)	78 (89%)	10 (11%)	5	24
10	CJ	88/92 (96%)	78 (89%)	10 (11%)	5	24
11	AK	90/99 (91%)	84 (93%)	6 (7%)	15	47
11	CK	90/99 (91%)	84 (93%)	6 (7%)	15	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	AL	104/111 (94%)	98 (94%)	6 (6%)	18	51
12	CL	104/111 (94%)	98 (94%)	6 (6%)	18	51
13	AM	94/101 (93%)	85 (90%)	9 (10%)	8	32
13	CM	94/101 (93%)	84 (89%)	10 (11%)	6	27
14	AN	49/50 (98%)	45 (92%)	4 (8%)	10	39
14	CN	49/50 (98%)	45 (92%)	4 (8%)	10	39
15	AO	79/80 (99%)	72 (91%)	7 (9%)	9	34
15	CO	79/80 (99%)	72 (91%)	7 (9%)	9	34
16	AP	72/74 (97%)	69 (96%)	3 (4%)	26	60
16	CP	72/74 (97%)	67 (93%)	5 (7%)	14	45
17	AQ	94/97 (97%)	86 (92%)	8 (8%)	10	37
17	CQ	94/97 (97%)	86 (92%)	8 (8%)	10	37
18	AR	61/77 (79%)	59 (97%)	2 (3%)	33	65
18	CR	61/77 (79%)	59 (97%)	2 (3%)	33	65
19	AS	72/80 (90%)	63 (88%)	9 (12%)	4	21
19	CS	72/80 (90%)	63 (88%)	9 (12%)	4	21
20	AT	76/82 (93%)	68 (90%)	8 (10%)	6	28
20	CT	76/82 (93%)	67 (88%)	9 (12%)	5	23
21	AU	19/22 (86%)	17 (90%)	2 (10%)	6	28
21	CU	19/22 (86%)	17 (90%)	2 (10%)	6	28
24	AY	78/78 (100%)	42 (54%)	36 (46%)	0	0
24	CY	12/78 (15%)	9 (75%)	3 (25%)	0	3
25	B0	66/67 (98%)	61 (92%)	5 (8%)	12	42
25	D0	66/67 (98%)	61 (92%)	5 (8%)	12	42
26	B1	78/83 (94%)	68 (87%)	10 (13%)	4	20
26	D1	78/83 (94%)	68 (87%)	10 (13%)	4	20
27	B2	66/67 (98%)	59 (89%)	7 (11%)	6	27
27	D2	66/67 (98%)	56 (85%)	10 (15%)	3	14
28	B3	51/52 (98%)	39 (76%)	12 (24%)	1	4
28	D3	51/52 (98%)	39 (76%)	12 (24%)	1	4
29	B4	49/63 (78%)	40 (82%)	9 (18%)	1	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	D4	49/63 (78%)	41 (84%)	8 (16%)	2	12
30	B5	51/52 (98%)	45 (88%)	6 (12%)	5	23
30	D5	51/52 (98%)	45 (88%)	6 (12%)	5	23
31	B6	43/52 (83%)	37 (86%)	6 (14%)	3	17
31	D6	43/52 (83%)	37 (86%)	6 (14%)	3	17
32	B7	41/42 (98%)	34 (83%)	7 (17%)	2	11
32	D7	41/42 (98%)	35 (85%)	6 (15%)	3	16
33	B8	53/55 (96%)	44 (83%)	9 (17%)	2	11
33	D8	53/55 (96%)	44 (83%)	9 (17%)	2	11
34	B9	33/34 (97%)	32 (97%)	1 (3%)	36	66
34	D9	33/34 (97%)	32 (97%)	1 (3%)	36	66
37	BC	61/181 (34%)	57 (93%)	4 (7%)	15	47
37	DC	61/181 (34%)	57 (93%)	4 (7%)	15	47
38	BD	213/218 (98%)	173 (81%)	40 (19%)	1	9
38	DD	213/218 (98%)	173 (81%)	40 (19%)	1	9
39	BE	165/166 (99%)	143 (87%)	22 (13%)	4	19
39	DE	165/166 (99%)	143 (87%)	22 (13%)	4	19
40	BF	165/166 (99%)	140 (85%)	25 (15%)	3	14
40	DF	165/166 (99%)	140 (85%)	25 (15%)	3	14
41	BG	155/156 (99%)	140 (90%)	15 (10%)	8	32
41	DG	155/156 (99%)	138 (89%)	17 (11%)	6	26
42	BH	137/148 (93%)	120 (88%)	17 (12%)	4	21
42	DH	137/148 (93%)	120 (88%)	17 (12%)	4	21
43	BI	121/124 (98%)	104 (86%)	17 (14%)	3	17
43	DI	121/124 (98%)	101 (84%)	20 (16%)	2	12
45	BN	117/119 (98%)	95 (81%)	22 (19%)	1	9
45	DN	117/119 (98%)	96 (82%)	21 (18%)	2	9
46	BO	100/100 (100%)	95 (95%)	5 (5%)	22	55
46	DO	100/100 (100%)	94 (94%)	6 (6%)	17	50
47	BP	112/116 (97%)	81 (72%)	31 (28%)	0	2
47	DP	112/116 (97%)	82 (73%)	30 (27%)	0	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
48	BQ	111/111 (100%)	104 (94%)	7 (6%)	16	48
48	DQ	111/111 (100%)	104 (94%)	7 (6%)	16	48
49	BR	100/101 (99%)	87 (87%)	13 (13%)	4	20
49	DR	100/101 (99%)	85 (85%)	15 (15%)	3	15
50	BS	77/88 (88%)	64 (83%)	13 (17%)	2	11
50	DS	77/88 (88%)	64 (83%)	13 (17%)	2	11
51	BT	120/127 (94%)	100 (83%)	20 (17%)	2	11
51	DT	120/127 (94%)	101 (84%)	19 (16%)	2	13
52	BU	92/94 (98%)	84 (91%)	8 (9%)	9	36
52	DU	92/94 (98%)	82 (89%)	10 (11%)	6	26
53	BV	82/82 (100%)	67 (82%)	15 (18%)	2	9
53	DV	82/82 (100%)	68 (83%)	14 (17%)	2	11
54	BW	91/92 (99%)	77 (85%)	14 (15%)	2	14
54	DW	91/92 (99%)	78 (86%)	13 (14%)	3	16
55	BX	74/78 (95%)	63 (85%)	11 (15%)	3	15
55	DX	74/78 (95%)	63 (85%)	11 (15%)	3	15
56	BY	84/91 (92%)	71 (84%)	13 (16%)	2	14
56	DY	84/91 (92%)	71 (84%)	13 (16%)	2	14
57	BZ	163/179 (91%)	145 (89%)	18 (11%)	6	26
57	DZ	163/179 (91%)	144 (88%)	19 (12%)	5	23
All	All	9806/10588 (93%)	8644 (88%)	1162 (12%)	5	23

5 of 1162 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
41	DG	82	LEU
57	DZ	28	MET
43	DI	5	LEU
41	DG	81	LYS
49	DR	34	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 325 such sidechains are listed below:

Mol	Chain	Res	Type
20	CT	90	GLN
46	DO	82	ASN
27	D2	71	ASN
39	DE	129	HIS
49	DR	71	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1505/1522 (98%)	207 (13%)	21 (1%)
1	CA	1505/1522 (98%)	236 (15%)	24 (1%)
22	AV	76/77 (98%)	18 (23%)	1 (1%)
22	AW	76/77 (98%)	14 (18%)	1 (1%)
22	CV	76/77 (98%)	20 (26%)	1 (1%)
22	CW	76/77 (98%)	8 (10%)	0
23	AX	15/25 (60%)	14 (93%)	10 (66%)
35	BA	2805/2848 (98%)	487 (17%)	58 (2%)
35	DA	2805/2848 (98%)	491 (17%)	58 (2%)
36	BB	118/122 (96%)	20 (16%)	1 (0%)
36	DB	118/122 (96%)	20 (16%)	1 (0%)
58	CX	8/25 (32%)	7 (87%)	5 (62%)
All	All	9183/9342 (98%)	1542 (16%)	181 (1%)

5 of 1542 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	4	U
1	AA	5	U
1	AA	6	G
1	AA	9	G
1	AA	31	G

5 of 181 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	CA	1504	G
35	DA	746	A
58	CX	14	A
35	DA	331	A
35	DA	1301	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	A3P	AA	1493	1	25,28,29	0.67	1 (4%)	37,42,45	1.54	4 (10%)
1	A3P	CA	1493	1	25,28,29	0.55	0	37,42,45	0.65	1 (2%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	A3P	AA	1493	1	-	2/12/30/31	0/3/3/3
1	A3P	CA	1493	1	-	3/12/30/31	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	1493	A3P	P1-O3'	-2.05	1.55	1.59

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1493	A3P	O2P-P1-O3'	-5.70	83.64	105.85
1	AA	1493	A3P	P1-O3'-C3'	-4.93	110.27	123.43
1	AA	1493	A3P	O3'-P1-O1P	4.47	125.27	109.33
1	CA	1493	A3P	O2P-P1-O1P	2.13	119.13	110.83
1	AA	1493	A3P	O2P-P1-O1P	2.12	119.09	110.83

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	CA	1493	A3P	C2'-C1'-N9-C8
1	AA	1493	A3P	C3'-O3'-P1-O3P
1	CA	1493	A3P	C4'-C5'-O5'-P2
1	CA	1493	A3P	O4'-C1'-N9-C8
1	AA	1493	A3P	C2'-C1'-N9-C8

There are no ring outliers.

2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	AA	1493	A3P	10	0
1	CA	1493	A3P	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2338 ligands modelled in this entry, 2338 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
13	AM	3

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Mol	Chain	Number of breaks
13	CM	3
9	CI	2
9	AI	2
31	B6	1
31	D6	1
41	BG	1
41	DG	1

The worst 5 of 14 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B6	46:HIS	C	47:THR	N	7.76
1	D6	46:HIS	C	47:THR	N	7.76
1	BG	112:PRO	C	113:ARG	N	4.73
1	DG	112:PRO	C	113:ARG	N	4.47
1	AM	69:GLU	C	70:LEU	N	4.25

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	1507/1522 (99%)	0.29	49 (3%)	49	30	54, 107, 196, 201	0
1	CA	1507/1522 (99%)	1.40	367 (24%)	2	2	60, 169, 201, 201	0
2	AB	235/256 (91%)	0.52	16 (6%)	23	15	77, 152, 197, 201	0
2	CB	235/256 (91%)	0.83	24 (10%)	12	8	90, 173, 201, 201	0
3	AC	207/239 (86%)	0.65	15 (7%)	21	14	83, 149, 188, 201	0
3	CC	207/239 (86%)	0.76	15 (7%)	21	14	106, 175, 201, 201	0
4	AD	208/209 (99%)	0.47	11 (5%)	32	20	65, 105, 149, 180	0
4	CD	208/209 (99%)	1.32	49 (23%)	2	2	85, 173, 201, 201	0
5	AE	151/162 (93%)	0.31	6 (3%)	42	26	70, 107, 155, 198	0
5	CE	151/162 (93%)	1.04	25 (16%)	4	3	89, 155, 197, 201	0
6	AF	101/101 (100%)	0.47	1 (0%)	79	63	70, 125, 163, 190	0
6	CF	101/101 (100%)	0.40	3 (2%)	52	33	65, 110, 155, 184	0
7	AG	155/156 (99%)	0.43	6 (3%)	43	27	85, 141, 184, 201	0
7	CG	155/156 (99%)	0.78	16 (10%)	12	8	86, 164, 200, 201	0
8	AH	138/138 (100%)	0.36	9 (6%)	25	16	66, 108, 151, 171	0
8	CH	138/138 (100%)	0.90	12 (8%)	16	11	79, 157, 189, 201	0
9	AI	127/128 (99%)	0.92	20 (15%)	5	4	94, 164, 200, 201	0
9	CI	127/128 (99%)	1.13	29 (22%)	2	2	115, 177, 201, 201	0
10	AJ	99/105 (94%)	1.07	13 (13%)	7	6	105, 169, 201, 201	0
10	CJ	99/105 (94%)	1.52	28 (28%)	1	1	125, 181, 201, 201	0
11	AK	119/129 (92%)	0.34	6 (5%)	34	22	60, 113, 168, 197	0
11	CK	119/129 (92%)	0.63	10 (8%)	17	11	78, 139, 188, 200	0
12	AL	125/135 (92%)	0.22	2 (1%)	70	51	59, 90, 144, 201	0
12	CL	125/135 (92%)	1.32	34 (27%)	1	1	63, 139, 187, 201	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AM	118/126 (93%)	0.76	8 (6%) 23 15	96, 152, 189, 201	0
13	CM	118/126 (93%)	0.95	20 (16%) 4 3	102, 165, 201, 201	0
14	AN	60/61 (98%)	1.01	7 (11%) 9 6	99, 153, 198, 201	0
14	CN	60/61 (98%)	1.52	18 (30%) 1 1	118, 171, 200, 201	0
15	AO	88/89 (98%)	0.22	1 (1%) 78 61	69, 102, 149, 171	0
15	CO	88/89 (98%)	0.58	6 (6%) 23 15	75, 123, 163, 176	0
16	AP	84/88 (95%)	0.31	2 (2%) 59 40	60, 92, 143, 195	0
16	CP	84/88 (95%)	1.57	25 (29%) 1 1	112, 172, 198, 201	0
17	AQ	100/105 (95%)	0.21	3 (3%) 52 33	63, 97, 134, 156	0
17	CQ	100/105 (95%)	0.86	6 (6%) 27 17	102, 142, 181, 195	0
18	AR	70/88 (79%)	0.38	1 (1%) 73 54	78, 116, 165, 178	0
18	CR	70/88 (79%)	0.45	2 (2%) 53 35	79, 120, 180, 196	0
19	AS	85/93 (91%)	0.53	2 (2%) 59 40	101, 164, 198, 201	0
19	CS	85/93 (91%)	1.03	16 (18%) 3 2	118, 176, 199, 201	0
20	AT	99/106 (93%)	0.41	3 (3%) 52 33	60, 104, 163, 191	0
20	CT	99/106 (93%)	1.07	15 (15%) 5 4	113, 169, 198, 201	0
21	AU	25/27 (92%)	0.91	3 (12%) 9 6	91, 151, 184, 201	0
21	CU	25/27 (92%)	2.22	9 (36%) 1 1	84, 159, 199, 201	0
22	AV	77/77 (100%)	0.13	2 (2%) 57 37	55, 106, 161, 194	0
22	AW	77/77 (100%)	0.97	7 (9%) 15 9	125, 201, 201, 201	0
22	CV	77/77 (100%)	0.96	9 (11%) 9 6	50, 131, 174, 182	0
22	CW	77/77 (100%)	0.99	7 (9%) 15 9	146, 201, 201, 201	0
23	AX	16/25 (64%)	0.94	3 (18%) 3 2	84, 199, 201, 201	0
24	AY	97/97 (100%)	0.92	12 (12%) 8 6	2, 149, 189, 201	1 (1%)
24	CY	16/97 (16%)	0.82	1 (6%) 26 17	130, 157, 201, 201	0
25	B0	84/85 (98%)	0.40	3 (3%) 46 28	51, 90, 164, 196	0
25	D0	84/85 (98%)	0.74	4 (4%) 35 22	70, 105, 166, 191	0
26	B1	94/98 (95%)	0.21	8 (8%) 16 11	44, 76, 145, 161	0
26	D1	94/98 (95%)	0.02	2 (2%) 63 43	41, 74, 139, 159	0
27	B2	71/72 (98%)	0.19	2 (2%) 55 35	65, 103, 150, 169	0
27	D2	71/72 (98%)	-0.20	1 (1%) 73 54	42, 71, 129, 195	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	B3	60/60 (100%)	0.07	0 100 100	42, 88, 148, 201	0
28	D3	60/60 (100%)	0.02	0 100 100	50, 87, 142, 200	0
29	B4	56/71 (78%)	0.43	1 (1%) 67 48	96, 160, 187, 197	0
29	D4	56/71 (78%)	0.73	2 (3%) 46 28	122, 176, 201, 201	0
30	B5	59/60 (98%)	0.32	4 (6%) 23 15	37, 70, 174, 181	0
30	D5	59/60 (98%)	0.36	3 (5%) 33 21	27, 75, 177, 201	0
31	B6	45/54 (83%)	1.06	8 (17%) 4 3	97, 141, 184, 187	0
31	D6	45/54 (83%)	1.25	7 (15%) 5 4	103, 161, 195, 199	0
32	B7	49/49 (100%)	-0.10	0 100 100	38, 55, 112, 194	0
32	D7	49/49 (100%)	-0.24	1 (2%) 65 45	21, 40, 108, 159	0
33	B8	64/65 (98%)	0.50	4 (6%) 26 17	32, 72, 132, 200	0
33	D8	64/65 (98%)	0.83	7 (10%) 10 7	41, 83, 148, 201	0
34	B9	36/37 (97%)	1.06	8 (22%) 2 2	83, 123, 168, 201	0
34	D9	36/37 (97%)	1.44	10 (27%) 1 1	91, 128, 167, 197	0
35	BA	2807/2848 (98%)	-0.14	65 (2%) 61 41	32, 74, 188, 201	0
35	DA	2807/2848 (98%)	0.08	85 (3%) 52 33	29, 77, 189, 201	0
36	BB	119/122 (97%)	0.55	4 (3%) 48 30	76, 130, 181, 201	0
36	DB	119/122 (97%)	0.84	12 (10%) 12 8	87, 151, 189, 200	0
37	BC	191/229 (83%)	0.89	19 (9%) 13 8	160, 198, 201, 201	0
37	DC	191/229 (83%)	0.94	23 (12%) 9 6	154, 197, 201, 201	0
38	BD	272/276 (98%)	0.09	7 (2%) 57 37	38, 71, 107, 184	0
38	DD	272/276 (98%)	0.27	8 (2%) 53 35	32, 68, 111, 185	0
39	BE	205/206 (99%)	0.29	11 (5%) 31 20	36, 83, 157, 201	0
39	DE	205/206 (99%)	0.49	13 (6%) 26 17	25, 91, 157, 201	0
40	BF	208/210 (99%)	0.06	2 (0%) 79 63	30, 73, 156, 186	0
40	DF	208/210 (99%)	0.17	6 (2%) 53 35	24, 78, 165, 196	0
41	BG	181/182 (99%)	0.48	7 (3%) 43 27	79, 142, 188, 201	0
41	DG	181/182 (99%)	0.61	11 (6%) 27 17	92, 155, 193, 201	0
42	BH	165/180 (91%)	0.82	18 (10%) 10 7	90, 157, 193, 201	0
42	DH	165/180 (91%)	0.59	11 (6%) 24 15	55, 112, 158, 182	0
43	BI	145/148 (97%)	1.66	49 (33%) 1 1	60, 161, 201, 201	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
43	DI	145/148 (97%)	0.95	15 (10%) 12 8	70, 130, 200, 201	0
44	BJ	0/131	-	-	-	-
44	DJ	0/131	-	-	-	-
45	BN	139/140 (99%)	0.21	5 (3%) 46 28	52, 88, 145, 201	0
45	DN	139/140 (99%)	0.09	3 (2%) 62 42	44, 79, 140, 189	0
46	BO	122/122 (100%)	-0.13	1 (0%) 82 67	42, 72, 101, 178	0
46	DO	122/122 (100%)	0.81	13 (10%) 11 7	59, 104, 154, 201	0
47	BP	146/150 (97%)	0.65	16 (10%) 10 7	26, 92, 150, 197	0
47	DP	146/150 (97%)	0.87	23 (15%) 5 4	35, 96, 170, 198	0
48	BQ	141/141 (100%)	0.31	5 (3%) 47 29	48, 89, 132, 201	0
48	DQ	141/141 (100%)	0.77	18 (12%) 7 6	53, 106, 159, 191	0
49	BR	117/118 (99%)	0.24	6 (5%) 33 21	39, 76, 125, 150	0
49	DR	117/118 (99%)	0.67	8 (6%) 23 15	53, 90, 147, 162	0
50	BS	99/112 (88%)	0.88	13 (13%) 7 6	75, 133, 182, 189	0
50	DS	99/112 (88%)	1.39	25 (25%) 1 2	95, 145, 196, 201	0
51	BT	138/146 (94%)	0.26	4 (2%) 53 35	51, 87, 182, 201	0
51	DT	138/146 (94%)	0.78	18 (13%) 7 6	68, 131, 194, 201	0
52	BU	117/118 (99%)	0.06	4 (3%) 48 30	37, 73, 137, 201	0
52	DU	117/118 (99%)	-0.03	4 (3%) 48 30	25, 62, 114, 174	0
53	BV	101/101 (100%)	0.33	4 (3%) 42 26	35, 103, 143, 201	0
53	DV	101/101 (100%)	0.07	4 (3%) 42 26	32, 80, 126, 180	0
54	BW	113/113 (100%)	0.03	2 (1%) 67 48	43, 70, 133, 201	0
54	DW	113/113 (100%)	-0.19	1 (0%) 81 64	37, 60, 118, 187	0
55	BX	93/96 (96%)	0.17	0 100 100	43, 89, 125, 140	0
55	DX	93/96 (96%)	-0.08	1 (1%) 78 61	43, 65, 114, 153	0
56	BY	101/110 (91%)	0.86	14 (13%) 6 5	63, 109, 182, 201	0
56	DY	101/110 (91%)	0.85	17 (16%) 4 3	54, 99, 176, 201	0
57	BZ	187/206 (90%)	0.27	4 (2%) 63 43	74, 121, 171, 201	0
57	DZ	187/206 (90%)	0.43	10 (5%) 32 20	76, 133, 187, 201	0
58	CX	8/25 (32%)	1.42	4 (50%) 0 1	106, 165, 200, 201	0
All	All	21297/22390 (95%)	0.46	1622 (7%) 20 13	2, 111, 198, 201	1 (0%)

The worst 5 of 1622 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
24	AY	46	ASP	16.2
14	CN	2	ALA	11.7
14	AN	2	ALA	8.3
50	DS	30	ARG	8.3
43	BI	119	PRO	7.6

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
1	A3P	CA	1493	26/27	0.56	0.14	191,200,203,203	0
1	A3P	AA	1493	26/27	0.83	0.12	151,182,188,189	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
59	MG	D3	101	1/1	-0.53	1.20	1,1,1,1	1
59	MG	DA	2944	1/1	-0.09	3.50	109,109,109,109	1
59	MG	DA	2950	1/1	-0.07	2.21	80,80,80,80	1
59	MG	DY	201	1/1	-0.06	0.23	168,168,168,168	0
59	MG	DA	2930	1/1	-0.04	0.84	1,1,1,1	1
59	MG	BA	3357	1/1	-0.01	0.33	78,78,78,78	1
59	MG	CA	1610	1/1	0.08	0.30	143,143,143,143	0
59	MG	AN	102	1/1	0.13	0.17	141,141,141,141	0
59	MG	DA	3345	1/1	0.14	1.28	25,25,25,25	1
59	MG	DA	3238	1/1	0.14	0.27	134,134,134,134	0
59	MG	AA	1712	1/1	0.15	0.30	188,188,188,188	0
59	MG	DA	3271	1/1	0.16	0.35	96,96,96,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	BT	201	1/1	0.21	0.29	117,117,117,117	0
59	MG	AA	1802	1/1	0.21	0.40	119,119,119,119	0
59	MG	DA	2931	1/1	0.23	1.52	151,151,151,151	1
59	MG	D6	102	1/1	0.26	0.26	97,97,97,97	0
59	MG	DA	2976	1/1	0.26	0.53	1,1,1,1	1
59	MG	BA	3316	1/1	0.26	0.84	98,98,98,98	0
59	MG	CA	1759	1/1	0.30	0.41	98,98,98,98	0
59	MG	CA	1777	1/1	0.31	0.20	125,125,125,125	0
59	MG	DA	3133	1/1	0.32	0.33	120,120,120,120	0
59	MG	BA	3120	1/1	0.33	0.34	101,101,101,101	0
59	MG	BA	2967	1/1	0.34	0.46	95,95,95,95	0
59	MG	AA	1605	1/1	0.35	0.31	152,152,152,152	0
59	MG	AA	1780	1/1	0.35	0.35	154,154,154,154	0
59	MG	DA	3131	1/1	0.35	0.43	154,154,154,154	0
59	MG	DA	3721	1/1	0.35	0.13	171,171,171,171	0
59	MG	BA	3585	1/1	0.35	0.54	143,143,143,143	0
59	MG	CC	301	1/1	0.36	0.14	117,117,117,117	0
59	MG	DA	3784	1/1	0.38	0.62	123,123,123,123	0
59	MG	AA	1972	1/1	0.40	0.58	98,98,98,98	1
59	MG	DA	2920	1/1	0.40	1.31	15,15,15,15	1
59	MG	DA	3689	1/1	0.40	0.14	123,123,123,123	0
59	MG	AA	1648	1/1	0.41	0.32	108,108,108,108	0
59	MG	DA	3686	1/1	0.41	0.35	107,107,107,107	0
59	MG	CV	106	1/1	0.41	0.20	101,101,101,101	0
59	MG	DA	3649	1/1	0.42	0.30	66,66,66,66	0
59	MG	AA	1604	1/1	0.42	0.25	118,118,118,118	0
59	MG	BA	3580	1/1	0.43	0.28	135,135,135,135	0
59	MG	BA	3112	1/1	0.43	0.31	101,101,101,101	0
59	MG	DA	3788	1/1	0.43	0.23	124,124,124,124	0
59	MG	BA	3205	1/1	0.43	0.38	78,78,78,78	0
59	MG	BA	3602	1/1	0.44	0.51	122,122,122,122	1
59	MG	BA	2951	1/1	0.44	0.22	142,142,142,142	0
59	MG	BA	3268	1/1	0.44	0.28	88,88,88,88	1
59	MG	DA	3125	1/1	0.44	0.35	118,118,118,118	0
59	MG	DA	3017	1/1	0.45	0.25	70,70,70,70	0
59	MG	DA	3418	1/1	0.45	0.31	88,88,88,88	0
59	MG	DA	3781	1/1	0.45	0.27	143,143,143,143	0
59	MG	CA	1658	1/1	0.46	0.18	97,97,97,97	0
59	MG	BA	3342	1/1	0.46	0.45	127,127,127,127	0
59	MG	DA	3374	1/1	0.46	0.42	91,91,91,91	0
59	MG	AA	1820	1/1	0.47	0.29	97,97,97,97	0
59	MG	DA	3779	1/1	0.47	0.33	122,122,122,122	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
59	MG	AA	1711	1/1	0.47	0.29	90,90,90,90	0
59	MG	DA	3769	1/1	0.48	0.30	142,142,142,142	0
59	MG	CA	1780	1/1	0.48	0.29	47,47,47,47	1
59	MG	DA	3419	1/1	0.48	0.72	122,122,122,122	0
59	MG	CA	1697	1/1	0.49	0.33	83,83,83,83	0
59	MG	DA	3571	1/1	0.49	0.34	96,96,96,96	0
59	MG	AQ	203	1/1	0.49	0.30	130,130,130,130	0
59	MG	D0	104	1/1	0.49	0.28	98,98,98,98	0
59	MG	BA	3245	1/1	0.49	0.28	116,116,116,116	0
59	MG	AV	104	1/1	0.49	0.15	133,133,133,133	0
59	MG	DA	3563	1/1	0.50	0.17	68,68,68,68	1
59	MG	BA	3005	1/1	0.50	0.75	105,105,105,105	0
59	MG	BA	3576	1/1	0.50	0.26	97,97,97,97	0
59	MG	DA	3349	1/1	0.50	1.07	141,141,141,141	0
59	MG	CA	1692	1/1	0.51	0.26	140,140,140,140	0
59	MG	DA	3634	1/1	0.51	0.22	83,83,83,83	0
59	MG	BA	3193	1/1	0.51	0.41	109,109,109,109	0
59	MG	BA	3379	1/1	0.51	0.49	114,114,114,114	0
59	MG	DA	3485	1/1	0.51	0.40	8,8,8,8	1
59	MG	BA	3059	1/1	0.51	0.33	98,98,98,98	0
59	MG	DA	3144	1/1	0.52	0.28	131,131,131,131	0
59	MG	DA	3515	1/1	0.52	0.53	108,108,108,108	0
59	MG	CA	1720	1/1	0.52	0.31	106,106,106,106	0
59	MG	AA	1627	1/1	0.52	0.23	142,142,142,142	0
59	MG	DA	3124	1/1	0.52	0.35	81,81,81,81	0
59	MG	AA	1642	1/1	0.53	0.38	108,108,108,108	0
59	MG	BA	3598	1/1	0.53	0.42	110,110,110,110	0
59	MG	BA	3095	1/1	0.53	0.40	95,95,95,95	0
59	MG	DA	3459	1/1	0.53	0.59	92,92,92,92	0
59	MG	DA	3479	1/1	0.53	0.35	127,127,127,127	0
59	MG	CA	1716	1/1	0.54	0.16	110,110,110,110	0
59	MG	AA	1666	1/1	0.54	0.45	127,127,127,127	0
59	MG	BA	3190	1/1	0.54	0.45	117,117,117,117	0
59	MG	DA	3203	1/1	0.54	0.28	112,112,112,112	0
59	MG	BA	3395	1/1	0.54	0.30	84,84,84,84	0
59	MG	DA	2906	1/1	0.54	0.48	93,93,93,93	1
59	MG	DA	3540	1/1	0.54	0.09	152,152,152,152	0
59	MG	DA	3113	1/1	0.54	0.41	109,109,109,109	0
59	MG	BA	3501	1/1	0.54	0.36	112,112,112,112	0
59	MG	BA	3570	1/1	0.54	0.34	115,115,115,115	0
59	MG	CA	1750	1/1	0.55	0.25	102,102,102,102	0
59	MG	AA	1801	1/1	0.55	0.37	130,130,130,130	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	DA	3035	1/1	0.55	0.26	84,84,84,84	0
59	MG	DA	3378	1/1	0.55	0.33	96,96,96,96	0
59	MG	AA	1792	1/1	0.55	0.22	102,102,102,102	0
59	MG	AA	1813	1/1	0.55	0.23	134,134,134,134	0
59	MG	CA	1747	1/1	0.55	0.27	79,79,79,79	0
59	MG	DA	3289	1/1	0.55	0.27	78,78,78,78	0
59	MG	BA	3043	1/1	0.56	0.49	80,80,80,80	0
59	MG	CA	1763	1/1	0.56	0.13	105,105,105,105	0
59	MG	BA	2963	1/1	0.56	0.46	113,113,113,113	0
59	MG	BA	3446	1/1	0.56	0.26	99,99,99,99	0
59	MG	AA	1900	1/1	0.56	0.11	128,128,128,128	0
59	MG	AA	1865	1/1	0.56	0.27	96,96,96,96	0
59	MG	DA	3145	1/1	0.56	0.54	120,120,120,120	0
59	MG	DA	3172	1/1	0.56	0.50	102,102,102,102	0
59	MG	BA	3234	1/1	0.56	0.41	90,90,90,90	0
59	MG	CA	1622	1/1	0.56	0.41	99,99,99,99	0
59	MG	CA	1756	1/1	0.56	0.19	87,87,87,87	0
59	MG	DA	3111	1/1	0.56	0.26	83,83,83,83	0
59	MG	DA	3390	1/1	0.57	0.51	60,60,60,60	1
59	MG	BA	3087	1/1	0.57	0.32	87,87,87,87	0
59	MG	AA	1868	1/1	0.57	0.26	100,100,100,100	0
59	MG	BA	2923	1/1	0.57	0.35	96,96,96,96	0
59	MG	CA	1685	1/1	0.57	0.26	92,92,92,92	0
59	MG	BA	3072	1/1	0.57	0.31	101,101,101,101	0
59	MG	DA	3240	1/1	0.57	0.19	128,128,128,128	0
59	MG	DA	3065	1/1	0.58	0.38	128,128,128,128	0
59	MG	DA	3075	1/1	0.58	0.26	98,98,98,98	0
59	MG	CA	1657	1/1	0.58	0.22	85,85,85,85	0
59	MG	AA	1938	1/1	0.58	0.55	124,124,124,124	0
59	MG	DA	3717	1/1	0.58	0.62	155,155,155,155	0
59	MG	AA	1968	1/1	0.58	0.32	95,95,95,95	0
59	MG	BA	3529	1/1	0.58	0.29	70,70,70,70	0
59	MG	BA	3044	1/1	0.58	0.49	64,64,64,64	0
59	MG	AA	1698	1/1	0.58	0.46	103,103,103,103	0
59	MG	AY	103	1/1	0.58	0.30	108,108,108,108	0
59	MG	DA	3049	1/1	0.58	0.66	96,96,96,96	0
59	MG	DB	204	1/1	0.58	0.24	110,110,110,110	0
59	MG	DA	3573	1/1	0.58	0.26	86,86,86,86	0
59	MG	AA	1883	1/1	0.59	0.24	58,58,58,58	0
59	MG	BA	3199	1/1	0.59	0.74	110,110,110,110	0
59	MG	DA	2939	1/1	0.59	0.62	1,1,1,1	1
59	MG	AA	1740	1/1	0.59	0.20	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	AA	1910	1/1	0.59	0.31	120,120,120,120	0
59	MG	DA	3615	1/1	0.59	0.27	86,86,86,86	0
59	MG	DA	3628	1/1	0.59	0.60	93,93,93,93	0
59	MG	DA	3322	1/1	0.59	0.45	89,89,89,89	0
59	MG	DA	2972	1/1	0.59	0.35	97,97,97,97	0
59	MG	DA	2925	1/1	0.59	0.47	108,108,108,108	0
59	MG	DA	3748	1/1	0.60	0.51	125,125,125,125	0
59	MG	BA	2987	1/1	0.60	0.33	104,104,104,104	0
59	MG	DA	3384	1/1	0.60	0.39	120,120,120,120	0
59	MG	AV	106	1/1	0.60	0.17	87,87,87,87	1
59	MG	AA	1953	1/1	0.60	0.18	120,120,120,120	0
59	MG	DA	2983	1/1	0.60	0.31	79,79,79,79	1
59	MG	AA	1771	1/1	0.60	0.29	95,95,95,95	0
59	MG	DA	3138	1/1	0.60	0.51	139,139,139,139	0
59	MG	DA	2961	1/1	0.61	0.41	126,126,126,126	0
59	MG	BA	3001	1/1	0.61	0.26	117,117,117,117	0
59	MG	BA	3346	1/1	0.61	0.25	71,71,71,71	0
59	MG	AA	1789	1/1	0.61	0.12	108,108,108,108	0
59	MG	CA	1689	1/1	0.61	0.15	96,96,96,96	1
59	MG	DA	3591	1/1	0.61	0.71	19,19,19,19	1
59	MG	DA	3266	1/1	0.61	0.36	57,57,57,57	0
59	MG	AA	1790	1/1	0.61	0.40	96,96,96,96	0
59	MG	BA	3383	1/1	0.61	0.34	126,126,126,126	0
59	MG	BA	3335	1/1	0.61	0.41	113,113,113,113	0
59	MG	DA	3066	1/1	0.61	0.23	113,113,113,113	0
59	MG	CA	1626	1/1	0.62	0.48	112,112,112,112	0
59	MG	BA	3480	1/1	0.62	0.29	55,55,55,55	0
59	MG	DA	2936	1/1	0.62	0.26	81,81,81,81	0
59	MG	BA	3303	1/1	0.62	0.17	88,88,88,88	0
59	MG	AA	1924	1/1	0.62	0.44	84,84,84,84	0
59	MG	BH	201	1/1	0.62	0.19	71,71,71,71	1
59	MG	BA	3146	1/1	0.62	0.39	113,113,113,113	0
59	MG	AA	1905	1/1	0.62	0.49	71,71,71,71	1
59	MG	DA	3640	1/1	0.62	0.53	81,81,81,81	1
59	MG	DA	3497	1/1	0.62	0.32	103,103,103,103	0
59	MG	BA	3287	1/1	0.62	0.26	104,104,104,104	0
59	MG	DA	3404	1/1	0.63	0.26	87,87,87,87	0
59	MG	BA	3350	1/1	0.63	0.60	118,118,118,118	0
59	MG	DA	2954	1/1	0.63	0.52	47,47,47,47	1
59	MG	DA	3673	1/1	0.63	0.34	116,116,116,116	0
59	MG	AA	1915	1/1	0.63	0.25	75,75,75,75	0
59	MG	CA	1721	1/1	0.63	0.87	111,111,111,111	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	CA	1725	1/1	0.63	0.27	76,76,76,76	1
59	MG	CA	1737	1/1	0.63	0.16	120,120,120,120	0
59	MG	CA	1741	1/1	0.63	0.49	106,106,106,106	0
59	MG	CA	1608	1/1	0.63	0.31	124,124,124,124	0
59	MG	DA	3143	1/1	0.63	0.41	113,113,113,113	0
59	MG	AA	1936	1/1	0.63	0.15	135,135,135,135	0
59	MG	DA	3376	1/1	0.63	0.54	93,93,93,93	0
59	MG	DA	2940	1/1	0.63	0.28	106,106,106,106	0
59	MG	DA	3150	1/1	0.63	0.15	98,98,98,98	0
59	MG	CA	1752	1/1	0.63	0.23	113,113,113,113	0
59	MG	CA	1700	1/1	0.64	0.34	104,104,104,104	0
59	MG	AA	1735	1/1	0.64	0.23	85,85,85,85	0
59	MG	CA	1719	1/1	0.64	0.24	95,95,95,95	0
59	MG	CA	1637	1/1	0.64	0.21	114,114,114,114	0
59	MG	DA	2928	1/1	0.64	0.17	61,61,61,61	1
59	MG	DA	3491	1/1	0.64	0.33	107,107,107,107	0
59	MG	DA	3337	1/1	0.64	0.31	90,90,90,90	0
59	MG	DA	3000	1/1	0.64	0.14	105,105,105,105	0
59	MG	DA	3517	1/1	0.64	0.20	107,107,107,107	0
59	MG	BA	3321	1/1	0.64	0.24	58,58,58,58	0
59	MG	BA	2993	1/1	0.64	0.47	86,86,86,86	0
59	MG	BA	2907	1/1	0.64	0.19	108,108,108,108	0
59	MG	CV	101	1/1	0.64	0.56	93,93,93,93	1
59	MG	AA	1722	1/1	0.64	0.23	116,116,116,116	0
59	MG	BA	3583	1/1	0.64	0.59	81,81,81,81	1
59	MG	BA	3132	1/1	0.64	0.27	81,81,81,81	0
59	MG	DA	2990	1/1	0.65	0.38	43,43,43,43	1
59	MG	BA	3213	1/1	0.65	0.53	135,135,135,135	0
59	MG	DA	3358	1/1	0.65	0.32	93,93,93,93	0
59	MG	DA	3770	1/1	0.65	0.17	85,85,85,85	1
59	MG	CA	1735	1/1	0.65	0.19	127,127,127,127	0
59	MG	CA	1695	1/1	0.65	0.43	110,110,110,110	0
59	MG	BA	3588	1/1	0.65	0.33	90,90,90,90	0
59	MG	AA	1705	1/1	0.65	0.28	105,105,105,105	0
59	MG	DA	3711	1/1	0.65	0.20	55,55,55,55	1
59	MG	CA	1770	1/1	0.65	0.21	54,54,54,54	1
59	MG	BA	3140	1/1	0.66	0.31	113,113,113,113	0
59	MG	CA	1646	1/1	0.66	0.34	102,102,102,102	0
59	MG	BA	3030	1/1	0.66	0.35	79,79,79,79	0
59	MG	AA	1758	1/1	0.66	0.32	98,98,98,98	0
59	MG	DA	3234	1/1	0.66	0.34	118,118,118,118	0
59	MG	CA	1671	1/1	0.66	0.29	99,99,99,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	DA	3464	1/1	0.66	0.27	62,62,62,62	1
59	MG	CJ	201	1/1	0.66	0.22	115,115,115,115	0
59	MG	BA	3272	1/1	0.66	0.52	126,126,126,126	0
59	MG	BA	3097	1/1	0.66	0.26	89,89,89,89	0
59	MG	AA	1776	1/1	0.66	0.48	119,119,119,119	0
59	MG	AA	1828	1/1	0.66	0.13	86,86,86,86	0
59	MG	D6	101	1/1	0.66	0.28	95,95,95,95	0
59	MG	BA	3391	1/1	0.66	0.43	91,91,91,91	1
59	MG	DA	2901	1/1	0.66	0.28	51,51,51,51	0
59	MG	DA	3137	1/1	0.66	0.21	70,70,70,70	0
59	MG	AV	102	1/1	0.66	0.49	106,106,106,106	0
59	MG	CA	1629	1/1	0.66	0.22	98,98,98,98	0
59	MG	DB	207	1/1	0.66	0.22	53,53,53,53	1
59	MG	DA	2991	1/1	0.66	0.17	44,44,44,44	1
59	MG	AD	303	1/1	0.67	0.25	134,134,134,134	0
59	MG	BA	3172	1/1	0.67	0.34	80,80,80,80	0
59	MG	DA	3021	1/1	0.67	0.47	87,87,87,87	0
59	MG	BA	3222	1/1	0.67	0.22	108,108,108,108	0
59	MG	AA	1966	1/1	0.67	0.11	99,99,99,99	0
59	MG	AA	1939	1/1	0.67	0.28	74,74,74,74	1
59	MG	CA	1773	1/1	0.67	0.21	106,106,106,106	0
59	MG	DA	3793	1/1	0.67	0.39	130,130,130,130	0
59	MG	DA	3366	1/1	0.67	0.48	9,9,9,9	1
59	MG	AA	1873	1/1	0.67	0.31	117,117,117,117	0
59	MG	DA	3079	1/1	0.67	0.41	127,127,127,127	0
59	MG	DA	3676	1/1	0.68	0.23	96,96,96,96	0
59	MG	BA	3218	1/1	0.68	0.18	111,111,111,111	0
59	MG	CA	1677	1/1	0.68	0.25	88,88,88,88	1
59	MG	DA	3706	1/1	0.68	0.33	66,66,66,66	0
59	MG	DA	3239	1/1	0.68	0.09	96,96,96,96	0
59	MG	BA	3113	1/1	0.68	0.12	95,95,95,95	0
59	MG	AA	1907	1/1	0.68	0.28	96,96,96,96	0
59	MG	DA	2908	1/1	0.68	0.29	97,97,97,97	0
59	MG	AA	1617	1/1	0.68	0.11	109,109,109,109	0
59	MG	DA	2923	1/1	0.68	0.12	94,94,94,94	0
59	MG	AA	1889	1/1	0.68	0.39	115,115,115,115	0
59	MG	CV	110	1/1	0.68	0.18	105,105,105,105	0
59	MG	DA	3476	1/1	0.68	0.34	120,120,120,120	0
59	MG	AH	201	1/1	0.68	0.32	102,102,102,102	0
59	MG	DA	2988	1/1	0.68	0.47	40,40,40,40	1
59	MG	DA	3661	1/1	0.68	0.27	100,100,100,100	0
59	MG	DA	3662	1/1	0.68	0.38	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
59	MG	BA	3150	1/1	0.68	0.41	145,145,145,145	0
59	MG	DA	3403	1/1	0.69	0.36	109,109,109,109	0
59	MG	BH	204	1/1	0.69	0.21	57,57,57,57	1
59	MG	BQ	201	1/1	0.69	0.15	72,72,72,72	0
59	MG	DA	3578	1/1	0.69	0.37	105,105,105,105	0
59	MG	BA	3394	1/1	0.69	0.22	85,85,85,85	0
59	MG	DA	3074	1/1	0.69	0.24	129,129,129,129	0
59	MG	AA	1935	1/1	0.69	0.26	96,96,96,96	0
59	MG	CA	1765	1/1	0.69	0.21	94,94,94,94	0
59	MG	AA	1857	1/1	0.69	0.11	57,57,57,57	0
59	MG	DA	3648	1/1	0.69	0.35	100,100,100,100	0
59	MG	BA	3358	1/1	0.69	0.18	100,100,100,100	0
59	MG	BA	3493	1/1	0.69	0.34	101,101,101,101	0
59	MG	BA	3276	1/1	0.69	0.11	125,125,125,125	0
59	MG	DA	3127	1/1	0.69	0.09	93,93,93,93	0
59	MG	AA	1964	1/1	0.69	0.47	106,106,106,106	0
59	MG	AA	1652	1/1	0.69	0.11	95,95,95,95	0
59	MG	BA	3003	1/1	0.70	0.29	75,75,75,75	0
59	MG	DA	3457	1/1	0.70	0.28	68,68,68,68	0
59	MG	CA	1668	1/1	0.70	0.17	94,94,94,94	0
59	MG	DA	3116	1/1	0.70	0.24	78,78,78,78	0
59	MG	DA	3123	1/1	0.70	0.46	91,91,91,91	0
59	MG	AO	102	1/1	0.70	0.21	77,77,77,77	0
59	MG	BA	3215	1/1	0.70	0.62	4,4,4,4	1
59	MG	BA	3364	1/1	0.70	0.98	66,66,66,66	1
59	MG	DA	3329	1/1	0.70	0.68	110,110,110,110	0
59	MG	BA	3216	1/1	0.70	0.18	73,73,73,73	0
59	MG	AX	101	1/1	0.70	0.21	113,113,113,113	0
59	MG	AA	1861	1/1	0.70	0.28	77,77,77,77	0
59	MG	B1	101	1/1	0.70	0.18	50,50,50,50	1
59	MG	CA	1698	1/1	0.70	0.30	73,73,73,73	1
59	MG	DA	2945	1/1	0.70	0.28	102,102,102,102	0
59	MG	AA	1747	1/1	0.70	0.17	119,119,119,119	0
59	MG	DA	3146	1/1	0.70	0.30	85,85,85,85	0
59	MG	BA	3409	1/1	0.70	0.14	104,104,104,104	0
59	MG	AA	1726	1/1	0.70	0.29	70,70,70,70	1
59	MG	BA	3471	1/1	0.70	0.37	96,96,96,96	0
59	MG	DA	3220	1/1	0.70	0.19	117,117,117,117	0
59	MG	DA	3081	1/1	0.70	0.29	75,75,75,75	0
59	MG	DA	3191	1/1	0.71	0.31	83,83,83,83	0
59	MG	BA	3284	1/1	0.71	0.44	97,97,97,97	0
59	MG	DA	3680	1/1	0.71	0.33	98,98,98,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	AA	1959	1/1	0.71	0.66	146,146,146,146	0
59	MG	AA	1891	1/1	0.71	0.20	54,54,54,54	1
59	MG	AA	1795	1/1	0.71	0.15	96,96,96,96	0
59	MG	DA	2921	1/1	0.71	0.65	114,114,114,114	0
59	MG	DA	3391	1/1	0.71	0.22	73,73,73,73	0
59	MG	CA	1641	1/1	0.71	0.25	84,84,84,84	0
59	MG	BA	3238	1/1	0.71	0.36	110,110,110,110	0
59	MG	AA	1662	1/1	0.71	0.23	68,68,68,68	0
59	MG	CA	1712	1/1	0.71	0.24	88,88,88,88	1
59	MG	DA	3443	1/1	0.71	0.49	133,133,133,133	0
59	MG	AA	1832	1/1	0.71	0.23	140,140,140,140	0
59	MG	AA	1757	1/1	0.71	0.45	111,111,111,111	0
59	MG	AA	1646	1/1	0.71	0.31	106,106,106,106	0
59	MG	DA	3168	1/1	0.71	0.33	100,100,100,100	0
59	MG	BA	3423	1/1	0.71	0.23	67,67,67,67	1
59	MG	DA	3189	1/1	0.71	0.35	80,80,80,80	0
59	MG	DB	211	1/1	0.71	0.21	80,80,80,80	0
59	MG	DA	3671	1/1	0.71	0.27	103,103,103,103	0
59	MG	DA	3134	1/1	0.72	0.10	74,74,74,74	0
59	MG	AA	1659	1/1	0.72	0.09	107,107,107,107	0
59	MG	DA	3462	1/1	0.72	0.36	78,78,78,78	0
59	MG	DA	3321	1/1	0.72	0.27	88,88,88,88	0
59	MG	AA	1614	1/1	0.72	0.33	113,113,113,113	0
59	MG	DA	2946	1/1	0.72	0.40	96,96,96,96	0
59	MG	DA	3068	1/1	0.72	0.14	51,51,51,51	0
59	MG	DA	2907	1/1	0.72	0.30	83,83,83,83	0
59	MG	BA	3286	1/1	0.72	0.20	57,57,57,57	0
59	MG	DA	2911	1/1	0.72	0.23	91,91,91,91	0
59	MG	BA	3592	1/1	0.72	0.18	100,100,100,100	0
59	MG	DA	3096	1/1	0.72	0.21	80,80,80,80	0
59	MG	DA	3727	1/1	0.72	0.14	70,70,70,70	1
59	MG	DA	3730	1/1	0.72	0.32	91,91,91,91	0
59	MG	BA	3015	1/1	0.72	0.16	105,105,105,105	0
59	MG	DA	3754	1/1	0.72	0.34	34,34,34,34	1
59	MG	CA	1746	1/1	0.72	0.19	85,85,85,85	0
59	MG	BA	3229	1/1	0.72	0.29	88,88,88,88	0
59	MG	AA	1632	1/1	0.72	0.33	97,97,97,97	0
59	MG	BA	3141	1/1	0.72	0.29	104,104,104,104	0
59	MG	BA	3210	1/1	0.72	0.46	106,106,106,106	0
59	MG	DA	3617	1/1	0.72	0.46	111,111,111,111	0
59	MG	AA	1948	1/1	0.72	0.30	114,114,114,114	0
59	MG	CA	1670	1/1	0.72	0.13	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	AA	1949	1/1	0.72	0.28	42,42,42,42	1
59	MG	DA	3269	1/1	0.72	0.21	44,44,44,44	0
59	MG	DF	302	1/1	0.72	0.30	98,98,98,98	0
59	MG	DA	3447	1/1	0.72	0.24	70,70,70,70	0
59	MG	AO	101	1/1	0.73	0.22	111,111,111,111	0
59	MG	DA	2958	1/1	0.73	0.84	59,59,59,59	1
59	MG	DA	3433	1/1	0.73	0.40	1,1,1,1	1
59	MG	BA	3117	1/1	0.73	0.43	98,98,98,98	0
59	MG	DA	3665	1/1	0.73	0.41	96,96,96,96	0
59	MG	AA	1756	1/1	0.73	0.22	91,91,91,91	0
59	MG	DA	3449	1/1	0.73	0.26	71,71,71,71	0
59	MG	DA	3253	1/1	0.73	0.28	52,52,52,52	0
59	MG	AA	1794	1/1	0.73	0.36	106,106,106,106	0
59	MG	CA	1679	1/1	0.73	0.10	65,65,65,65	1
59	MG	CA	1680	1/1	0.73	0.34	102,102,102,102	0
59	MG	DA	3696	1/1	0.73	0.44	80,80,80,80	0
59	MG	AA	1821	1/1	0.73	0.34	65,65,65,65	0
59	MG	DA	3297	1/1	0.73	0.31	53,53,53,53	0
59	MG	AA	1970	1/1	0.73	0.18	107,107,107,107	0
59	MG	CA	1609	1/1	0.73	0.28	93,93,93,93	0
59	MG	DA	3723	1/1	0.73	0.22	101,101,101,101	0
59	MG	DA	3495	1/1	0.73	0.27	75,75,75,75	0
59	MG	BA	3539	1/1	0.73	0.13	97,97,97,97	1
59	MG	AA	1761	1/1	0.73	0.34	83,83,83,83	0
59	MG	DA	3025	1/1	0.73	0.43	108,108,108,108	0
59	MG	BA	3380	1/1	0.73	0.36	133,133,133,133	0
59	MG	AA	1831	1/1	0.73	0.49	89,89,89,89	0
59	MG	CA	1705	1/1	0.73	0.15	62,62,62,62	0
59	MG	BA	3312	1/1	0.73	0.24	53,53,53,53	0
59	MG	DA	3165	1/1	0.73	0.08	121,121,121,121	0
59	MG	AA	1765	1/1	0.73	0.13	107,107,107,107	1
59	MG	CA	1642	1/1	0.73	0.15	85,85,85,85	0
59	MG	AA	1673	1/1	0.73	0.32	90,90,90,90	0
59	MG	CA	1650	1/1	0.73	0.22	79,79,79,79	0
59	MG	BA	2904	1/1	0.73	0.37	104,104,104,104	0
59	MG	DA	3637	1/1	0.73	0.33	88,88,88,88	0
59	MG	BA	3336	1/1	0.73	0.14	99,99,99,99	0
59	MG	AA	1943	1/1	0.74	0.25	60,60,60,60	1
59	MG	DA	3712	1/1	0.74	0.54	108,108,108,108	0
59	MG	CA	1644	1/1	0.74	0.20	92,92,92,92	0
59	MG	BA	3092	1/1	0.74	0.37	101,101,101,101	0
59	MG	AA	1836	1/1	0.74	0.22	114,114,114,114	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	DA	3208	1/1	0.74	0.27	91,91,91,91	0
59	MG	AL	203	1/1	0.74	0.22	81,81,81,81	0
59	MG	BA	3098	1/1	0.74	0.22	62,62,62,62	0
59	MG	BA	3339	1/1	0.74	0.54	63,63,63,63	1
59	MG	AA	1932	1/1	0.74	0.23	82,82,82,82	0
59	MG	BA	3400	1/1	0.74	0.20	87,87,87,87	0
59	MG	AA	1762	1/1	0.74	0.20	74,74,74,74	0
59	MG	AA	1942	1/1	0.74	0.35	98,98,98,98	0
59	MG	DA	3498	1/1	0.74	0.24	82,82,82,82	0
59	MG	DA	3786	1/1	0.74	0.36	144,144,144,144	0
59	MG	DA	2917	1/1	0.74	0.30	89,89,89,89	0
59	MG	CA	1723	1/1	0.74	0.22	82,82,82,82	0
59	MG	BA	3440	1/1	0.74	0.34	72,72,72,72	0
59	MG	CA	1726	1/1	0.74	0.30	107,107,107,107	0
59	MG	BA	3301	1/1	0.74	0.23	67,67,67,67	0
59	MG	DA	3439	1/1	0.74	0.14	54,54,54,54	1
59	MG	DO	201	1/1	0.74	0.17	117,117,117,117	0
59	MG	BA	3083	1/1	0.74	0.32	80,80,80,80	0
59	MG	BA	2961	1/1	0.75	0.13	79,79,79,79	0
59	MG	AA	1624	1/1	0.75	0.21	98,98,98,98	0
59	MG	BA	3196	1/1	0.75	0.34	64,64,64,64	0
59	MG	DA	3344	1/1	0.75	0.37	75,75,75,75	0
59	MG	DA	3481	1/1	0.75	0.39	73,73,73,73	0
59	MG	AA	1715	1/1	0.75	0.18	126,126,126,126	0
59	MG	BA	3548	1/1	0.75	0.15	92,92,92,92	0
59	MG	DA	3170	1/1	0.75	0.15	98,98,98,98	0
59	MG	D9	101	1/1	0.75	0.21	92,92,92,92	1
59	MG	DA	3369	1/1	0.75	0.27	95,95,95,95	0
59	MG	BA	3567	1/1	0.75	0.16	76,76,76,76	0
59	MG	BA	3331	1/1	0.75	0.50	92,92,92,92	0
59	MG	CA	1627	1/1	0.75	0.11	71,71,71,71	0
59	MG	BA	3265	1/1	0.75	0.14	66,66,66,66	0
59	MG	DA	3567	1/1	0.75	0.26	98,98,98,98	0
59	MG	DA	3117	1/1	0.75	0.17	88,88,88,88	0
59	MG	DA	3221	1/1	0.75	0.34	77,77,77,77	0
59	MG	DA	3577	1/1	0.75	0.46	92,92,92,92	0
59	MG	CA	1632	1/1	0.75	0.17	94,94,94,94	0
59	MG	BA	3016	1/1	0.75	0.23	66,66,66,66	0
59	MG	BA	2986	1/1	0.75	0.24	52,52,52,52	0
59	MG	AA	1717	1/1	0.75	0.32	120,120,120,120	0
59	MG	BA	3415	1/1	0.75	0.22	69,69,69,69	1
59	MG	DA	3436	1/1	0.75	0.29	104,104,104,104	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	BA	2929	1/1	0.75	0.21	90,90,90,90	0
59	MG	BA	3102	1/1	0.75	0.32	64,64,64,64	0
59	MG	BA	3354	1/1	0.75	0.30	76,76,76,76	0
59	MG	BA	3165	1/1	0.75	0.38	77,77,77,77	0
59	MG	DA	3455	1/1	0.75	0.22	71,71,71,71	0
59	MG	CA	1663	1/1	0.75	0.20	97,97,97,97	0
59	MG	AA	1739	1/1	0.75	0.34	73,73,73,73	1
59	MG	DA	3597	1/1	0.76	0.17	66,66,66,66	0
59	MG	BA	2927	1/1	0.76	0.36	83,83,83,83	1
59	MG	CA	1662	1/1	0.76	0.13	79,79,79,79	0
59	MG	DA	3002	1/1	0.76	0.12	78,78,78,78	0
59	MG	DA	3630	1/1	0.76	0.28	99,99,99,99	0
59	MG	BA	3596	1/1	0.76	0.28	107,107,107,107	0
59	MG	DA	3148	1/1	0.76	0.49	120,120,120,120	0
59	MG	BA	3248	1/1	0.76	0.30	101,101,101,101	0
59	MG	DA	3158	1/1	0.76	0.28	130,130,130,130	0
59	MG	AA	1971	1/1	0.76	0.15	125,125,125,125	0
59	MG	AA	1827	1/1	0.76	0.18	85,85,85,85	0
59	MG	DA	3042	1/1	0.76	0.17	60,60,60,60	0
59	MG	BA	3460	1/1	0.76	0.35	40,40,40,40	0
59	MG	AA	1656	1/1	0.76	0.19	98,98,98,98	1
59	MG	AA	1730	1/1	0.76	0.16	77,77,77,77	1
59	MG	DA	3196	1/1	0.76	0.24	100,100,100,100	0
59	MG	DA	3067	1/1	0.76	0.24	106,106,106,106	0
59	MG	BA	3116	1/1	0.76	0.21	81,81,81,81	0
59	MG	DA	3073	1/1	0.76	0.29	64,64,64,64	0
59	MG	BA	3498	1/1	0.76	0.80	85,85,85,85	1
59	MG	AA	1625	1/1	0.76	0.44	73,73,73,73	1
59	MG	CA	1619	1/1	0.76	0.11	116,116,116,116	0
59	MG	BA	3361	1/1	0.76	0.45	105,105,105,105	0
59	MG	DA	3714	1/1	0.76	0.28	109,109,109,109	0
59	MG	DA	3470	1/1	0.76	0.26	75,75,75,75	0
59	MG	DA	3094	1/1	0.76	0.19	87,87,87,87	0
59	MG	BA	3051	1/1	0.76	0.17	68,68,68,68	0
59	MG	DA	3105	1/1	0.76	0.29	92,92,92,92	0
59	MG	DA	3728	1/1	0.76	0.55	46,46,46,46	1
59	MG	BA	3540	1/1	0.76	0.81	66,66,66,66	1
59	MG	CC	302	1/1	0.76	0.12	114,114,114,114	0
59	MG	CH	201	1/1	0.76	0.09	37,37,37,37	1
59	MG	BA	2977	1/1	0.76	0.62	93,93,93,93	0
59	MG	BA	3554	1/1	0.76	0.14	109,109,109,109	0
59	MG	DA	3506	1/1	0.76	0.50	73,73,73,73	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	AA	1720	1/1	0.76	0.32	37,37,37,37	1
59	MG	DA	3783	1/1	0.76	0.25	90,90,90,90	0
59	MG	AA	1887	1/1	0.76	0.24	72,72,72,72	0
59	MG	CV	112	1/1	0.76	0.15	69,69,69,69	0
59	MG	DA	3552	1/1	0.76	0.38	120,120,120,120	0
59	MG	AA	1640	1/1	0.76	0.56	127,127,127,127	0
59	MG	BA	3318	1/1	0.76	0.24	63,63,63,63	0
59	MG	DA	3346	1/1	0.76	0.22	59,59,59,59	0
59	MG	BA	2914	1/1	0.76	0.53	106,106,106,106	0
59	MG	DA	3135	1/1	0.76	0.20	51,51,51,51	0
59	MG	BA	3153	1/1	0.76	0.19	93,93,93,93	0
59	MG	AA	1945	1/1	0.76	0.32	94,94,94,94	1
59	MG	DA	2942	1/1	0.77	1.04	27,27,27,27	1
59	MG	AQ	202	1/1	0.77	0.15	97,97,97,97	0
59	MG	AA	1800	1/1	0.77	0.38	114,114,114,114	0
59	MG	AA	1769	1/1	0.77	0.18	101,101,101,101	0
59	MG	DA	3453	1/1	0.77	0.27	84,84,84,84	0
59	MG	AA	1937	1/1	0.77	0.17	58,58,58,58	0
59	MG	AA	1630	1/1	0.77	0.21	57,57,57,57	0
59	MG	CV	109	1/1	0.77	0.14	95,95,95,95	0
59	MG	DA	3668	1/1	0.77	0.13	93,93,93,93	0
59	MG	DA	2960	1/1	0.77	0.37	57,57,57,57	1
59	MG	AA	1743	1/1	0.77	0.26	87,87,87,87	0
59	MG	DA	3467	1/1	0.77	0.58	109,109,109,109	0
59	MG	BA	3244	1/1	0.77	0.28	88,88,88,88	0
59	MG	BA	3594	1/1	0.77	0.24	83,83,83,83	0
59	MG	DA	2981	1/1	0.77	0.30	127,127,127,127	0
59	MG	DA	3691	1/1	0.77	0.16	59,59,59,59	0
59	MG	AA	1908	1/1	0.77	0.17	65,65,65,65	0
59	MG	BA	3154	1/1	0.77	0.22	54,54,54,54	0
59	MG	BA	2992	1/1	0.77	0.10	50,50,50,50	1
59	MG	BA	3094	1/1	0.77	0.21	32,32,32,32	0
59	MG	AA	1881	1/1	0.77	0.18	98,98,98,98	0
59	MG	AA	1833	1/1	0.77	0.15	87,87,87,87	0
59	MG	DA	3719	1/1	0.77	0.24	73,73,73,73	0
59	MG	DA	3015	1/1	0.77	0.34	81,81,81,81	0
59	MG	AA	1946	1/1	0.77	0.24	77,77,77,77	0
59	MG	BA	3502	1/1	0.77	1.20	132,132,132,132	0
59	MG	DA	3526	1/1	0.77	0.27	11,11,11,11	1
59	MG	DA	3538	1/1	0.77	0.33	118,118,118,118	0
59	MG	CA	1758	1/1	0.77	0.14	126,126,126,126	0
59	MG	DA	3549	1/1	0.77	0.17	97,97,97,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	DA	3030	1/1	0.77	0.35	59,59,59,59	0
59	MG	DA	3555	1/1	0.77	0.34	105,105,105,105	0
59	MG	BA	3513	1/1	0.77	0.21	77,77,77,77	0
59	MG	DA	3566	1/1	0.77	0.12	106,106,106,106	0
59	MG	AA	1922	1/1	0.77	0.09	82,82,82,82	0
59	MG	AA	1713	1/1	0.77	0.17	70,70,70,70	0
59	MG	AA	1952	1/1	0.77	0.43	97,97,97,97	0
59	MG	CA	1771	1/1	0.77	0.28	96,96,96,96	0
59	MG	BA	3545	1/1	0.77	0.33	79,79,79,79	0
59	MG	CA	1774	1/1	0.77	0.29	111,111,111,111	1
59	MG	AA	1781	1/1	0.77	0.17	111,111,111,111	0
59	MG	CA	1779	1/1	0.77	0.28	102,102,102,102	0
59	MG	BA	3387	1/1	0.77	0.15	87,87,87,87	0
59	MG	BA	3039	1/1	0.77	0.42	81,81,81,81	0
59	MG	DA	3214	1/1	0.77	0.39	102,102,102,102	0
59	MG	AA	1697	1/1	0.78	0.38	76,76,76,76	0
59	MG	DA	3261	1/1	0.78	0.40	34,34,34,34	1
59	MG	D7	104	1/1	0.78	0.57	82,82,82,82	1
59	MG	DA	3651	1/1	0.78	0.75	93,93,93,93	0
59	MG	BA	3045	1/1	0.78	0.20	75,75,75,75	0
59	MG	CA	1601	1/1	0.78	0.12	96,96,96,96	0
59	MG	CA	1605	1/1	0.78	0.24	49,49,49,49	1
59	MG	DA	3666	1/1	0.78	0.27	66,66,66,66	0
59	MG	DA	3468	1/1	0.78	0.43	76,76,76,76	0
59	MG	AA	1850	1/1	0.78	0.53	89,89,89,89	0
59	MG	BA	2922	1/1	0.78	0.41	95,95,95,95	0
59	MG	DA	3478	1/1	0.78	0.30	112,112,112,112	0
59	MG	BA	3564	1/1	0.78	0.45	113,113,113,113	0
59	MG	DA	3326	1/1	0.78	0.16	63,63,63,63	0
59	MG	AA	1772	1/1	0.78	0.21	85,85,85,85	0
59	MG	DA	3330	1/1	0.78	0.41	1,1,1,1	1
59	MG	DA	3695	1/1	0.78	0.27	81,81,81,81	0
59	MG	CA	1620	1/1	0.78	0.18	87,87,87,87	0
59	MG	BA	3138	1/1	0.78	0.14	60,60,60,60	0
59	MG	AA	1727	1/1	0.78	0.20	84,84,84,84	1
59	MG	AA	1729	1/1	0.78	0.13	50,50,50,50	0
59	MG	AA	1904	1/1	0.78	0.15	81,81,81,81	0
59	MG	DA	3516	1/1	0.78	0.54	97,97,97,97	0
59	MG	CA	1703	1/1	0.78	0.19	82,82,82,82	0
59	MG	DA	3059	1/1	0.78	0.29	77,77,77,77	0
59	MG	BA	3491	1/1	0.78	0.13	70,70,70,70	0
59	MG	BA	3149	1/1	0.78	0.30	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	CA	1639	1/1	0.78	0.14	95,95,95,95	0
59	MG	AA	1709	1/1	0.78	0.28	85,85,85,85	1
59	MG	DA	3382	1/1	0.78	0.11	101,101,101,101	0
59	MG	DA	3556	1/1	0.78	0.42	97,97,97,97	0
59	MG	DA	3071	1/1	0.78	0.33	71,71,71,71	0
59	MG	AA	1906	1/1	0.78	0.29	65,65,65,65	1
59	MG	BA	3019	1/1	0.78	0.31	66,66,66,66	0
59	MG	DA	3780	1/1	0.78	0.25	77,77,77,77	0
59	MG	AA	1750	1/1	0.78	0.18	54,54,54,54	1
59	MG	CA	1724	1/1	0.78	0.24	102,102,102,102	0
59	MG	AA	1677	1/1	0.78	0.17	76,76,76,76	1
59	MG	BA	3605	1/1	0.78	0.33	79,79,79,79	0
59	MG	DA	3421	1/1	0.78	0.26	71,71,71,71	0
59	MG	DA	2957	1/1	0.78	0.29	47,47,47,47	0
59	MG	CA	1730	1/1	0.78	0.10	106,106,106,106	0
59	MG	BB	206	1/1	0.78	0.25	90,90,90,90	1
59	MG	DB	209	1/1	0.78	0.18	95,95,95,95	0
59	MG	DA	3235	1/1	0.78	0.23	110,110,110,110	0
59	MG	D1	101	1/1	0.78	0.10	75,75,75,75	0
59	MG	BA	3532	1/1	0.78	0.33	88,88,88,88	0
59	MG	BA	2981	1/1	0.78	0.29	80,80,80,80	0
59	MG	AA	1637	1/1	0.79	0.26	78,78,78,78	1
59	MG	BA	3233	1/1	0.79	0.21	73,73,73,73	0
59	MG	BA	2970	1/1	0.79	0.36	101,101,101,101	0
59	MG	CA	1708	1/1	0.79	0.16	64,64,64,64	1
59	MG	CA	1659	1/1	0.79	0.34	100,100,100,100	0
59	MG	AA	1686	1/1	0.79	0.16	81,81,81,81	0
59	MG	CA	1766	1/1	0.79	0.17	118,118,118,118	0
59	MG	BA	3477	1/1	0.79	0.72	128,128,128,128	0
59	MG	BA	3550	1/1	0.79	0.20	103,103,103,103	0
59	MG	AA	1787	1/1	0.79	0.17	109,109,109,109	0
59	MG	BB	204	1/1	0.79	0.12	109,109,109,109	0
59	MG	DA	3736	1/1	0.79	0.23	77,77,77,77	1
59	MG	DA	3417	1/1	0.79	0.25	48,48,48,48	1
59	MG	AA	1803	1/1	0.79	0.12	98,98,98,98	0
59	MG	AA	1736	1/1	0.79	0.27	101,101,101,101	0
59	MG	DA	2912	1/1	0.79	0.24	68,68,68,68	0
59	MG	CA	1636	1/1	0.79	0.21	77,77,77,77	0
59	MG	DA	2982	1/1	0.79	0.47	97,97,97,97	0
59	MG	DA	3531	1/1	0.79	0.21	82,82,82,82	0
59	MG	DA	3534	1/1	0.79	0.44	73,73,73,73	1
59	MG	CA	1681	1/1	0.79	0.13	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	BA	3259	1/1	0.79	0.17	59,59,59,59	0
59	MG	DA	3787	1/1	0.79	0.33	95,95,95,95	0
59	MG	BN	201	1/1	0.79	0.20	64,64,64,64	0
59	MG	CA	1739	1/1	0.79	0.17	104,104,104,104	0
59	MG	DA	3343	1/1	0.79	0.25	69,69,69,69	0
59	MG	DA	2927	1/1	0.79	1.15	1,1,1,1	1
59	MG	BA	2908	1/1	0.79	0.16	84,84,84,84	0
59	MG	BA	3192	1/1	0.79	0.42	90,90,90,90	0
59	MG	DA	3693	1/1	0.79	0.21	33,33,33,33	1
59	MG	AA	1798	1/1	0.79	0.14	114,114,114,114	0
59	MG	BA	3430	1/1	0.79	0.15	68,68,68,68	0
59	MG	DA	3667	1/1	0.80	0.36	46,46,46,46	1
59	MG	AA	1742	1/1	0.80	0.10	63,63,63,63	1
59	MG	BA	2984	1/1	0.80	0.17	92,92,92,92	0
59	MG	DA	3510	1/1	0.80	0.10	59,59,59,59	0
59	MG	AA	1775	1/1	0.80	0.18	92,92,92,92	0
59	MG	DA	3197	1/1	0.80	0.17	67,67,67,67	0
59	MG	DA	3682	1/1	0.80	0.43	103,103,103,103	0
59	MG	BA	3115	1/1	0.80	0.52	93,93,93,93	0
59	MG	DA	3519	1/1	0.80	0.12	77,77,77,77	0
59	MG	BA	3071	1/1	0.80	0.51	110,110,110,110	0
59	MG	AA	1834	1/1	0.80	0.23	94,94,94,94	0
59	MG	BA	3313	1/1	0.80	0.24	70,70,70,70	0
59	MG	CA	1762	1/1	0.80	0.16	95,95,95,95	0
59	MG	AA	1805	1/1	0.80	0.13	102,102,102,102	0
59	MG	BA	3084	1/1	0.80	0.24	88,88,88,88	0
59	MG	BA	3246	1/1	0.80	0.16	68,68,68,68	0
59	MG	DA	2989	1/1	0.80	0.21	83,83,83,83	0
59	MG	BA	3522	1/1	0.80	0.30	74,74,74,74	0
59	MG	DA	3241	1/1	0.80	0.91	34,34,34,34	1
59	MG	DA	3252	1/1	0.80	0.20	87,87,87,87	0
59	MG	BA	3031	1/1	0.80	0.19	58,58,58,58	0
59	MG	DA	3569	1/1	0.80	0.46	102,102,102,102	0
59	MG	BA	3258	1/1	0.80	0.40	69,69,69,69	0
59	MG	BA	3536	1/1	0.80	0.21	73,73,73,73	0
59	MG	BE	301	1/1	0.80	0.25	88,88,88,88	0
59	MG	CA	1648	1/1	0.80	0.33	90,90,90,90	0
59	MG	DA	3583	1/1	0.80	0.24	64,64,64,64	0
59	MG	BA	3037	1/1	0.80	0.32	64,64,64,64	0
59	MG	DA	3291	1/1	0.80	0.24	88,88,88,88	0
59	MG	BH	202	1/1	0.80	0.09	95,95,95,95	0
59	MG	AY	102	1/1	0.80	0.27	104,104,104,104	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	DA	3618	1/1	0.80	0.30	72,72,72,72	0
59	MG	BA	3340	1/1	0.80	0.53	99,99,99,99	0
59	MG	BA	3422	1/1	0.80	0.12	68,68,68,68	0
59	MG	DA	3632	1/1	0.80	0.20	56,56,56,56	0
59	MG	CJ	202	1/1	0.80	0.10	130,130,130,130	0
59	MG	BA	3040	1/1	0.80	0.33	79,79,79,79	0
59	MG	DA	3062	1/1	0.80	0.31	88,88,88,88	0
59	MG	AA	1965	1/1	0.80	0.33	97,97,97,97	0
59	MG	DA	3151	1/1	0.80	0.34	73,73,73,73	0
59	MG	AA	1886	1/1	0.80	0.43	84,84,84,84	0
59	MG	BA	3566	1/1	0.80	0.39	66,66,66,66	1
59	MG	CA	1675	1/1	0.80	0.29	93,93,93,93	0
59	MG	BA	3353	1/1	0.80	0.39	107,107,107,107	0
59	MG	DA	2953	1/1	0.80	0.33	99,99,99,99	0
59	MG	CA	1686	1/1	0.81	0.17	74,74,74,74	0
59	MG	BA	3556	1/1	0.81	0.29	116,116,116,116	0
59	MG	BA	3558	1/1	0.81	0.21	78,78,78,78	0
59	MG	AA	1876	1/1	0.81	0.19	92,92,92,92	1
59	MG	AA	1880	1/1	0.81	0.25	102,102,102,102	0
59	MG	CA	1621	1/1	0.81	0.13	89,89,89,89	0
59	MG	AA	1793	1/1	0.81	0.17	75,75,75,75	0
59	MG	BA	3569	1/1	0.81	0.60	113,113,113,113	0
59	MG	DA	3224	1/1	0.81	0.26	85,85,85,85	0
59	MG	DA	3642	1/1	0.81	0.34	88,88,88,88	0
59	MG	AA	1676	1/1	0.81	0.12	68,68,68,68	0
59	MG	BA	3575	1/1	0.81	0.31	92,92,92,92	0
59	MG	AA	1917	1/1	0.81	0.27	78,78,78,78	0
59	MG	DA	3086	1/1	0.81	0.12	60,60,60,60	0
59	MG	AA	1950	1/1	0.81	0.34	81,81,81,81	0
59	MG	BA	3008	1/1	0.81	0.29	123,123,123,123	0
59	MG	DA	3098	1/1	0.81	0.16	86,86,86,86	0
59	MG	CV	104	1/1	0.81	0.08	86,86,86,86	0
59	MG	DA	3107	1/1	0.81	0.11	103,103,103,103	0
59	MG	AA	1920	1/1	0.81	0.10	73,73,73,73	0
59	MG	BA	3174	1/1	0.81	0.25	83,83,83,83	0
59	MG	BA	3482	1/1	0.81	0.63	144,144,144,144	0
59	MG	DA	3272	1/1	0.81	0.20	79,79,79,79	1
59	MG	DA	2969	1/1	0.81	0.29	98,98,98,98	0
59	MG	BA	2950	1/1	0.81	0.14	55,55,55,55	1
59	MG	DA	3489	1/1	0.81	0.19	59,59,59,59	1
59	MG	DA	3293	1/1	0.81	0.20	70,70,70,70	0
59	MG	AA	1835	1/1	0.81	0.37	102,102,102,102	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	DA	3316	1/1	0.81	0.24	59,59,59,59	1
59	MG	AA	1737	1/1	0.81	0.28	69,69,69,69	0
59	MG	DA	3505	1/1	0.81	0.36	125,125,125,125	0
59	MG	DA	3710	1/1	0.81	0.43	92,92,92,92	0
59	MG	BA	3274	1/1	0.81	0.31	83,83,83,83	0
59	MG	DA	3324	1/1	0.81	0.26	66,66,66,66	1
59	MG	DA	3512	1/1	0.81	0.52	104,104,104,104	0
59	MG	DA	3716	1/1	0.81	0.45	103,103,103,103	0
59	MG	BA	3604	1/1	0.81	0.51	82,82,82,82	0
59	MG	AA	1738	1/1	0.81	0.34	59,59,59,59	0
59	MG	BA	3505	1/1	0.81	0.43	95,95,95,95	0
59	MG	BA	3035	1/1	0.81	0.32	42,42,42,42	0
59	MG	AA	1755	1/1	0.81	0.17	34,34,34,34	1
59	MG	AA	1635	1/1	0.81	0.47	108,108,108,108	0
59	MG	BA	3293	1/1	0.81	0.17	82,82,82,82	0
59	MG	DA	3009	1/1	0.81	0.42	83,83,83,83	0
59	MG	BA	3300	1/1	0.81	0.21	71,71,71,71	0
59	MG	CA	1754	1/1	0.81	0.10	78,78,78,78	1
59	MG	DA	3756	1/1	0.81	0.39	106,106,106,106	0
59	MG	DA	3550	1/1	0.81	0.60	86,86,86,86	0
59	MG	CA	1672	1/1	0.81	0.17	92,92,92,92	0
59	MG	DA	3023	1/1	0.81	0.21	41,41,41,41	0
59	MG	DA	3372	1/1	0.81	0.14	82,82,82,82	0
59	MG	BA	2976	1/1	0.81	0.16	97,97,97,97	0
59	MG	DA	3153	1/1	0.81	0.20	68,68,68,68	0
59	MG	DA	3154	1/1	0.81	0.20	58,58,58,58	0
59	MG	AA	1902	1/1	0.81	0.11	90,90,90,90	0
59	MG	AA	1829	1/1	0.81	0.34	91,91,91,91	0
59	MG	DA	3036	1/1	0.81	0.32	76,76,76,76	0
59	MG	AA	1634	1/1	0.81	0.20	70,70,70,70	1
59	MG	AA	1691	1/1	0.81	0.36	90,90,90,90	0
59	MG	DB	205	1/1	0.81	0.20	82,82,82,82	0
59	MG	BA	3058	1/1	0.81	0.26	74,74,74,74	0
59	MG	DA	3584	1/1	0.81	0.22	80,80,80,80	0
59	MG	DA	3587	1/1	0.81	0.34	74,74,74,74	0
59	MG	DA	3590	1/1	0.81	0.17	67,67,67,67	0
59	MG	DA	3407	1/1	0.81	0.34	77,77,77,77	1
59	MG	DA	3409	1/1	0.81	0.14	53,53,53,53	1
59	MG	CA	1738	1/1	0.82	0.09	80,80,80,80	0
59	MG	DA	3624	1/1	0.82	0.19	71,71,71,71	0
59	MG	BA	3591	1/1	0.82	0.53	93,93,93,93	0
59	MG	CA	1654	1/1	0.82	0.17	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	CA	1743	1/1	0.82	0.20	81,81,81,81	0
59	MG	CA	1655	1/1	0.82	0.13	84,84,84,84	0
59	MG	DA	3446	1/1	0.82	0.19	52,52,52,52	0
59	MG	BA	3004	1/1	0.82	0.27	84,84,84,84	0
59	MG	AA	1809	1/1	0.82	0.27	92,92,92,92	0
59	MG	DA	3643	1/1	0.82	0.21	113,113,113,113	0
59	MG	BA	2935	1/1	0.82	0.60	102,102,102,102	0
59	MG	BA	3010	1/1	0.82	0.41	95,95,95,95	0
59	MG	AA	1955	1/1	0.82	0.32	64,64,64,64	1
59	MG	BA	3494	1/1	0.82	0.25	77,77,77,77	0
59	MG	AA	1956	1/1	0.82	0.30	58,58,58,58	0
59	MG	DA	2938	1/1	0.82	0.50	17,17,17,17	1
59	MG	BA	3500	1/1	0.82	0.21	79,79,79,79	0
59	MG	AA	1958	1/1	0.82	0.19	106,106,106,106	0
59	MG	DA	3091	1/1	0.82	0.66	119,119,119,119	0
59	MG	AA	1768	1/1	0.82	0.38	107,107,107,107	0
59	MG	BA	3186	1/1	0.82	0.15	81,81,81,81	0
59	MG	BA	3511	1/1	0.82	0.22	73,73,73,73	0
59	MG	AA	1814	1/1	0.82	0.30	77,77,77,77	0
59	MG	DA	3483	1/1	0.82	0.32	55,55,55,55	0
59	MG	DA	2949	1/1	0.82	0.35	98,98,98,98	1
59	MG	DA	3487	1/1	0.82	0.45	42,42,42,42	1
59	MG	DA	3109	1/1	0.82	0.18	90,90,90,90	0
59	MG	AA	1745	1/1	0.82	0.32	50,50,50,50	1
59	MG	BA	3365	1/1	0.82	0.23	112,112,112,112	0
59	MG	BA	3104	1/1	0.82	0.34	78,78,78,78	0
59	MG	BA	3109	1/1	0.82	0.16	35,35,35,35	0
59	MG	AA	1786	1/1	0.82	0.15	123,123,123,123	0
59	MG	AA	1941	1/1	0.82	0.20	63,63,63,63	0
59	MG	AA	1621	1/1	0.82	0.40	98,98,98,98	0
59	MG	AA	1681	1/1	0.82	0.18	106,106,106,106	0
59	MG	DA	3130	1/1	0.82	0.37	108,108,108,108	0
59	MG	AA	1703	1/1	0.82	0.11	44,44,44,44	1
59	MG	DA	3338	1/1	0.82	0.31	68,68,68,68	0
59	MG	DA	3340	1/1	0.82	0.33	96,96,96,96	0
59	MG	DA	3522	1/1	0.82	0.37	56,56,56,56	0
59	MG	DA	3132	1/1	0.82	0.28	49,49,49,49	0
59	MG	BA	3399	1/1	0.82	0.69	146,146,146,146	0
59	MG	AA	1894	1/1	0.82	0.18	90,90,90,90	0
59	MG	BA	3401	1/1	0.82	0.23	75,75,75,75	0
59	MG	DA	3347	1/1	0.82	0.14	71,71,71,71	0
59	MG	BA	3561	1/1	0.82	0.27	122,122,122,122	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	DA	3352	1/1	0.82	0.18	58,58,58,58	0
59	MG	DA	3767	1/1	0.82	0.27	67,67,67,67	0
59	MG	DA	2986	1/1	0.82	0.35	142,142,142,142	0
59	MG	DA	2987	1/1	0.82	0.28	68,68,68,68	0
59	MG	CA	1714	1/1	0.82	0.28	83,83,83,83	0
59	MG	BA	3122	1/1	0.82	0.33	106,106,106,106	0
59	MG	CA	1717	1/1	0.82	0.21	78,78,78,78	0
59	MG	BA	3127	1/1	0.82	0.15	71,71,71,71	0
59	MG	AA	1895	1/1	0.82	0.22	72,72,72,72	0
59	MG	AA	1725	1/1	0.82	0.30	70,70,70,70	1
59	MG	BA	3325	1/1	0.82	0.23	84,84,84,84	0
59	MG	BA	3327	1/1	0.82	0.31	59,59,59,59	0
59	MG	BA	3445	1/1	0.82	0.58	111,111,111,111	0
59	MG	DA	3401	1/1	0.82	0.38	65,65,65,65	0
59	MG	AA	1927	1/1	0.82	0.19	113,113,113,113	0
59	MG	BA	3458	1/1	0.82	0.42	104,104,104,104	0
59	MG	DA	2905	1/1	0.82	0.09	80,80,80,80	0
59	MG	DA	3028	1/1	0.82	0.33	79,79,79,79	0
59	MG	CA	1732	1/1	0.82	0.10	70,70,70,70	0
59	MG	AA	1777	1/1	0.82	0.31	115,115,115,115	0
59	MG	BA	3239	1/1	0.82	0.14	77,77,77,77	0
59	MG	DA	2967	1/1	0.83	1.36	35,35,35,35	1
59	MG	DA	3360	1/1	0.83	0.28	99,99,99,99	0
59	MG	B6	101	1/1	0.83	0.13	111,111,111,111	0
59	MG	DA	3659	1/1	0.83	0.44	88,88,88,88	0
59	MG	DA	3503	1/1	0.83	0.15	59,59,59,59	0
59	MG	AA	1807	1/1	0.83	0.17	61,61,61,61	0
59	MG	BA	3345	1/1	0.83	0.28	37,37,37,37	0
59	MG	AA	1754	1/1	0.83	0.12	124,124,124,124	0
59	MG	DA	3101	1/1	0.83	0.54	97,97,97,97	0
59	MG	BA	3453	1/1	0.83	0.10	120,120,120,120	0
59	MG	AA	1860	1/1	0.83	0.31	61,61,61,61	0
59	MG	CA	1753	1/1	0.83	0.09	103,103,103,103	0
59	MG	AA	1797	1/1	0.83	0.15	76,76,76,76	0
59	MG	DA	3520	1/1	0.83	0.23	103,103,103,103	0
59	MG	CA	1755	1/1	0.83	0.28	100,100,100,100	0
59	MG	BA	3080	1/1	0.83	0.39	83,83,83,83	0
59	MG	DA	2909	1/1	0.83	0.35	83,83,83,83	0
59	MG	BA	2973	1/1	0.83	0.26	85,85,85,85	0
59	MG	DA	3406	1/1	0.83	1.24	38,38,38,38	1
59	MG	DA	3539	1/1	0.83	0.23	70,70,70,70	0
59	MG	DA	3248	1/1	0.83	0.09	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	DA	3548	1/1	0.83	0.28	50,50,50,50	1
59	MG	DA	2993	1/1	0.83	0.49	96,96,96,96	0
59	MG	BA	2917	1/1	0.83	0.22	84,84,84,84	0
59	MG	BA	3018	1/1	0.83	0.20	38,38,38,38	0
59	MG	DA	3553	1/1	0.83	0.37	68,68,68,68	0
59	MG	BA	3485	1/1	0.83	0.36	103,103,103,103	0
59	MG	AA	1912	1/1	0.83	0.15	57,57,57,57	1
59	MG	DA	3718	1/1	0.83	0.30	92,92,92,92	0
59	MG	DA	3561	1/1	0.83	0.23	81,81,81,81	1
59	MG	DA	3432	1/1	0.83	0.65	86,86,86,86	1
59	MG	BA	3225	1/1	0.83	0.15	62,62,62,62	0
59	MG	CA	1635	1/1	0.83	0.15	93,93,93,93	0
59	MG	AA	1710	1/1	0.83	0.19	77,77,77,77	0
59	MG	AX	102	1/1	0.83	0.06	87,87,87,87	0
59	MG	DA	3572	1/1	0.83	0.23	56,56,56,56	1
59	MG	DA	3744	1/1	0.83	0.11	93,93,93,93	1
59	MG	AA	1611	1/1	0.83	0.10	66,66,66,66	0
59	MG	DA	3750	1/1	0.83	0.24	84,84,84,84	0
59	MG	DA	3751	1/1	0.83	0.27	82,82,82,82	0
59	MG	BA	3384	1/1	0.83	0.43	95,95,95,95	0
59	MG	DA	3304	1/1	0.83	0.34	84,84,84,84	0
59	MG	DA	3761	1/1	0.83	0.29	96,96,96,96	0
59	MG	DA	3311	1/1	0.83	0.43	96,96,96,96	0
59	MG	AA	1919	1/1	0.83	0.14	78,78,78,78	0
59	MG	BA	3597	1/1	0.83	0.31	53,53,53,53	1
59	MG	CA	1784	1/1	0.83	0.25	76,76,76,76	0
59	MG	BA	2939	1/1	0.83	0.20	80,80,80,80	0
59	MG	BA	2945	1/1	0.83	0.25	113,113,113,113	0
59	MG	DA	3602	1/1	0.83	0.20	76,76,76,76	0
59	MG	DA	3607	1/1	0.83	0.30	104,104,104,104	0
59	MG	BA	3105	1/1	0.83	0.37	79,79,79,79	0
59	MG	BA	3326	1/1	0.83	0.30	77,77,77,77	0
59	MG	BA	2994	1/1	0.83	0.26	80,80,80,80	0
59	MG	BA	3111	1/1	0.83	0.16	79,79,79,79	0
59	MG	BA	3403	1/1	0.83	0.08	69,69,69,69	0
59	MG	BE	304	1/1	0.83	0.16	46,46,46,46	1
59	MG	BA	3405	1/1	0.83	0.24	44,44,44,44	0
59	MG	BA	3254	1/1	0.83	0.32	93,93,93,93	0
59	MG	AA	1848	1/1	0.83	0.33	117,117,117,117	0
59	MG	DA	3179	1/1	0.83	0.27	66,66,66,66	0
59	MG	DN	203	1/1	0.83	0.18	64,64,64,64	1
59	MG	BA	3338	1/1	0.83	0.30	97,97,97,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	DP	206	1/1	0.83	0.23	82,82,82,82	0
59	MG	BA	3002	1/1	0.83	0.35	83,83,83,83	0
59	MG	AA	1728	1/1	0.84	0.16	78,78,78,78	0
59	MG	BA	3006	1/1	0.84	0.24	68,68,68,68	0
59	MG	AA	1870	1/1	0.84	0.29	73,73,73,73	0
59	MG	DA	3650	1/1	0.84	0.14	106,106,106,106	0
59	MG	CA	1660	1/1	0.84	0.14	99,99,99,99	0
59	MG	AA	1767	1/1	0.84	0.26	77,77,77,77	0
59	MG	AA	1874	1/1	0.84	0.06	111,111,111,111	0
59	MG	BA	3241	1/1	0.84	0.10	44,44,44,44	0
59	MG	DA	3664	1/1	0.84	0.24	85,85,85,85	0
59	MG	AA	1969	1/1	0.84	0.31	83,83,83,83	0
59	MG	BA	3421	1/1	0.84	0.26	68,68,68,68	0
59	MG	AA	1663	1/1	0.84	0.16	95,95,95,95	0
59	MG	CA	1674	1/1	0.84	0.12	90,90,90,90	0
59	MG	BA	2975	1/1	0.84	0.28	57,57,57,57	0
59	MG	BA	3555	1/1	0.84	0.31	60,60,60,60	0
59	MG	BA	3159	1/1	0.84	0.24	72,72,72,72	0
59	MG	DA	2922	1/1	0.84	0.29	65,65,65,65	0
59	MG	BA	3096	1/1	0.84	0.38	102,102,102,102	0
59	MG	AA	1810	1/1	0.84	0.17	71,71,71,71	0
59	MG	DA	3688	1/1	0.84	0.17	107,107,107,107	1
59	MG	DA	3163	1/1	0.84	0.15	49,49,49,49	0
59	MG	AA	1944	1/1	0.84	0.20	76,76,76,76	0
59	MG	DA	3692	1/1	0.84	0.30	61,61,61,61	0
59	MG	DA	3363	1/1	0.84	0.21	69,69,69,69	0
59	MG	CA	1618	1/1	0.84	0.28	79,79,79,79	0
59	MG	DA	3524	1/1	0.84	0.13	61,61,61,61	0
59	MG	BA	3032	1/1	0.84	0.49	88,88,88,88	0
59	MG	CA	1691	1/1	0.84	0.15	103,103,103,103	0
59	MG	AA	1716	1/1	0.84	0.26	82,82,82,82	0
59	MG	DA	2937	1/1	0.84	0.27	63,63,63,63	1
59	MG	AA	1631	1/1	0.84	0.24	85,85,85,85	0
59	MG	AA	1839	1/1	0.84	0.24	74,74,74,74	0
59	MG	AA	1843	1/1	0.84	0.18	99,99,99,99	0
59	MG	DA	3388	1/1	0.84	0.20	78,78,78,78	0
59	MG	BA	3479	1/1	0.84	0.21	133,133,133,133	0
59	MG	CA	1628	1/1	0.84	0.13	88,88,88,88	0
59	MG	DA	3210	1/1	0.84	0.37	71,71,71,71	0
59	MG	BA	3578	1/1	0.84	0.20	76,76,76,76	0
59	MG	DA	3076	1/1	0.84	0.23	75,75,75,75	0
59	MG	CA	1630	1/1	0.84	0.10	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	AA	1751	1/1	0.84	0.11	104,104,104,104	0
59	MG	DA	3737	1/1	0.84	0.30	74,74,74,74	0
59	MG	DA	3739	1/1	0.84	0.21	95,95,95,95	0
59	MG	DA	3408	1/1	0.84	0.13	41,41,41,41	0
59	MG	DA	3231	1/1	0.84	0.24	98,98,98,98	0
59	MG	BA	3203	1/1	0.84	0.19	75,75,75,75	0
59	MG	AA	1667	1/1	0.84	0.12	49,49,49,49	0
59	MG	BA	3367	1/1	0.84	0.53	96,96,96,96	0
59	MG	DA	3095	1/1	0.84	0.26	42,42,42,42	0
59	MG	DA	3424	1/1	0.84	0.35	84,84,84,84	0
59	MG	DA	3762	1/1	0.84	0.17	99,99,99,99	0
59	MG	CM	202	1/1	0.84	0.20	151,151,151,151	0
59	MG	DA	3581	1/1	0.84	0.26	88,88,88,88	1
59	MG	BA	3206	1/1	0.84	0.36	59,59,59,59	0
59	MG	DA	2959	1/1	0.84	0.30	61,61,61,61	0
59	MG	DA	3250	1/1	0.84	0.12	69,69,69,69	0
59	MG	AA	1822	1/1	0.84	0.35	60,60,60,60	0
59	MG	DA	3106	1/1	0.84	0.10	77,77,77,77	0
59	MG	BA	3046	1/1	0.84	0.08	90,90,90,90	0
59	MG	DA	2962	1/1	0.84	0.28	84,84,84,84	0
59	MG	CV	107	1/1	0.84	0.27	115,115,115,115	0
59	MG	AA	1791	1/1	0.84	0.17	93,93,93,93	0
59	MG	BA	3386	1/1	0.84	0.38	72,72,72,72	0
59	MG	DA	3286	1/1	0.84	0.08	112,112,112,112	0
59	MG	DA	3461	1/1	0.84	0.29	77,77,77,77	0
59	MG	DA	3288	1/1	0.84	0.16	60,60,60,60	0
59	MG	CA	1647	1/1	0.84	0.13	77,77,77,77	0
59	MG	CY	101	1/1	0.84	0.05	143,143,143,143	0
59	MG	DA	3633	1/1	0.84	0.23	75,75,75,75	0
59	MG	AA	1898	1/1	0.84	0.21	65,65,65,65	0
59	MG	AA	1763	1/1	0.84	0.23	88,88,88,88	0
59	MG	BA	3061	1/1	0.84	0.25	63,63,63,63	0
59	MG	AA	1804	1/1	0.84	0.28	90,90,90,90	0
59	MG	DA	3155	1/1	0.85	0.44	78,78,78,78	0
59	MG	BA	3211	1/1	0.85	0.14	67,67,67,67	0
59	MG	DA	3159	1/1	0.85	0.26	85,85,85,85	0
59	MG	DA	3047	1/1	0.85	0.42	88,88,88,88	0
59	MG	CA	1624	1/1	0.85	0.19	86,86,86,86	0
59	MG	DA	2935	1/1	0.85	0.82	12,12,12,12	1
59	MG	BA	3330	1/1	0.85	0.41	88,88,88,88	0
59	MG	AA	1918	1/1	0.85	0.17	64,64,64,64	0
59	MG	BA	3497	1/1	0.85	0.44	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	DA	3679	1/1	0.85	0.14	51,51,51,51	0
59	MG	DA	3185	1/1	0.85	0.09	79,79,79,79	0
59	MG	CA	1701	1/1	0.85	0.14	83,83,83,83	0
59	MG	DA	3684	1/1	0.85	0.24	82,82,82,82	0
59	MG	DA	3190	1/1	0.85	0.21	97,97,97,97	0
59	MG	BA	3581	1/1	0.85	0.40	95,95,95,95	0
59	MG	AA	1644	1/1	0.85	0.21	84,84,84,84	0
59	MG	BA	3270	1/1	0.85	0.11	60,60,60,60	0
59	MG	AA	1774	1/1	0.85	0.33	120,120,120,120	0
59	MG	DA	3205	1/1	0.85	0.20	130,130,130,130	0
59	MG	BA	3590	1/1	0.85	0.12	90,90,90,90	0
59	MG	BA	3217	1/1	0.85	0.12	72,72,72,72	0
59	MG	AA	1830	1/1	0.85	0.15	86,86,86,86	0
59	MG	DA	2951	1/1	0.85	0.40	102,102,102,102	0
59	MG	AA	1840	1/1	0.85	0.29	76,76,76,76	0
59	MG	BA	3512	1/1	0.85	0.14	51,51,51,51	0
59	MG	AA	1925	1/1	0.85	0.09	72,72,72,72	0
59	MG	BA	3411	1/1	0.85	0.21	76,76,76,76	0
59	MG	AA	1869	1/1	0.85	0.35	75,75,75,75	0
59	MG	BA	3290	1/1	0.85	0.22	86,86,86,86	0
59	MG	AA	1723	1/1	0.85	0.10	91,91,91,91	0
59	MG	AA	1782	1/1	0.85	0.12	103,103,103,103	0
59	MG	D0	102	1/1	0.85	0.14	75,75,75,75	0
59	MG	BA	3123	1/1	0.85	0.29	105,105,105,105	0
59	MG	BA	3544	1/1	0.85	0.18	62,62,62,62	0
59	MG	BA	2971	1/1	0.85	0.47	92,92,92,92	0
59	MG	DA	3112	1/1	0.85	0.14	87,87,87,87	0
59	MG	DA	3438	1/1	0.85	0.26	76,76,76,76	0
59	MG	BA	3308	1/1	0.85	0.34	53,53,53,53	1
59	MG	BA	3194	1/1	0.85	0.16	67,67,67,67	0
59	MG	DA	3745	1/1	0.85	0.22	56,56,56,56	0
59	MG	D7	103	1/1	0.85	0.80	69,69,69,69	0
59	MG	DA	2984	1/1	0.85	0.31	66,66,66,66	1
59	MG	BA	3553	1/1	0.85	0.13	106,106,106,106	0
59	MG	BA	3450	1/1	0.85	0.27	60,60,60,60	0
59	MG	DA	3594	1/1	0.85	0.15	63,63,63,63	1
59	MG	CA	1745	1/1	0.85	0.13	112,112,112,112	0
59	MG	BO	201	1/1	0.85	0.26	88,88,88,88	0
59	MG	DA	3766	1/1	0.85	0.32	100,100,100,100	0
59	MG	AA	1825	1/1	0.85	0.29	71,71,71,71	0
59	MG	DA	3608	1/1	0.85	0.31	61,61,61,61	0
59	MG	DA	3292	1/1	0.85	0.45	106,106,106,106	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	BR	203	1/1	0.85	0.30	83,83,83,83	0
59	MG	AA	1856	1/1	0.85	0.28	80,80,80,80	0
59	MG	DA	3619	1/1	0.85	0.11	69,69,69,69	0
59	MG	DA	3466	1/1	0.85	0.30	40,40,40,40	0
59	MG	BA	3557	1/1	0.85	0.35	37,37,37,37	1
59	MG	DA	3001	1/1	0.85	0.07	79,79,79,79	0
59	MG	AA	1690	1/1	0.85	0.11	81,81,81,81	1
59	MG	DA	3320	1/1	0.85	0.11	78,78,78,78	0
59	MG	BA	3560	1/1	0.85	0.37	83,83,83,83	0
59	MG	DA	3139	1/1	0.85	0.21	89,89,89,89	0
59	MG	BA	3320	1/1	0.85	0.31	92,92,92,92	0
59	MG	BA	3382	1/1	0.85	0.08	77,77,77,77	0
59	MG	CA	1615	1/1	0.85	0.37	104,104,104,104	0
59	MG	CA	1684	1/1	0.85	0.17	64,64,64,64	0
59	MG	BA	2928	1/1	0.85	0.32	116,116,116,116	0
59	MG	AC	302	1/1	0.85	0.12	163,163,163,163	0
59	MG	DA	2926	1/1	0.85	0.13	45,45,45,45	1
59	MG	BA	3385	1/1	0.85	0.21	63,63,63,63	1
59	MG	BA	2982	1/1	0.85	0.07	58,58,58,58	1
59	MG	BA	3128	1/1	0.86	0.18	92,92,92,92	0
59	MG	DA	3255	1/1	0.86	0.27	51,51,51,51	0
59	MG	BA	3070	1/1	0.86	0.27	108,108,108,108	0
59	MG	AA	1748	1/1	0.86	0.26	23,23,23,23	1
59	MG	BA	3223	1/1	0.86	0.09	80,80,80,80	0
59	MG	CA	1602	1/1	0.86	0.11	76,76,76,76	0
59	MG	CA	1603	1/1	0.86	0.20	112,112,112,112	0
59	MG	DA	3645	1/1	0.86	0.14	78,78,78,78	0
59	MG	AA	1678	1/1	0.86	0.22	76,76,76,76	0
59	MG	BA	3076	1/1	0.86	0.16	30,30,30,30	0
59	MG	BA	3145	1/1	0.86	0.13	89,89,89,89	0
59	MG	BA	2911	1/1	0.86	0.18	94,94,94,94	0
59	MG	DA	3474	1/1	0.86	0.42	99,99,99,99	0
59	MG	CA	1611	1/1	0.86	0.15	86,86,86,86	0
59	MG	DA	2975	1/1	0.86	0.20	56,56,56,56	0
59	MG	DA	3128	1/1	0.86	0.13	86,86,86,86	0
59	MG	BA	3414	1/1	0.86	0.17	67,67,67,67	0
59	MG	DA	3308	1/1	0.86	0.27	103,103,103,103	0
59	MG	AA	1724	1/1	0.86	0.17	86,86,86,86	1
59	MG	BA	2916	1/1	0.86	0.23	78,78,78,78	0
59	MG	BA	3333	1/1	0.86	0.30	72,72,72,72	0
59	MG	BA	3334	1/1	0.86	0.21	60,60,60,60	0
59	MG	AA	1872	1/1	0.86	0.18	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	BA	3017	1/1	0.86	0.35	93,93,93,93	0
59	MG	BA	3443	1/1	0.86	0.18	76,76,76,76	0
59	MG	DA	3501	1/1	0.86	0.20	59,59,59,59	0
59	MG	AA	1619	1/1	0.86	0.15	111,111,111,111	0
59	MG	AA	1704	1/1	0.86	0.18	84,84,84,84	0
59	MG	BA	3020	1/1	0.86	0.15	103,103,103,103	0
59	MG	BA	3173	1/1	0.86	0.21	102,102,102,102	1
59	MG	BA	3455	1/1	0.86	0.25	65,65,65,65	0
59	MG	DA	3513	1/1	0.86	0.16	95,95,95,95	0
59	MG	DA	3147	1/1	0.86	0.24	90,90,90,90	0
59	MG	BA	3255	1/1	0.86	0.19	55,55,55,55	0
59	MG	BA	2978	1/1	0.86	0.30	75,75,75,75	0
59	MG	DA	3518	1/1	0.86	0.35	62,62,62,62	1
59	MG	DA	3005	1/1	0.86	0.09	69,69,69,69	0
59	MG	CA	1729	1/1	0.86	0.17	88,88,88,88	0
59	MG	BA	3463	1/1	0.86	0.28	66,66,66,66	0
59	MG	BA	3185	1/1	0.86	0.16	75,75,75,75	0
59	MG	DA	3355	1/1	0.86	0.10	80,80,80,80	0
59	MG	DA	3357	1/1	0.86	0.11	64,64,64,64	0
59	MG	CA	1733	1/1	0.86	0.07	76,76,76,76	0
59	MG	BA	3472	1/1	0.86	0.44	100,100,100,100	0
59	MG	BA	2924	1/1	0.86	0.14	73,73,73,73	0
59	MG	AA	1854	1/1	0.86	0.12	71,71,71,71	0
59	MG	DA	3544	1/1	0.86	0.18	62,62,62,62	0
59	MG	AA	1903	1/1	0.86	0.11	79,79,79,79	0
59	MG	DA	2916	1/1	0.86	0.18	57,57,57,57	0
59	MG	DA	3373	1/1	0.86	0.51	75,75,75,75	0
59	MG	AA	1610	1/1	0.86	0.24	77,77,77,77	0
59	MG	DA	3173	1/1	0.86	0.16	48,48,48,48	0
59	MG	AA	1645	1/1	0.86	0.37	56,56,56,56	1
59	MG	CA	1649	1/1	0.86	0.24	92,92,92,92	0
59	MG	BA	3487	1/1	0.86	0.18	64,64,64,64	0
59	MG	AA	1718	1/1	0.86	0.16	98,98,98,98	0
59	MG	DA	3389	1/1	0.86	0.81	145,145,145,145	0
59	MG	BA	3278	1/1	0.86	0.33	71,71,71,71	0
59	MG	CA	1656	1/1	0.86	0.14	73,73,73,73	0
59	MG	DA	3400	1/1	0.86	0.19	63,63,63,63	1
59	MG	BA	3198	1/1	0.86	0.20	102,102,102,102	0
59	MG	AA	1951	1/1	0.86	0.16	82,82,82,82	0
59	MG	BA	2948	1/1	0.86	0.10	64,64,64,64	0
59	MG	BA	2998	1/1	0.86	0.18	54,54,54,54	0
59	MG	DA	2934	1/1	0.86	0.20	48,48,48,48	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	DA	3211	1/1	0.86	0.18	65,65,65,65	0
59	MG	BA	3000	1/1	0.86	0.07	80,80,80,80	0
59	MG	DA	3585	1/1	0.86	0.15	78,78,78,78	0
59	MG	BB	203	1/1	0.86	0.28	59,59,59,59	0
59	MG	CA	1760	1/1	0.86	0.06	52,52,52,52	1
59	MG	BA	2949	1/1	0.86	0.25	102,102,102,102	0
59	MG	DA	3228	1/1	0.86	0.19	79,79,79,79	0
59	MG	BA	3504	1/1	0.86	0.18	59,59,59,59	0
59	MG	CA	1764	1/1	0.86	0.07	82,82,82,82	0
59	MG	DB	202	1/1	0.86	0.28	55,55,55,55	0
59	MG	AA	1885	1/1	0.86	0.27	57,57,57,57	0
59	MG	DA	3092	1/1	0.86	0.60	106,106,106,106	0
59	MG	AA	1615	1/1	0.86	0.33	67,67,67,67	0
59	MG	BA	3307	1/1	0.86	0.32	75,75,75,75	0
59	MG	DA	3442	1/1	0.86	0.29	71,71,71,71	0
59	MG	DD	303	1/1	0.86	0.20	64,64,64,64	0
59	MG	AA	1607	1/1	0.86	0.22	73,73,73,73	0
59	MG	DN	201	1/1	0.86	0.08	19,19,19,19	1
59	MG	DN	202	1/1	0.86	0.12	78,78,78,78	0
59	MG	DA	3621	1/1	0.86	0.24	76,76,76,76	1
59	MG	BA	3392	1/1	0.86	0.29	87,87,87,87	0
59	MG	BA	3528	1/1	0.86	0.18	73,73,73,73	0
59	MG	BA	3064	1/1	0.86	0.18	45,45,45,45	0
59	MG	CA	1690	1/1	0.87	0.28	60,60,60,60	0
59	MG	AA	1707	1/1	0.87	0.21	97,97,97,97	0
59	MG	DA	3629	1/1	0.87	0.17	45,45,45,45	0
59	MG	BA	3207	1/1	0.87	0.19	43,43,43,43	0
59	MG	CA	1693	1/1	0.87	0.19	73,73,73,73	0
59	MG	DA	3263	1/1	0.87	0.34	125,125,125,125	0
59	MG	BA	3133	1/1	0.87	0.25	57,57,57,57	0
59	MG	CA	1696	1/1	0.87	0.20	79,79,79,79	0
59	MG	BA	3454	1/1	0.87	0.22	64,64,64,64	0
59	MG	DA	3460	1/1	0.87	0.12	73,73,73,73	0
59	MG	BA	3086	1/1	0.87	0.11	123,123,123,123	0
59	MG	AA	1708	1/1	0.87	0.16	65,65,65,65	1
59	MG	BA	3565	1/1	0.87	0.33	79,79,79,79	0
59	MG	CS	101	1/1	0.87	0.07	97,97,97,97	1
59	MG	BA	3089	1/1	0.87	0.21	33,33,33,33	0
59	MG	AA	1683	1/1	0.87	0.19	47,47,47,47	1
59	MG	DA	3653	1/1	0.87	0.09	82,82,82,82	0
59	MG	DA	3654	1/1	0.87	0.13	78,78,78,78	0
59	MG	BA	3093	1/1	0.87	0.11	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	DA	3295	1/1	0.87	0.29	99,99,99,99	0
59	MG	DA	3475	1/1	0.87	0.12	115,115,115,115	0
59	MG	CA	1625	1/1	0.87	0.10	62,62,62,62	0
59	MG	DA	3477	1/1	0.87	0.45	76,76,76,76	0
59	MG	DA	3300	1/1	0.87	0.07	67,67,67,67	0
59	MG	CV	108	1/1	0.87	0.29	101,101,101,101	0
59	MG	DA	3306	1/1	0.87	0.10	56,56,56,56	0
59	MG	DA	3669	1/1	0.87	0.24	39,39,39,39	0
59	MG	DA	3307	1/1	0.87	0.28	77,77,77,77	0
59	MG	BA	3366	1/1	0.87	0.22	71,71,71,71	0
59	MG	BA	3148	1/1	0.87	0.28	106,106,106,106	0
59	MG	DA	3314	1/1	0.87	0.19	71,71,71,71	0
59	MG	BA	3370	1/1	0.87	0.36	105,105,105,105	0
59	MG	DA	3317	1/1	0.87	0.19	62,62,62,62	0
59	MG	AA	1851	1/1	0.87	0.15	62,62,62,62	0
59	MG	DA	3685	1/1	0.87	0.09	69,69,69,69	0
59	MG	AA	1685	1/1	0.87	0.32	30,30,30,30	1
59	MG	D0	103	1/1	0.87	0.13	74,74,74,74	0
59	MG	DA	3502	1/1	0.87	0.33	74,74,74,74	0
59	MG	AA	1699	1/1	0.87	0.16	71,71,71,71	0
59	MG	AA	1734	1/1	0.87	0.12	9,9,9,9	1
59	MG	BA	3309	1/1	0.87	0.11	58,58,58,58	0
59	MG	BA	3311	1/1	0.87	0.12	80,80,80,80	0
59	MG	AX	103	1/1	0.87	0.42	112,112,112,112	0
59	MG	AA	1638	1/1	0.87	0.29	119,119,119,119	0
59	MG	BA	3170	1/1	0.87	0.15	56,56,56,56	0
59	MG	DA	3341	1/1	0.87	0.23	62,62,62,62	0
59	MG	D8	101	1/1	0.87	0.07	74,74,74,74	0
59	MG	DA	3004	1/1	0.87	0.56	122,122,122,122	0
59	MG	CA	1731	1/1	0.87	0.08	76,76,76,76	0
59	MG	BA	3317	1/1	0.87	0.40	64,64,64,64	1
59	MG	DA	3521	1/1	0.87	0.28	99,99,99,99	0
59	MG	DA	2902	1/1	0.87	0.26	42,42,42,42	0
59	MG	BA	3595	1/1	0.87	0.35	65,65,65,65	0
59	MG	DA	3351	1/1	0.87	0.09	77,77,77,77	0
59	MG	DA	3724	1/1	0.87	0.25	73,73,73,73	0
59	MG	DA	3530	1/1	0.87	0.38	122,122,122,122	0
59	MG	AA	1674	1/1	0.87	0.08	48,48,48,48	0
59	MG	DA	3353	1/1	0.87	0.17	84,84,84,84	0
59	MG	DA	3022	1/1	0.87	0.13	71,71,71,71	0
59	MG	BA	3050	1/1	0.87	0.17	73,73,73,73	0
59	MG	AI	201	1/1	0.87	0.12	163,163,163,163	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	DA	3167	1/1	0.87	0.14	40,40,40,40	0
59	MG	DA	3026	1/1	0.87	0.26	60,60,60,60	0
59	MG	BA	3600	1/1	0.87	0.23	63,63,63,63	0
59	MG	DA	3171	1/1	0.87	0.13	71,71,71,71	0
59	MG	BA	3011	1/1	0.87	0.43	107,107,107,107	0
59	MG	BA	3603	1/1	0.87	0.23	74,74,74,74	0
59	MG	BA	3013	1/1	0.87	0.27	60,60,60,60	0
59	MG	DA	3758	1/1	0.87	0.41	95,95,95,95	0
59	MG	BA	3014	1/1	0.87	0.12	79,79,79,79	0
59	MG	BA	3607	1/1	0.87	0.43	95,95,95,95	0
59	MG	BA	3251	1/1	0.87	0.36	100,100,100,100	0
59	MG	BA	3519	1/1	0.87	0.30	88,88,88,88	0
59	MG	AA	1863	1/1	0.87	0.26	80,80,80,80	0
59	MG	BA	3524	1/1	0.87	0.24	103,103,103,103	0
59	MG	DA	3778	1/1	0.87	0.16	115,115,115,115	0
59	MG	BA	3065	1/1	0.87	0.18	50,50,50,50	0
59	MG	BA	3256	1/1	0.87	0.51	122,122,122,122	0
59	MG	B7	101	1/1	0.87	0.42	93,93,93,93	0
59	MG	BA	3535	1/1	0.87	0.14	81,81,81,81	0
59	MG	DA	3072	1/1	0.87	0.15	81,81,81,81	0
59	MG	DA	3212	1/1	0.87	0.28	105,105,105,105	0
59	MG	BA	2985	1/1	0.87	0.44	84,84,84,84	0
59	MG	DA	3219	1/1	0.87	0.23	62,62,62,62	0
59	MG	BA	3263	1/1	0.87	0.30	76,76,76,76	0
59	MG	AA	1962	1/1	0.87	0.29	65,65,65,65	0
59	MG	BA	3424	1/1	0.87	0.19	64,64,64,64	0
59	MG	DA	3078	1/1	0.87	0.23	73,73,73,73	0
59	MG	BA	3429	1/1	0.87	0.30	67,67,67,67	0
59	MG	BA	3267	1/1	0.87	0.25	94,94,94,94	0
59	MG	DA	3423	1/1	0.87	0.11	51,51,51,51	1
59	MG	BA	3431	1/1	0.87	0.30	79,79,79,79	0
59	MG	BA	2905	1/1	0.87	0.19	52,52,52,52	0
59	MG	DA	3614	1/1	0.87	0.22	100,100,100,100	0
59	MG	AA	1749	1/1	0.87	0.08	74,74,74,74	1
59	MG	AA	1609	1/1	0.87	0.20	59,59,59,59	0
59	MG	CA	1775	1/1	0.87	0.11	70,70,70,70	1
59	MG	CA	1776	1/1	0.87	0.20	83,83,83,83	0
59	MG	DA	2948	1/1	0.87	0.26	75,75,75,75	0
59	MG	BA	3142	1/1	0.88	0.10	67,67,67,67	0
59	MG	DA	3325	1/1	0.88	0.37	109,109,109,109	0
59	MG	BA	3143	1/1	0.88	0.62	149,149,149,149	0
59	MG	DA	3157	1/1	0.88	0.09	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	BA	3507	1/1	0.88	0.18	55,55,55,55	0
59	MG	DA	3335	1/1	0.88	0.14	48,48,48,48	0
59	MG	BA	3509	1/1	0.88	0.33	58,58,58,58	0
59	MG	DA	3027	1/1	0.88	0.30	69,69,69,69	0
59	MG	AA	1752	1/1	0.88	0.08	51,51,51,51	1
59	MG	AA	1633	1/1	0.88	0.40	72,72,72,72	1
59	MG	AA	1684	1/1	0.88	0.08	87,87,87,87	0
59	MG	AA	1866	1/1	0.88	0.09	74,74,74,74	0
59	MG	BA	3025	1/1	0.88	0.12	83,83,83,83	0
59	MG	AA	1779	1/1	0.88	0.14	114,114,114,114	0
59	MG	BA	2930	1/1	0.88	0.08	85,85,85,85	0
59	MG	B5	101	1/1	0.88	0.24	83,83,83,83	0
59	MG	BA	3160	1/1	0.88	0.17	49,49,49,49	0
59	MG	DA	3507	1/1	0.88	0.11	5,5,5,5	1
59	MG	DA	2933	1/1	0.88	0.23	51,51,51,51	0
59	MG	BA	3533	1/1	0.88	0.31	83,83,83,83	0
59	MG	AA	1940	1/1	0.88	0.13	86,86,86,86	0
59	MG	DA	3192	1/1	0.88	0.39	70,70,70,70	0
59	MG	BA	2943	1/1	0.88	0.22	92,92,92,92	1
59	MG	BA	3171	1/1	0.88	0.15	29,29,29,29	0
59	MG	AL	206	1/1	0.88	0.13	53,53,53,53	1
59	MG	DA	3365	1/1	0.88	0.13	92,92,92,92	0
59	MG	BU	201	1/1	0.88	0.21	46,46,46,46	0
59	MG	BA	3101	1/1	0.88	0.28	79,79,79,79	0
59	MG	BA	2901	1/1	0.88	0.15	113,113,113,113	0
59	MG	DA	2943	1/1	0.88	0.07	71,71,71,71	1
59	MG	DA	3525	1/1	0.88	0.41	63,63,63,63	0
59	MG	BA	3547	1/1	0.88	0.16	78,78,78,78	0
59	MG	BA	3180	1/1	0.88	0.23	42,42,42,42	0
59	MG	CA	1607	1/1	0.88	0.13	94,94,94,94	0
59	MG	AA	1628	1/1	0.88	0.13	84,84,84,84	0
59	MG	DA	3535	1/1	0.88	0.30	52,52,52,52	0
59	MG	BA	3434	1/1	0.88	0.27	68,68,68,68	0
59	MG	BA	2996	1/1	0.88	0.27	68,68,68,68	0
59	MG	DA	3093	1/1	0.88	0.39	67,67,67,67	0
59	MG	DA	3541	1/1	0.88	0.28	96,96,96,96	0
59	MG	BA	3187	1/1	0.88	0.30	37,37,37,37	0
59	MG	AA	1626	1/1	0.88	0.29	89,89,89,89	0
59	MG	DA	3395	1/1	0.88	0.26	83,83,83,83	0
59	MG	BA	3349	1/1	0.88	0.20	68,68,68,68	0
59	MG	DA	3236	1/1	0.88	0.26	63,63,63,63	0
59	MG	CA	1702	1/1	0.88	0.09	104,104,104,104	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	BA	3448	1/1	0.88	0.34	40,40,40,40	0
59	MG	DA	3405	1/1	0.88	0.12	63,63,63,63	0
59	MG	DA	3735	1/1	0.88	0.17	90,90,90,90	0
59	MG	BA	3191	1/1	0.88	0.40	78,78,78,78	0
59	MG	BA	3110	1/1	0.88	0.13	55,55,55,55	0
59	MG	AA	1731	1/1	0.88	0.22	81,81,81,81	0
59	MG	BA	3047	1/1	0.88	0.33	89,89,89,89	0
59	MG	DA	3411	1/1	0.88	0.20	67,67,67,67	1
59	MG	DA	2965	1/1	0.88	0.28	52,52,52,52	0
59	MG	BA	2955	1/1	0.88	0.38	84,84,84,84	0
59	MG	BA	3359	1/1	0.88	0.48	101,101,101,101	0
59	MG	DA	3574	1/1	0.88	0.30	70,70,70,70	1
59	MG	DA	3755	1/1	0.88	0.34	128,128,128,128	0
59	MG	BA	2957	1/1	0.88	0.26	81,81,81,81	0
59	MG	BA	3363	1/1	0.88	0.39	92,92,92,92	0
59	MG	BA	3573	1/1	0.88	0.27	75,75,75,75	0
59	MG	DA	3429	1/1	0.88	0.17	23,23,23,23	1
59	MG	BA	2958	1/1	0.88	0.16	46,46,46,46	0
59	MG	BA	3285	1/1	0.88	0.42	96,96,96,96	0
59	MG	DA	3435	1/1	0.88	0.17	47,47,47,47	0
59	MG	BA	2959	1/1	0.88	0.20	65,65,65,65	0
59	MG	DA	3777	1/1	0.88	0.15	70,70,70,70	0
59	MG	DA	3276	1/1	0.88	0.22	58,58,58,58	0
59	MG	AA	1732	1/1	0.88	0.09	52,52,52,52	0
59	MG	BA	3368	1/1	0.88	0.12	62,62,62,62	0
59	MG	DA	3600	1/1	0.88	0.22	30,30,30,30	0
59	MG	CA	1638	1/1	0.88	0.25	61,61,61,61	0
59	MG	D7	101	1/1	0.88	0.34	89,89,89,89	0
59	MG	D7	102	1/1	0.88	0.21	75,75,75,75	0
59	MG	BA	3484	1/1	0.88	0.34	94,94,94,94	0
59	MG	BA	3063	1/1	0.88	0.16	59,59,59,59	0
59	MG	DA	3791	1/1	0.88	0.39	76,76,76,76	0
59	MG	AA	1852	1/1	0.88	0.24	56,56,56,56	0
59	MG	BA	3299	1/1	0.88	0.29	66,66,66,66	0
59	MG	BA	2965	1/1	0.88	0.25	84,84,84,84	0
59	MG	DA	3305	1/1	0.88	0.37	52,52,52,52	0
59	MG	AA	1812	1/1	0.88	0.52	70,70,70,70	0
59	MG	DA	3627	1/1	0.88	0.11	70,70,70,70	0
59	MG	AA	1721	1/1	0.88	0.06	111,111,111,111	0
59	MG	AA	1788	1/1	0.88	0.08	80,80,80,80	0
59	MG	DD	304	1/1	0.88	0.19	97,97,97,97	0
59	MG	DD	305	1/1	0.88	0.41	1,1,1,1	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	DE	302	1/1	0.88	0.07	39,39,39,39	1
59	MG	BA	3499	1/1	0.88	0.15	43,43,43,43	0
59	MG	DA	3013	1/1	0.88	0.28	68,68,68,68	0
59	MG	DA	3014	1/1	0.88	0.23	108,108,108,108	0
59	MG	BA	2972	1/1	0.88	0.30	63,63,63,63	1
59	MG	BA	2920	1/1	0.88	0.13	42,42,42,42	0
59	MG	DA	3152	1/1	0.88	0.42	108,108,108,108	0
59	MG	DR	202	1/1	0.88	0.15	65,65,65,65	1
59	MG	AA	1815	1/1	0.88	0.15	76,76,76,76	0
59	MG	BA	3118	1/1	0.89	0.16	59,59,59,59	0
59	MG	AV	107	1/1	0.89	0.14	58,58,58,58	0
59	MG	DA	3302	1/1	0.89	0.27	57,57,57,57	0
59	MG	AA	1687	1/1	0.89	0.07	101,101,101,101	0
59	MG	BA	3406	1/1	0.89	0.22	52,52,52,52	0
59	MG	AC	301	1/1	0.89	0.18	173,173,173,173	0
59	MG	BA	3029	1/1	0.89	0.26	92,92,92,92	0
59	MG	AA	1700	1/1	0.89	0.17	90,90,90,90	0
59	MG	BA	3130	1/1	0.89	0.17	62,62,62,62	0
59	MG	DA	3312	1/1	0.89	0.22	48,48,48,48	0
59	MG	BA	3416	1/1	0.89	0.26	58,58,58,58	0
59	MG	BA	3417	1/1	0.89	0.13	68,68,68,68	0
59	MG	DA	3006	1/1	0.89	0.28	107,107,107,107	0
59	MG	DA	3657	1/1	0.89	0.14	59,59,59,59	0
59	MG	BA	3082	1/1	0.89	0.33	90,90,90,90	0
59	MG	BA	2997	1/1	0.89	0.20	82,82,82,82	0
59	MG	BA	3526	1/1	0.89	0.25	76,76,76,76	0
59	MG	DA	3486	1/1	0.89	0.25	38,38,38,38	0
59	MG	CA	1748	1/1	0.89	0.12	102,102,102,102	0
59	MG	AA	1689	1/1	0.89	0.14	82,82,82,82	1
59	MG	DA	3019	1/1	0.89	0.66	92,92,92,92	0
59	MG	DA	3494	1/1	0.89	0.28	41,41,41,41	0
59	MG	BA	3204	1/1	0.89	0.53	71,71,71,71	0
59	MG	DA	3670	1/1	0.89	0.42	88,88,88,88	0
59	MG	CA	1664	1/1	0.89	0.10	91,91,91,91	0
59	MG	DA	3156	1/1	0.89	0.31	73,73,73,73	0
59	MG	BA	3034	1/1	0.89	0.12	51,51,51,51	0
59	MG	AA	1818	1/1	0.89	0.09	60,60,60,60	0
59	MG	BA	3281	1/1	0.89	0.70	94,94,94,94	0
59	MG	AA	1957	1/1	0.89	0.26	75,75,75,75	0
59	MG	BA	3437	1/1	0.89	0.14	60,60,60,60	0
59	MG	AA	1855	1/1	0.89	0.12	69,69,69,69	0
59	MG	CA	1761	1/1	0.89	0.10	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	DA	3511	1/1	0.89	0.30	83,83,83,83	0
59	MG	CA	1676	1/1	0.89	0.06	88,88,88,88	0
59	MG	DA	3037	1/1	0.89	0.33	58,58,58,58	0
59	MG	DA	3040	1/1	0.89	0.35	81,81,81,81	0
59	MG	BA	3541	1/1	0.89	0.51	82,82,82,82	0
59	MG	AA	1764	1/1	0.89	0.26	65,65,65,65	0
59	MG	BA	3212	1/1	0.89	0.31	52,52,52,52	0
59	MG	DA	3052	1/1	0.89	0.30	68,68,68,68	0
59	MG	DA	3708	1/1	0.89	0.34	100,100,100,100	0
59	MG	AA	1753	1/1	0.89	0.11	110,110,110,110	0
59	MG	CA	1769	1/1	0.89	0.12	68,68,68,68	0
59	MG	DA	3064	1/1	0.89	0.16	51,51,51,51	0
59	MG	DA	3195	1/1	0.89	0.35	96,96,96,96	0
59	MG	AA	1744	1/1	0.89	0.14	80,80,80,80	0
59	MG	BA	2940	1/1	0.89	0.18	63,63,63,63	0
59	MG	BA	3007	1/1	0.89	0.15	93,93,93,93	0
59	MG	BA	2942	1/1	0.89	0.57	110,110,110,110	0
59	MG	DA	3207	1/1	0.89	0.20	84,84,84,84	0
59	MG	DA	3070	1/1	0.89	0.06	59,59,59,59	0
59	MG	DA	3536	1/1	0.89	0.10	37,37,37,37	1
59	MG	BA	3049	1/1	0.89	0.16	66,66,66,66	0
59	MG	BA	3457	1/1	0.89	0.23	72,72,72,72	0
59	MG	BA	3304	1/1	0.89	0.29	90,90,90,90	0
59	MG	DA	3733	1/1	0.89	0.11	43,43,43,43	0
59	MG	DA	3383	1/1	0.89	0.18	135,135,135,135	0
59	MG	AA	1838	1/1	0.89	0.36	80,80,80,80	0
59	MG	DA	3387	1/1	0.89	0.12	77,77,77,77	0
59	MG	BA	3462	1/1	0.89	0.23	28,28,28,28	0
59	MG	BA	3375	1/1	0.89	0.47	74,74,74,74	0
59	MG	BA	3465	1/1	0.89	0.28	37,37,37,37	0
59	MG	DA	3222	1/1	0.89	0.17	79,79,79,79	0
59	MG	DA	3223	1/1	0.89	0.20	37,37,37,37	0
59	MG	BA	3378	1/1	0.89	0.22	79,79,79,79	0
59	MG	DA	3753	1/1	0.89	0.41	83,83,83,83	0
59	MG	DA	2947	1/1	0.89	0.14	86,86,86,86	0
59	MG	AA	1618	1/1	0.89	0.24	78,78,78,78	0
59	MG	BA	2947	1/1	0.89	0.27	45,45,45,45	0
59	MG	BA	3568	1/1	0.89	0.18	58,58,58,58	0
59	MG	BA	3168	1/1	0.89	0.24	24,24,24,24	0
59	MG	CM	203	1/1	0.89	0.07	123,123,123,123	0
59	MG	CQ	201	1/1	0.89	0.08	98,98,98,98	1
59	MG	AA	1929	1/1	0.89	0.20	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	CS	102	1/1	0.89	0.09	102,102,102,102	0
59	MG	DA	3100	1/1	0.89	0.21	67,67,67,67	0
59	MG	DA	3776	1/1	0.89	0.13	58,58,58,58	0
59	MG	CA	1707	1/1	0.89	0.13	79,79,79,79	0
59	MG	BA	3060	1/1	0.89	0.32	98,98,98,98	0
59	MG	DA	3582	1/1	0.89	0.49	47,47,47,47	1
59	MG	DA	3420	1/1	0.89	0.13	100,100,100,100	0
59	MG	AV	101	1/1	0.89	0.23	52,52,52,52	1
59	MG	BA	3062	1/1	0.89	0.14	61,61,61,61	0
59	MG	DA	3108	1/1	0.89	0.18	81,81,81,81	0
59	MG	AA	1668	1/1	0.89	0.16	78,78,78,78	0
59	MG	BA	3388	1/1	0.89	0.62	100,100,100,100	0
59	MG	DA	3592	1/1	0.89	0.32	58,58,58,58	0
59	MG	DA	3789	1/1	0.89	0.27	68,68,68,68	0
59	MG	BA	3492	1/1	0.89	0.12	31,31,31,31	1
59	MG	DA	3270	1/1	0.89	0.24	55,55,55,55	0
59	MG	BA	3582	1/1	0.89	0.24	63,63,63,63	0
59	MG	DA	2974	1/1	0.89	0.33	47,47,47,47	1
59	MG	DA	3605	1/1	0.89	0.22	63,63,63,63	0
59	MG	DA	3274	1/1	0.89	0.16	73,73,73,73	0
59	MG	DB	208	1/1	0.89	0.10	86,86,86,86	0
59	MG	DA	3440	1/1	0.89	0.07	50,50,50,50	1
59	MG	BA	3176	1/1	0.89	0.14	50,50,50,50	0
59	MG	DA	3283	1/1	0.89	0.16	65,65,65,65	0
59	MG	D0	101	1/1	0.89	0.13	16,16,16,16	1
59	MG	BA	3178	1/1	0.89	0.26	79,79,79,79	0
59	MG	DE	301	1/1	0.89	0.06	67,67,67,67	0
59	MG	AA	1643	1/1	0.89	0.14	92,92,92,92	0
59	MG	DA	3620	1/1	0.89	0.11	70,70,70,70	0
59	MG	DA	3451	1/1	0.89	0.23	80,80,80,80	1
59	MG	AA	1641	1/1	0.89	0.15	68,68,68,68	1
59	MG	DA	3454	1/1	0.89	0.17	35,35,35,35	0
59	MG	BA	3253	1/1	0.89	0.22	52,52,52,52	1
59	MG	DP	205	1/1	0.89	0.25	63,63,63,63	0
59	MG	D2	101	1/1	0.89	0.14	62,62,62,62	0
59	MG	BA	3069	1/1	0.89	0.41	100,100,100,100	0
59	MG	DA	3296	1/1	0.89	0.23	46,46,46,46	1
59	MG	CA	1767	1/1	0.90	0.20	73,73,73,73	0
59	MG	BA	3226	1/1	0.90	0.24	78,78,78,78	0
59	MG	DA	3652	1/1	0.90	0.14	74,74,74,74	0
59	MG	BA	3373	1/1	0.90	0.21	56,56,56,56	0
59	MG	DA	3488	1/1	0.90	0.10	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	DA	3656	1/1	0.90	0.19	75,75,75,75	0
59	MG	DA	3175	1/1	0.90	0.11	28,28,28,28	0
59	MG	DA	3177	1/1	0.90	0.10	71,71,71,71	0
59	MG	BA	3374	1/1	0.90	0.26	74,74,74,74	0
59	MG	DA	3180	1/1	0.90	0.17	115,115,115,115	0
59	MG	DA	3184	1/1	0.90	0.13	63,63,63,63	0
59	MG	BA	3552	1/1	0.90	0.14	54,54,54,54	1
59	MG	BA	2933	1/1	0.90	0.11	36,36,36,36	0
59	MG	AA	1923	1/1	0.90	0.34	55,55,55,55	0
59	MG	AA	1719	1/1	0.90	0.42	76,76,76,76	1
59	MG	BA	3236	1/1	0.90	0.32	86,86,86,86	0
59	MG	AA	1811	1/1	0.90	0.19	49,49,49,49	0
59	MG	BA	3067	1/1	0.90	0.10	34,34,34,34	0
59	MG	DA	3672	1/1	0.90	0.25	74,74,74,74	0
59	MG	DA	3509	1/1	0.90	0.23	39,39,39,39	0
59	MG	DA	3354	1/1	0.90	0.17	52,52,52,52	0
59	MG	CA	1781	1/1	0.90	0.07	74,74,74,74	0
59	MG	DA	3200	1/1	0.90	0.23	62,62,62,62	0
59	MG	DA	3202	1/1	0.90	0.13	70,70,70,70	0
59	MG	BA	3177	1/1	0.90	0.27	45,45,45,45	0
59	MG	DA	3361	1/1	0.90	0.20	42,42,42,42	0
59	MG	AA	1796	1/1	0.90	0.11	61,61,61,61	0
59	MG	BA	3562	1/1	0.90	0.29	71,71,71,71	0
59	MG	CD	302	1/1	0.90	0.07	68,68,68,68	0
59	MG	BA	3473	1/1	0.90	0.54	87,87,87,87	0
59	MG	AA	1783	1/1	0.90	0.36	73,73,73,73	0
59	MG	AI	202	1/1	0.90	0.08	117,117,117,117	0
59	MG	DA	3694	1/1	0.90	0.26	107,107,107,107	0
59	MG	DA	3080	1/1	0.90	0.08	56,56,56,56	0
59	MG	BA	3121	1/1	0.90	0.51	125,125,125,125	0
59	MG	BA	3324	1/1	0.90	0.20	63,63,63,63	0
59	MG	DA	3707	1/1	0.90	0.16	55,55,55,55	1
59	MG	DA	3379	1/1	0.90	0.14	72,72,72,72	0
59	MG	AL	201	1/1	0.90	0.11	87,87,87,87	0
59	MG	BA	3393	1/1	0.90	0.24	104,104,104,104	0
59	MG	CA	1710	1/1	0.90	0.15	51,51,51,51	0
59	MG	BA	3486	1/1	0.90	0.12	54,54,54,54	0
59	MG	BA	3188	1/1	0.90	0.10	58,58,58,58	0
59	MG	CV	105	1/1	0.90	0.10	82,82,82,82	0
59	MG	BA	3189	1/1	0.90	0.22	62,62,62,62	0
59	MG	DA	2966	1/1	0.90	0.87	51,51,51,51	1
59	MG	DA	3542	1/1	0.90	0.10	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	AA	1875	1/1	0.90	0.19	62,62,62,62	0
59	MG	CA	1718	1/1	0.90	0.16	87,87,87,87	0
59	MG	BA	2991	1/1	0.90	0.13	60,60,60,60	1
59	MG	CA	1634	1/1	0.90	0.07	97,97,97,97	0
59	MG	AL	204	1/1	0.90	0.11	90,90,90,90	0
59	MG	DA	3732	1/1	0.90	0.21	67,67,67,67	0
59	MG	DA	3245	1/1	0.90	0.17	78,78,78,78	0
59	MG	CA	1722	1/1	0.90	0.11	73,73,73,73	0
59	MG	BA	3496	1/1	0.90	0.17	44,44,44,44	0
59	MG	DA	3558	1/1	0.90	0.21	88,88,88,88	0
59	MG	AA	1651	1/1	0.90	0.09	76,76,76,76	0
59	MG	DA	3743	1/1	0.90	0.23	50,50,50,50	1
59	MG	BA	3260	1/1	0.90	0.18	77,77,77,77	0
59	MG	AA	1701	1/1	0.90	0.24	77,77,77,77	0
59	MG	DA	3414	1/1	0.90	0.42	121,121,121,121	0
59	MG	DA	3415	1/1	0.90	0.29	41,41,41,41	0
59	MG	BA	2953	1/1	0.90	0.49	84,84,84,84	0
59	MG	BA	2910	1/1	0.90	0.26	83,83,83,83	1
59	MG	CA	1643	1/1	0.90	0.14	80,80,80,80	0
59	MG	BA	3412	1/1	0.90	0.20	95,95,95,95	0
59	MG	AA	1675	1/1	0.90	0.13	52,52,52,52	1
59	MG	BA	3091	1/1	0.90	0.26	62,62,62,62	0
59	MG	DA	3760	1/1	0.90	0.14	52,52,52,52	0
59	MG	BA	2999	1/1	0.90	0.18	86,86,86,86	0
59	MG	DA	2999	1/1	0.90	0.14	91,91,91,91	0
59	MG	AA	1661	1/1	0.90	0.14	34,34,34,34	1
59	MG	DA	3277	1/1	0.90	0.12	42,42,42,42	0
59	MG	DA	3279	1/1	0.90	0.26	70,70,70,70	0
59	MG	DA	3282	1/1	0.90	0.13	31,31,31,31	0
59	MG	BA	3275	1/1	0.90	0.07	38,38,38,38	0
59	MG	CA	1652	1/1	0.90	0.33	78,78,78,78	0
59	MG	BA	3599	1/1	0.90	0.11	83,83,83,83	0
59	MG	DA	3441	1/1	0.90	0.24	55,55,55,55	0
59	MG	AA	1695	1/1	0.90	0.07	65,65,65,65	0
59	MG	BA	3352	1/1	0.90	0.12	72,72,72,72	0
59	MG	DA	3007	1/1	0.90	0.15	57,57,57,57	0
59	MG	AA	1963	1/1	0.90	0.31	74,74,74,74	0
59	MG	DA	3785	1/1	0.90	0.56	35,35,35,35	1
59	MG	DA	3294	1/1	0.90	0.07	80,80,80,80	1
59	MG	BA	3426	1/1	0.90	0.30	77,77,77,77	0
59	MG	DA	3612	1/1	0.90	0.13	77,77,77,77	0
59	MG	CA	1749	1/1	0.90	0.24	16,16,16,16	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	DA	3790	1/1	0.90	0.45	29,29,29,29	1
59	MG	BA	3523	1/1	0.90	0.32	122,122,122,122	0
59	MG	DA	3792	1/1	0.90	0.19	77,77,77,77	0
59	MG	BA	3147	1/1	0.90	0.20	72,72,72,72	0
59	MG	DA	3796	1/1	0.90	0.39	95,95,95,95	1
59	MG	DB	201	1/1	0.90	0.14	59,59,59,59	0
59	MG	DA	2910	1/1	0.90	0.21	68,68,68,68	0
59	MG	AA	1911	1/1	0.90	0.08	55,55,55,55	0
59	MG	AA	1778	1/1	0.90	0.17	84,84,84,84	0
59	MG	BA	3433	1/1	0.90	0.11	61,61,61,61	0
59	MG	BA	2966	1/1	0.90	0.26	64,64,64,64	0
59	MG	BA	3435	1/1	0.90	0.44	70,70,70,70	0
59	MG	AA	1602	1/1	0.90	0.11	71,71,71,71	0
59	MG	AA	1650	1/1	0.90	0.15	73,73,73,73	0
59	MG	BA	3103	1/1	0.90	0.19	69,69,69,69	0
59	MG	DA	3631	1/1	0.90	0.24	41,41,41,41	0
59	MG	AA	1890	1/1	0.90	0.16	78,78,78,78	0
59	MG	DA	3473	1/1	0.90	0.30	38,38,38,38	0
59	MG	AA	1867	1/1	0.90	0.10	65,65,65,65	0
59	MG	DA	3636	1/1	0.90	0.08	50,50,50,50	0
59	MG	DA	3161	1/1	0.90	0.34	61,61,61,61	0
59	MG	AA	1845	1/1	0.90	0.24	53,53,53,53	0
59	MG	BR	201	1/1	0.90	0.21	47,47,47,47	1
59	MG	DA	3166	1/1	0.90	0.12	30,30,30,30	0
59	MG	AA	1680	1/1	0.90	0.16	75,75,75,75	0
59	MG	DA	3043	1/1	0.90	0.17	80,80,80,80	0
59	MG	DW	201	1/1	0.90	0.08	36,36,36,36	1
59	MG	DA	3046	1/1	0.90	0.28	95,95,95,95	0
59	MG	DA	2977	1/1	0.91	0.27	60,60,60,60	0
59	MG	DA	3230	1/1	0.91	0.28	94,94,94,94	0
59	MG	DA	2980	1/1	0.91	0.20	69,69,69,69	0
59	MG	DA	3233	1/1	0.91	0.23	152,152,152,152	0
59	MG	BA	3608	1/1	0.91	0.22	31,31,31,31	0
59	MG	DA	3380	1/1	0.91	0.21	43,43,43,43	0
59	MG	BB	202	1/1	0.91	0.36	62,62,62,62	0
59	MG	BA	3452	1/1	0.91	0.35	45,45,45,45	0
59	MG	BA	3135	1/1	0.91	0.21	86,86,86,86	0
59	MG	BA	3055	1/1	0.91	0.50	92,92,92,92	0
59	MG	BD	305	1/1	0.91	0.29	168,168,168,168	0
59	MG	BA	3249	1/1	0.91	0.25	79,79,79,79	0
59	MG	BA	3543	1/1	0.91	0.20	71,71,71,71	0
59	MG	DA	3121	1/1	0.91	0.16	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	BA	3057	1/1	0.91	0.14	68,68,68,68	0
59	MG	CA	1751	1/1	0.91	0.12	69,69,69,69	1
59	MG	BA	2990	1/1	0.91	0.21	77,77,77,77	0
59	MG	BH	203	1/1	0.91	0.29	75,75,75,75	0
59	MG	DA	2903	1/1	0.91	0.11	43,43,43,43	0
59	MG	DA	2904	1/1	0.91	0.51	66,66,66,66	0
59	MG	DA	3703	1/1	0.91	0.12	41,41,41,41	0
59	MG	BA	3546	1/1	0.91	0.35	83,83,83,83	0
59	MG	DA	3268	1/1	0.91	0.11	35,35,35,35	0
59	MG	AA	1608	1/1	0.91	0.17	58,58,58,58	0
59	MG	AA	1692	1/1	0.91	0.08	89,89,89,89	0
59	MG	BA	2938	1/1	0.91	0.08	64,64,64,64	1
59	MG	AA	1658	1/1	0.91	0.12	106,106,106,106	0
59	MG	DA	3713	1/1	0.91	0.10	67,67,67,67	0
59	MG	DA	3008	1/1	0.91	0.10	70,70,70,70	0
59	MG	AA	1806	1/1	0.91	0.12	81,81,81,81	0
59	MG	BA	3028	1/1	0.91	0.14	58,58,58,58	0
59	MG	DA	3278	1/1	0.91	0.14	57,57,57,57	0
59	MG	AA	1926	1/1	0.91	0.12	59,59,59,59	0
59	MG	DA	2914	1/1	0.91	0.18	83,83,83,83	0
59	MG	BA	3107	1/1	0.91	0.45	87,87,87,87	0
59	MG	AA	1620	1/1	0.91	0.23	71,71,71,71	0
59	MG	DA	3425	1/1	0.91	0.15	56,56,56,56	0
59	MG	DA	3428	1/1	0.91	0.19	65,65,65,65	0
59	MG	DA	3287	1/1	0.91	0.12	66,66,66,66	0
59	MG	DA	2918	1/1	0.91	0.23	91,91,91,91	0
59	MG	DA	3576	1/1	0.91	0.41	87,87,87,87	0
59	MG	DA	2919	1/1	0.91	0.18	57,57,57,57	0
59	MG	BA	2944	1/1	0.91	0.15	43,43,43,43	0
59	MG	DA	3580	1/1	0.91	0.11	34,34,34,34	0
59	MG	AL	202	1/1	0.91	0.10	73,73,73,73	0
59	MG	AA	1660	1/1	0.91	0.12	82,82,82,82	0
59	MG	CA	1768	1/1	0.91	0.07	71,71,71,71	0
59	MG	BA	3162	1/1	0.91	0.19	41,41,41,41	0
59	MG	AA	1859	1/1	0.91	0.09	44,44,44,44	0
59	MG	DA	3034	1/1	0.91	0.22	98,98,98,98	0
59	MG	BA	3344	1/1	0.91	0.24	45,45,45,45	0
59	MG	AA	1759	1/1	0.91	0.18	51,51,51,51	0
59	MG	BA	3077	1/1	0.91	0.24	71,71,71,71	0
59	MG	DA	3593	1/1	0.91	0.08	61,61,61,61	0
59	MG	BA	3348	1/1	0.91	0.25	61,61,61,61	0
59	MG	B0	102	1/1	0.91	0.10	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	BA	3282	1/1	0.91	0.21	47,47,47,47	0
59	MG	DA	3601	1/1	0.91	0.07	39,39,39,39	0
59	MG	BA	3283	1/1	0.91	0.15	58,58,58,58	0
59	MG	DA	3764	1/1	0.91	0.29	75,75,75,75	0
59	MG	DA	3765	1/1	0.91	0.29	69,69,69,69	0
59	MG	BA	2979	1/1	0.91	0.18	66,66,66,66	0
59	MG	BA	3420	1/1	0.91	0.31	71,71,71,71	0
59	MG	DA	3169	1/1	0.91	0.46	67,67,67,67	0
59	MG	CA	1783	1/1	0.91	0.08	83,83,83,83	0
59	MG	DA	3775	1/1	0.91	0.31	86,86,86,86	0
59	MG	DA	3613	1/1	0.91	0.07	56,56,56,56	1
59	MG	AA	1847	1/1	0.91	0.07	76,76,76,76	0
59	MG	BA	3224	1/1	0.91	0.28	79,79,79,79	0
59	MG	DA	3463	1/1	0.91	0.22	83,83,83,83	0
59	MG	AA	1603	1/1	0.91	0.29	74,74,74,74	0
59	MG	DA	3174	1/1	0.91	0.23	93,93,93,93	0
59	MG	DA	3782	1/1	0.91	0.22	51,51,51,51	0
59	MG	BA	3085	1/1	0.91	0.53	68,68,68,68	0
59	MG	CA	1709	1/1	0.91	0.11	85,85,85,85	1
59	MG	BA	3360	1/1	0.91	0.20	80,80,80,80	0
59	MG	BA	2983	1/1	0.91	0.14	63,63,63,63	0
59	MG	BA	3586	1/1	0.91	0.22	86,86,86,86	0
59	MG	DA	3334	1/1	0.91	0.11	56,56,56,56	0
59	MG	BA	3587	1/1	0.91	0.25	47,47,47,47	0
59	MG	BA	3508	1/1	0.91	0.16	39,39,39,39	0
59	MG	BA	3230	1/1	0.91	0.19	85,85,85,85	0
59	MG	BA	3231	1/1	0.91	0.18	28,28,28,28	0
59	MG	BA	3432	1/1	0.91	0.27	59,59,59,59	0
59	MG	DA	3635	1/1	0.91	0.21	31,31,31,31	0
59	MG	DA	3797	1/1	0.91	0.17	56,56,56,56	0
59	MG	CV	103	1/1	0.91	0.08	67,67,67,67	0
59	MG	BA	3124	1/1	0.91	0.25	62,62,62,62	0
59	MG	CA	1640	1/1	0.91	0.10	76,76,76,76	0
59	MG	BA	3518	1/1	0.91	0.36	64,64,64,64	0
59	MG	DA	3201	1/1	0.91	0.07	62,62,62,62	0
59	MG	DA	3348	1/1	0.91	0.19	43,43,43,43	0
59	MG	BA	3179	1/1	0.91	0.12	66,66,66,66	0
59	MG	DA	3350	1/1	0.91	0.28	34,34,34,34	0
59	MG	DA	3083	1/1	0.91	0.22	104,104,104,104	0
59	MG	DA	3084	1/1	0.91	0.19	57,57,57,57	0
59	MG	DA	3085	1/1	0.91	0.08	68,68,68,68	0
59	MG	AA	1901	1/1	0.91	0.32	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	DA	3087	1/1	0.91	0.17	33,33,33,33	0
59	MG	AA	1849	1/1	0.91	0.11	80,80,80,80	0
59	MG	DF	303	1/1	0.91	0.10	22,22,22,22	1
59	MG	BA	3369	1/1	0.91	0.15	65,65,65,65	0
59	MG	BA	3129	1/1	0.91	0.33	42,42,42,42	0
59	MG	BA	3240	1/1	0.91	0.27	55,55,55,55	0
59	MG	AA	1823	1/1	0.91	0.19	68,68,68,68	0
59	MG	BA	3447	1/1	0.91	0.13	90,90,90,90	0
59	MG	CA	1651	1/1	0.91	0.09	84,84,84,84	0
59	MG	DR	201	1/1	0.91	0.10	108,108,108,108	0
59	MG	DA	3368	1/1	0.91	0.45	104,104,104,104	0
59	MG	BA	2902	1/1	0.91	0.10	79,79,79,79	0
59	MG	BA	2988	1/1	0.91	0.12	35,35,35,35	0
59	MG	BA	3201	1/1	0.92	0.09	50,50,50,50	0
59	MG	AA	1914	1/1	0.92	0.10	56,56,56,56	0
59	MG	DA	3480	1/1	0.92	0.21	87,87,87,87	0
59	MG	DA	3323	1/1	0.92	0.29	58,58,58,58	0
59	MG	BA	2921	1/1	0.92	0.07	51,51,51,51	0
59	MG	AA	1671	1/1	0.92	0.51	107,107,107,107	0
59	MG	AA	1639	1/1	0.92	0.28	79,79,79,79	0
59	MG	DA	3039	1/1	0.92	0.32	88,88,88,88	0
59	MG	BA	3514	1/1	0.92	0.18	76,76,76,76	0
59	MG	BA	3269	1/1	0.92	0.10	63,63,63,63	0
59	MG	AA	1877	1/1	0.92	0.20	61,61,61,61	0
59	MG	DA	3663	1/1	0.92	0.23	55,55,55,55	0
59	MG	DA	3493	1/1	0.92	0.10	90,90,90,90	0
59	MG	BA	3208	1/1	0.92	0.18	27,27,27,27	0
59	MG	BA	3209	1/1	0.92	0.16	61,61,61,61	0
59	MG	DA	3176	1/1	0.92	0.25	37,37,37,37	0
59	MG	DA	3048	1/1	0.92	0.37	63,63,63,63	0
59	MG	DA	3342	1/1	0.92	0.15	58,58,58,58	0
59	MG	BA	3609	1/1	0.92	0.17	56,56,56,56	0
59	MG	DA	3050	1/1	0.92	0.29	40,40,40,40	0
59	MG	AA	1784	1/1	0.92	0.12	92,92,92,92	0
59	MG	AA	1702	1/1	0.92	0.14	64,64,64,64	0
59	MG	BA	3527	1/1	0.92	0.37	86,86,86,86	0
59	MG	DA	3508	1/1	0.92	0.07	88,88,88,88	0
59	MG	BA	3277	1/1	0.92	0.22	44,44,44,44	0
59	MG	CA	1673	1/1	0.92	0.14	62,62,62,62	0
59	MG	BD	304	1/1	0.92	0.17	49,49,49,49	0
59	MG	BA	3021	1/1	0.92	0.25	78,78,78,78	0
59	MG	BA	3157	1/1	0.92	0.18	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	B5	102	1/1	0.92	0.08	32,32,32,32	1
59	MG	DA	3198	1/1	0.92	0.23	31,31,31,31	0
59	MG	BA	3534	1/1	0.92	0.32	56,56,56,56	0
59	MG	BA	3026	1/1	0.92	0.23	105,105,105,105	0
59	MG	BA	3027	1/1	0.92	0.30	74,74,74,74	0
59	MG	CA	1683	1/1	0.92	0.24	60,60,60,60	0
59	MG	CA	1778	1/1	0.92	0.15	88,88,88,88	0
59	MG	DA	3362	1/1	0.92	0.20	39,39,39,39	0
59	MG	BA	3538	1/1	0.92	0.09	37,37,37,37	0
59	MG	BA	3439	1/1	0.92	0.18	37,37,37,37	0
59	MG	AA	1921	1/1	0.92	0.17	86,86,86,86	0
59	MG	DA	3527	1/1	0.92	0.08	46,46,46,46	0
59	MG	BA	3220	1/1	0.92	0.23	54,54,54,54	0
59	MG	BA	3542	1/1	0.92	0.21	102,102,102,102	0
59	MG	DA	3370	1/1	0.92	0.29	68,68,68,68	0
59	MG	BA	3221	1/1	0.92	0.22	42,42,42,42	0
59	MG	DA	3218	1/1	0.92	0.27	130,130,130,130	0
59	MG	DA	3537	1/1	0.92	0.38	56,56,56,56	0
59	MG	BA	2995	1/1	0.92	0.28	84,84,84,84	0
59	MG	AA	1882	1/1	0.92	0.15	57,57,57,57	0
59	MG	BA	3298	1/1	0.92	0.17	67,67,67,67	0
59	MG	BA	2968	1/1	0.92	0.32	72,72,72,72	0
59	MG	AA	1770	1/1	0.92	0.27	76,76,76,76	0
59	MG	CA	1604	1/1	0.92	0.07	63,63,63,63	0
59	MG	DA	3546	1/1	0.92	0.69	11,11,11,11	1
59	MG	DA	3547	1/1	0.92	0.29	89,89,89,89	0
59	MG	DA	3227	1/1	0.92	0.24	73,73,73,73	0
59	MG	BA	3119	1/1	0.92	0.14	30,30,30,30	0
59	MG	CA	1606	1/1	0.92	0.08	60,60,60,60	0
59	MG	BA	3227	1/1	0.92	0.14	78,78,78,78	0
59	MG	DA	3232	1/1	0.92	0.24	59,59,59,59	0
59	MG	BA	3033	1/1	0.92	0.11	69,69,69,69	0
59	MG	CA	1704	1/1	0.92	0.08	71,71,71,71	0
59	MG	CV	102	1/1	0.92	0.15	92,92,92,92	0
59	MG	DA	3559	1/1	0.92	0.31	74,74,74,74	0
59	MG	DA	3397	1/1	0.92	0.24	72,72,72,72	0
59	MG	DA	3746	1/1	0.92	0.27	71,71,71,71	0
59	MG	DA	3747	1/1	0.92	0.22	38,38,38,38	1
59	MG	DA	2968	1/1	0.92	0.13	1,1,1,1	1
59	MG	DA	3749	1/1	0.92	0.32	80,80,80,80	1
59	MG	BA	3376	1/1	0.92	0.18	68,68,68,68	1
59	MG	DA	2970	1/1	0.92	0.17	41,41,41,41	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	DA	3568	1/1	0.92	0.15	73,73,73,73	0
59	MG	AA	1826	1/1	0.92	0.15	83,83,83,83	0
59	MG	AA	1947	1/1	0.92	0.32	79,79,79,79	0
59	MG	DA	3242	1/1	0.92	0.21	31,31,31,31	0
59	MG	DA	3757	1/1	0.92	0.27	86,86,86,86	0
59	MG	DA	3244	1/1	0.92	0.16	29,29,29,29	0
59	MG	DA	3759	1/1	0.92	0.25	49,49,49,49	0
59	MG	CA	1613	1/1	0.92	0.12	73,73,73,73	0
59	MG	DA	3575	1/1	0.92	0.30	89,89,89,89	0
59	MG	AA	1837	1/1	0.92	0.12	75,75,75,75	0
59	MG	DA	3249	1/1	0.92	0.16	68,68,68,68	0
59	MG	CA	1616	1/1	0.92	0.09	62,62,62,62	0
59	MG	DA	2979	1/1	0.92	0.14	42,42,42,42	0
59	MG	DA	3114	1/1	0.92	0.31	55,55,55,55	0
59	MG	BA	3381	1/1	0.92	0.22	42,42,42,42	0
59	MG	CA	1715	1/1	0.92	0.06	80,80,80,80	0
59	MG	DA	3771	1/1	0.92	0.43	71,71,71,71	0
59	MG	DA	3119	1/1	0.92	0.16	66,66,66,66	0
59	MG	AA	1669	1/1	0.92	0.16	50,50,50,50	0
59	MG	AA	1694	1/1	0.92	0.12	56,56,56,56	1
59	MG	DA	3588	1/1	0.92	0.18	83,83,83,83	0
59	MG	BA	3181	1/1	0.92	0.20	42,42,42,42	0
59	MG	BA	3315	1/1	0.92	0.32	74,74,74,74	0
59	MG	DA	3126	1/1	0.92	0.14	60,60,60,60	0
59	MG	BA	3475	1/1	0.92	0.16	59,59,59,59	0
59	MG	BA	3183	1/1	0.92	0.08	54,54,54,54	0
59	MG	DA	3596	1/1	0.92	0.12	54,54,54,54	1
59	MG	DA	3275	1/1	0.92	0.13	63,63,63,63	0
59	MG	DA	3598	1/1	0.92	0.28	83,83,83,83	0
59	MG	BA	3184	1/1	0.92	0.19	38,38,38,38	0
59	MG	BA	3042	1/1	0.92	0.54	103,103,103,103	0
59	MG	BA	3389	1/1	0.92	0.23	56,56,56,56	0
59	MG	D5	103	1/1	0.92	0.16	88,88,88,88	0
59	MG	DA	3280	1/1	0.92	0.12	58,58,58,58	0
59	MG	DA	2997	1/1	0.92	0.21	43,43,43,43	0
59	MG	DA	3609	1/1	0.92	0.30	63,63,63,63	0
59	MG	DA	3794	1/1	0.92	0.21	79,79,79,79	0
59	MG	DA	3611	1/1	0.92	0.37	31,31,31,31	0
59	MG	BA	3390	1/1	0.92	0.16	65,65,65,65	0
59	MG	BA	3243	1/1	0.92	0.26	25,25,25,25	0
59	MG	AA	1909	1/1	0.92	0.05	87,87,87,87	1
59	MG	BA	3323	1/1	0.92	0.22	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	DA	3142	1/1	0.92	0.14	90,90,90,90	0
59	MG	BA	3488	1/1	0.92	0.38	66,66,66,66	1
59	MG	BA	3579	1/1	0.92	0.35	71,71,71,71	0
59	MG	BA	3088	1/1	0.92	0.39	62,62,62,62	0
59	MG	AA	1817	1/1	0.92	0.08	71,71,71,71	0
59	MG	BA	3397	1/1	0.92	0.16	75,75,75,75	0
59	MG	AD	302	1/1	0.92	0.08	96,96,96,96	0
59	MG	DA	3149	1/1	0.92	0.15	26,26,26,26	0
59	MG	BA	2980	1/1	0.92	0.14	47,47,47,47	0
59	MG	BA	3137	1/1	0.92	0.13	43,43,43,43	0
59	MG	DE	303	1/1	0.92	0.08	42,42,42,42	0
59	MG	CA	1742	1/1	0.92	0.15	81,81,81,81	0
59	MG	BA	2915	1/1	0.92	0.24	70,70,70,70	0
59	MG	BA	3404	1/1	0.92	0.19	34,34,34,34	0
59	MG	BA	3139	1/1	0.92	0.21	27,27,27,27	0
59	MG	AA	1766	1/1	0.92	0.18	74,74,74,74	0
59	MG	AA	1844	1/1	0.92	0.20	107,107,107,107	0
59	MG	DP	204	1/1	0.92	0.06	15,15,15,15	0
59	MG	DA	3472	1/1	0.92	0.44	79,79,79,79	1
59	MG	BA	2918	1/1	0.92	0.16	76,76,76,76	1
59	MG	BA	3337	1/1	0.92	0.19	37,37,37,37	0
59	MG	DA	2913	1/1	0.92	0.41	15,15,15,15	1
59	MG	BA	3053	1/1	0.92	0.42	62,62,62,62	0
59	MG	DA	3164	1/1	0.92	0.24	55,55,55,55	0
59	MG	CC	303	1/1	0.93	0.15	113,113,113,113	0
59	MG	DA	3254	1/1	0.93	0.11	59,59,59,59	0
59	MG	DA	3533	1/1	0.93	0.23	100,100,100,100	0
59	MG	DA	3683	1/1	0.93	0.22	46,46,46,46	0
59	MG	CA	1633	1/1	0.93	0.08	70,70,70,70	0
59	MG	BA	2937	1/1	0.93	0.24	40,40,40,40	0
59	MG	DA	3262	1/1	0.93	0.20	59,59,59,59	1
59	MG	DA	3392	1/1	0.93	0.08	81,81,81,81	0
59	MG	DA	3393	1/1	0.93	0.09	6,6,6,6	1
59	MG	DA	3032	1/1	0.93	0.37	34,34,34,34	0
59	MG	DA	3265	1/1	0.93	0.46	82,82,82,82	0
59	MG	AA	1931	1/1	0.93	0.15	87,87,87,87	0
59	MG	AA	1682	1/1	0.93	0.43	104,104,104,104	0
59	MG	CM	201	1/1	0.93	0.06	131,131,131,131	0
59	MG	DA	3545	1/1	0.93	0.07	58,58,58,58	0
59	MG	DA	3698	1/1	0.93	0.06	25,25,25,25	0
59	MG	DA	3700	1/1	0.93	0.15	59,59,59,59	0
59	MG	BA	3108	1/1	0.93	0.27	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	BA	3341	1/1	0.93	0.21	33,33,33,33	0
59	MG	BA	2909	1/1	0.93	0.16	50,50,50,50	0
59	MG	BA	3343	1/1	0.93	0.20	32,32,32,32	0
59	MG	AA	1934	1/1	0.93	0.10	68,68,68,68	0
59	MG	AA	1913	1/1	0.93	0.10	72,72,72,72	0
59	MG	BA	3464	1/1	0.93	0.21	43,43,43,43	0
59	MG	DA	3413	1/1	0.93	0.28	84,84,84,84	0
59	MG	BA	2912	1/1	0.93	0.24	57,57,57,57	0
59	MG	BA	3466	1/1	0.93	0.17	38,38,38,38	0
59	MG	BB	201	1/1	0.93	0.20	46,46,46,46	0
59	MG	BA	3468	1/1	0.93	0.16	36,36,36,36	0
59	MG	DA	3160	1/1	0.93	0.19	68,68,68,68	0
59	MG	DA	3053	1/1	0.93	0.13	33,33,33,33	0
59	MG	DA	3722	1/1	0.93	0.16	86,86,86,86	0
59	MG	DA	3056	1/1	0.93	0.21	65,65,65,65	0
59	MG	DA	3058	1/1	0.93	0.13	32,32,32,32	0
59	MG	DA	3725	1/1	0.93	0.11	71,71,71,71	0
59	MG	BA	3295	1/1	0.93	0.37	51,51,51,51	0
59	MG	DA	2955	1/1	0.93	0.19	34,34,34,34	1
59	MG	DA	3729	1/1	0.93	0.32	96,96,96,96	0
59	MG	DA	2956	1/1	0.93	0.09	38,38,38,38	0
59	MG	DA	3731	1/1	0.93	0.17	45,45,45,45	1
59	MG	BA	3075	1/1	0.93	0.28	87,87,87,87	0
59	MG	BB	205	1/1	0.93	0.07	69,69,69,69	1
59	MG	BA	3036	1/1	0.93	0.25	98,98,98,98	0
59	MG	AA	1897	1/1	0.93	0.12	68,68,68,68	0
59	MG	AA	1773	1/1	0.93	0.06	50,50,50,50	0
59	MG	DA	3298	1/1	0.93	0.13	65,65,65,65	0
59	MG	DA	3299	1/1	0.93	0.26	75,75,75,75	0
59	MG	AA	1879	1/1	0.93	0.14	74,74,74,74	0
59	MG	DA	3301	1/1	0.93	0.06	32,32,32,32	0
59	MG	BA	3407	1/1	0.93	0.12	64,64,64,64	0
59	MG	DA	3303	1/1	0.93	0.12	54,54,54,54	0
59	MG	DA	3445	1/1	0.93	0.28	55,55,55,55	0
59	MG	BA	3408	1/1	0.93	0.29	73,73,73,73	0
59	MG	CA	1740	1/1	0.93	0.15	85,85,85,85	0
59	MG	BA	3355	1/1	0.93	0.17	26,26,26,26	0
59	MG	DA	3752	1/1	0.93	0.30	96,96,96,96	0
59	MG	AA	1606	1/1	0.93	0.13	77,77,77,77	0
59	MG	CA	1661	1/1	0.93	0.06	65,65,65,65	0
59	MG	DA	3309	1/1	0.93	0.36	76,76,76,76	0
59	MG	DA	3181	1/1	0.93	0.21	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	BA	3164	1/1	0.93	0.31	44,44,44,44	0
59	MG	BA	3413	1/1	0.93	0.38	73,73,73,73	0
59	MG	DA	3187	1/1	0.93	0.26	44,44,44,44	0
59	MG	DA	3188	1/1	0.93	0.16	31,31,31,31	0
59	MG	AA	1816	1/1	0.93	0.21	64,64,64,64	0
59	MG	BP	204	1/1	0.93	0.09	24,24,24,24	1
59	MG	BA	3167	1/1	0.93	0.15	36,36,36,36	0
59	MG	BA	3310	1/1	0.93	0.13	68,68,68,68	0
59	MG	DA	3193	1/1	0.93	0.13	68,68,68,68	0
59	MG	BA	3362	1/1	0.93	0.23	43,43,43,43	0
59	MG	BA	3563	1/1	0.93	0.21	80,80,80,80	0
59	MG	DA	3088	1/1	0.93	0.09	65,65,65,65	0
59	MG	AA	1696	1/1	0.93	0.09	90,90,90,90	0
59	MG	DA	3331	1/1	0.93	0.11	45,45,45,45	1
59	MG	BA	3495	1/1	0.93	0.16	69,69,69,69	0
59	MG	BA	2952	1/1	0.93	0.27	96,96,96,96	0
59	MG	DA	2985	1/1	0.93	0.14	39,39,39,39	0
59	MG	BA	3012	1/1	0.93	0.27	34,34,34,34	0
59	MG	AA	1622	1/1	0.93	0.17	70,70,70,70	0
59	MG	BA	3125	1/1	0.93	0.15	70,70,70,70	0
59	MG	DA	3622	1/1	0.93	0.08	58,58,58,58	0
59	MG	DA	3099	1/1	0.93	0.19	67,67,67,67	0
59	MG	BA	2954	1/1	0.93	0.09	59,59,59,59	0
59	MG	BA	3571	1/1	0.93	0.28	77,77,77,77	0
59	MG	AA	1853	1/1	0.93	0.19	74,74,74,74	0
59	MG	AL	205	1/1	0.93	0.09	47,47,47,47	1
59	MG	AA	1819	1/1	0.93	0.05	75,75,75,75	0
59	MG	DA	2998	1/1	0.93	0.22	49,49,49,49	0
59	MG	CA	1688	1/1	0.93	0.04	79,79,79,79	0
59	MG	DA	3492	1/1	0.93	0.38	62,62,62,62	0
59	MG	BA	3577	1/1	0.93	0.21	38,38,38,38	0
59	MG	BA	3219	1/1	0.93	0.36	57,57,57,57	0
59	MG	BA	2989	1/1	0.93	0.26	82,82,82,82	0
59	MG	DA	3496	1/1	0.93	0.17	83,83,83,83	0
59	MG	DA	3003	1/1	0.93	0.14	36,36,36,36	0
59	MG	DA	3225	1/1	0.93	0.18	32,32,32,32	0
59	MG	DA	3226	1/1	0.93	0.31	54,54,54,54	0
59	MG	AA	1623	1/1	0.93	0.33	66,66,66,66	0
59	MG	AA	1785	1/1	0.93	0.06	108,108,108,108	0
59	MG	DA	3359	1/1	0.93	0.13	64,64,64,64	0
59	MG	CA	1694	1/1	0.93	0.12	93,93,93,93	0
59	MG	BA	3182	1/1	0.93	0.10	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	BA	3328	1/1	0.93	0.26	76,76,76,76	0
59	MG	BA	3584	1/1	0.93	0.17	65,65,65,65	0
59	MG	DA	3655	1/1	0.93	0.43	91,91,91,91	0
59	MG	DA	3011	1/1	0.93	0.29	40,40,40,40	0
59	MG	BA	3329	1/1	0.93	0.18	1,1,1,1	1
59	MG	BA	2962	1/1	0.93	0.18	70,70,70,70	0
59	MG	AA	1601	1/1	0.93	0.06	74,74,74,74	0
59	MG	DA	3016	1/1	0.93	0.19	51,51,51,51	0
59	MG	AA	1858	1/1	0.93	0.13	60,60,60,60	0
59	MG	AA	1846	1/1	0.93	0.27	45,45,45,45	0
59	MG	DA	3020	1/1	0.93	0.17	52,52,52,52	0
59	MG	DA	3375	1/1	0.93	0.18	57,57,57,57	0
59	MG	BA	3280	1/1	0.93	0.23	38,38,38,38	0
59	MG	DP	202	1/1	0.93	0.18	49,49,49,49	1
59	MG	BA	3449	1/1	0.93	0.11	69,69,69,69	0
59	MG	DA	3247	1/1	0.93	0.31	41,41,41,41	0
59	MG	AT	201	1/1	0.93	0.06	76,76,76,76	1
59	MG	CA	1631	1/1	0.93	0.08	59,59,59,59	0
59	MG	BA	3451	1/1	0.93	0.08	55,55,55,55	0
59	MG	DT	201	1/1	0.93	0.05	5,5,5,5	1
59	MG	DU	201	1/1	0.93	0.13	68,68,68,68	0
59	MG	DU	203	1/1	0.93	0.21	36,36,36,36	0
59	MG	DA	3140	1/1	0.93	0.54	77,77,77,77	0
59	MG	DA	3528	1/1	0.93	0.14	80,80,80,80	0
60	ZN	CD	301	1/1	0.93	0.20	151,151,151,151	0
59	MG	BA	3197	1/1	0.94	0.23	54,54,54,54	0
59	MG	AA	1893	1/1	0.94	0.20	56,56,56,56	0
59	MG	DA	3377	1/1	0.94	0.11	16,16,16,16	0
59	MG	DA	3595	1/1	0.94	0.37	75,75,75,75	0
59	MG	DA	3284	1/1	0.94	0.14	25,25,25,25	0
59	MG	DA	3031	1/1	0.94	0.26	51,51,51,51	0
59	MG	DA	3194	1/1	0.94	0.30	92,92,92,92	0
59	MG	BA	3175	1/1	0.94	0.20	25,25,25,25	0
59	MG	CA	1706	1/1	0.94	0.06	47,47,47,47	0
59	MG	BA	3291	1/1	0.94	0.28	41,41,41,41	0
59	MG	DA	3604	1/1	0.94	0.23	39,39,39,39	0
59	MG	BA	3476	1/1	0.94	0.11	58,58,58,58	0
59	MG	DA	3606	1/1	0.94	0.10	88,88,88,88	1
59	MG	BA	2931	1/1	0.94	0.13	44,44,44,44	0
59	MG	BA	2906	1/1	0.94	0.21	92,92,92,92	0
59	MG	BA	3297	1/1	0.94	0.08	34,34,34,34	0
59	MG	DA	3610	1/1	0.94	0.20	112,112,112,112	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	CA	1713	1/1	0.94	0.11	65,65,65,65	1
59	MG	DA	3204	1/1	0.94	0.16	70,70,70,70	0
59	MG	BY	201	1/1	0.94	0.08	50,50,50,50	0
59	MG	DA	3740	1/1	0.94	0.08	50,50,50,50	0
59	MG	DA	3045	1/1	0.94	0.08	47,47,47,47	0
59	MG	DA	3396	1/1	0.94	0.25	62,62,62,62	0
59	MG	BA	3052	1/1	0.94	0.13	64,64,64,64	0
59	MG	DA	3398	1/1	0.94	0.12	31,31,31,31	1
59	MG	DA	3399	1/1	0.94	0.16	62,62,62,62	0
59	MG	DA	3209	1/1	0.94	0.20	50,50,50,50	0
59	MG	BA	3483	1/1	0.94	0.33	60,60,60,60	0
59	MG	DA	2973	1/1	0.94	0.15	21,21,21,21	0
59	MG	BA	3436	1/1	0.94	0.06	62,62,62,62	0
59	MG	DA	3626	1/1	0.94	0.09	34,34,34,34	0
59	MG	AA	1657	1/1	0.94	0.06	77,77,77,77	0
59	MG	BA	3537	1/1	0.94	0.15	28,28,28,28	0
59	MG	BA	3264	1/1	0.94	0.21	42,42,42,42	0
59	MG	BA	3054	1/1	0.94	0.15	100,100,100,100	0
59	MG	BA	3266	1/1	0.94	0.09	65,65,65,65	0
59	MG	BA	3489	1/1	0.94	0.05	22,22,22,22	0
59	MG	BA	3490	1/1	0.94	0.26	19,19,19,19	0
59	MG	DA	3313	1/1	0.94	0.20	101,101,101,101	0
59	MG	CA	1665	1/1	0.94	0.15	79,79,79,79	0
59	MG	BA	3444	1/1	0.94	0.24	69,69,69,69	0
59	MG	DA	3763	1/1	0.94	0.10	62,62,62,62	1
59	MG	CA	1728	1/1	0.94	0.11	88,88,88,88	0
59	MG	BA	3081	1/1	0.94	0.27	64,64,64,64	0
59	MG	DA	3641	1/1	0.94	0.49	68,68,68,68	0
59	MG	CA	1614	1/1	0.94	0.21	72,72,72,72	0
59	MG	AA	1760	1/1	0.94	0.23	45,45,45,45	0
59	MG	DA	3529	1/1	0.94	0.06	42,42,42,42	0
59	MG	DA	3647	1/1	0.94	0.28	36,36,36,36	0
59	MG	DA	3773	1/1	0.94	0.12	90,90,90,90	0
59	MG	BA	3371	1/1	0.94	0.11	63,63,63,63	0
59	MG	BA	3372	1/1	0.94	0.20	70,70,70,70	0
59	MG	DA	2924	1/1	0.94	0.08	65,65,65,65	0
59	MG	DA	3427	1/1	0.94	0.29	78,78,78,78	0
59	MG	BA	3155	1/1	0.94	0.17	29,29,29,29	0
59	MG	DA	2996	1/1	0.94	0.49	71,71,71,71	1
59	MG	DA	3431	1/1	0.94	0.20	38,38,38,38	0
59	MG	AA	1733	1/1	0.94	0.07	71,71,71,71	0
59	MG	DA	3237	1/1	0.94	0.19	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	CP	101	1/1	0.94	0.05	81,81,81,81	0
59	MG	BA	3551	1/1	0.94	0.23	82,82,82,82	0
59	MG	AA	1871	1/1	0.94	0.31	144,144,144,144	0
59	MG	DA	3543	1/1	0.94	0.15	71,71,71,71	0
59	MG	AA	1670	1/1	0.94	0.09	28,28,28,28	1
59	MG	DA	3082	1/1	0.94	0.13	82,82,82,82	0
59	MG	DA	3243	1/1	0.94	0.27	64,64,64,64	0
59	MG	BA	3377	1/1	0.94	0.16	59,59,59,59	0
59	MG	DA	3162	1/1	0.94	0.37	122,122,122,122	0
59	MG	BA	2941	1/1	0.94	0.15	62,62,62,62	0
59	MG	BA	3242	1/1	0.94	0.38	60,60,60,60	0
59	MG	CA	1744	1/1	0.94	0.11	57,57,57,57	0
59	MG	BA	3503	1/1	0.94	0.16	65,65,65,65	1
59	MG	DA	3450	1/1	0.94	0.14	100,100,100,100	0
59	MG	BA	3041	1/1	0.94	0.13	37,37,37,37	0
59	MG	DA	3675	1/1	0.94	0.18	39,39,39,39	0
59	MG	DA	3557	1/1	0.94	0.10	64,64,64,64	0
59	MG	DA	3089	1/1	0.94	0.13	81,81,81,81	0
59	MG	BA	3559	1/1	0.94	0.16	45,45,45,45	0
59	MG	DA	3681	1/1	0.94	0.06	28,28,28,28	0
59	MG	DB	210	1/1	0.94	0.14	56,56,56,56	0
59	MG	AA	1973	1/1	0.94	0.15	69,69,69,69	0
59	MG	DD	301	1/1	0.94	0.21	57,57,57,57	0
59	MG	DA	3456	1/1	0.94	0.34	56,56,56,56	0
59	MG	DA	3258	1/1	0.94	0.12	48,48,48,48	0
59	MG	DA	3010	1/1	0.94	0.25	49,49,49,49	0
59	MG	DD	306	1/1	0.94	0.09	60,60,60,60	0
59	MG	BA	2925	1/1	0.94	0.24	33,33,33,33	0
59	MG	BA	3461	1/1	0.94	0.24	41,41,41,41	0
59	MG	CV	111	1/1	0.94	0.07	71,71,71,71	0
59	MG	DA	3690	1/1	0.94	0.13	62,62,62,62	0
59	MG	BA	2913	1/1	0.94	0.33	51,51,51,51	0
59	MG	DA	3267	1/1	0.94	0.28	62,62,62,62	0
59	MG	DA	3465	1/1	0.94	0.18	26,26,26,26	0
59	MG	AA	1612	1/1	0.94	0.05	55,55,55,55	0
59	MG	AA	1706	1/1	0.94	0.06	44,44,44,44	1
59	MG	BA	2964	1/1	0.94	0.11	96,96,96,96	0
59	MG	DA	3103	1/1	0.94	0.12	60,60,60,60	0
59	MG	BA	3048	1/1	0.94	0.13	90,90,90,90	0
59	MG	DA	3182	1/1	0.94	0.06	73,73,73,73	0
59	MG	DA	3367	1/1	0.94	0.31	28,28,28,28	1
59	MG	BF	301	1/1	0.94	0.15	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	CA	1757	1/1	0.94	0.07	83,83,83,83	0
59	MG	BA	3467	1/1	0.94	0.17	93,93,93,93	0
59	MG	DA	3371	1/1	0.94	0.05	59,59,59,59	1
59	MG	BA	3425	1/1	0.94	0.23	48,48,48,48	0
59	MG	BA	3520	1/1	0.94	0.08	80,80,80,80	0
59	MG	BA	3521	1/1	0.94	0.33	119,119,119,119	0
59	MG	DA	3701	1/1	0.95	0.10	55,55,55,55	0
59	MG	BD	302	1/1	0.95	0.09	52,52,52,52	0
59	MG	DA	3704	1/1	0.95	0.23	74,74,74,74	0
59	MG	DA	3051	1/1	0.95	0.19	36,36,36,36	0
59	MG	BD	303	1/1	0.95	0.10	35,35,35,35	0
59	MG	CA	1699	1/1	0.95	0.08	64,64,64,64	0
59	MG	BA	3517	1/1	0.95	0.24	98,98,98,98	0
59	MG	BA	2919	1/1	0.95	0.15	44,44,44,44	1
59	MG	BA	3262	1/1	0.95	0.07	50,50,50,50	0
59	MG	DA	3579	1/1	0.95	0.17	110,110,110,110	0
59	MG	BA	3305	1/1	0.95	0.17	28,28,28,28	0
59	MG	DA	3063	1/1	0.95	0.07	50,50,50,50	0
59	MG	BA	3474	1/1	0.95	0.32	53,53,53,53	0
59	MG	AD	304	1/1	0.95	0.21	135,135,135,135	0
59	MG	BA	3158	1/1	0.95	0.12	33,33,33,33	0
59	MG	AA	1842	1/1	0.95	0.08	58,58,58,58	0
59	MG	CA	1772	1/1	0.95	0.09	79,79,79,79	0
59	MG	BA	3478	1/1	0.95	0.28	28,28,28,28	0
59	MG	AA	1714	1/1	0.95	0.20	66,66,66,66	0
59	MG	BA	2946	1/1	0.95	0.14	49,49,49,49	0
59	MG	DA	3356	1/1	0.95	0.28	32,32,32,32	0
59	MG	BP	201	1/1	0.95	0.05	24,24,24,24	0
59	MG	DA	3251	1/1	0.95	0.11	53,53,53,53	0
59	MG	BA	3481	1/1	0.95	0.17	59,59,59,59	0
59	MG	BA	3531	1/1	0.95	0.29	53,53,53,53	0
59	MG	BA	3195	1/1	0.95	0.31	85,85,85,85	0
59	MG	DA	3077	1/1	0.95	0.22	68,68,68,68	0
59	MG	AA	1665	1/1	0.95	0.27	60,60,60,60	0
59	MG	DA	3364	1/1	0.95	0.15	59,59,59,59	0
59	MG	BR	204	1/1	0.95	0.08	26,26,26,26	0
59	MG	DA	3603	1/1	0.95	0.09	60,60,60,60	0
59	MG	DA	3482	1/1	0.95	0.27	37,37,37,37	1
59	MG	DA	3741	1/1	0.95	0.20	43,43,43,43	0
59	MG	BA	3068	1/1	0.95	0.29	59,59,59,59	0
59	MG	DA	3484	1/1	0.95	0.36	58,58,58,58	0
59	MG	DA	2995	1/1	0.95	0.07	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	BA	3099	1/1	0.95	0.13	30,30,30,30	0
59	MG	AV	105	1/1	0.95	0.04	80,80,80,80	0
59	MG	AI	203	1/1	0.95	0.10	138,138,138,138	0
59	MG	BA	2974	1/1	0.95	0.23	38,38,38,38	0
59	MG	BA	3134	1/1	0.95	0.06	65,65,65,65	0
59	MG	AA	1967	1/1	0.95	0.13	67,67,67,67	0
59	MG	BA	3279	1/1	0.95	0.18	59,59,59,59	0
59	MG	AA	1864	1/1	0.95	0.10	67,67,67,67	0
59	MG	DA	3090	1/1	0.95	0.10	35,35,35,35	0
59	MG	DA	2929	1/1	0.95	0.13	10,10,10,10	1
59	MG	BA	3023	1/1	0.95	0.10	64,64,64,64	0
59	MG	BA	3593	1/1	0.95	0.07	41,41,41,41	0
59	MG	DA	3500	1/1	0.95	0.13	84,84,84,84	0
59	MG	DA	2932	1/1	0.95	0.76	1,1,1,1	1
59	MG	AA	1799	1/1	0.95	0.09	80,80,80,80	0
59	MG	DA	3625	1/1	0.95	0.24	29,29,29,29	0
59	MG	DA	3183	1/1	0.95	0.11	94,94,94,94	0
59	MG	DA	3504	1/1	0.95	0.09	60,60,60,60	0
59	MG	DA	3281	1/1	0.95	0.23	31,31,31,31	0
59	MG	DA	3385	1/1	0.95	0.09	43,43,43,43	0
59	MG	DA	3386	1/1	0.95	0.26	99,99,99,99	0
59	MG	CA	1669	1/1	0.95	0.06	57,57,57,57	0
59	MG	DA	3097	1/1	0.95	0.15	69,69,69,69	0
59	MG	AA	1616	1/1	0.95	0.17	61,61,61,61	0
59	MG	DA	3285	1/1	0.95	0.17	37,37,37,37	0
59	MG	DA	3772	1/1	0.95	0.07	69,69,69,69	0
59	MG	AA	1746	1/1	0.95	0.15	66,66,66,66	0
59	MG	DA	3012	1/1	0.95	0.21	30,30,30,30	0
59	MG	DA	3514	1/1	0.95	0.12	82,82,82,82	0
59	MG	DA	3639	1/1	0.95	0.17	37,37,37,37	0
59	MG	CA	1734	1/1	0.95	0.14	56,56,56,56	0
59	MG	CA	1612	1/1	0.95	0.13	58,58,58,58	0
59	MG	DA	3290	1/1	0.95	0.17	32,32,32,32	0
59	MG	DA	3104	1/1	0.95	0.07	63,63,63,63	0
59	MG	CA	1736	1/1	0.95	0.07	60,60,60,60	0
59	MG	BA	2932	1/1	0.95	0.22	63,63,63,63	0
59	MG	BA	3410	1/1	0.95	0.36	42,42,42,42	0
59	MG	AA	1928	1/1	0.95	0.20	42,42,42,42	0
59	MG	DA	3402	1/1	0.95	0.21	16,16,16,16	0
59	MG	B0	101	1/1	0.95	0.43	73,73,73,73	0
59	MG	CA	1617	1/1	0.95	0.04	66,66,66,66	0
59	MG	DA	3199	1/1	0.95	0.14	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	CA	1678	1/1	0.95	0.05	45,45,45,45	1
59	MG	BA	3601	1/1	0.95	0.42	79,79,79,79	0
59	MG	BA	3250	1/1	0.95	0.07	51,51,51,51	0
59	MG	DA	3115	1/1	0.95	0.33	39,39,39,39	0
59	MG	BA	3114	1/1	0.95	0.08	80,80,80,80	0
59	MG	CA	1682	1/1	0.95	0.26	53,53,53,53	0
59	MG	DA	3206	1/1	0.95	0.11	66,66,66,66	0
59	MG	BA	3292	1/1	0.95	0.12	29,29,29,29	0
59	MG	DA	2952	1/1	0.95	0.16	44,44,44,44	0
59	MG	AA	1878	1/1	0.95	0.08	76,76,76,76	0
59	MG	CA	1623	1/1	0.95	0.04	81,81,81,81	0
59	MG	DB	206	1/1	0.95	0.08	65,65,65,65	1
59	MG	DA	3310	1/1	0.95	0.15	90,90,90,90	1
59	MG	BA	3606	1/1	0.95	0.18	65,65,65,65	0
59	MG	CA	1687	1/1	0.95	0.05	63,63,63,63	0
59	MG	DA	3213	1/1	0.95	0.25	67,67,67,67	0
59	MG	BA	3056	1/1	0.95	0.37	156,156,156,156	0
59	MG	DA	3315	1/1	0.95	0.17	77,77,77,77	0
59	MG	DD	302	1/1	0.95	0.16	53,53,53,53	0
59	MG	DA	3216	1/1	0.95	0.14	36,36,36,36	0
59	MG	DA	3674	1/1	0.95	0.35	55,55,55,55	0
59	MG	D1	102	1/1	0.95	0.16	80,80,80,80	0
59	MG	DA	3430	1/1	0.95	0.11	25,25,25,25	0
59	MG	DA	3129	1/1	0.95	0.29	72,72,72,72	0
59	MG	DA	3038	1/1	0.95	0.24	32,32,32,32	0
59	MG	DA	3551	1/1	0.95	0.19	53,53,53,53	0
59	MG	AA	1930	1/1	0.95	0.06	64,64,64,64	0
59	MG	AA	1741	1/1	0.95	0.14	54,54,54,54	0
59	MG	BA	3257	1/1	0.95	0.40	42,42,42,42	0
59	MG	BA	3510	1/1	0.95	0.26	41,41,41,41	0
59	MG	DA	2963	1/1	0.95	0.04	39,39,39,39	1
59	MG	DA	3687	1/1	0.95	0.09	43,43,43,43	0
59	MG	DA	3328	1/1	0.95	0.15	34,34,34,34	0
59	MG	DA	3136	1/1	0.95	0.28	97,97,97,97	0
59	MG	DA	3560	1/1	0.95	0.06	58,58,58,58	0
59	MG	AA	1636	1/1	0.95	0.14	53,53,53,53	0
59	MG	AA	1841	1/1	0.95	0.19	42,42,42,42	0
59	MG	DA	3564	1/1	0.95	0.18	42,42,42,42	0
59	MG	DA	3332	1/1	0.95	0.17	26,26,26,26	0
59	MG	DA	3333	1/1	0.95	0.25	55,55,55,55	0
59	MG	DU	202	1/1	0.95	0.28	8,8,8,8	1
59	MG	DA	3229	1/1	0.95	0.06	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	BA	3469	1/1	0.95	0.28	102,102,102,102	0
59	MG	DA	3699	1/1	0.95	0.07	62,62,62,62	0
59	MG	BA	3470	1/1	0.95	0.15	35,35,35,35	0
59	MG	DA	3458	1/1	0.96	0.39	59,59,59,59	0
59	MG	DA	3638	1/1	0.96	0.15	21,21,21,21	0
59	MG	BA	3347	1/1	0.96	0.19	30,30,30,30	0
59	MG	CA	1711	1/1	0.96	0.06	65,65,65,65	1
59	MG	AA	1629	1/1	0.96	0.17	80,80,80,80	0
59	MG	AA	1960	1/1	0.96	0.07	72,72,72,72	0
59	MG	AN	103	1/1	0.96	0.15	147,147,147,147	0
59	MG	BA	3351	1/1	0.96	0.14	26,26,26,26	0
59	MG	BA	3066	1/1	0.96	0.30	57,57,57,57	0
59	MG	AA	1824	1/1	0.96	0.11	83,83,83,83	0
59	MG	DA	3554	1/1	0.96	0.06	95,95,95,95	0
59	MG	DA	3018	1/1	0.96	0.05	76,76,76,76	0
59	MG	AA	1892	1/1	0.96	0.10	75,75,75,75	0
59	MG	AQ	201	1/1	0.96	0.06	97,97,97,97	1
59	MG	BA	3356	1/1	0.96	0.16	45,45,45,45	0
59	MG	BA	3161	1/1	0.96	0.12	39,39,39,39	0
59	MG	BA	2934	1/1	0.96	0.24	57,57,57,57	0
59	MG	BA	3100	1/1	0.96	0.06	47,47,47,47	0
59	MG	BA	3022	1/1	0.96	0.05	43,43,43,43	0
59	MG	BA	3549	1/1	0.96	0.16	84,84,84,84	0
59	MG	DA	3660	1/1	0.96	0.34	78,78,78,78	0
59	MG	BA	3166	1/1	0.96	0.43	89,89,89,89	0
59	MG	DA	3029	1/1	0.96	0.11	30,30,30,30	0
59	MG	CA	1782	1/1	0.96	0.10	52,52,52,52	0
59	MG	DA	3394	1/1	0.96	0.09	63,63,63,63	0
59	MG	DA	3570	1/1	0.96	0.08	62,62,62,62	0
59	MG	BA	2956	1/1	0.96	0.05	37,37,37,37	1
59	MG	DA	3319	1/1	0.96	0.17	47,47,47,47	0
59	MG	DA	3102	1/1	0.96	0.10	86,86,86,86	0
59	MG	BA	3200	1/1	0.96	0.04	31,31,31,31	0
59	MG	BA	3073	1/1	0.96	0.23	52,52,52,52	0
59	MG	BA	3169	1/1	0.96	0.16	24,24,24,24	0
59	MG	DA	3774	1/1	0.96	0.23	84,84,84,84	0
59	MG	BA	3459	1/1	0.96	0.13	44,44,44,44	0
59	MG	DA	3178	1/1	0.96	0.11	29,29,29,29	0
59	MG	BA	3074	1/1	0.96	0.15	36,36,36,36	0
59	MG	AA	1884	1/1	0.96	0.04	89,89,89,89	0
59	MG	AA	1672	1/1	0.96	0.06	77,77,77,77	0
59	MG	AA	1916	1/1	0.96	0.04	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	DA	2978	1/1	0.96	0.18	33,33,33,33	0
59	MG	B5	103	1/1	0.96	0.18	36,36,36,36	0
59	MG	DA	3256	1/1	0.96	0.30	42,42,42,42	0
59	MG	DA	3586	1/1	0.96	0.30	34,34,34,34	0
59	MG	DA	3410	1/1	0.96	0.29	25,25,25,25	0
59	MG	DA	3044	1/1	0.96	0.10	78,78,78,78	0
59	MG	DA	3412	1/1	0.96	0.32	42,42,42,42	0
59	MG	DA	3260	1/1	0.96	0.32	33,33,33,33	0
59	MG	DA	3336	1/1	0.96	0.21	31,31,31,31	0
59	MG	AA	1613	1/1	0.96	0.26	74,74,74,74	0
59	MG	AA	1896	1/1	0.96	0.06	78,78,78,78	0
59	MG	BA	3332	1/1	0.96	0.13	19,19,19,19	0
59	MG	BD	301	1/1	0.96	0.25	25,25,25,25	0
59	MG	BA	3418	1/1	0.96	0.21	69,69,69,69	0
59	MG	DA	3795	1/1	0.96	0.20	25,25,25,25	0
59	MG	BA	3515	1/1	0.96	0.16	47,47,47,47	1
59	MG	DA	3422	1/1	0.96	0.38	63,63,63,63	0
59	MG	BA	3516	1/1	0.96	0.32	64,64,64,64	0
59	MG	BA	3419	1/1	0.96	0.20	49,49,49,49	0
59	MG	DB	203	1/1	0.96	0.06	30,30,30,30	1
59	MG	BA	3288	1/1	0.96	0.31	38,38,38,38	0
59	MG	DA	3426	1/1	0.96	0.19	28,28,28,28	0
59	MG	AV	103	1/1	0.96	0.05	72,72,72,72	0
59	MG	DA	3702	1/1	0.96	0.11	80,80,80,80	0
59	MG	AA	1954	1/1	0.96	0.27	67,67,67,67	0
59	MG	DA	3273	1/1	0.96	0.29	54,54,54,54	0
59	MG	BA	3252	1/1	0.96	0.15	75,75,75,75	0
59	MG	DA	3060	1/1	0.96	0.27	77,77,77,77	0
59	MG	DA	3061	1/1	0.96	0.10	67,67,67,67	0
59	MG	DA	3709	1/1	0.96	0.08	61,61,61,61	0
59	MG	DA	2992	1/1	0.96	0.38	103,103,103,103	0
59	MG	BA	3572	1/1	0.96	0.27	68,68,68,68	0
59	MG	DA	3523	1/1	0.96	0.11	34,34,34,34	0
59	MG	DA	2994	1/1	0.96	0.19	60,60,60,60	0
59	MG	BA	3144	1/1	0.96	0.15	73,73,73,73	0
59	MG	BA	3294	1/1	0.96	0.20	73,73,73,73	0
59	MG	BA	3214	1/1	0.96	0.29	85,85,85,85	0
59	MG	BA	3525	1/1	0.96	0.07	44,44,44,44	0
59	MG	DA	3069	1/1	0.96	0.05	50,50,50,50	0
59	MG	DA	3720	1/1	0.96	0.08	66,66,66,66	0
59	MG	BA	3427	1/1	0.96	0.16	63,63,63,63	0
59	MG	BP	203	1/1	0.96	0.11	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	DA	3623	1/1	0.96	0.09	28,28,28,28	0
59	MG	DP	201	1/1	0.96	0.06	36,36,36,36	1
59	MG	DA	3532	1/1	0.96	0.15	79,79,79,79	0
59	MG	BA	3009	1/1	0.96	0.23	80,80,80,80	0
59	MG	DA	2941	1/1	0.96	0.05	27,27,27,27	1
59	MG	DA	3448	1/1	0.96	0.06	55,55,55,55	0
59	MG	BA	2903	1/1	0.96	0.26	37,37,37,37	0
59	MG	AA	1862	1/1	0.96	0.26	65,65,65,65	0
59	MG	DA	3215	1/1	0.96	0.21	69,69,69,69	0
59	MG	DA	3452	1/1	0.96	0.18	30,30,30,30	0
59	MG	AA	1888	1/1	0.96	0.12	58,58,58,58	0
59	MG	AA	1647	1/1	0.96	0.10	35,35,35,35	0
59	MG	BR	205	1/1	0.96	0.08	76,76,76,76	0
59	MG	AA	1933	1/1	0.96	0.17	67,67,67,67	0
59	MG	BA	3152	1/1	0.96	0.16	34,34,34,34	0
59	MG	DA	3469	1/1	0.97	0.17	65,65,65,65	0
59	MG	DA	3644	1/1	0.97	0.16	54,54,54,54	0
59	MG	DA	3217	1/1	0.97	0.43	69,69,69,69	0
59	MG	DA	3646	1/1	0.97	0.28	57,57,57,57	0
59	MG	DA	3471	1/1	0.97	0.16	63,63,63,63	0
59	MG	DA	3416	1/1	0.97	0.17	35,35,35,35	0
59	MG	BA	3402	1/1	0.97	0.28	37,37,37,37	0
59	MG	AY	101	1/1	0.97	0.35	6,6,6,6	1
59	MG	BA	2926	1/1	0.97	0.10	20,20,20,20	0
59	MG	DA	3318	1/1	0.97	0.05	59,59,59,59	0
59	MG	BA	3428	1/1	0.97	0.43	72,72,72,72	0
59	MG	BA	3456	1/1	0.97	0.27	33,33,33,33	0
59	MG	BA	3228	1/1	0.97	0.45	99,99,99,99	0
59	MG	BA	2969	1/1	0.97	0.10	41,41,41,41	0
59	MG	CA	1653	1/1	0.97	0.18	39,39,39,39	0
59	MG	DA	3658	1/1	0.97	0.09	53,53,53,53	0
59	MG	BA	3273	1/1	0.97	0.27	31,31,31,31	0
59	MG	DA	3054	1/1	0.97	0.05	69,69,69,69	0
59	MG	DA	3726	1/1	0.97	0.10	65,65,65,65	0
59	MG	DA	3055	1/1	0.97	0.22	51,51,51,51	0
59	MG	BP	202	1/1	0.97	0.13	69,69,69,69	1
59	MG	DA	3057	1/1	0.97	0.15	32,32,32,32	0
59	MG	DA	3186	1/1	0.97	0.06	42,42,42,42	0
59	MG	DA	3381	1/1	0.97	0.34	43,43,43,43	0
59	MG	BA	2960	1/1	0.97	0.31	84,84,84,84	0
59	MG	DA	3490	1/1	0.97	0.08	29,29,29,29	1
59	MG	AA	1679	1/1	0.97	0.20	53,53,53,53	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	CA	1727	1/1	0.97	0.10	74,74,74,74	0
59	MG	DA	3437	1/1	0.97	0.05	12,12,12,12	1
59	MG	DA	3738	1/1	0.97	0.10	89,89,89,89	0
59	MG	BA	3574	1/1	0.97	0.12	53,53,53,53	0
59	MG	BA	3232	1/1	0.97	0.19	64,64,64,64	0
59	MG	BA	3079	1/1	0.97	0.08	37,37,37,37	0
59	MG	DA	3742	1/1	0.97	0.27	51,51,51,51	0
59	MG	BA	3163	1/1	0.97	0.21	35,35,35,35	0
59	MG	AA	1808	1/1	0.97	0.23	57,57,57,57	0
59	MG	DA	3499	1/1	0.97	0.21	90,90,90,90	0
59	MG	DA	3678	1/1	0.97	0.20	100,100,100,100	0
59	MG	BA	3302	1/1	0.97	0.45	69,69,69,69	0
59	MG	BA	3106	1/1	0.97	0.04	35,35,35,35	0
59	MG	BU	202	1/1	0.97	0.12	39,39,39,39	0
59	MG	CA	1667	1/1	0.97	0.10	66,66,66,66	0
59	MG	DA	3110	1/1	0.97	0.19	200,200,200,200	0
59	MG	BA	3441	1/1	0.97	0.06	40,40,40,40	0
59	MG	DA	3246	1/1	0.97	0.10	32,32,32,32	0
59	MG	DA	2915	1/1	0.97	0.16	48,48,48,48	0
59	MG	DA	3565	1/1	0.97	0.16	54,54,54,54	0
59	MG	BA	3442	1/1	0.97	0.27	65,65,65,65	0
59	MG	AA	1899	1/1	0.97	0.09	63,63,63,63	0
59	MG	BA	3136	1/1	0.97	0.12	34,34,34,34	0
59	MG	BA	3151	1/1	0.97	0.09	65,65,65,65	0
59	MG	BA	3024	1/1	0.97	0.12	79,79,79,79	0
59	MG	DP	203	1/1	0.97	0.17	53,53,53,53	0
59	MG	DA	3118	1/1	0.97	0.05	63,63,63,63	0
59	MG	BA	3396	1/1	0.97	0.23	86,86,86,86	0
59	MG	DA	3120	1/1	0.97	0.24	106,106,106,106	0
59	MG	AA	1649	1/1	0.97	0.06	63,63,63,63	0
59	MG	DA	3257	1/1	0.97	0.32	29,29,29,29	0
59	MG	AA	1961	1/1	0.97	0.19	87,87,87,87	0
59	MG	DA	3259	1/1	0.97	0.22	32,32,32,32	0
59	MG	AX	104	1/1	0.97	0.17	43,43,43,43	0
59	MG	BA	3156	1/1	0.97	0.17	27,27,27,27	0
59	MG	DU	204	1/1	0.97	0.12	19,19,19,19	0
59	MG	BE	302	1/1	0.97	0.06	30,30,30,30	0
59	MG	BA	3506	1/1	0.97	0.06	42,42,42,42	0
59	MG	D5	102	1/1	0.97	0.07	63,63,63,63	0
59	MG	DA	3715	1/1	0.98	0.11	64,64,64,64	0
59	MG	BA	3314	1/1	0.98	0.28	29,29,29,29	0
59	MG	BA	3438	1/1	0.98	0.09	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	DA	3677	1/1	0.98	0.13	45,45,45,45	0
59	MG	DA	3122	1/1	0.98	0.40	38,38,38,38	0
59	MG	BA	3271	1/1	0.98	0.16	29,29,29,29	0
59	MG	BA	3237	1/1	0.98	0.11	58,58,58,58	0
59	MG	D5	101	1/1	0.98	0.15	48,48,48,48	0
59	MG	DA	3434	1/1	0.98	0.33	44,44,44,44	0
59	MG	DA	3041	1/1	0.98	0.12	78,78,78,78	0
59	MG	DA	3339	1/1	0.98	0.34	37,37,37,37	0
59	MG	AA	1655	1/1	0.98	0.04	101,101,101,101	0
59	MG	DA	3768	1/1	0.98	0.04	58,58,58,58	1
59	MG	DA	2964	1/1	0.98	0.29	54,54,54,54	0
59	MG	BA	3261	1/1	0.98	0.12	41,41,41,41	0
59	MG	BR	202	1/1	0.98	0.04	24,24,24,24	0
59	MG	BA	3319	1/1	0.98	0.28	33,33,33,33	0
59	MG	BA	3078	1/1	0.98	0.10	18,18,18,18	0
59	MG	DA	3616	1/1	0.98	0.21	51,51,51,51	0
59	MG	BA	3289	1/1	0.98	0.21	39,39,39,39	0
59	MG	DE	304	1/1	0.98	0.14	22,22,22,22	0
59	MG	DF	301	1/1	0.98	0.10	17,17,17,17	1
59	MG	DA	3734	1/1	0.98	0.08	74,74,74,74	0
59	MG	DA	3444	1/1	0.98	0.34	31,31,31,31	0
59	MG	BA	3202	1/1	0.98	0.07	24,24,24,24	0
59	MG	BA	3306	1/1	0.98	0.24	57,57,57,57	0
59	MG	AA	1653	1/1	0.98	0.04	68,68,68,68	1
59	MG	DA	3024	1/1	0.98	0.13	92,92,92,92	0
59	MG	BE	303	1/1	0.98	0.11	22,22,22,22	0
59	MG	CA	1645	1/1	0.98	0.12	50,50,50,50	0
59	MG	BA	3131	1/1	0.98	0.13	43,43,43,43	0
59	MG	DA	3589	1/1	0.98	0.32	47,47,47,47	0
59	MG	DA	3141	1/1	0.98	0.17	99,99,99,99	0
59	MG	AA	1654	1/1	0.98	0.13	58,58,58,58	1
59	MG	DA	3705	1/1	0.98	0.17	58,58,58,58	0
59	MG	AA	1693	1/1	0.98	0.05	56,56,56,56	1
59	MG	BA	2936	1/1	0.98	0.28	43,43,43,43	0
59	MG	BA	3398	1/1	0.98	0.26	53,53,53,53	0
59	MG	DA	3327	1/1	0.98	0.04	39,39,39,39	1
59	MG	AA	1664	1/1	0.98	0.04	17,17,17,17	1
59	MG	DA	3033	1/1	0.98	0.07	50,50,50,50	0
59	MG	BA	3589	1/1	0.98	0.07	41,41,41,41	0
59	MG	DA	3599	1/1	0.98	0.09	39,39,39,39	0
60	ZN	AD	301	1/1	0.98	0.12	106,106,106,106	0
59	MG	BA	3247	1/1	0.98	0.15	62,62,62,62	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	BA	3322	1/1	0.99	0.25	24,24,24,24	0
59	MG	BA	3126	1/1	0.99	0.04	36,36,36,36	0
59	MG	CA	1666	1/1	0.99	0.03	63,63,63,63	0
59	MG	DA	2971	1/1	0.99	0.03	20,20,20,20	0
59	MG	BA	3090	1/1	0.99	0.05	27,27,27,27	0
59	MG	AP	101	1/1	0.99	0.05	93,93,93,93	0
59	MG	DA	3264	1/1	0.99	0.08	47,47,47,47	1
59	MG	DA	3562	1/1	0.99	0.03	25,25,25,25	1
59	MG	AA	1688	1/1	0.99	0.04	22,22,22,22	1
59	MG	BA	3530	1/1	0.99	0.08	33,33,33,33	0
59	MG	DA	3697	1/1	0.99	0.09	32,32,32,32	0
59	MG	BA	3235	1/1	0.99	0.08	40,40,40,40	0
60	ZN	AD	305	1/1	0.99	0.10	88,88,88,88	0
60	ZN	AN	101	1/1	0.99	0.03	153,153,153,153	0
59	MG	BA	3038	1/1	0.99	0.03	17,17,17,17	0
59	MG	BA	3296	1/1	1.00	0.23	27,27,27,27	0

6.5 Other polymers

There are no such residues in this entry.