



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 26, 2019 – 01:29 PM EDT

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

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.0 (224370), CSD as540be (2019)
Xtriage (Phenix) : 1.13
EDS : 2.3.2
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.3.2

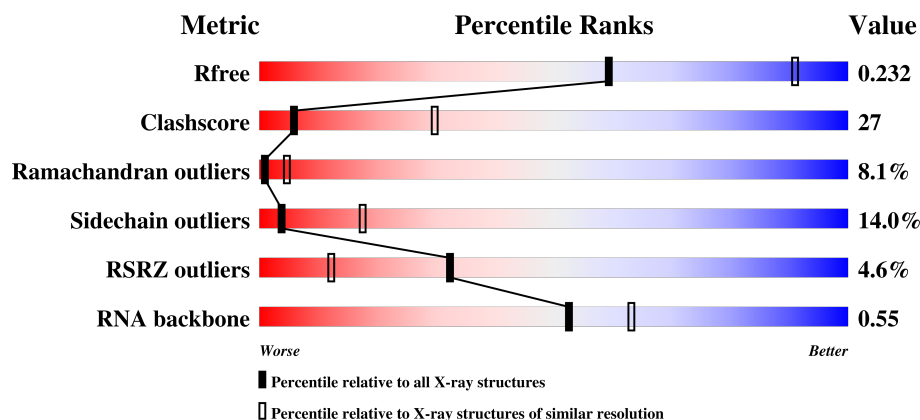
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	111664	1851 (3.00-3.00)
Clashscore	122126	2167 (3.00-3.00)
Ramachandran outliers	120053	2101 (3.00-3.00)
Sidechain outliers	120020	2104 (3.00-3.00)
RSRZ outliers	108989	1751 (3.00-3.00)
RNA backbone	2636	1017 (3.30-2.70)

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

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

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




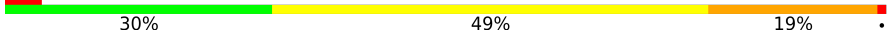

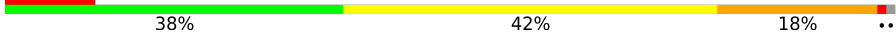
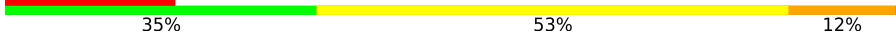
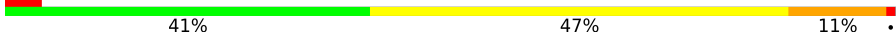
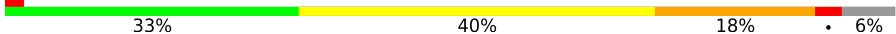
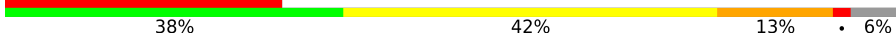
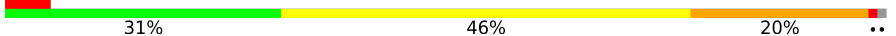
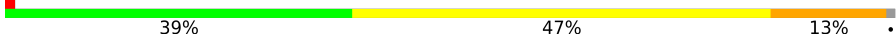
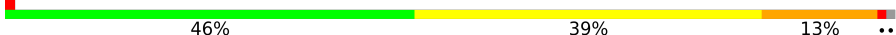
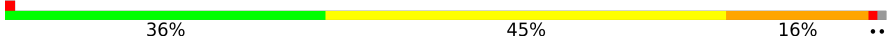


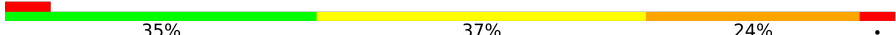
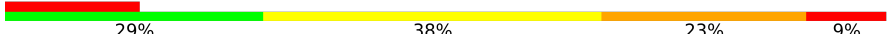

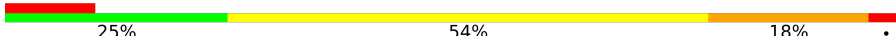





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Mol	Chain	Length	Quality of chain
15	CR	89	
16	AS	88	
16	CS	88	
17	AT	105	
17	CT	105	
18	AU	88	
18	CU	88	
19	AV	93	
19	CV	93	
20	AW	106	
20	CW	106	
21	AX	27	
21	CX	27	
22	AB	85	
22	AD	85	
22	CB	85	
22	CD	85	
23	AC	77	
23	CC	77	
24	A1	16	
24	C1	16	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

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

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

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	AA	1613	-	-	-	X
55	MG	AA	1643	-	-	-	X
55	MG	AA	1666	-	-	-	X
55	MG	AA	1683	-	-	-	X
55	MG	AA	1726	-	-	-	X
55	MG	AA	1728	-	-	-	X
55	MG	AA	1736	-	-	-	X
55	MG	AA	1750	-	-	-	X
55	MG	AA	1758	-	-	-	X
55	MG	AA	1768	-	-	-	X
55	MG	AA	1772	-	-	-	X
55	MG	AA	1775	-	-	-	X
55	MG	AA	1785	-	-	-	X
55	MG	AA	1791	-	-	-	X
55	MG	AA	1800	-	-	-	X
55	MG	AA	1804	-	-	-	X
55	MG	AA	1805	-	-	-	X
55	MG	AA	1806	-	-	-	X
55	MG	AA	1809	-	-	-	X
55	MG	AA	1815	-	-	-	X
55	MG	AA	1818	-	-	-	X
55	MG	AC	107	-	-	-	X
55	MG	BA	3041	-	-	-	X
55	MG	BA	3069	-	-	-	X
55	MG	BA	3078	-	-	-	X
55	MG	BA	3100	-	-	-	X
55	MG	BA	3122	-	-	-	X

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

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

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

2 Entry composition

There are 56 unique types of molecules in this entry. The entry contains 299676 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1502	Total	C	N	O	P	0	0	0
			32284	14370	5982	10431	1501			
1	CA	1502	Total	C	N	O	P	0	0	0
			32287	14370	5982	10433	1502			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 24 is a RNA chain called MRNA.

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

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

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

There are 14 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	AD	3	Total 3	Mg 3	0	0
55	DD	3	Total 3	Mg 3	0	0
55	D0	1	Total 1	Mg 1	0	0
55	CC	9	Total 9	Mg 9	0	0
55	DE	1	Total 1	Mg 1	0	0
55	B3	3	Total 3	Mg 3	0	0
55	DA	488	Total 488	Mg 488	0	0
55	D5	2	Total 2	Mg 2	0	0
55	B7	1	Total 1	Mg 1	0	0
55	AG	2	Total 2	Mg 2	0	0
55	BO	2	Total 2	Mg 2	0	0
55	D1	1	Total 1	Mg 1	0	0
55	CB	4	Total 4	Mg 4	0	0
55	AC	8	Total 8	Mg 8	0	0
55	CD	1	Total 1	Mg 1	0	0
55	BD	1	Total 1	Mg 1	0	0
55	B0	1	Total 1	Mg 1	0	0
55	BW	1	Total 1	Mg 1	0	0
55	CK	1	Total 1	Mg 1	0	0
55	DB	20	Total 20	Mg 20	0	0

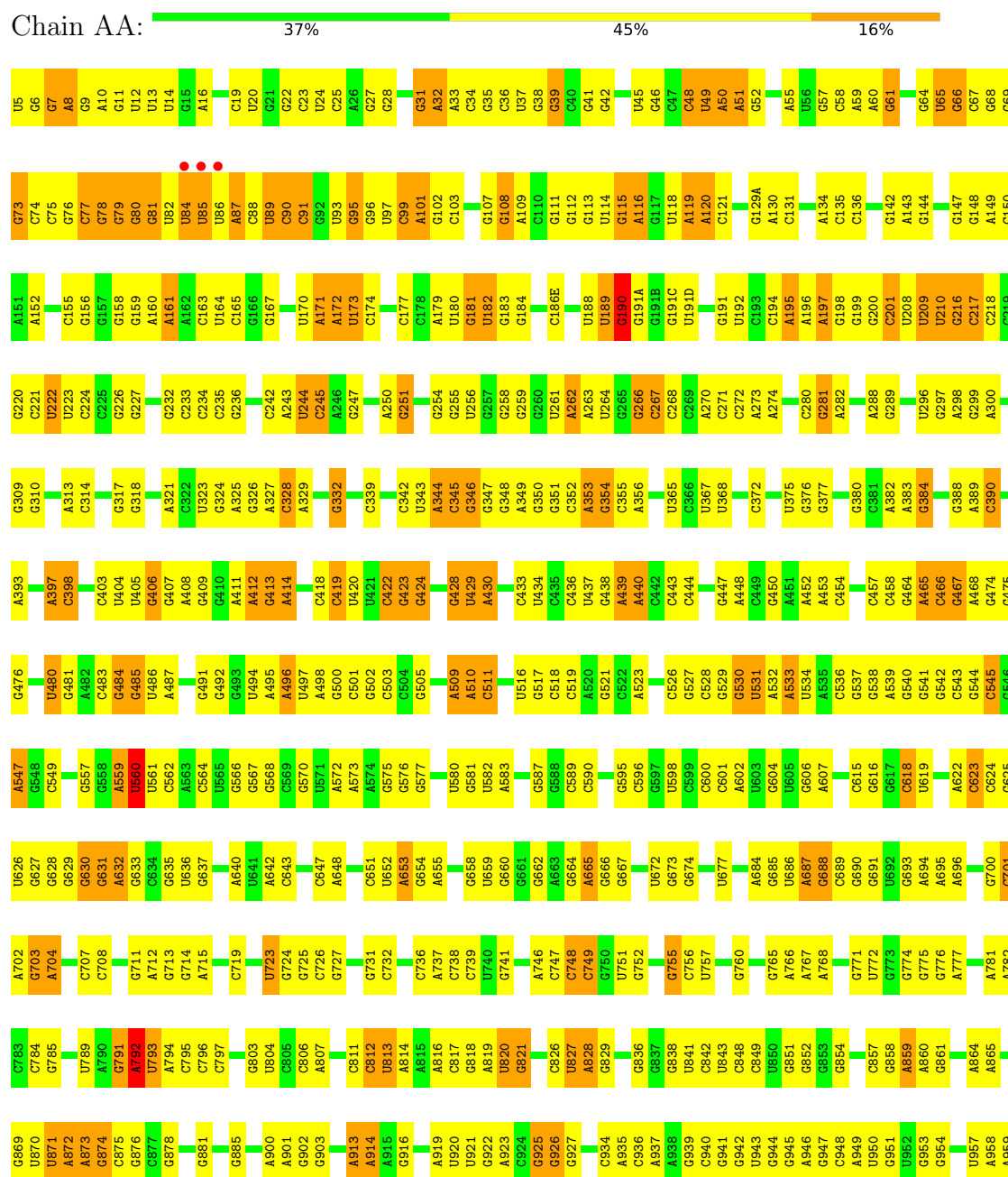
- Molecule 56 is ZINC ION (three-letter code: ZN) (formula: Zn).

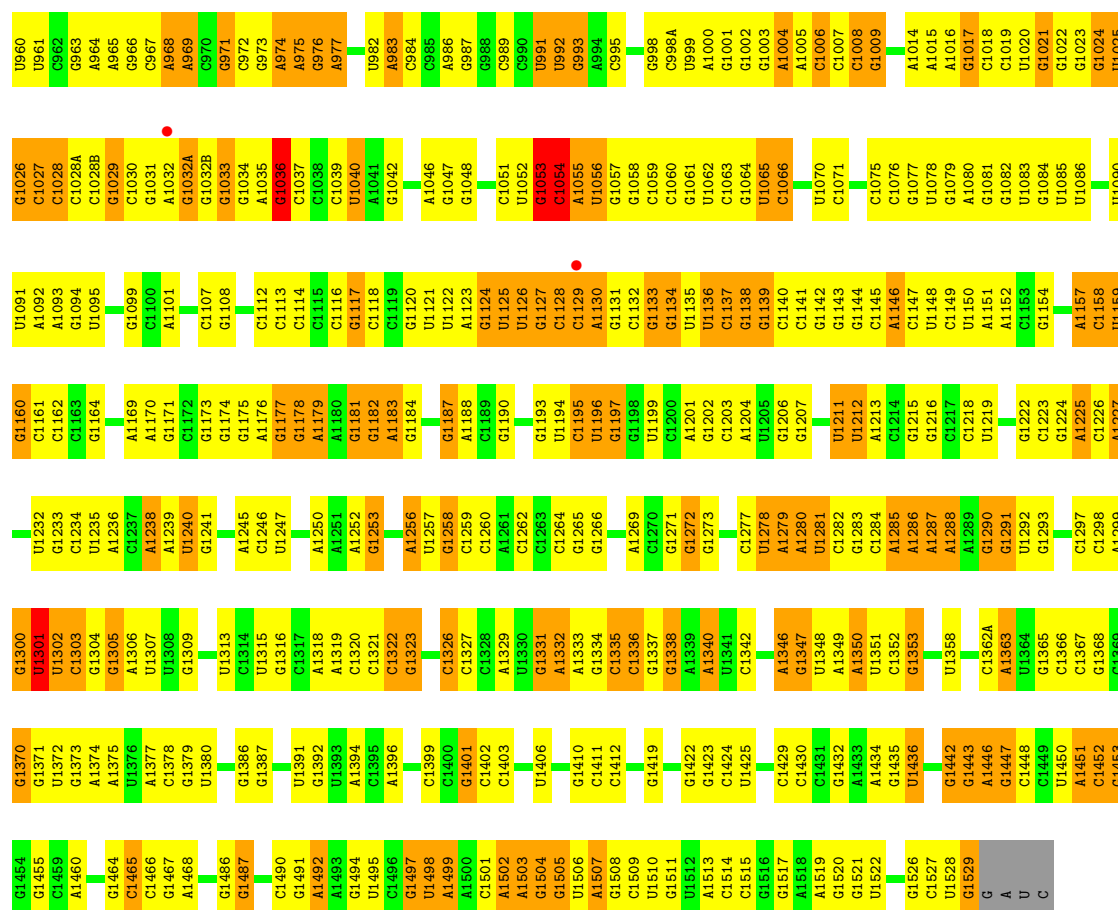
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	AG	1	Total 1	Zn 1	0	0
56	AQ	1	Total 1	Zn 1	0	0
56	CQ	1	Total 1	Zn 1	0	0
56	CG	1	Total 1	Zn 1	0	0

3 Residue-property plots

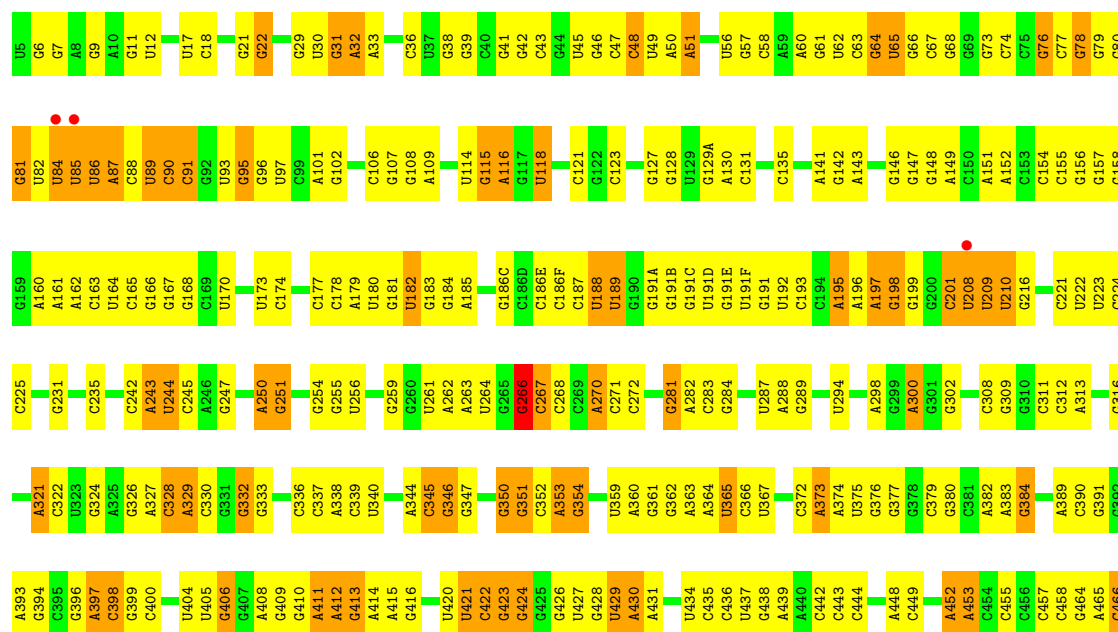
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

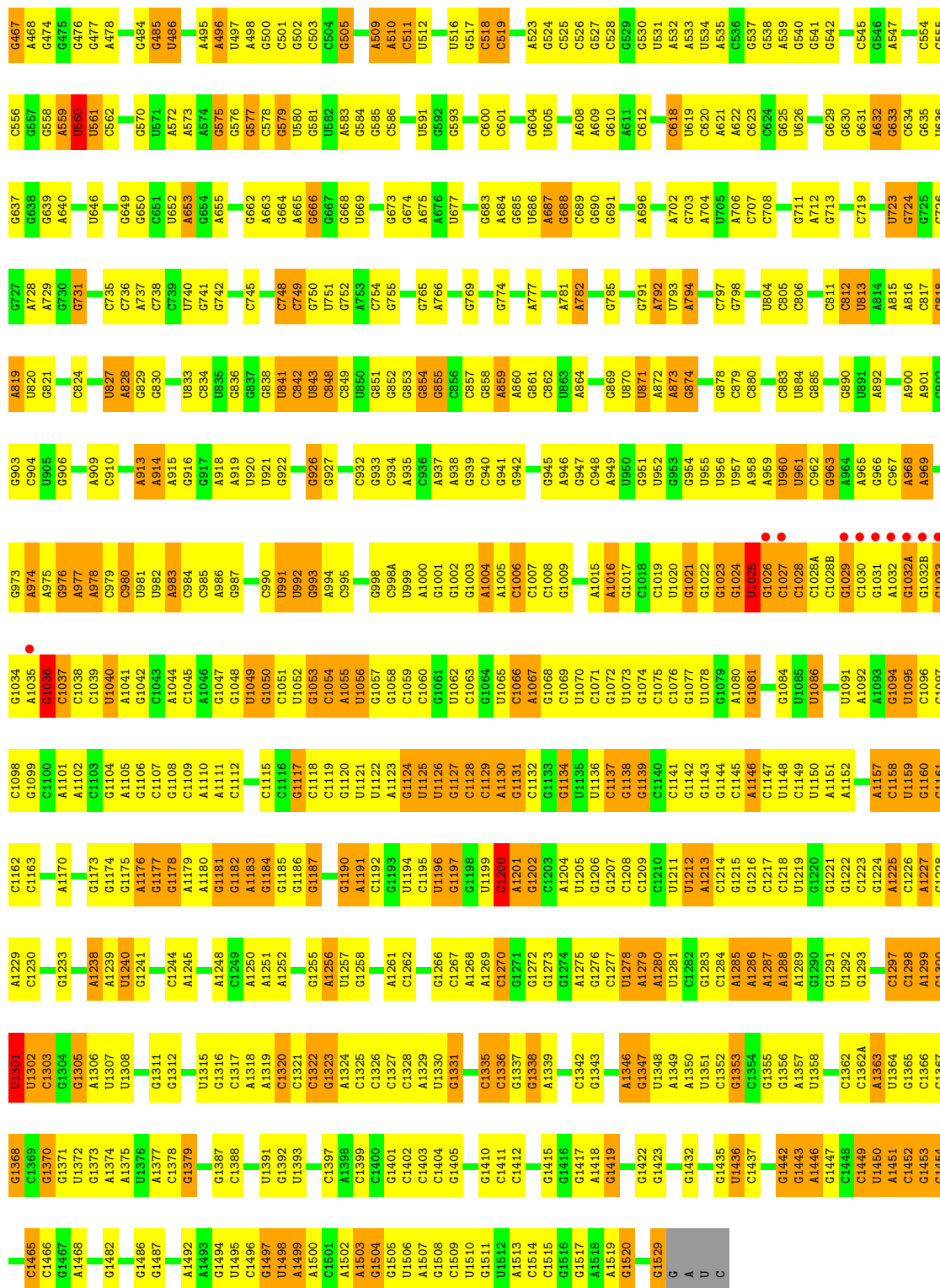
- Molecule 1: 16S ribosomal RNA

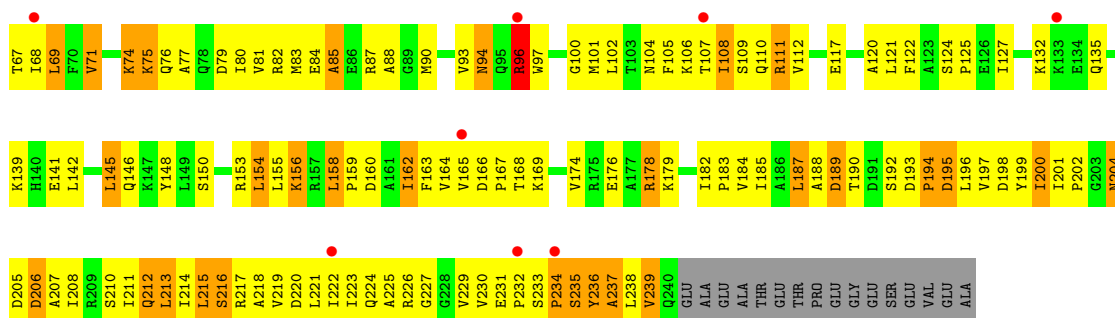




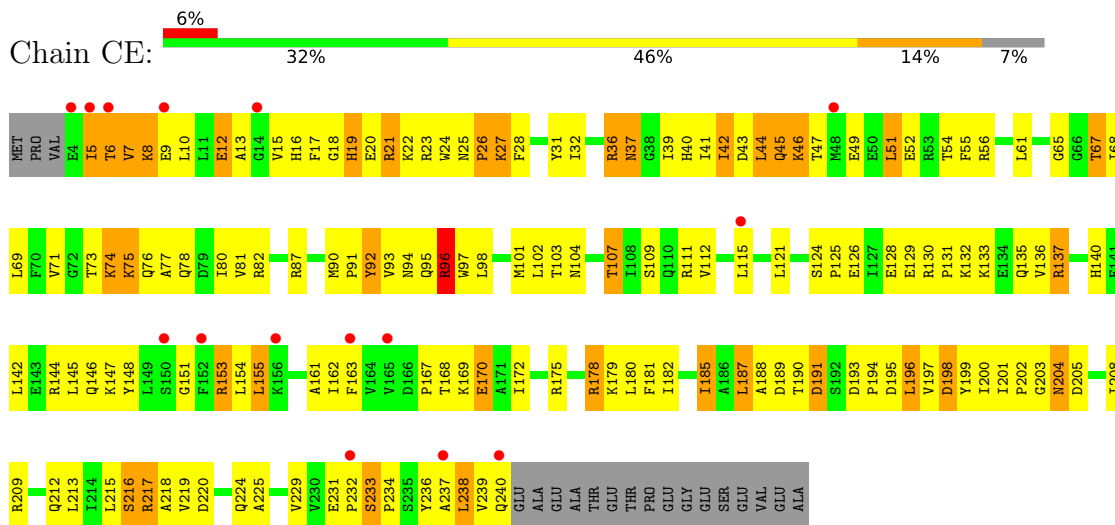
• Molecule 1: 16S ribosomal RNA



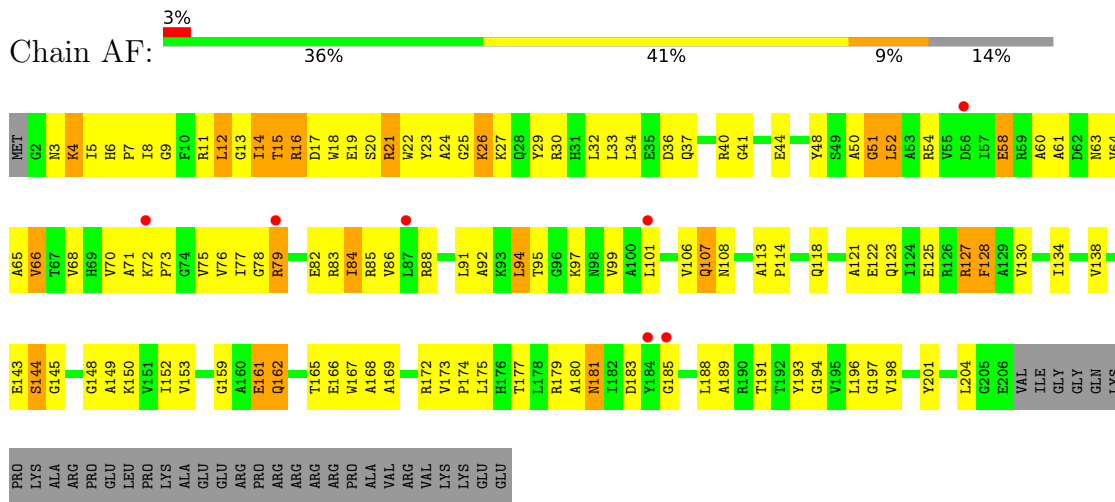




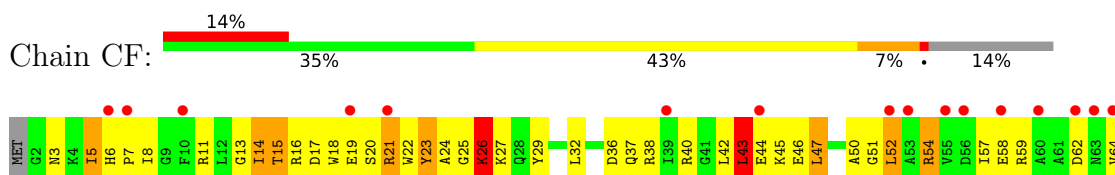
• Molecule 2: 30S RIBOSOMAL PROTEIN S2

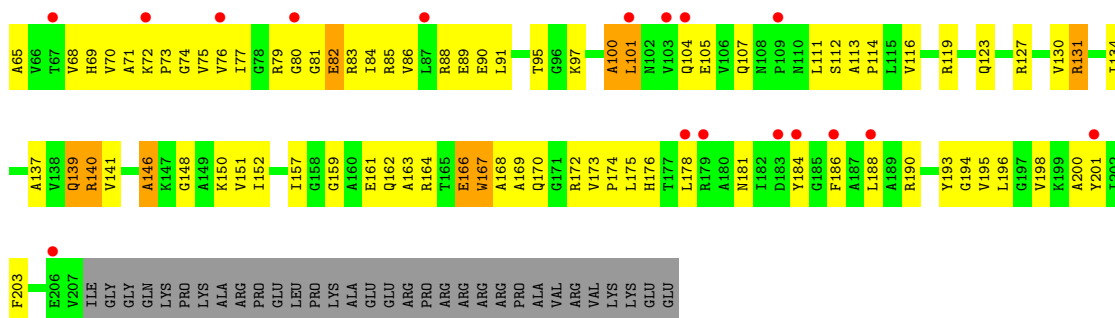


• Molecule 3: 30S RIBOSOMAL PROTEIN S3



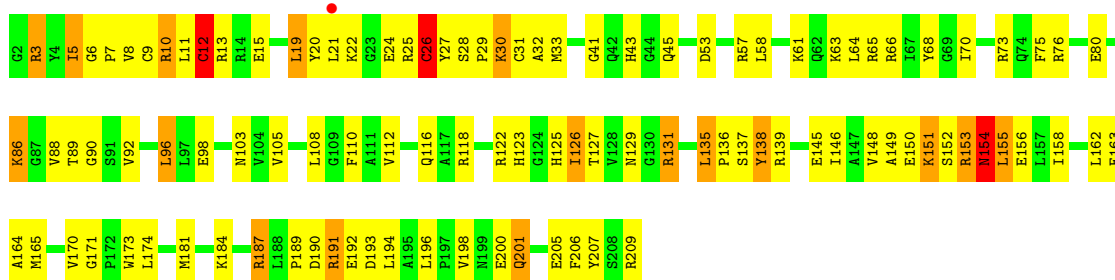
• Molecule 3: 30S RIBOSOMAL PROTEIN S3





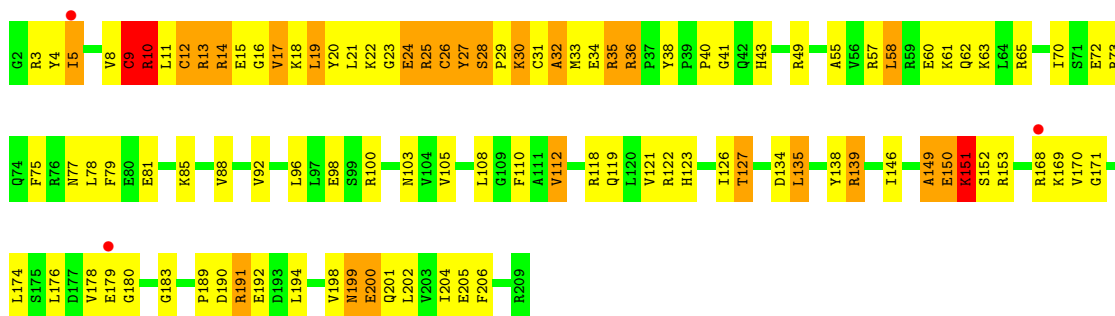
• Molecule 4: 30S RIBOSOMAL PROTEIN S4

Chain AG: 50% 41% 8%



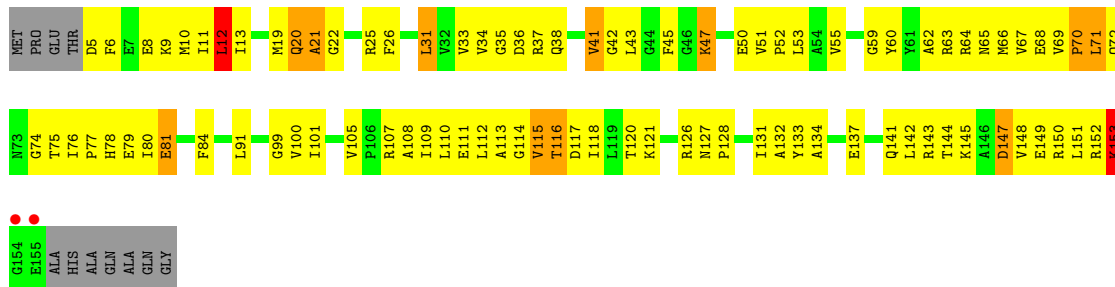
• Molecule 4: 30S RIBOSOMAL PROTEIN S4

Chain CG: 50% 37% 12%



• Molecule 5: 30S RIBOSOMAL PROTEIN S5

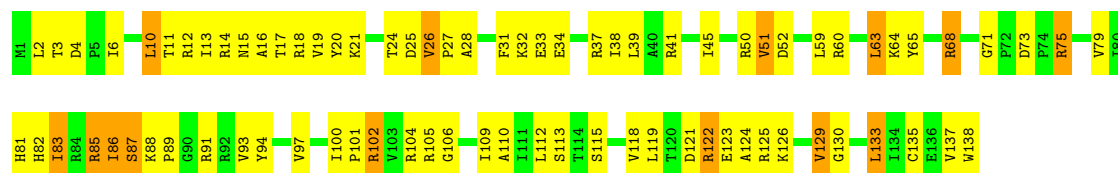
Chain AH: 36% 49% 7% 7%



• Molecule 5: 30S RIBOSOMAL PROTEIN S5

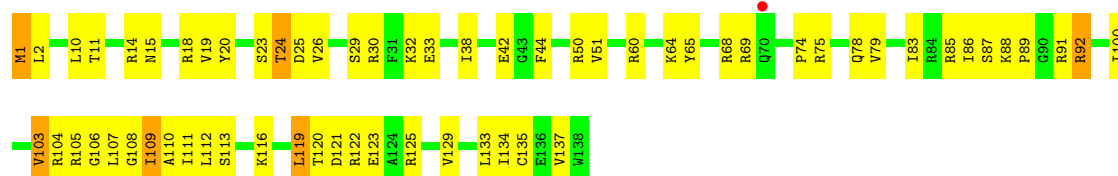
- Molecule 8: 30S RIBOSOMAL PROTEIN S8

Chain AK: 



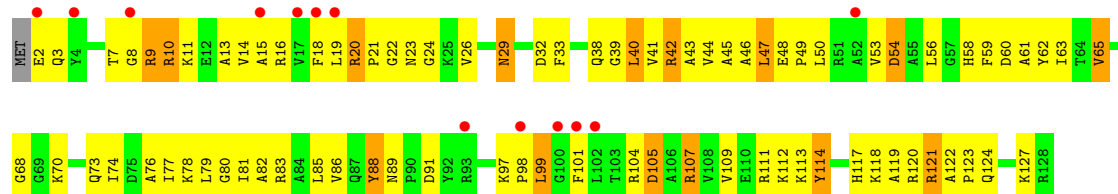
- Molecule 8: 30S RIBOSOMAL PROTEIN S8

Chain CK: 



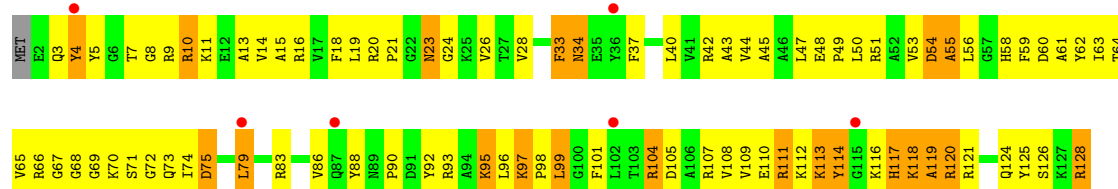
- Molecule 9: 30S RIBOSOMAL PROTEIN S9

Chain AL: 



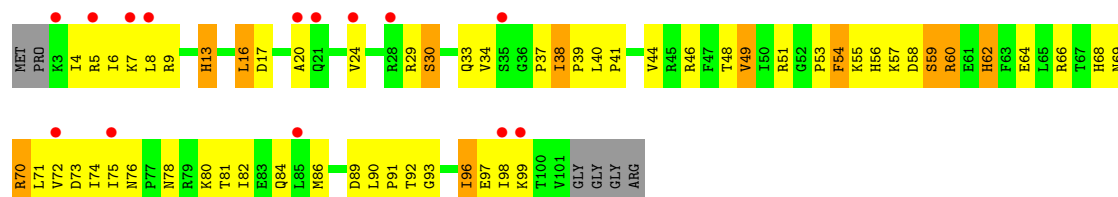
- Molecule 9: 30S RIBOSOMAL PROTEIN S9

Chain CL: 

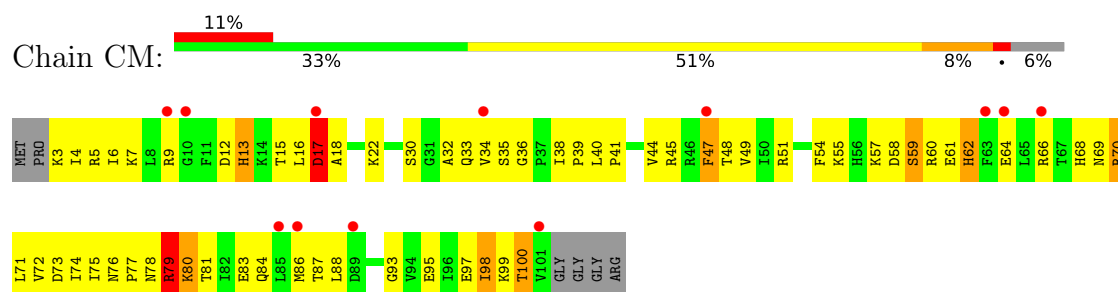


- Molecule 10: 30S RIBOSOMAL PROTEIN S10

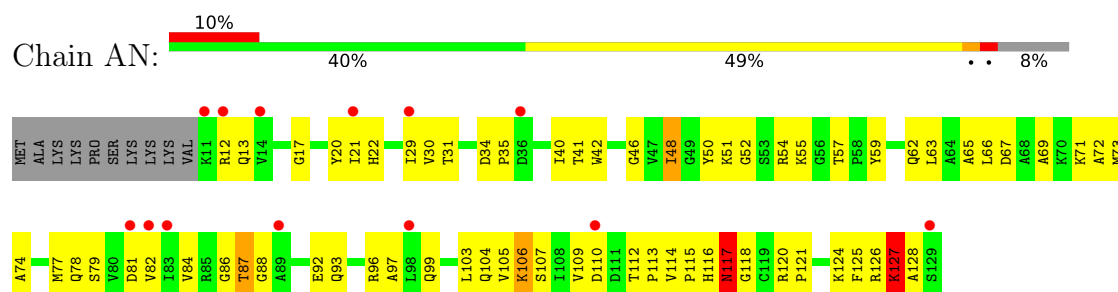
Chain AM: 



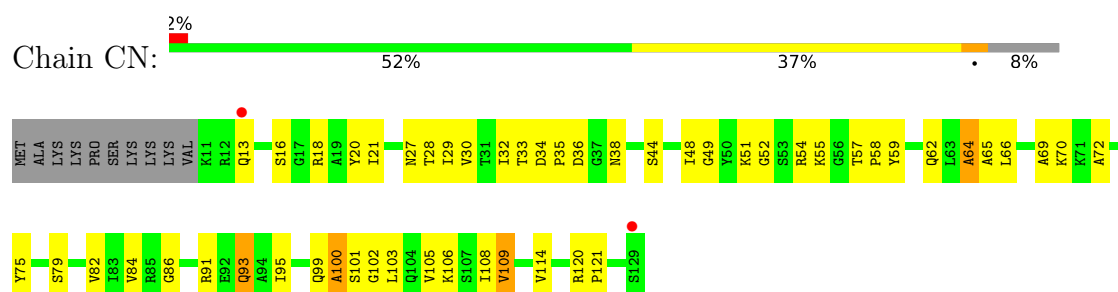
- Molecule 10: 30S RIBOSOMAL PROTEIN S10



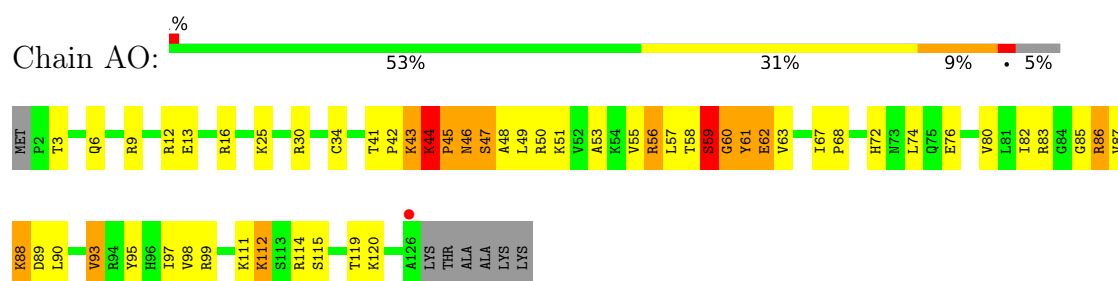
- Molecule 11: 30S RIBOSOMAL PROTEIN S11



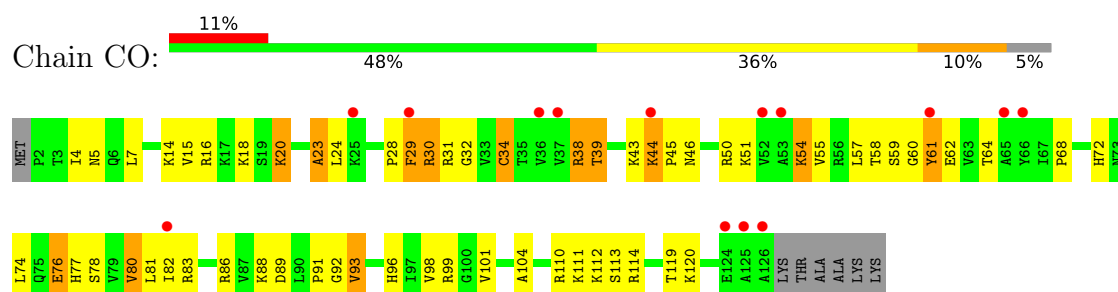
- Molecule 11: 30S RIBOSOMAL PROTEIN S11



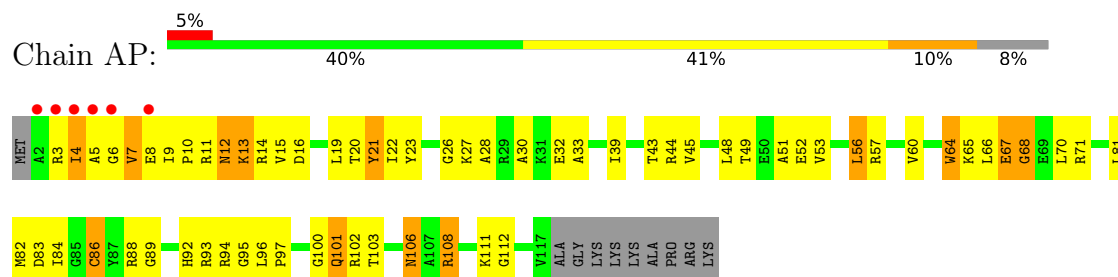
- Molecule 12: 30S RIBOSOMAL PROTEIN S12



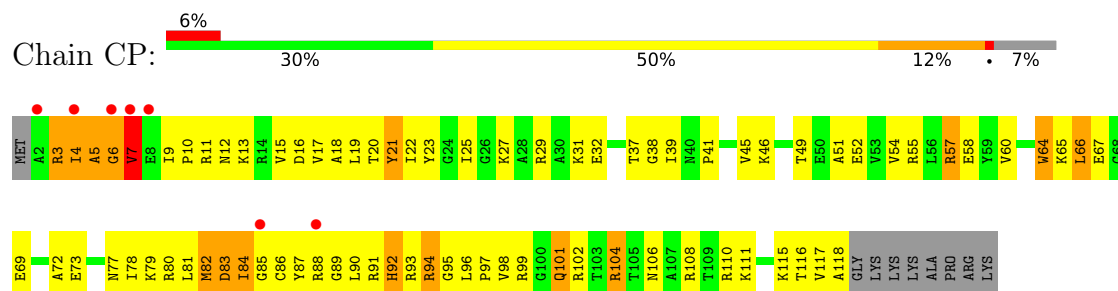
- Molecule 12: 30S RIBOSOMAL PROTEIN S12



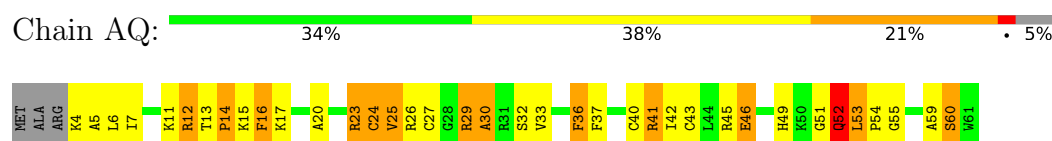
- Molecule 13: 30S RIBOSOMAL PROTEIN S13



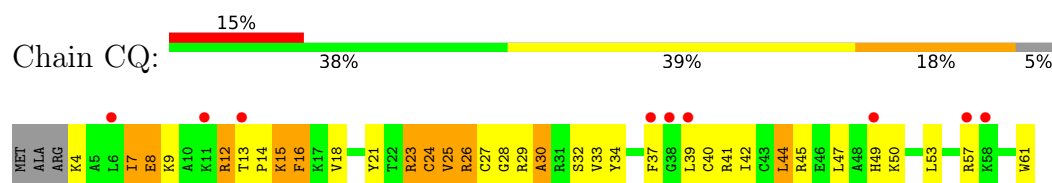
- Molecule 13: 30S RIBOSOMAL PROTEIN S13



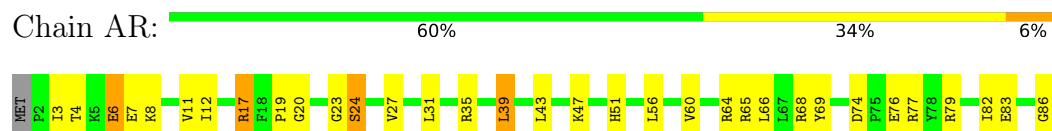
- Molecule 14: 30S RIBOSOMAL PROTEIN S14



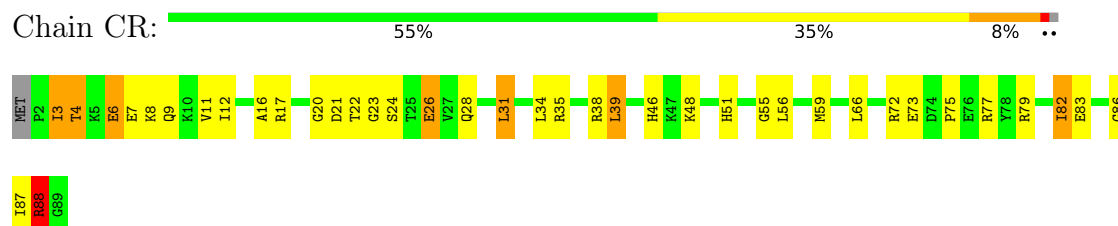
- Molecule 14: 30S RIBOSOMAL PROTEIN S14



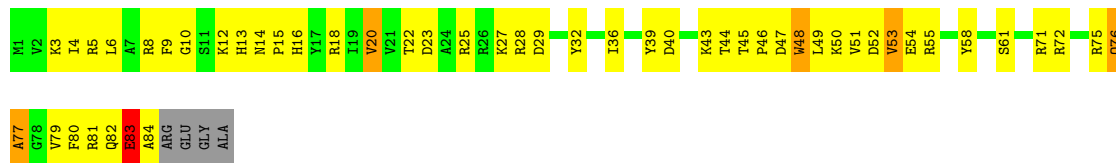
- Molecule 15: 30S RIBOSOMAL PROTEIN S15



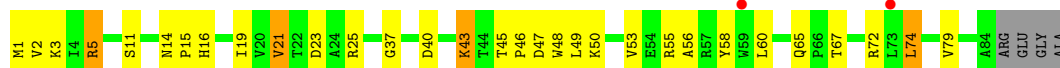
- Molecule 15: 30S RIBOSOMAL PROTEIN S15



• Molecule 16: 30S RIBOSOMAL PROTEIN S16

Chain AS:  39% 50% 6% • 5%

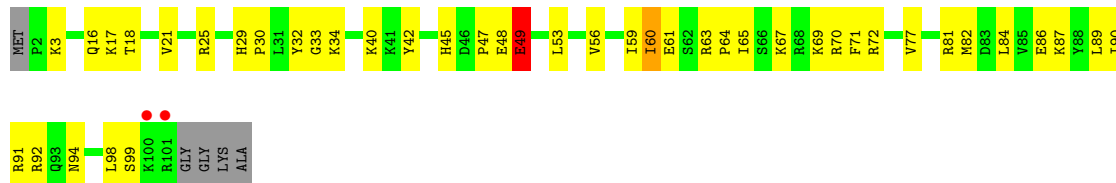
• Molecule 16: 30S RIBOSOMAL PROTEIN S16

Chain CS:  2% 60% 31% 5% 5%

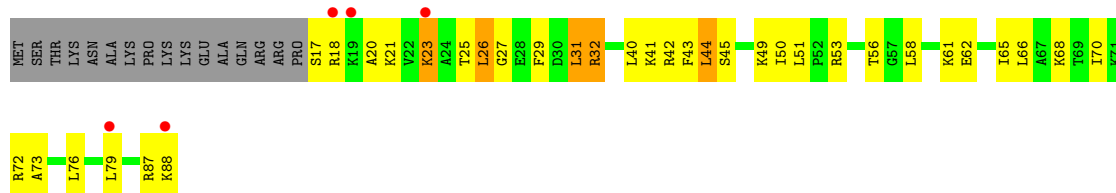
• Molecule 17: 30S RIBOSOMAL PROTEIN S17

Chain AT:  2% 48% 38% 9% • 5%

• Molecule 17: 30S RIBOSOMAL PROTEIN S17

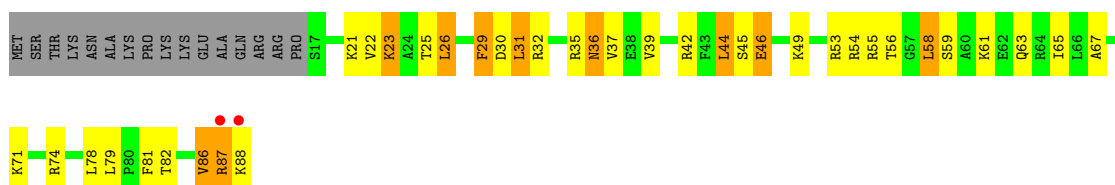
Chain CT:  2% 54% 39% • 5%

• Molecule 18: 30S RIBOSOMAL PROTEIN S18

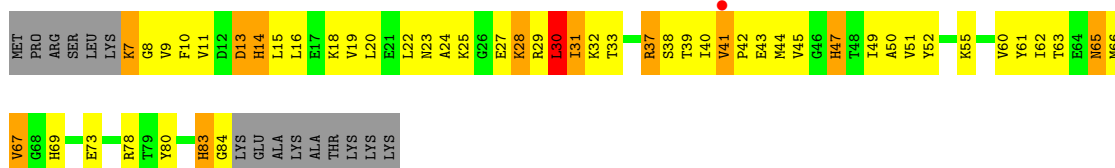
Chain AU:  6% 42% 34% 6% 18%

• Molecule 18: 30S RIBOSOMAL PROTEIN S18

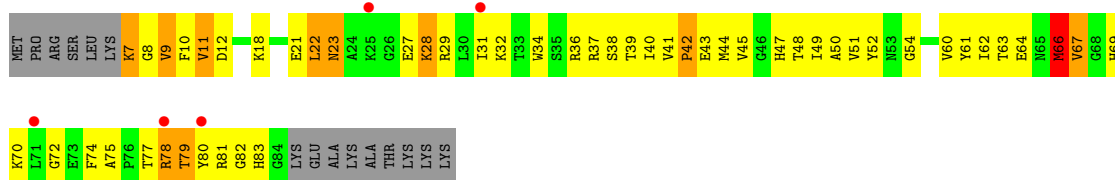
Chain CU:  2% 40% 31% 11% 18%



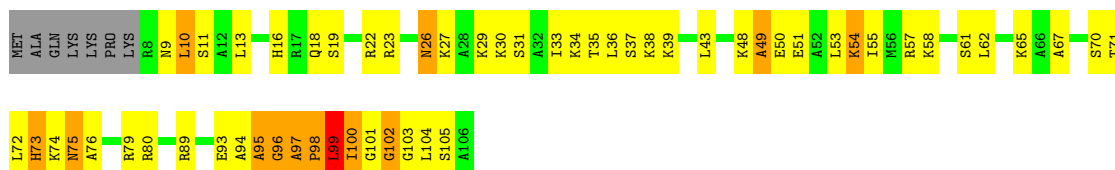
• Molecule 19: 30S RIBOSOMAL PROTEIN S19



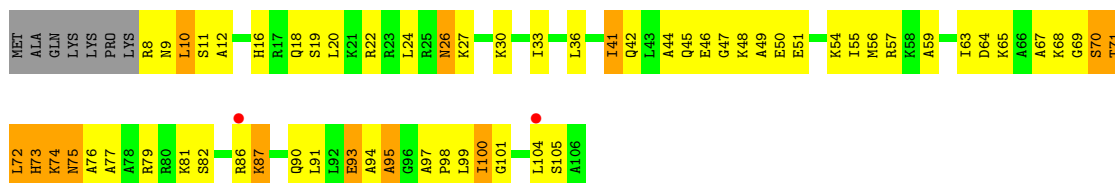
• Molecule 19: 30S RIBOSOMAL PROTEIN S19



• Molecule 20: 30S RIBOSOMAL PROTEIN S20

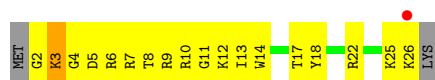


• Molecule 20: 30S RIBOSOMAL PROTEIN S20



• Molecule 21: 30S RIBOSOMAL PROTEIN THX

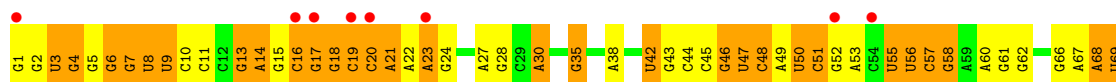
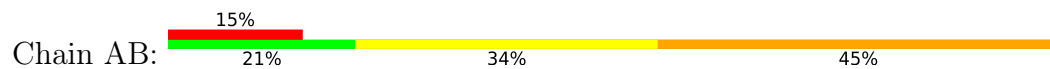




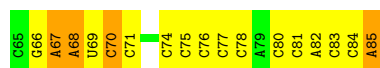
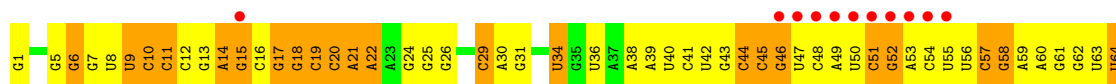
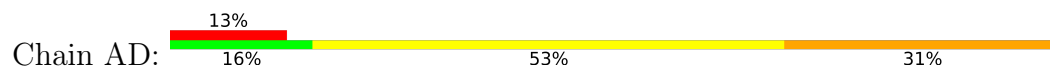
• Molecule 21: 30S RIBOSOMAL PROTEIN THX



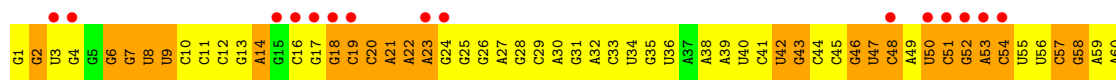
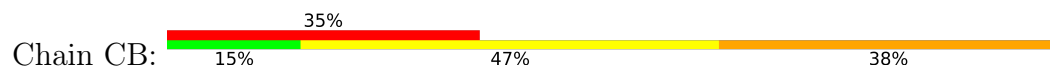
• Molecule 22: TRNA-TYR



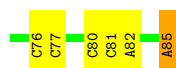
• Molecule 22: TRNA-TYR



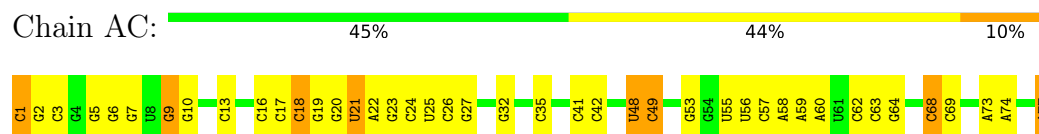
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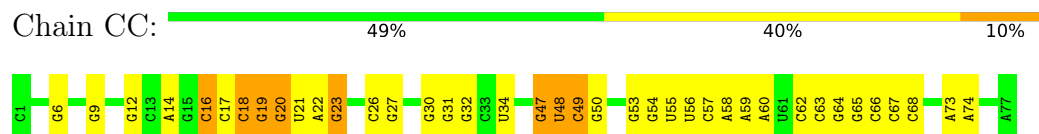
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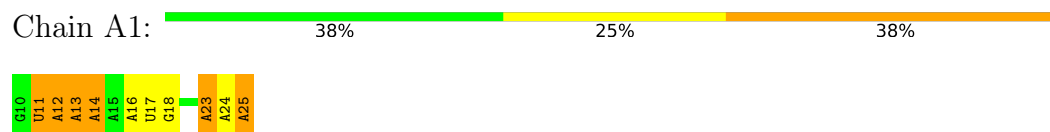
• Molecule 23: TRNA-FMET



- Molecule 23: TRNA-FMET



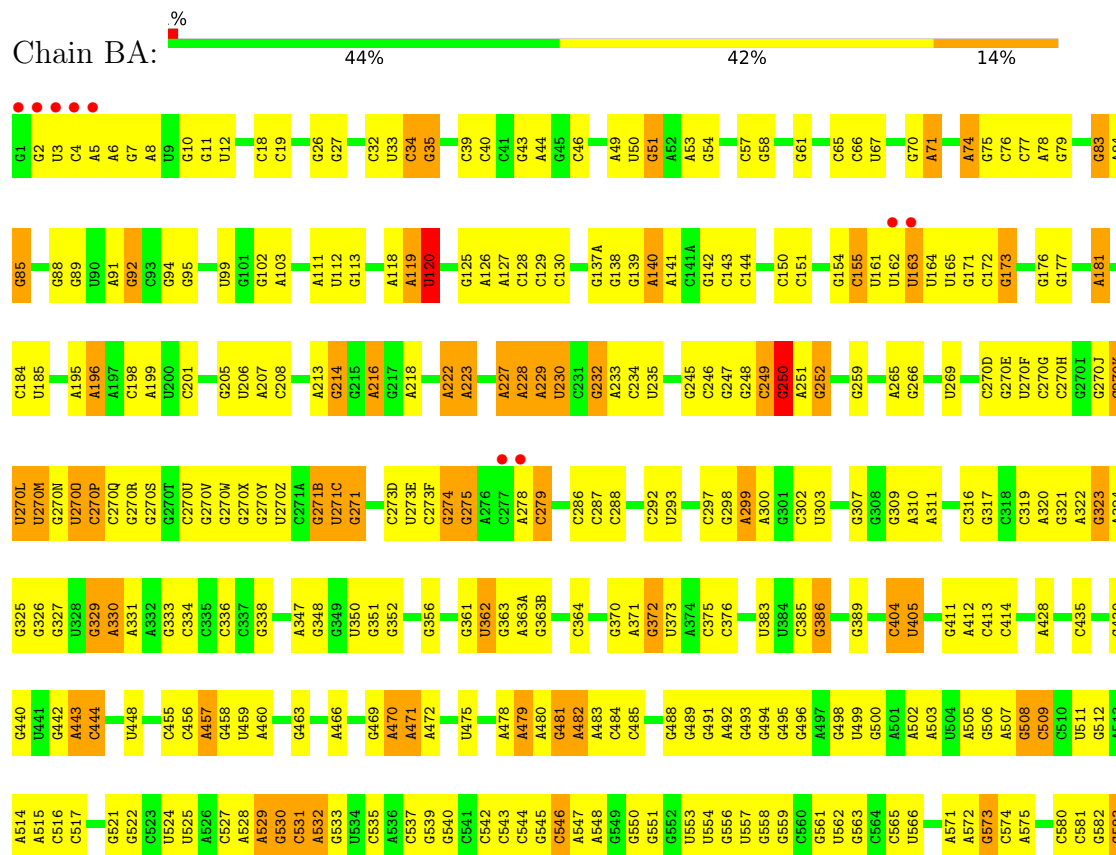
- Molecule 24: MRNA



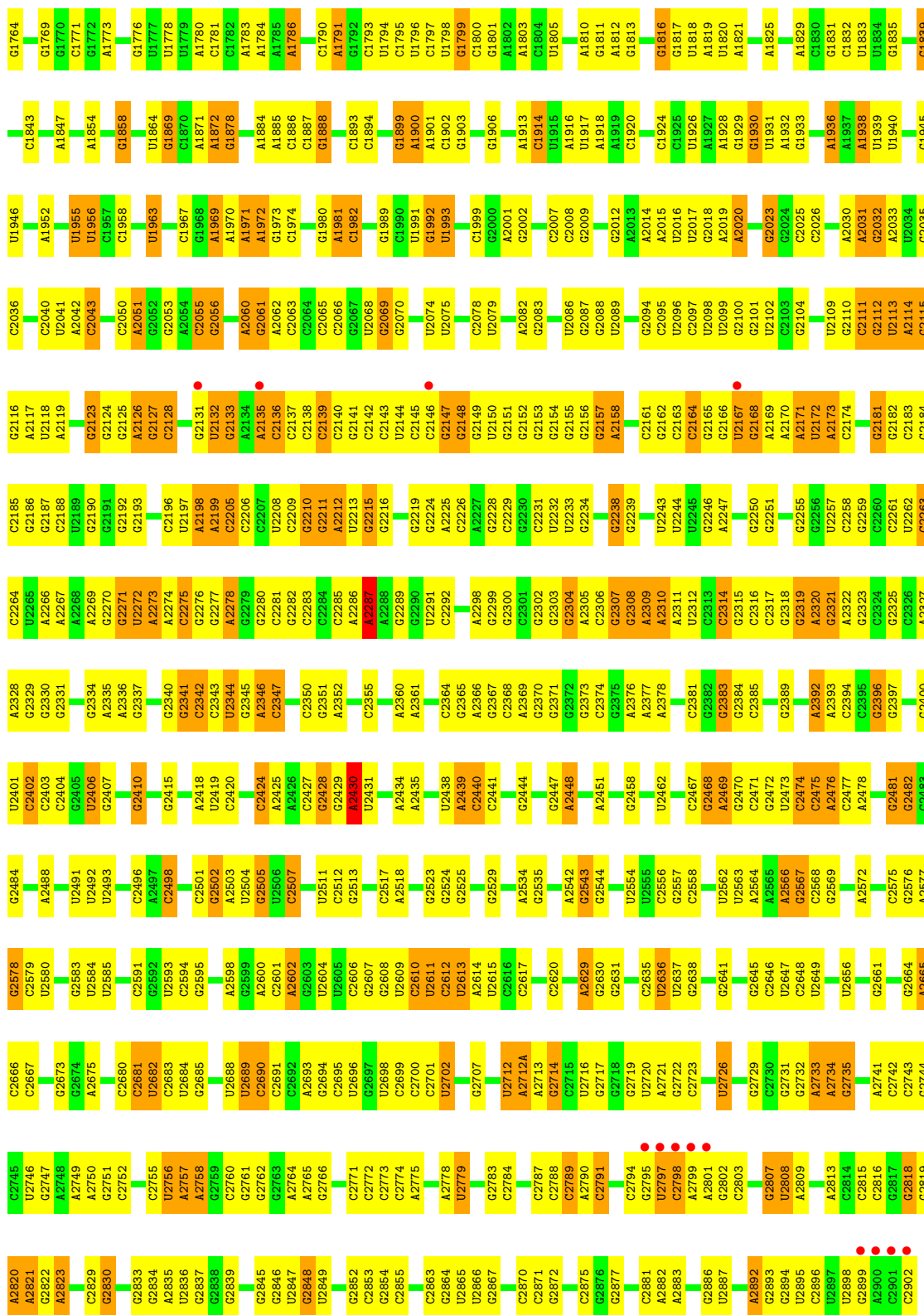
- Molecule 24: MRNA



- Molecule 25: RNA (2912-MER)

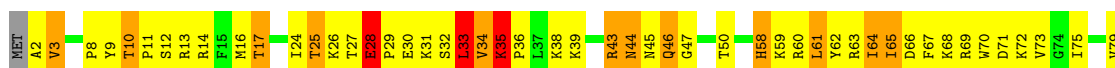


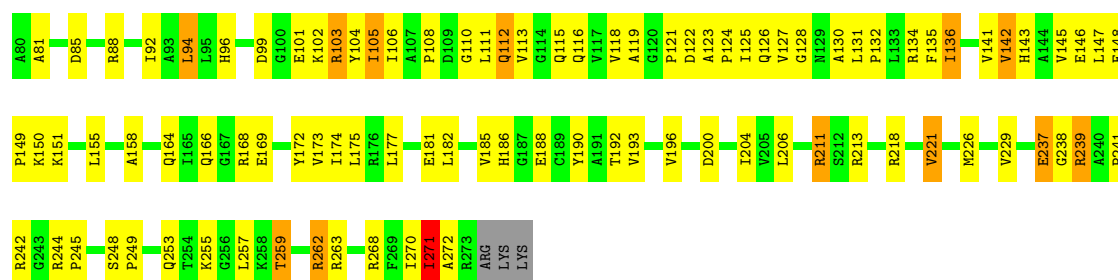
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C1674	C1675	A1578	A1579	A1507	G1421	A1352	U1263	C1185	G1106	A1045	C886	C967	G733	A654J	C592
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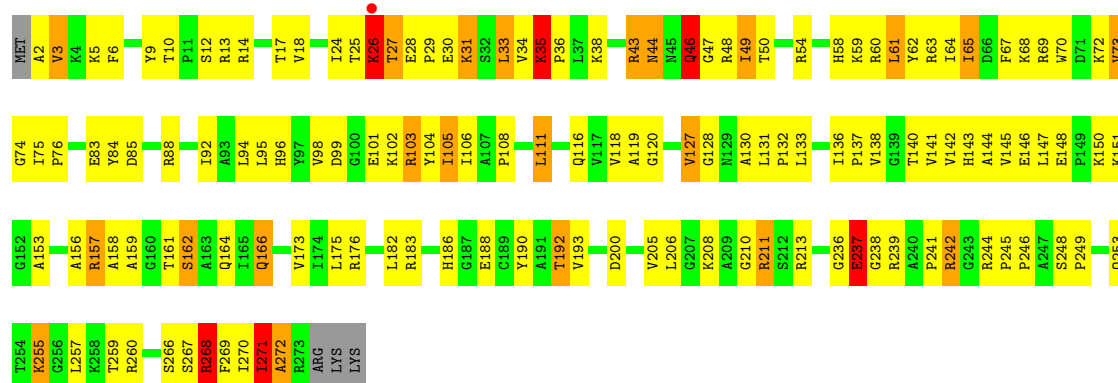
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C2324	G2165	G2104	G2021	G1929	A1815	G1728	G1635	A1536	A1469	A1393	U1312	C1225	C1153
G2326	U2167	C2105	U2022	G1930	G1817	A1729	G1635	C1537	A1460	U1394	G1314	G1226	G1154
C2327	G2168	C2107	G2023	A1936	U1818	U1730	G1638	G1538	G1461	A1395	G1315	G1227	A1155
A2328	A2169	C2108	G2024	A1937	A1819	G1731	U1639	U1539	C1464	U1396	U1316	G1228	A1156
G2329	A2170	C2111	C2025	A1938	U1820	A1732	C1640	A1542	C1467	U1397	A1317	G1229	U1159
G2330	U2172	G2112	G2026	U1939	A1821	C1735	C1640	A1543	G1467	C1398	U1318	G1230	G1160
C2331	U2172	U2113	G2027	U1940	G1826	C1741	G1645	A1544	C1468	G1401	U1323	G1231	C1161
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G2333	C2174	G2115	A2031	C1942	A1829	G1748	G1647	C1548	A1469	C1403	G1325	A1241	G1163
G2334	C2175	G2116	G2032	U1943	C1830	A1749	G1648	C1549	A1470	C1404	U1326	U1248	G1164
A2335	U2180	U2117	A2033	U1944	G1831	G1753	G1649	C1550	A1471	U1405	G1327	G1249	U1165
G2336	G2181	U2118	U2034	U1945	C1832	C1754	G1650	C1551	A1472	U1406	G1328	U1250	U1167
G2337	G2182	A2119	G2035	U1946	G1833	A1755	G1651	C1552	A1473	U1407	U1329	C1251	G1168
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G2341	G2184	G2121	A2042	U1951	C1843	U1757	A1653	C1556	C1476	C1409	C1331	G1253	G1170
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G2379	G2234	C2151	U2086	G2002	U1915	U1805	C1710	A1610	G1525	C1450	A1385	G1303	A1220
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G2384	U2244	G2156	G2094	G2010	C1914	A1810	U1716	A1618	A1528				
G2385	G2250	G2157	C2097	G2012	U1915	U1805	C1710	A1610	G1525				
G2386	G2251	A2158	U2098	A2013	A1916	A1810	C1712	A1618	G1527				
U2387	G2252	G2160	U2099	A2014	A1916	A1810	C1712	A1618	G1527				
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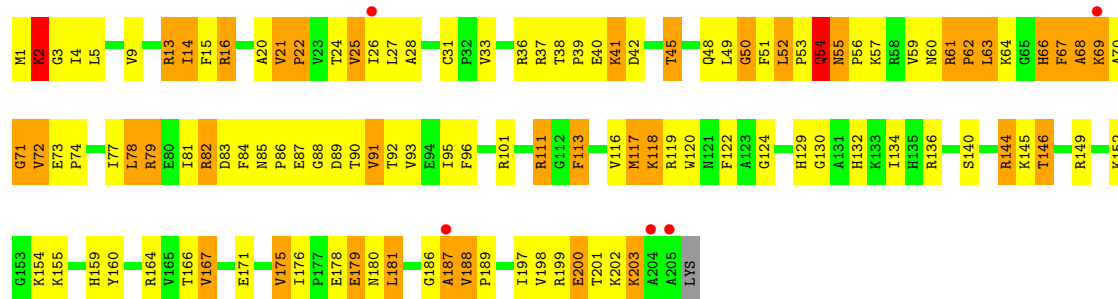
• Molecule 27: 50S ribosomal protein L2

Chain DD: 48% 41% 8% ..



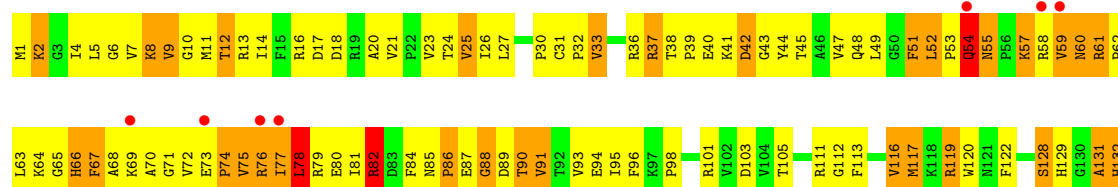
• Molecule 28: 50S ribosomal protein L3

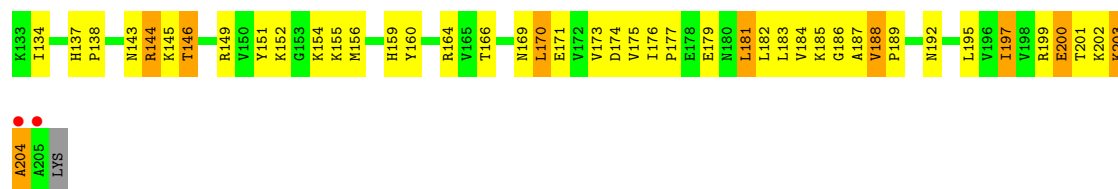
Chain BE: 2% 43% 37% 18% .



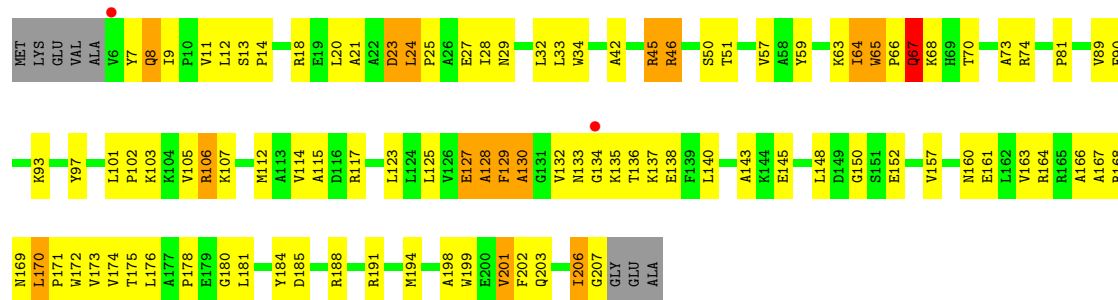
• Molecule 28: 50S ribosomal protein L3

Chain DE: 4% 30% 49% 19% .

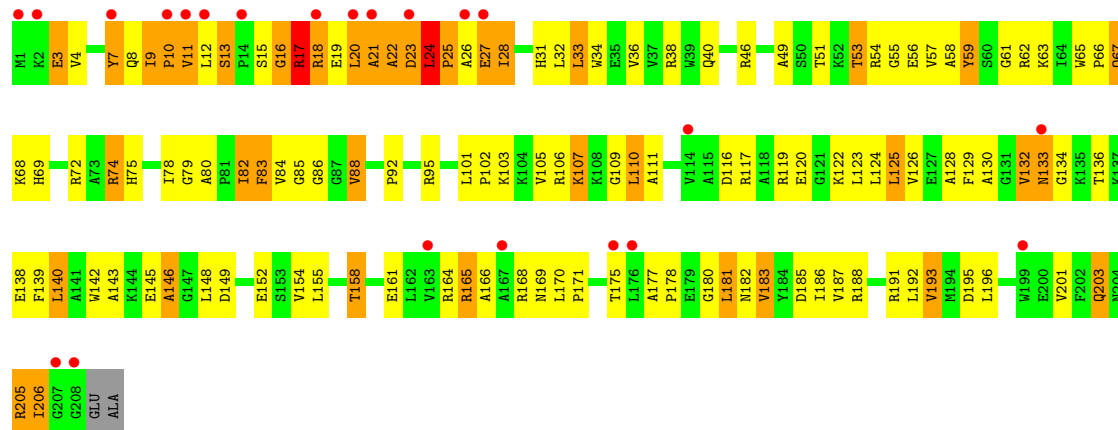




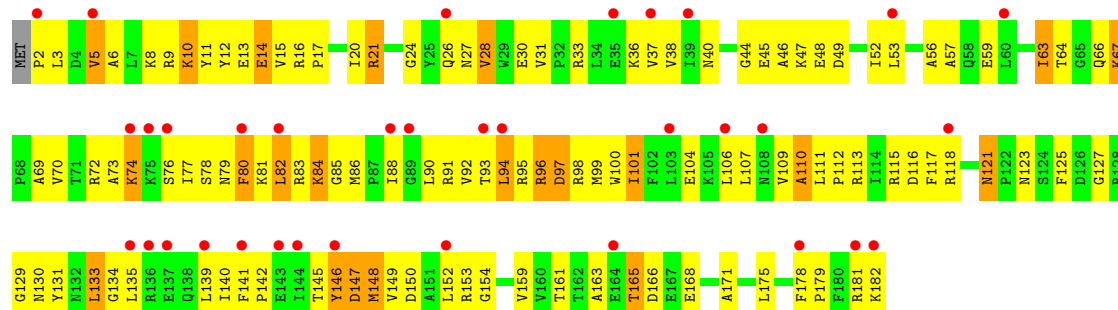
• Molecule 29: 50S ribosomal protein L4



• Molecule 29: 50S ribosomal protein L4



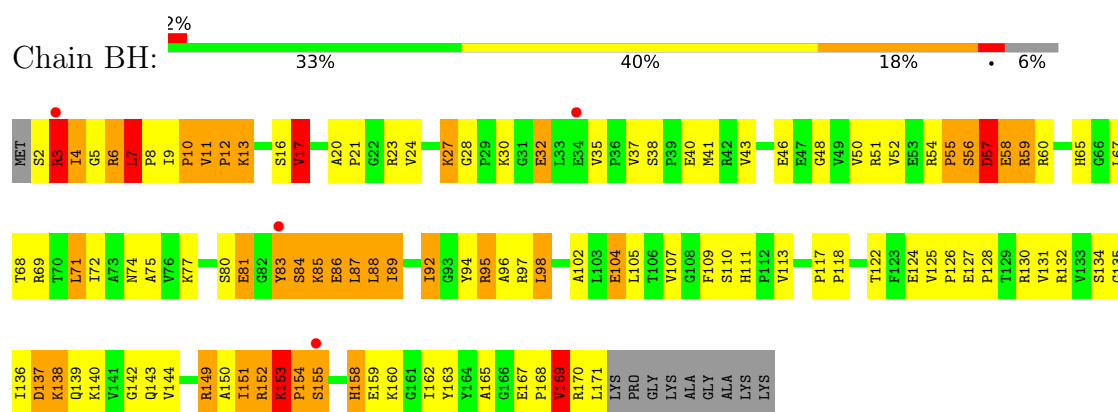
• Molecule 30: 50S ribosomal protein L5



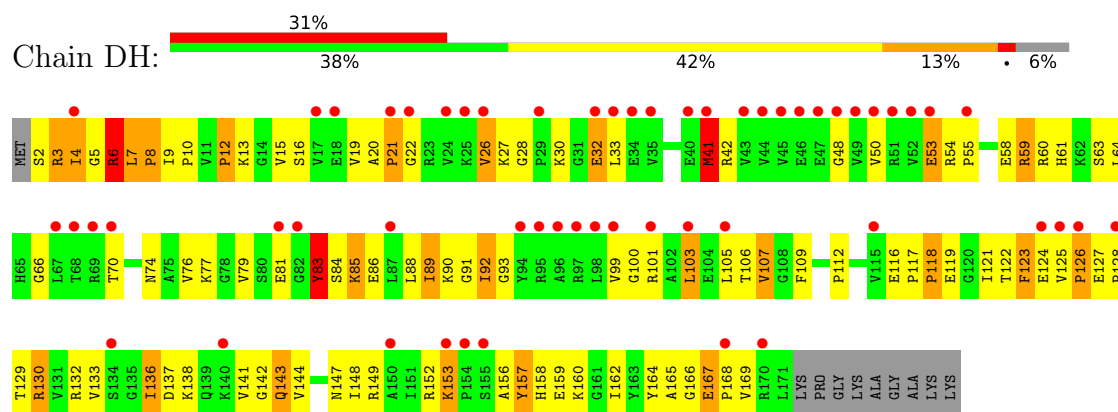
- Molecule 30: 50S ribosomal protein L5



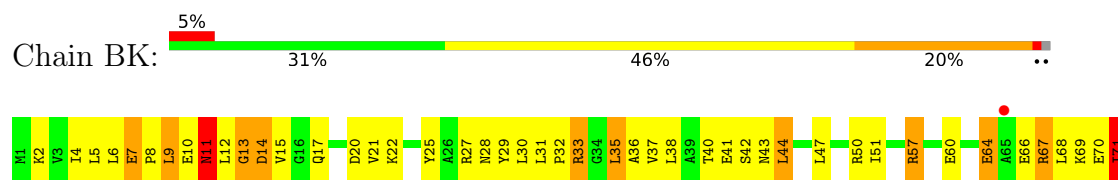
- Molecule 31: 50S ribosomal protein L6

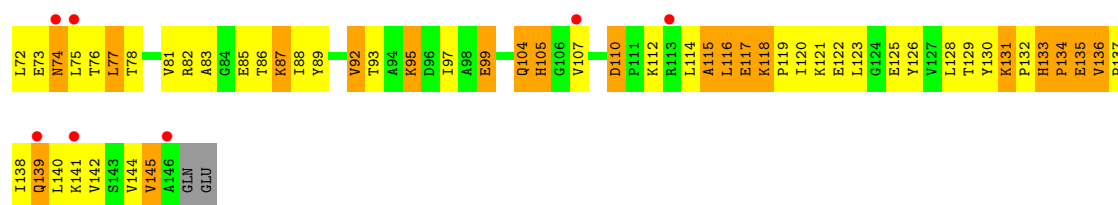


- Molecule 31: 50S ribosomal protein L6

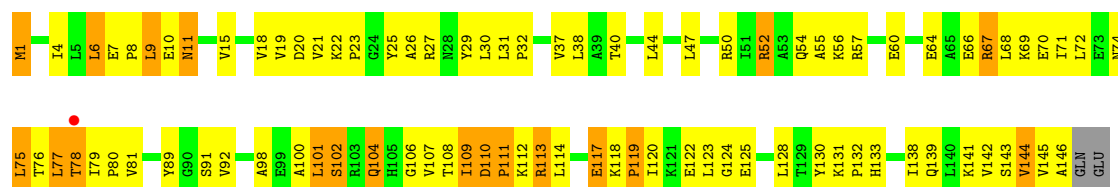


- Molecule 32: 50S ribosomal protein L9

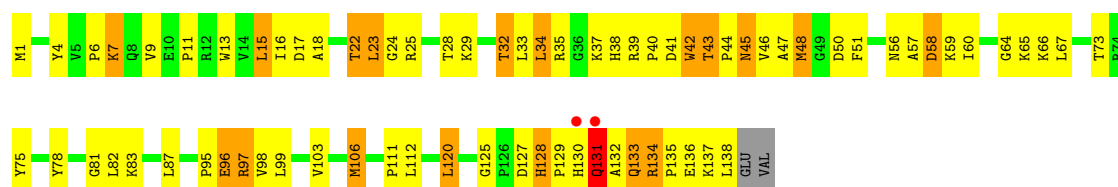




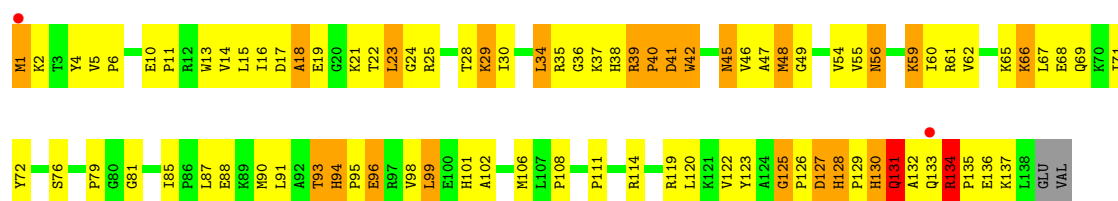
• Molecule 32: 50S ribosomal protein L9



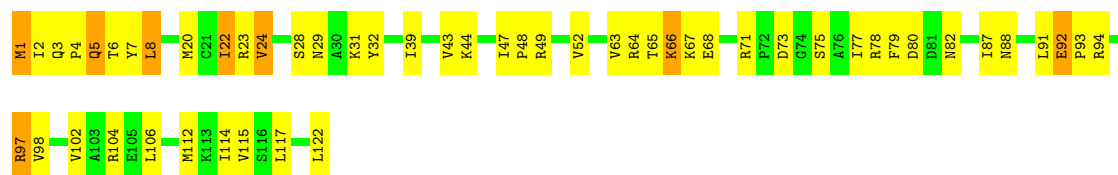
• Molecule 33: 50S ribosomal protein L13



• Molecule 33: 50S ribosomal protein L13

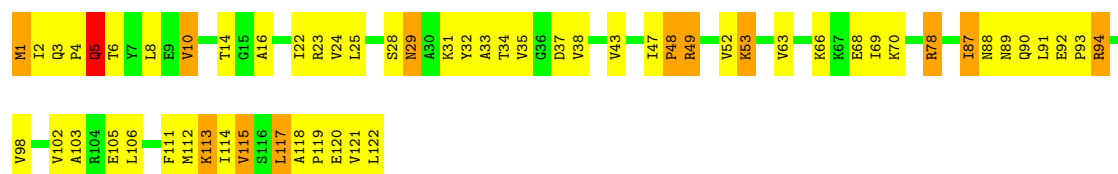


• Molecule 34: 50S ribosomal protein L14

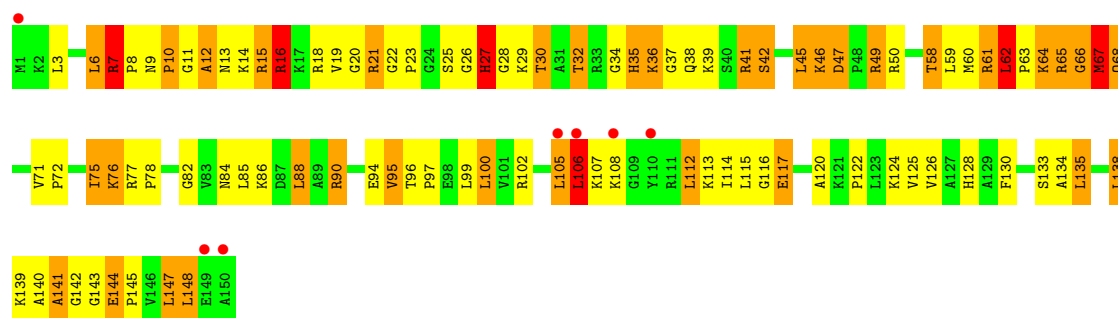


• Molecule 34: 50S ribosomal protein L14

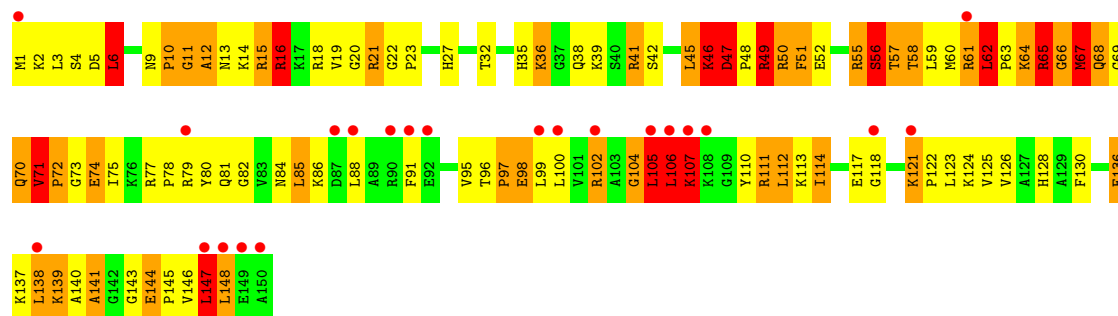




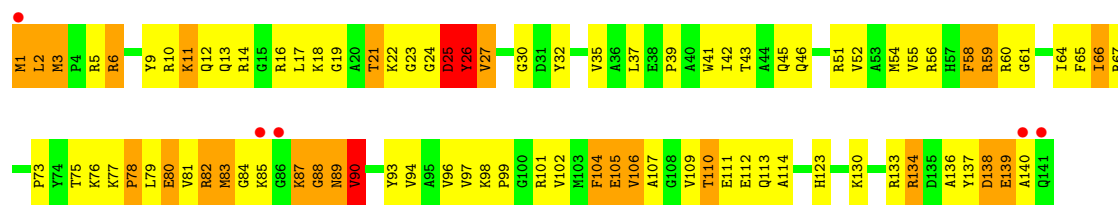
• Molecule 35: 50S ribosomal protein L15



• Molecule 35: 50S ribosomal protein L15

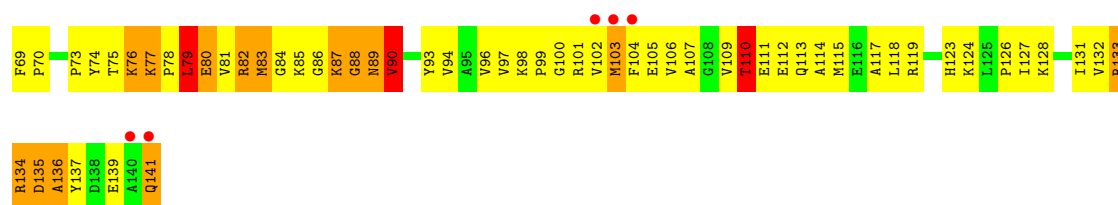


• Molecule 36: 50S ribosomal protein L16



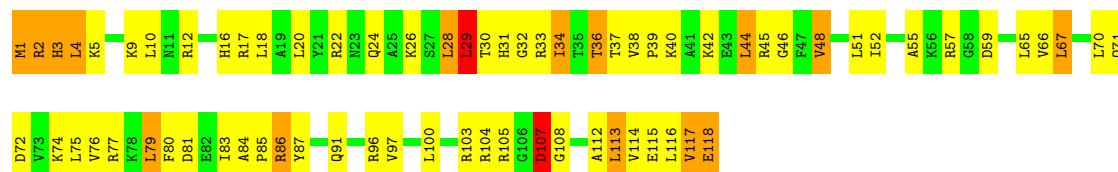
• Molecule 36: 50S ribosomal protein L16





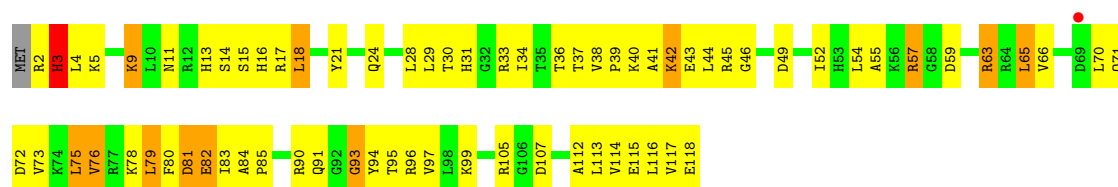
- Molecule 37: 50S ribosomal protein L17

Chain B0: 40% 46% 13%



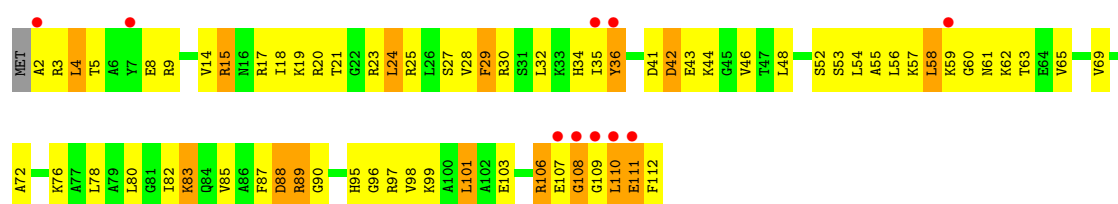
- Molecule 37: 50S ribosomal protein L17

Chain D0: 39% 49% 10%



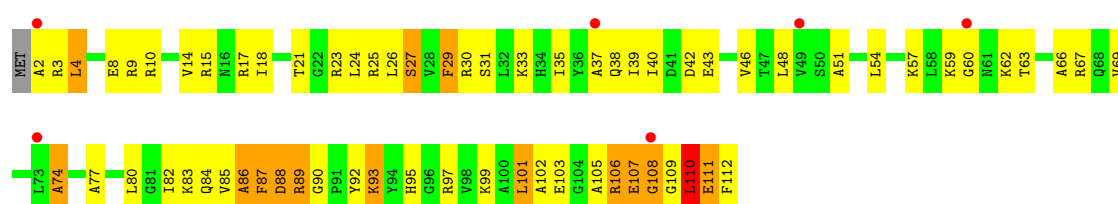
- Molecule 38: 50S ribosomal protein L18

Chain BQ: 9% 38% 48% 13%

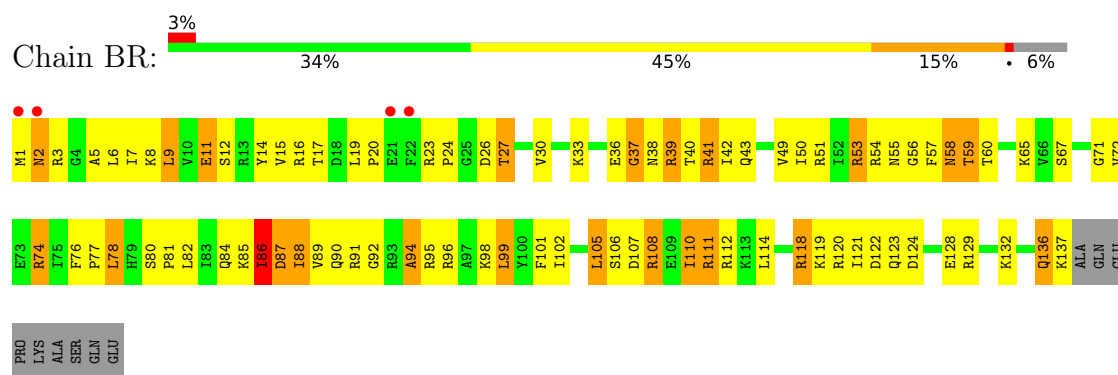


- Molecule 38: 50S ribosomal protein L18

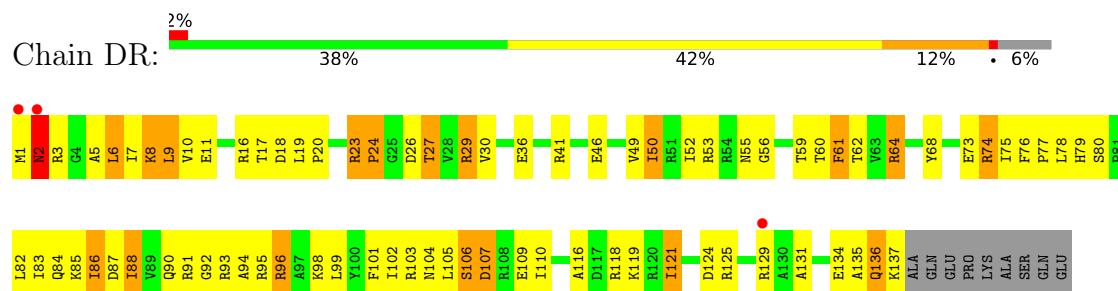
Chain DQ: 5% 39% 46% 13%



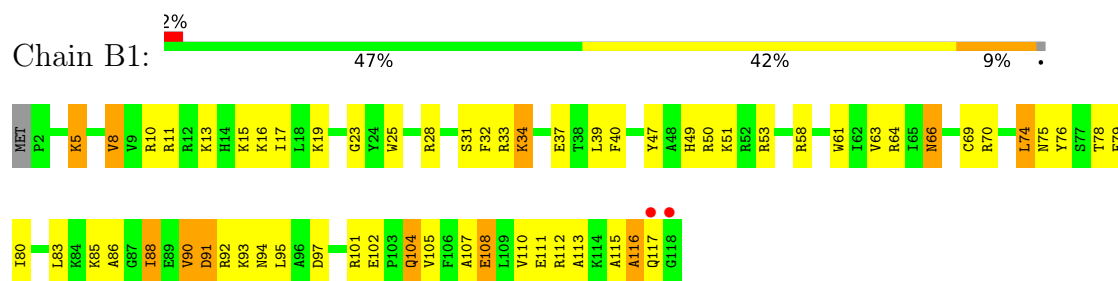
- Molecule 39: 50S ribosomal protein L19



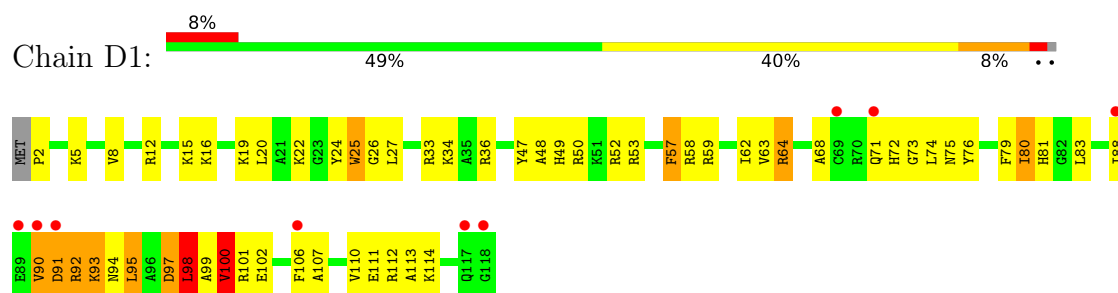
- Molecule 39: 50S ribosomal protein L19



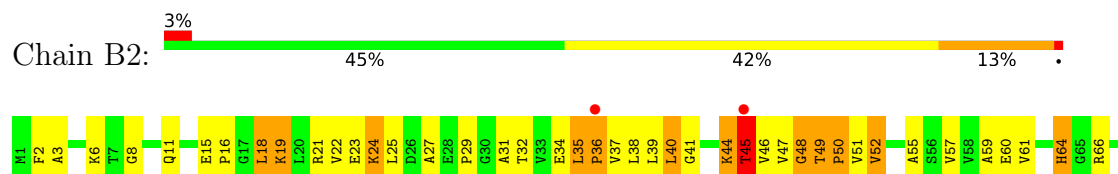
- Molecule 40: 50S ribosomal protein L20

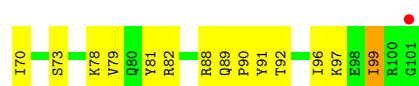


- Molecule 40: 50S ribosomal protein L20

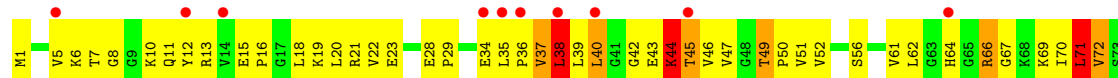


- Molecule 41: 50S ribosomal protein L21

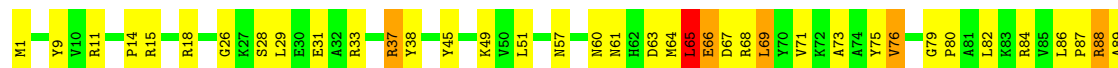




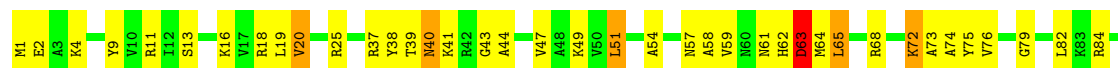
• Molecule 41: 50S ribosomal protein L21



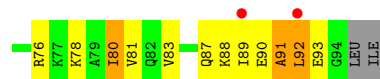
• Molecule 42: 50S ribosomal protein L22



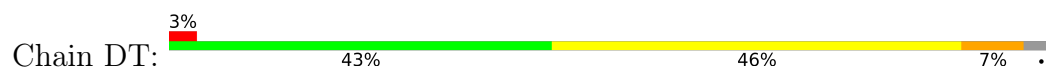
• Molecule 42: 50S ribosomal protein L22

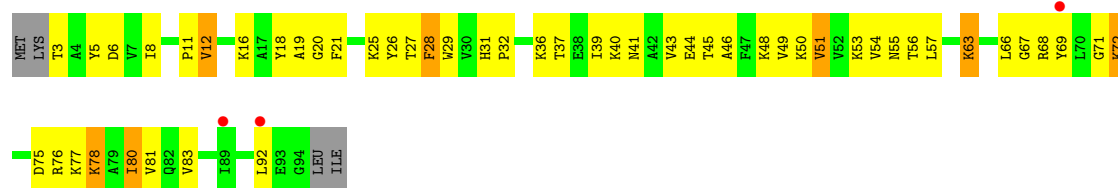


• Molecule 43: 50S ribosomal protein L23



• Molecule 43: 50S ribosomal protein L23





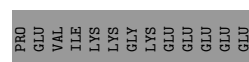
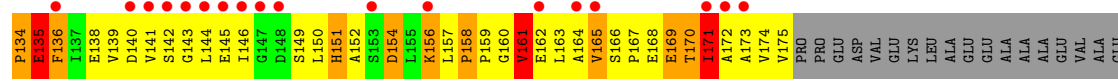
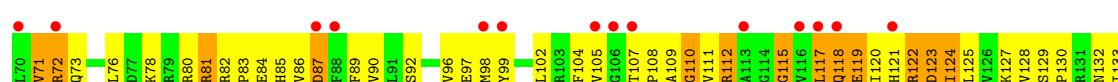
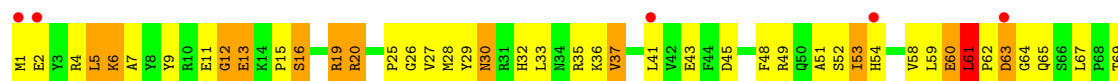
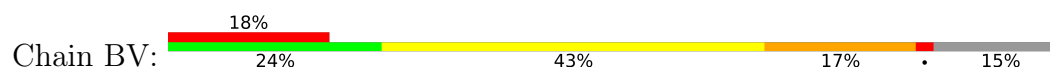
• Molecule 44: 50S ribosomal protein L24



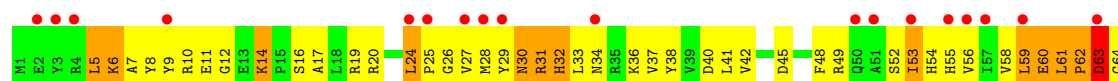
• Molecule 44: 50S ribosomal protein L24

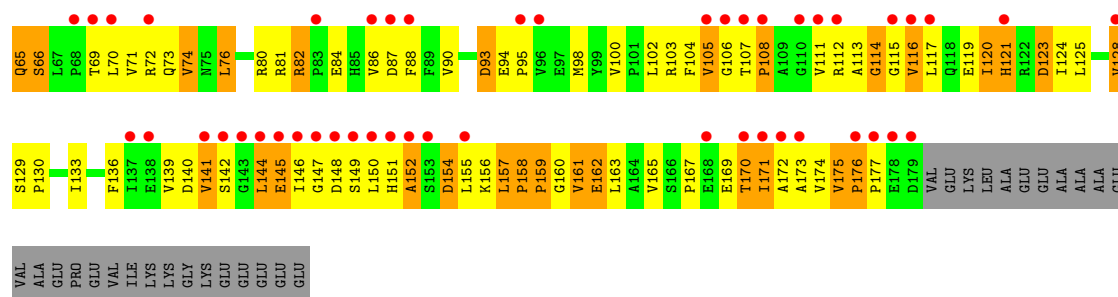


• Molecule 45: 50S ribosomal protein L25

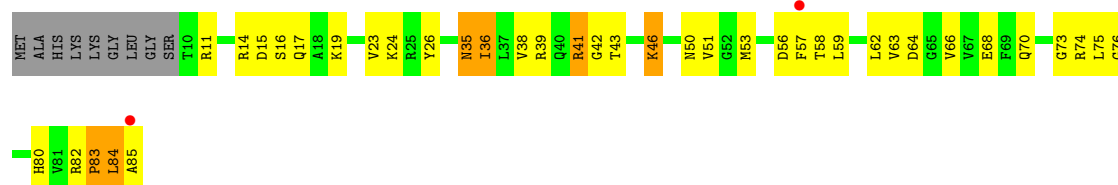
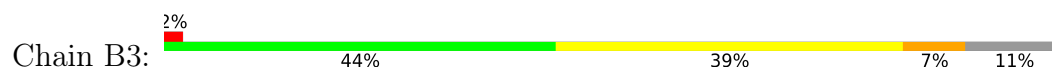


• Molecule 45: 50S ribosomal protein L25

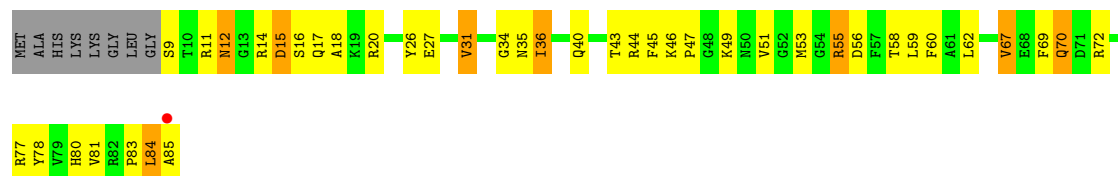
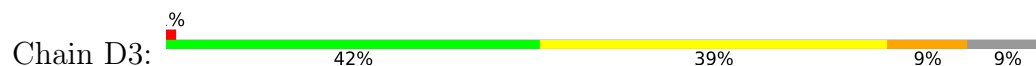




• Molecule 46: 50S ribosomal protein L27



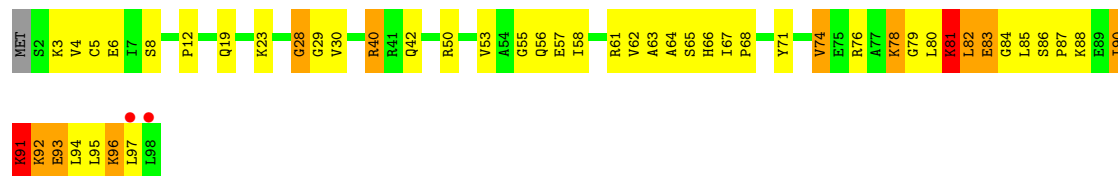
• Molecule 46: 50S ribosomal protein L27



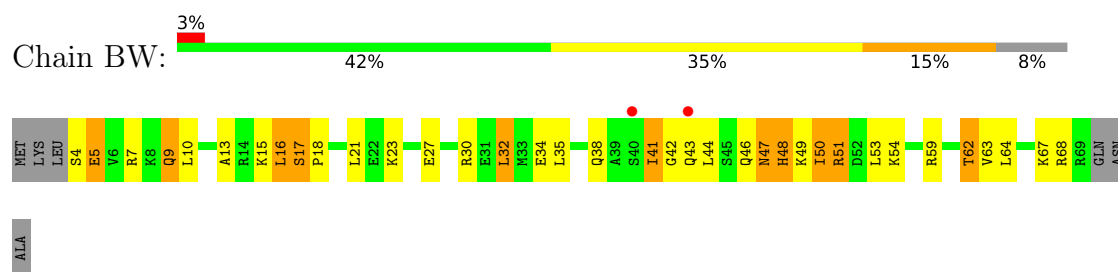
• Molecule 47: 50S ribosomal protein L28



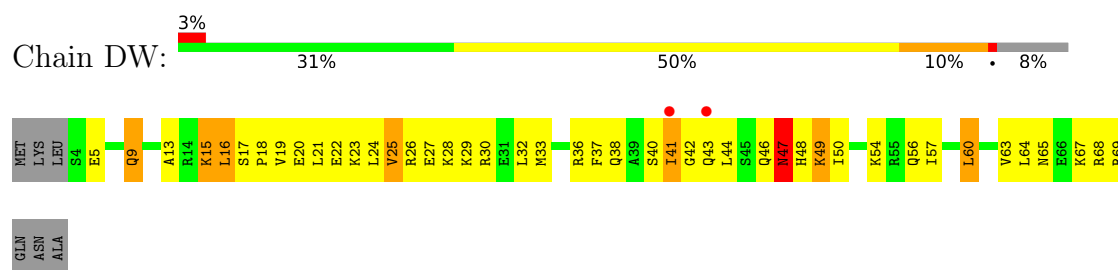
• Molecule 47: 50S ribosomal protein L28



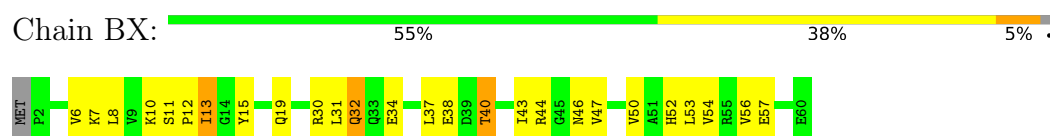
• Molecule 48: 50S ribosomal protein L29



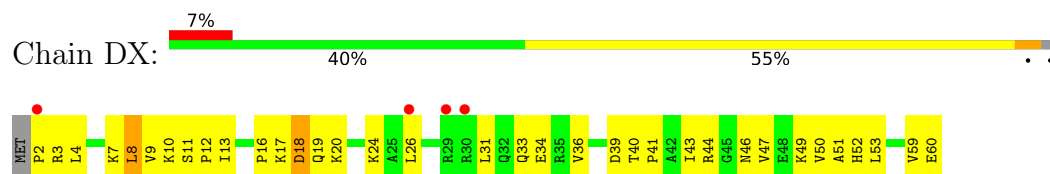
- Molecule 48: 50S ribosomal protein L29



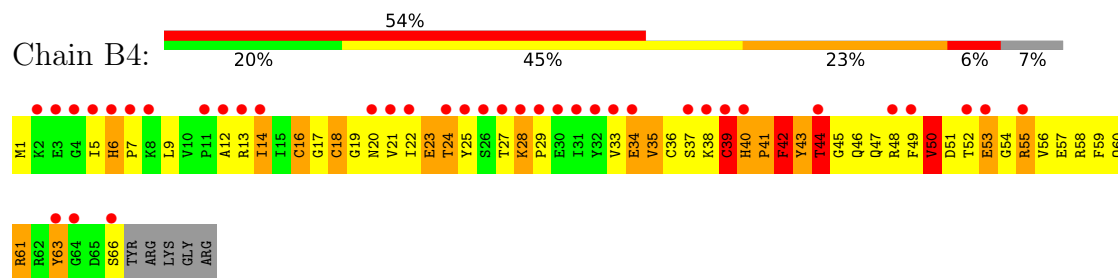
- Molecule 49: 50S ribosomal protein L30



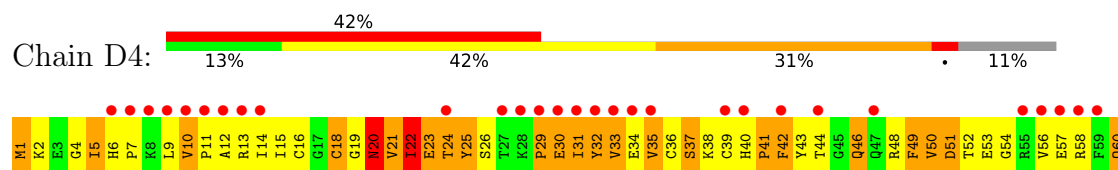
- Molecule 49: 50S ribosomal protein L30

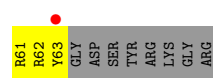


- Molecule 50: 50S ribosomal protein L31

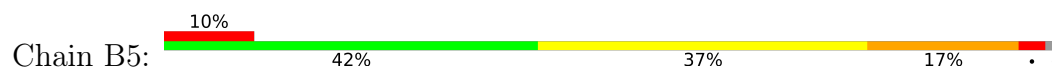


- Molecule 50: 50S ribosomal protein L31





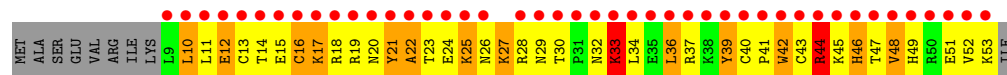
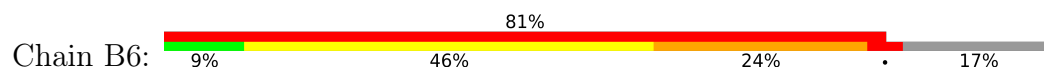
• Molecule 51: 50S ribosomal protein L32



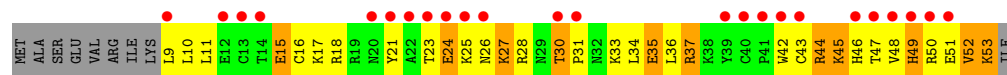
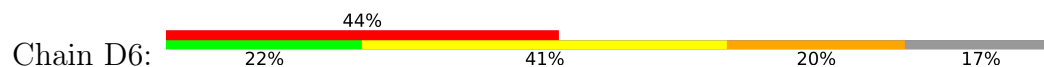
• Molecule 51: 50S ribosomal protein L32



• Molecule 52: 50S ribosomal protein L33



• Molecule 52: 50S ribosomal protein L33



• Molecule 53: 50S ribosomal protein L34



• Molecule 53: 50S ribosomal protein L34



• Molecule 54: 50S ribosomal protein L35





● Molecule 54: 50S ribosomal protein L35



4 Data and refinement statistics

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

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

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 [i](#)

5.1 Standard geometry [i](#)

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

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

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

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

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

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

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

All (2) bond length outliers are listed below:

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

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

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

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
31	BH	153	LYS	Peptide

5.2 Too-close contacts [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	32284	0	16296	1132	1
1	CA	32287	0	16295	1151	1
2	AE	1924	0	1975	160	0
2	CE	1924	0	1975	155	0
3	AF	1605	0	1668	115	0
3	CF	1612	0	1677	117	0
4	AG	1703	0	1763	116	0
4	CG	1703	0	1763	116	0
5	AH	1155	0	1213	75	0
5	CH	1155	0	1213	63	0

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

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

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

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

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 27.

The worst 5 of 13379 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:DO:46:LYS:HD3	35:DO:51:PHE:CD1	1.38	1.55
54:B8:34:TRP:CB	54:B8:35:GLN:HB2	1.34	1.55
50:B4:37:SER:HB3	50:B4:42:PHE:CD1	1.40	1.52
35:DO:71:VAL:HG13	35:DO:72:PRO:CD	1.44	1.47
35:BO:19:VAL:HG23	35:BO:27:HIS:CB	1.45	1.46

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:85:U:O2'	31:DH:100:GLY:O[3_555]	1.97	0.23
1:CA:86:U:O2'	25:DA:276:A:OP2[3_545]	2.19	0.01

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AE	235/256 (92%)	170 (72%)	44 (19%)	21 (9%)	1	4
2	CE	235/256 (92%)	161 (68%)	48 (20%)	26 (11%)	0	2
3	AF	203/239 (85%)	157 (77%)	36 (18%)	10 (5%)	2	14
3	CF	204/239 (85%)	151 (74%)	40 (20%)	13 (6%)	1	8
4	AG	206/208 (99%)	169 (82%)	29 (14%)	8 (4%)	3	19
4	CG	206/208 (99%)	167 (81%)	24 (12%)	15 (7%)	1	6
5	AH	149/162 (92%)	128 (86%)	16 (11%)	5 (3%)	4	22
5	CH	149/162 (92%)	129 (87%)	18 (12%)	2 (1%)	13	49
6	AI	99/101 (98%)	88 (89%)	8 (8%)	3 (3%)	5	26
6	CI	99/101 (98%)	92 (93%)	7 (7%)	0	100	100
7	AJ	153/156 (98%)	127 (83%)	21 (14%)	5 (3%)	4	23
7	CJ	153/156 (98%)	131 (86%)	16 (10%)	6 (4%)	3	19
8	AK	136/138 (99%)	113 (83%)	15 (11%)	8 (6%)	2	10
8	CK	136/138 (99%)	116 (85%)	17 (12%)	3 (2%)	7	34
9	AL	125/128 (98%)	90 (72%)	26 (21%)	9 (7%)	1	6
9	CL	125/128 (98%)	86 (69%)	30 (24%)	9 (7%)	1	6
10	AM	97/105 (92%)	77 (79%)	17 (18%)	3 (3%)	4	25
10	CM	97/105 (92%)	79 (81%)	13 (13%)	5 (5%)	2	13
11	AN	117/129 (91%)	101 (86%)	11 (9%)	5 (4%)	3	17
11	CN	117/129 (91%)	97 (83%)	16 (14%)	4 (3%)	4	22
12	AO	123/132 (93%)	104 (85%)	7 (6%)	12 (10%)	1	3
12	CO	123/132 (93%)	96 (78%)	21 (17%)	6 (5%)	2	14
13	AP	114/126 (90%)	76 (67%)	26 (23%)	12 (10%)	0	2
13	CP	115/126 (91%)	83 (72%)	18 (16%)	14 (12%)	0	1
14	AQ	56/61 (92%)	37 (66%)	7 (12%)	12 (21%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	CQ	56/61 (92%)	39 (70%)	9 (16%)	8 (14%)	0	1
15	AR	86/89 (97%)	68 (79%)	14 (16%)	4 (5%)	2	15
15	CR	86/89 (97%)	82 (95%)	2 (2%)	2 (2%)	7	33
16	AS	82/88 (93%)	64 (78%)	13 (16%)	5 (6%)	1	9
16	CS	82/88 (93%)	72 (88%)	10 (12%)	0	100	100
17	AT	98/105 (93%)	83 (85%)	9 (9%)	6 (6%)	1	9
17	CT	98/105 (93%)	85 (87%)	10 (10%)	3 (3%)	4	25
18	AU	70/88 (80%)	53 (76%)	13 (19%)	4 (6%)	2	11
18	CU	70/88 (80%)	60 (86%)	7 (10%)	3 (4%)	3	17
19	AV	76/93 (82%)	56 (74%)	12 (16%)	8 (10%)	0	2
19	CV	76/93 (82%)	53 (70%)	16 (21%)	7 (9%)	1	3
20	AW	97/106 (92%)	75 (77%)	14 (14%)	8 (8%)	1	4
20	CW	97/106 (92%)	72 (74%)	16 (16%)	9 (9%)	1	3
21	AX	23/27 (85%)	19 (83%)	2 (9%)	2 (9%)	1	4
21	CX	23/27 (85%)	18 (78%)	2 (9%)	3 (13%)	0	1
27	BD	270/276 (98%)	227 (84%)	30 (11%)	13 (5%)	2	15
27	DD	270/276 (98%)	226 (84%)	32 (12%)	12 (4%)	3	16
28	BE	203/206 (98%)	146 (72%)	34 (17%)	23 (11%)	0	2
28	DE	203/206 (98%)	134 (66%)	40 (20%)	29 (14%)	0	1
29	BF	200/210 (95%)	177 (88%)	14 (7%)	9 (4%)	3	16
29	DF	206/210 (98%)	153 (74%)	30 (15%)	23 (11%)	0	2
30	BG	179/182 (98%)	139 (78%)	27 (15%)	13 (7%)	1	6
30	DG	179/182 (98%)	140 (78%)	28 (16%)	11 (6%)	1	9
31	BH	168/180 (93%)	113 (67%)	20 (12%)	35 (21%)	0	0
31	DH	168/180 (93%)	108 (64%)	36 (21%)	24 (14%)	0	1
32	BK	144/148 (97%)	90 (62%)	39 (27%)	15 (10%)	0	2
32	DK	144/148 (97%)	98 (68%)	36 (25%)	10 (7%)	1	6
33	BM	136/140 (97%)	107 (79%)	21 (15%)	8 (6%)	2	10
33	DM	136/140 (97%)	106 (78%)	16 (12%)	14 (10%)	0	2
34	BN	120/122 (98%)	114 (95%)	4 (3%)	2 (2%)	10	42
34	DN	120/122 (98%)	106 (88%)	10 (8%)	4 (3%)	4	23

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

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

5 of 913 Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AE	205/220 (93%)	165 (80%)	40 (20%)	1	8
2	CE	205/220 (93%)	180 (88%)	25 (12%)	5	23
3	AF	159/188 (85%)	141 (89%)	18 (11%)	6	26
3	CF	160/188 (85%)	143 (89%)	17 (11%)	7	29
4	AG	180/180 (100%)	160 (89%)	20 (11%)	7	27
4	CG	180/180 (100%)	160 (89%)	20 (11%)	7	27
5	AH	116/123 (94%)	97 (84%)	19 (16%)	2	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	CH	116/123 (94%)	102 (88%)	14 (12%)	5	23
6	AI	90/90 (100%)	80 (89%)	10 (11%)	7	27
6	CI	90/90 (100%)	81 (90%)	9 (10%)	8	31
7	AJ	126/127 (99%)	106 (84%)	20 (16%)	3	13
7	CJ	126/127 (99%)	105 (83%)	21 (17%)	2	12
8	AK	119/119 (100%)	106 (89%)	13 (11%)	7	27
8	CK	119/119 (100%)	111 (93%)	8 (7%)	18	52
9	AL	98/99 (99%)	86 (88%)	12 (12%)	5	23
9	CL	98/99 (99%)	81 (83%)	17 (17%)	2	11
10	AM	89/92 (97%)	79 (89%)	10 (11%)	6	26
10	CM	89/92 (97%)	78 (88%)	11 (12%)	5	22
11	AN	90/99 (91%)	79 (88%)	11 (12%)	5	23
11	CN	90/99 (91%)	85 (94%)	5 (6%)	23	60
12	AO	104/109 (95%)	95 (91%)	9 (9%)	11	40
12	CO	104/109 (95%)	94 (90%)	10 (10%)	9	34
13	AP	94/101 (93%)	87 (93%)	7 (7%)	15	47
13	CP	94/101 (93%)	83 (88%)	11 (12%)	6	24
14	AQ	48/50 (96%)	42 (88%)	6 (12%)	5	22
14	CQ	48/50 (96%)	44 (92%)	4 (8%)	12	42
15	AR	79/80 (99%)	73 (92%)	6 (8%)	14	46
15	CR	79/80 (99%)	67 (85%)	12 (15%)	3	15
16	AS	72/74 (97%)	68 (94%)	4 (6%)	23	60
16	CS	72/74 (97%)	64 (89%)	8 (11%)	7	27
17	AT	95/97 (98%)	85 (90%)	10 (10%)	7	29
17	CT	95/97 (98%)	92 (97%)	3 (3%)	42	78
18	AU	63/77 (82%)	57 (90%)	6 (10%)	9	35
18	CU	63/77 (82%)	51 (81%)	12 (19%)	1	9
19	AV	67/80 (84%)	55 (82%)	12 (18%)	2	10
19	CV	67/80 (84%)	58 (87%)	9 (13%)	4	19
20	AW	76/82 (93%)	68 (90%)	8 (10%)	7	29
20	CW	76/82 (93%)	66 (87%)	10 (13%)	4	20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	AX	20/22 (91%)	20 (100%)	0	100	100
21	CX	20/22 (91%)	20 (100%)	0	100	100
27	BD	214/218 (98%)	178 (83%)	36 (17%)	2	12
27	DD	214/218 (98%)	181 (85%)	33 (15%)	3	14
28	BE	165/166 (99%)	135 (82%)	30 (18%)	2	10
28	DE	165/166 (99%)	139 (84%)	26 (16%)	3	14
29	BF	161/166 (97%)	141 (88%)	20 (12%)	5	22
29	DF	165/166 (99%)	140 (85%)	25 (15%)	3	15
30	BG	155/156 (99%)	135 (87%)	20 (13%)	5	20
30	DG	155/156 (99%)	139 (90%)	16 (10%)	8	30
31	BH	142/148 (96%)	122 (86%)	20 (14%)	4	17
31	DH	142/148 (96%)	124 (87%)	18 (13%)	5	21
32	BK	122/124 (98%)	101 (83%)	21 (17%)	2	11
32	DK	122/124 (98%)	106 (87%)	16 (13%)	4	20
33	BM	117/119 (98%)	98 (84%)	19 (16%)	2	13
33	DM	117/119 (98%)	97 (83%)	20 (17%)	2	11
34	BN	100/100 (100%)	92 (92%)	8 (8%)	13	43
34	DN	100/100 (100%)	87 (87%)	13 (13%)	4	20
35	BO	116/116 (100%)	84 (72%)	32 (28%)	0	2
35	DO	116/116 (100%)	80 (69%)	36 (31%)	0	1
36	BP	111/111 (100%)	94 (85%)	17 (15%)	3	14
36	DP	111/111 (100%)	89 (80%)	22 (20%)	1	8
37	B0	101/101 (100%)	85 (84%)	16 (16%)	3	14
37	D0	100/101 (99%)	82 (82%)	18 (18%)	2	10
38	BQ	87/88 (99%)	73 (84%)	14 (16%)	2	13
38	DQ	87/88 (99%)	79 (91%)	8 (9%)	10	37
39	BR	120/127 (94%)	99 (82%)	21 (18%)	2	10
39	DR	120/127 (94%)	102 (85%)	18 (15%)	3	15
40	B1	93/94 (99%)	85 (91%)	8 (9%)	11	40
40	D1	93/94 (99%)	82 (88%)	11 (12%)	6	24
41	B2	82/82 (100%)	70 (85%)	12 (15%)	3	16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
41	D2	82/82 (100%)	69 (84%)	13 (16%)	3	13
42	BS	92/92 (100%)	79 (86%)	13 (14%)	4	17
42	DS	92/92 (100%)	76 (83%)	16 (17%)	2	11
43	BT	74/78 (95%)	65 (88%)	9 (12%)	5	23
43	DT	74/78 (95%)	63 (85%)	11 (15%)	3	15
44	BU	85/91 (93%)	72 (85%)	13 (15%)	3	14
44	DU	85/91 (93%)	67 (79%)	18 (21%)	1	6
45	BV	154/179 (86%)	126 (82%)	28 (18%)	2	10
45	DV	158/179 (88%)	138 (87%)	20 (13%)	5	21
46	B3	61/67 (91%)	57 (93%)	4 (7%)	18	53
46	D3	62/67 (92%)	55 (89%)	7 (11%)	6	26
47	BZ	82/83 (99%)	69 (84%)	13 (16%)	3	13
47	DZ	82/83 (99%)	68 (83%)	14 (17%)	2	11
48	BW	62/67 (92%)	51 (82%)	11 (18%)	2	10
48	DW	62/67 (92%)	51 (82%)	11 (18%)	2	10
49	BX	51/52 (98%)	46 (90%)	5 (10%)	9	33
49	DX	51/52 (98%)	48 (94%)	3 (6%)	21	58
50	B4	59/63 (94%)	49 (83%)	10 (17%)	2	12
50	D4	57/63 (90%)	46 (81%)	11 (19%)	1	8
51	B5	51/52 (98%)	42 (82%)	9 (18%)	2	10
51	D5	51/52 (98%)	41 (80%)	10 (20%)	1	8
52	B6	44/52 (85%)	34 (77%)	10 (23%)	1	4
52	D6	44/52 (85%)	40 (91%)	4 (9%)	10	37
53	B7	38/42 (90%)	33 (87%)	5 (13%)	4	20
53	D7	38/42 (90%)	33 (87%)	5 (13%)	4	20
54	B8	50/55 (91%)	37 (74%)	13 (26%)	0	3
54	D8	50/55 (91%)	41 (82%)	9 (18%)	2	10
All	All	9565/9996 (96%)	8229 (86%)	1336 (14%)	4	17

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

Mol	Chain	Res	Type
47	BZ	26	ARG

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

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

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

5.3.3 RNA ⓘ

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

5 of 1909 RNA backbone outliers are listed below:

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

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Mol	Chain	Res	Type
1	AA	32	A

5 of 232 RNA pucker outliers are listed below:

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

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
22	MIA	AB	38	22	22,31,32	1.40	1 (4%)	26,44,47	2.33	9 (34%)
22	MIA	AD	38	22	22,31,32	1.47	1 (4%)	26,44,47	2.73	10 (38%)
22	MIA	CB	38	22	22,31,32	1.49	1 (4%)	26,44,47	2.37	9 (34%)
22	MIA	CD	38	22	22,31,32	1.48	2 (9%)	26,44,47	2.79	10 (38%)

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

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

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	CB	38	MIA	C13-C14	6.21	1.50	1.32
22	CD	38	MIA	C13-C14	5.99	1.49	1.32
22	AD	38	MIA	C13-C14	5.95	1.49	1.32
22	AB	38	MIA	C13-C14	5.88	1.49	1.32
22	CD	38	MIA	O5'-C5'	-2.00	1.42	1.44

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	CD	38	MIA	C11-S10-C2	10.25	109.88	102.29
22	AD	38	MIA	C11-S10-C2	9.76	109.51	102.29
22	CB	38	MIA	C11-S10-C2	7.61	107.92	102.29
22	AB	38	MIA	C11-S10-C2	5.99	106.72	102.29
22	AB	38	MIA	C12-C13-C14	-5.75	115.77	127.10

There are no chirality outliers.

5 of 23 torsion outliers are listed below:

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

There are no ring outliers.

4 monomers are involved in 11 short contacts:

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 1608 ligands modelled in this entry, 1608 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	1502/1506 (99%)	-0.36	5 (0%) 93 83	54, 99, 183, 246	0
1	CA	1502/1506 (99%)	-0.28	13 (0%) 84 62	59, 100, 182, 245	0
2	AE	237/256 (92%)	0.24	11 (4%) 32 12	98, 139, 177, 190	0
2	CE	237/256 (92%)	0.57	15 (6%) 20 6	106, 152, 189, 209	0
3	AF	205/239 (85%)	0.29	7 (3%) 45 19	88, 113, 149, 158	0
3	CF	206/239 (86%)	1.03	33 (16%) 1 0	101, 135, 165, 180	0
4	AG	208/208 (100%)	-0.32	1 (0%) 90 74	81, 107, 131, 143	0
4	CG	208/208 (100%)	0.24	3 (1%) 75 49	75, 95, 123, 135	0
5	AH	151/162 (93%)	0.01	2 (1%) 77 51	78, 99, 125, 164	0
5	CH	151/162 (93%)	0.19	2 (1%) 77 51	84, 106, 131, 167	0
6	AI	101/101 (100%)	0.44	5 (4%) 29 11	67, 99, 115, 141	0
6	CI	101/101 (100%)	-0.07	0 100 100	76, 96, 115, 153	0
7	AJ	155/156 (99%)	0.40	12 (7%) 13 4	96, 114, 143, 161	0
7	CJ	155/156 (99%)	0.05	6 (3%) 39 16	100, 119, 147, 158	0
8	AK	138/138 (100%)	-0.28	0 100 100	81, 103, 117, 132	0
8	CK	138/138 (100%)	0.02	1 (0%) 87 68	81, 109, 125, 136	0
9	AL	127/128 (99%)	0.51	13 (10%) 7 2	83, 138, 159, 166	0
9	CL	127/128 (99%)	0.09	6 (4%) 31 12	95, 147, 165, 171	0
10	AM	99/105 (94%)	0.77	14 (14%) 2 1	81, 140, 167, 178	0
10	CM	99/105 (94%)	0.83	12 (12%) 4 1	103, 154, 174, 180	0
11	AN	119/129 (92%)	0.77	13 (10%) 5 2	62, 95, 130, 161	0
11	CN	119/129 (92%)	0.21	2 (1%) 70 41	74, 99, 133, 164	0
12	AO	125/132 (94%)	-0.22	1 (0%) 86 64	59, 75, 107, 162	0
12	CO	125/132 (94%)	0.62	14 (11%) 5 1	63, 91, 126, 166	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AP	116/126 (92%)	0.23	6 (5%) 27 10	75, 124, 143, 155	0
13	CP	117/126 (92%)	0.19	7 (5%) 22 7	91, 145, 161, 169	0
14	AQ	58/61 (95%)	-0.15	0 100 100	87, 103, 120, 127	0
14	CQ	58/61 (95%)	1.17	9 (15%) 2 0	108, 125, 150, 154	0
15	AR	88/89 (98%)	-0.14	0 100 100	70, 94, 116, 120	0
15	CR	88/89 (98%)	-0.06	0 100 100	67, 96, 124, 136	0
16	AS	84/88 (95%)	-0.36	0 100 100	87, 109, 134, 174	0
16	CS	84/88 (95%)	0.32	2 (2%) 59 30	76, 91, 118, 157	0
17	AT	100/105 (95%)	-0.35	2 (2%) 65 36	80, 102, 118, 129	0
17	CT	100/105 (95%)	0.03	2 (2%) 65 36	75, 100, 126, 144	0
18	AU	72/88 (81%)	0.56	5 (6%) 17 5	77, 97, 135, 164	0
18	CU	72/88 (81%)	0.17	2 (2%) 53 24	85, 103, 149, 172	0
19	AV	78/93 (83%)	0.12	1 (1%) 77 51	97, 120, 145, 156	0
19	CV	78/93 (83%)	0.55	5 (6%) 19 6	128, 152, 178, 186	0
20	AW	99/106 (93%)	-0.17	0 100 100	97, 121, 148, 153	0
20	CW	99/106 (93%)	0.21	2 (2%) 65 36	86, 106, 141, 153	0
21	AX	25/27 (92%)	0.21	1 (4%) 38 15	97, 107, 121, 153	0
21	CX	25/27 (92%)	0.78	2 (8%) 12 4	101, 129, 150, 171	0
22	AB	84/85 (98%)	0.73	13 (15%) 2 0	76, 148, 167, 178	0
22	AD	84/85 (98%)	0.30	11 (13%) 3 1	70, 147, 206, 218	0
22	CB	84/85 (98%)	1.60	30 (35%) 0 0	92, 155, 171, 179	0
22	CD	84/85 (98%)	-0.64	0 100 100	74, 147, 207, 212	0
23	AC	77/77 (100%)	-0.42	0 100 100	66, 91, 135, 155	0
23	CC	77/77 (100%)	-0.59	0 100 100	79, 104, 143, 165	0
24	A1	16/16 (100%)	-0.21	0 100 100	66, 97, 168, 177	0
24	C1	16/16 (100%)	-0.18	0 100 100	75, 107, 176, 183	0
25	BA	2912/2912 (100%)	-0.04	42 (1%) 75 49	39, 68, 206, 243	0
25	DA	2907/2912 (99%)	-0.18	66 (2%) 60 31	49, 82, 226, 247	0
26	BB	122/122 (100%)	-0.27	1 (0%) 86 64	65, 92, 113, 183	0
26	DB	122/122 (100%)	-0.46	2 (1%) 72 44	78, 110, 139, 198	0
27	BD	272/276 (98%)	0.03	0 100 100	39, 59, 82, 104	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
27	DD	272/276 (98%)	-0.08	1 (0%) 92 78	45, 67, 87, 120	0
28	BE	205/206 (99%)	0.11	5 (2%) 59 30	44, 77, 125, 150	0
28	DE	205/206 (99%)	0.07	9 (4%) 34 13	56, 93, 144, 157	0
29	BF	202/210 (96%)	0.08	2 (0%) 82 59	42, 75, 110, 127	0
29	DF	208/210 (99%)	0.84	22 (10%) 6 2	53, 93, 155, 185	0
30	BG	181/182 (99%)	0.94	34 (18%) 1 0	79, 105, 136, 146	0
30	DG	181/182 (99%)	0.37	8 (4%) 34 13	96, 128, 157, 168	0
31	BH	170/180 (94%)	0.13	4 (2%) 59 30	71, 105, 126, 151	0
31	DH	170/180 (94%)	1.56	56 (32%) 0 0	143, 193, 217, 231	0
32	BK	146/148 (98%)	0.46	8 (5%) 25 9	72, 120, 141, 153	0
32	DK	146/148 (98%)	-0.20	1 (0%) 87 68	73, 120, 147, 151	0
33	BM	138/140 (98%)	0.08	2 (1%) 75 49	58, 79, 115, 136	0
33	DM	138/140 (98%)	0.12	2 (1%) 75 49	72, 104, 137, 147	0
34	BN	122/122 (100%)	-0.07	0 100 100	55, 71, 87, 93	0
34	DN	122/122 (100%)	0.04	0 100 100	66, 85, 103, 110	0
35	BO	150/150 (100%)	0.32	7 (4%) 31 12	45, 82, 109, 167	0
35	DO	150/150 (100%)	0.85	22 (14%) 2 1	45, 93, 136, 174	0
36	BP	141/141 (100%)	0.17	5 (3%) 44 18	55, 77, 105, 140	0
36	DP	141/141 (100%)	0.43	14 (9%) 7 2	58, 100, 130, 154	0
37	B0	118/118 (100%)	0.01	0 100 100	53, 74, 96, 106	0
37	D0	117/118 (99%)	0.03	1 (0%) 84 62	62, 81, 100, 117	0
38	BQ	111/112 (99%)	0.73	10 (9%) 9 3	71, 91, 116, 130	0
38	DQ	111/112 (99%)	0.24	6 (5%) 26 9	73, 109, 135, 157	0
39	BR	137/146 (93%)	0.15	4 (2%) 51 23	66, 85, 135, 167	0
39	DR	137/146 (93%)	0.07	3 (2%) 62 33	73, 94, 154, 184	0
40	B1	117/118 (99%)	0.00	2 (1%) 70 41	50, 70, 98, 140	0
40	D1	117/118 (99%)	0.49	9 (7%) 13 4	60, 99, 137, 155	0
41	B2	101/101 (100%)	0.08	3 (2%) 50 22	46, 91, 116, 128	0
41	D2	101/101 (100%)	0.97	14 (13%) 2 1	63, 122, 139, 150	0
42	BS	113/113 (100%)	-0.04	1 (0%) 84 62	44, 67, 99, 152	0
42	DS	113/113 (100%)	0.16	2 (1%) 68 39	61, 75, 109, 161	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
43	BT	92/96 (95%)	0.35	3 (3%) 46 20	54, 69, 95, 112	0
43	DT	92/96 (95%)	0.22	3 (3%) 46 20	65, 81, 109, 122	0
44	BU	102/110 (92%)	0.48	5 (4%) 29 11	70, 94, 144, 165	0
44	DU	102/110 (92%)	1.47	27 (26%) 0 0	78, 111, 162, 172	0
45	BV	175/206 (84%)	1.29	37 (21%) 1 0	79, 120, 189, 194	0
45	DV	179/206 (86%)	1.88	65 (36%) 0 0	111, 152, 207, 219	0
46	B3	76/85 (89%)	0.16	2 (2%) 56 27	51, 72, 92, 125	0
46	D3	77/85 (90%)	-0.04	1 (1%) 77 51	64, 87, 110, 151	0
47	BZ	97/98 (98%)	0.44	8 (8%) 11 3	48, 71, 115, 155	0
47	DZ	97/98 (98%)	-0.07	2 (2%) 63 34	54, 74, 126, 152	0
48	BW	66/72 (91%)	0.35	2 (3%) 50 22	59, 79, 95, 127	0
48	DW	66/72 (91%)	0.40	2 (3%) 50 22	75, 99, 121, 134	0
49	BX	59/60 (98%)	-0.03	0 100 100	61, 77, 112, 131	0
49	DX	59/60 (98%)	0.58	4 (6%) 17 5	76, 103, 136, 159	0
50	B4	66/71 (92%)	2.42	38 (57%) 0 0	112, 153, 176, 181	0
50	D4	63/71 (88%)	1.98	30 (47%) 0 0	141, 181, 191, 201	0
51	B5	59/60 (98%)	0.38	6 (10%) 7 2	43, 81, 156, 165	0
51	D5	59/60 (98%)	0.82	8 (13%) 3 1	61, 84, 169, 188	0
52	B6	45/54 (83%)	5.94	44 (97%) 0 0	117, 148, 164, 173	0
52	D6	45/54 (83%)	2.59	24 (53%) 0 0	131, 164, 181, 185	0
53	B7	45/49 (91%)	-0.03	0 100 100	38, 48, 68, 85	0
53	D7	45/49 (91%)	0.00	0 100 100	52, 59, 74, 94	0
54	B8	60/65 (92%)	0.35	2 (3%) 46 20	51, 68, 88, 115	0
54	D8	60/65 (92%)	0.34	3 (5%) 29 11	64, 80, 106, 132	0
All	All	21100/21658 (97%)	0.13	975 (4%) 32 12	38, 95, 177, 247	0

The worst 5 of 975 RSRZ outliers are listed below:

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

6.2 Non-standard residues in protein, DNA, RNA chains [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
22	MIA	AD	38	29/30	0.92	0.18	98,122,141,145	0
22	MIA	CB	38	29/30	0.94	0.19	63,95,112,126	0
22	MIA	CD	38	29/30	0.94	0.21	101,121,146,154	0
22	MIA	AB	38	29/30	0.96	0.18	65,78,90,93	0

6.3 Carbohydrates [i](#)

There are no carbohydrates 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
55	MG	DA	3229	1/1	-0.26	0.38	118,118,118,118	0
55	MG	AA	1758	1/1	-0.20	0.45	165,165,165,165	0
55	MG	DA	3407	1/1	-0.02	0.23	103,103,103,103	0
55	MG	CA	1786	1/1	0.06	0.27	111,111,111,111	0
55	MG	AD	101	1/1	0.09	0.32	154,154,154,154	0
55	MG	BA	3380	1/1	0.12	0.43	98,98,98,98	0
55	MG	CA	1803	1/1	0.19	0.24	103,103,103,103	0
55	MG	AA	1788	1/1	0.26	0.27	98,98,98,98	0
55	MG	DA	3176	1/1	0.30	0.54	105,105,105,105	0
55	MG	D1	201	1/1	0.31	0.26	89,89,89,89	0
55	MG	DA	3397	1/1	0.35	0.19	105,105,105,105	0
55	MG	AA	1643	1/1	0.42	0.53	127,127,127,127	0
55	MG	CA	1816	1/1	0.44	0.31	102,102,102,102	0
55	MG	DA	3330	1/1	0.45	0.65	100,100,100,100	0
55	MG	AA	1666	1/1	0.47	0.43	103,103,103,103	0
55	MG	CA	1806	1/1	0.47	0.27	103,103,103,103	0
55	MG	BA	3503	1/1	0.48	0.46	111,111,111,111	0
55	MG	AA	1735	1/1	0.49	0.20	102,102,102,102	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

6.5 Other polymers ⓘ

There are no such residues in this entry.