



wwPDB X-ray Structure Validation Summary Report ⓘ

May 21, 2020 – 03:27 am BST

PDB ID : 4V9A
Title : Crystal Structure of the 70S ribosome with tetracycline.
Authors : Jenner, L.; Yusupov, M.; Yusupova, G.
Deposited on : 2012-07-18
Resolution : 3.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

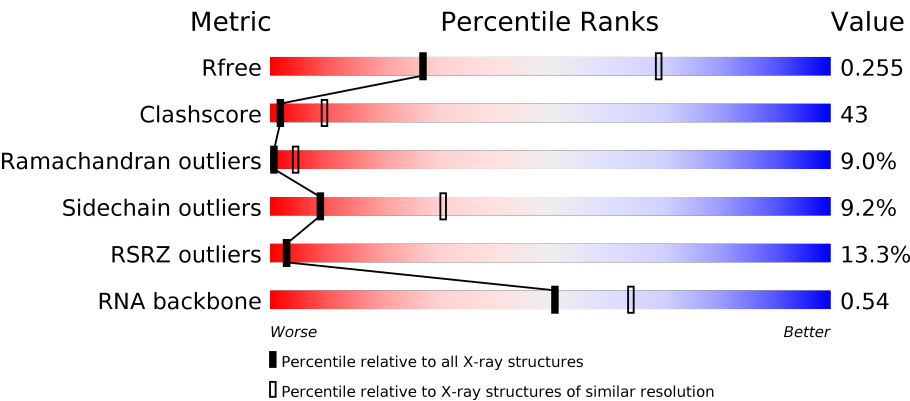
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)
RNA backbone	3102	1117 (3.70-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	<div><div>25%58%17%</div></div>
1	CA	1506	<div><div>25%59%16%</div></div>
2	AE	256	<div><div>23%22%56%14%7%</div></div>
2	CE	256	<div><div>38%20%54%18%7%</div></div>

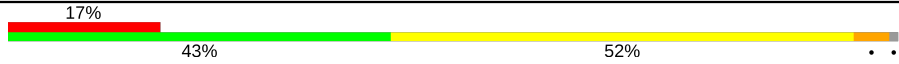
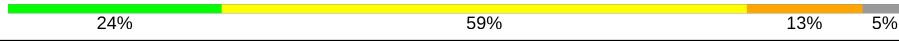

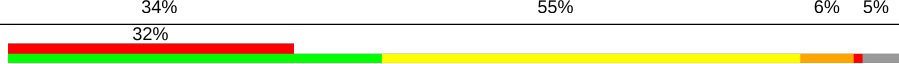
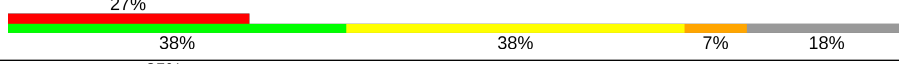
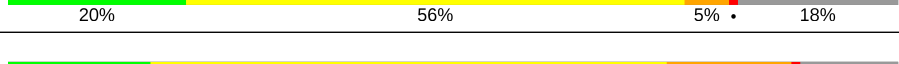
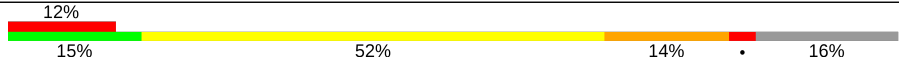
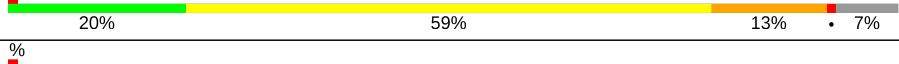
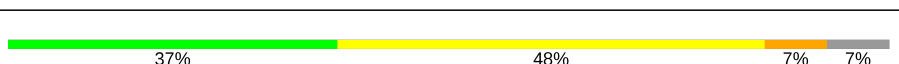
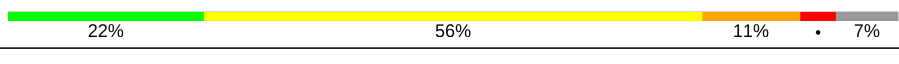
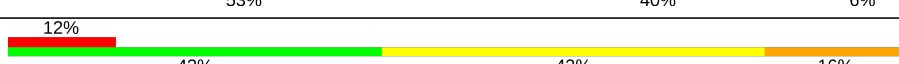

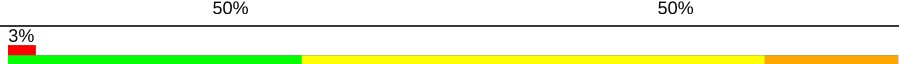


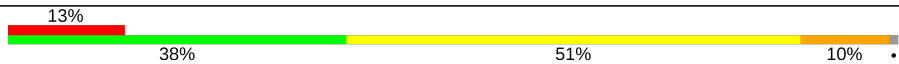

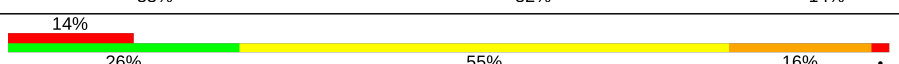



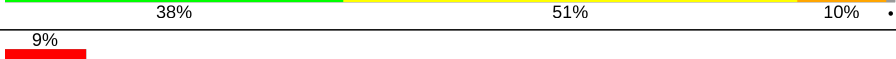

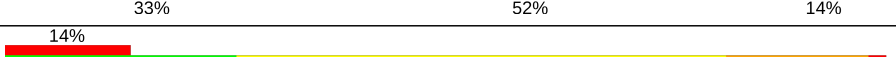
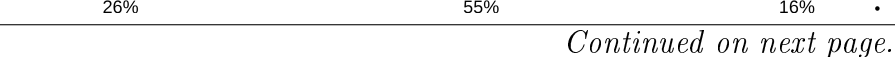
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Mol	Chain	Length	Quality of chain
3	AF	239	
3	CF	239	
4	AG	208	
4	CG	208	
5	AH	162	
5	CH	162	
6	AI	101	
6	CI	101	
7	AJ	156	
7	CJ	156	
8	AK	138	
8	CK	138	
9	AL	128	
9	CL	128	
10	AM	105	
10	CM	105	
11	AN	129	
11	CN	129	
12	AO	128	
12	CO	128	
13	AP	126	
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	AC	77	
22	CC	77	
23	A1	4	
23	C1	4	
24	BA	2912	
24	DA	2912	
25	BB	122	
25	DB	122	
26	BD	276	
26	DD	276	
27	BE	206	
27	DE	206	

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Mol	Chain	Length	Quality of chain
28	BF	210	
28	DF	210	
29	BG	182	
29	DG	182	
30	BH	180	
30	DH	180	
31	BK	148	
31	DK	148	
32	BM	140	
32	DM	140	
33	BN	122	
33	DN	122	
34	BO	150	
34	DO	150	
35	BP	141	
35	DP	141	
36	B0	118	
36	D0	118	
37	BQ	112	
37	DQ	112	
38	BR	146	
38	DR	146	
39	B1	118	
39	D1	118	
40	B2	101	

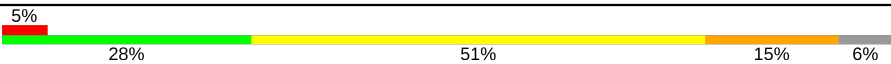
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Mol	Chain	Length	Quality of chain
40	D2	101	
41	BS	113	
41	DS	113	
42	BT	96	
42	DT	96	
43	BU	110	
43	DU	110	
44	BV	206	
44	DV	206	
45	B3	85	
45	D3	85	
46	BZ	98	
46	DZ	98	
47	BW	72	
47	DW	72	
48	BX	60	
48	DX	60	
49	B4	71	
49	D4	71	
50	B5	60	
50	D5	60	
51	B6	54	
51	D6	54	
52	B7	49	
52	D7	49	

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Mol	Chain	Length	Quality of chain
53	B8	65	
53	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
54	MG	AA	1662	-	-	-	X
54	MG	AA	1674	-	-	-	X
54	MG	AA	1676	-	-	-	X
54	MG	AA	1683	-	-	-	X
54	MG	AA	1694	-	-	-	X
54	MG	AA	1724	-	-	-	X
54	MG	AA	1730	-	-	-	X
54	MG	AA	1748	-	-	-	X
54	MG	AA	1750	-	-	-	X
54	MG	AA	1751	-	-	-	X
54	MG	AA	1752	-	-	-	X
54	MG	AA	1770	-	-	-	X
54	MG	AA	1773	-	-	-	X
54	MG	AA	1790	-	-	-	X
54	MG	AA	1805	-	-	-	X
54	MG	AA	1809	-	-	-	X
54	MG	AA	1810	-	-	-	X
54	MG	AA	1820	-	-	-	X
54	MG	AC	108	-	-	-	X
54	MG	B6	101	-	-	-	X
54	MG	BA	3056	-	-	-	X
54	MG	BA	3069	-	-	-	X
54	MG	BA	3075	-	-	-	X
54	MG	BA	3084	-	-	-	X
54	MG	BA	3095	-	-	-	X
54	MG	BA	3096	-	-	-	X
54	MG	BA	3119	-	-	-	X
54	MG	BA	3188	-	-	-	X
54	MG	BA	3191	-	-	-	X
54	MG	BA	3204	-	-	-	X
54	MG	BA	3212	-	-	-	X
54	MG	BA	3214	-	-	-	X
54	MG	BA	3228	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
54	MG	BA	3245	-	-	-	X
54	MG	BA	3251	-	-	-	X
54	MG	BA	3275	-	-	-	X
54	MG	BA	3285	-	-	-	X
54	MG	BA	3292	-	-	-	X
54	MG	BA	3296	-	-	-	X
54	MG	BA	3319	-	-	-	X
54	MG	BA	3329	-	-	-	X
54	MG	BA	3340	-	-	-	X
54	MG	BA	3357	-	-	-	X
54	MG	BA	3361	-	-	-	X
54	MG	BA	3365	-	-	-	X
54	MG	BA	3368	-	-	-	X
54	MG	BA	3369	-	-	-	X
54	MG	BA	3370	-	-	-	X
54	MG	BA	3376	-	-	-	X
54	MG	BA	3395	-	-	-	X
54	MG	BA	3396	-	-	-	X
54	MG	BA	3398	-	-	-	X
54	MG	BA	3406	-	-	-	X
54	MG	BA	3407	-	-	-	X
54	MG	BA	3411	-	-	-	X
54	MG	BA	3421	-	-	-	X
54	MG	BA	3424	-	-	-	X
54	MG	BA	3429	-	-	-	X
54	MG	BA	3431	-	-	-	X
54	MG	BA	3442	-	-	-	X
54	MG	BA	3443	-	-	-	X
54	MG	BA	3446	-	-	-	X
54	MG	BA	3449	-	-	-	X
54	MG	BA	3455	-	-	-	X
54	MG	BA	3458	-	-	-	X
54	MG	BA	3465	-	-	-	X
54	MG	BA	3493	-	-	-	X
54	MG	BA	3496	-	-	-	X
54	MG	BA	3505	-	-	-	X
54	MG	BA	3509	-	-	-	X
54	MG	BA	3526	-	-	-	X
54	MG	BA	3527	-	-	-	X
54	MG	BA	3534	-	-	-	X
54	MG	BA	3535	-	-	-	X
54	MG	BA	3539	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
54	MG	BA	3540	-	-	-	X
54	MG	BA	3541	-	-	-	X
54	MG	BA	3564	-	-	-	X
54	MG	BA	3576	-	-	-	X
54	MG	BA	3612	-	-	-	X
54	MG	BA	3618	-	-	-	X
54	MG	BA	3626	-	-	-	X
54	MG	BB	211	-	-	-	X
54	MG	BB	214	-	-	-	X
54	MG	BE	304	-	-	-	X
54	MG	CA	1602	-	-	-	X
54	MG	CA	1604	-	-	-	X
54	MG	CA	1622	-	-	-	X
54	MG	CA	1630	-	-	-	X
54	MG	CA	1644	-	-	-	X
54	MG	CA	1650	-	-	-	X
54	MG	CA	1695	-	-	-	X
54	MG	CA	1705	-	-	-	X
54	MG	CA	1707	-	-	-	X
54	MG	CA	1716	-	-	-	X
54	MG	CA	1723	-	-	-	X
54	MG	CA	1731	-	-	-	X
54	MG	CA	1747	-	-	-	X
54	MG	CA	1750	-	-	-	X
54	MG	CA	1751	-	-	-	X
54	MG	CA	1758	-	-	-	X
54	MG	CA	1778	-	-	-	X
54	MG	CA	1794	-	-	-	X
54	MG	DA	3002	-	-	-	X
54	MG	DA	3018	-	-	-	X
54	MG	DA	3037	-	-	-	X
54	MG	DA	3074	-	-	-	X
54	MG	DA	3104	-	-	-	X
54	MG	DA	3135	-	-	-	X
54	MG	DA	3158	-	-	-	X
54	MG	DA	3172	-	-	-	X
54	MG	DA	3239	-	-	-	X
54	MG	DA	3256	-	-	-	X
54	MG	DA	3291	-	-	-	X
54	MG	DA	3293	-	-	-	X
54	MG	DA	3295	-	-	-	X
54	MG	DA	3301	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
54	MG	DA	3310	-	-	-	X
54	MG	DA	3318	-	-	-	X
54	MG	DA	3320	-	-	-	X
54	MG	DA	3333	-	-	-	X
54	MG	DA	3339	-	-	-	X
54	MG	DA	3354	-	-	-	X
54	MG	DA	3367	-	-	-	X
54	MG	DA	3410	-	-	-	X
54	MG	DA	3424	-	-	-	X
54	MG	DA	3478	-	-	-	X
54	MG	DA	3486	-	-	-	X
54	MG	DA	3523	-	-	-	X
56	ZN	CG	303	-	-	X	-

2 Entry composition

There are 56 unique types of molecules in this entry. The entry contains 292440 atoms, of which 1 is hydrogen and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AV	83	Total	C	N	O	S	0	0	0
			665	424	124	115	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-FMET.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AC	77	Total	C	N	O	P	0	0	0
			1640	732	298	534	76			
22	CC	77	Total	C	N	O	P	0	0	0
			1640	732	298	534	76			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AC	17A	C	U	CONFLICT	GB AP008226.1
AC	50	U	C	CONFLICT	GB AP008226.1
AC	51	C	G	CONFLICT	GB AP008226.1
AC	63	G	C	CONFLICT	GB AP008226.1
CC	17A	C	U	CONFLICT	GB AP008226.1
CC	50	U	C	CONFLICT	GB AP008226.1
CC	51	C	G	CONFLICT	GB AP008226.1
CC	63	G	C	CONFLICT	GB AP008226.1

- Molecule 23 is a RNA chain called MRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	A1	4	Total	C	N	O	P	0	0	0
			85	38	14	29	4			
23	C1	4	Total	C	N	O	P	0	0	0
			85	38	14	29	4			

- Molecule 24 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	BA	2912	Total	C	N	O	P	0	0	0
			62707	27911	11722	20163	2911			
24	DA	2909	Total	C	N	O	P	0	0	0
			62647	27884	11716	20139	2908			

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	158	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 25 is a RNA chain called 5S RIBOSOMAL RNA.

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

- Molecule 26 is a protein called 50S ribosomal protein L2.

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

- Molecule 27 is a protein called 50S ribosomal protein L3.

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

- Molecule 28 is a protein called 50S ribosomal protein L4.

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

- Molecule 29 is a protein called 50S ribosomal protein L5.

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

- Molecule 30 is a protein called 50S ribosomal protein L6.

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

- Molecule 31 is a protein called 50S ribosomal protein L9.

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

- Molecule 32 is a protein called 50S ribosomal protein L13.

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

- Molecule 33 is a protein called 50S ribosomal protein L14.

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

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

- Molecule 34 is a protein called 50S ribosomal protein L15.

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

- Molecule 35 is a protein called 50S ribosomal protein L16.

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

- Molecule 36 is a protein called 50S ribosomal protein L17.

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

- Molecule 37 is a protein called 50S ribosomal protein L18.

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

- Molecule 38 is a protein called 50S ribosomal protein L19.

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

- Molecule 39 is a protein called 50S ribosomal protein L20.

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

- Molecule 40 is a protein called 50S ribosomal protein L21.

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

- Molecule 41 is a protein called 50S ribosomal protein L22.

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

- Molecule 42 is a protein called 50S ribosomal protein L23.

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

- Molecule 43 is a protein called 50S ribosomal protein L24.

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

- Molecule 44 is a protein called 50S ribosomal protein L25.

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

- Molecule 45 is a protein called 50S ribosomal protein L27.

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

- Molecule 46 is a protein called 50S ribosomal protein L28.

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

- Molecule 47 is a protein called 50S ribosomal protein L29.

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

- Molecule 48 is a protein called 50S ribosomal protein L30.

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

- Molecule 49 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	B4	66	Total	C	N	O	S	0	0	0
			533	335	96	97	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	D4	63	Total	C	N	O	S	0	0	0
			515	326	93	91	5			

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

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

- Molecule 51 is a protein called 50S ribosomal protein L33.

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

- Molecule 52 is a protein called 50S ribosomal protein L34.

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

- Molecule 53 is a protein called 50S ribosomal protein L35.

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

- Molecule 54 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	BA	627	Total	Mg	0	0
			627	627		
54	CA	204	Total	Mg	0	0
			204	204		

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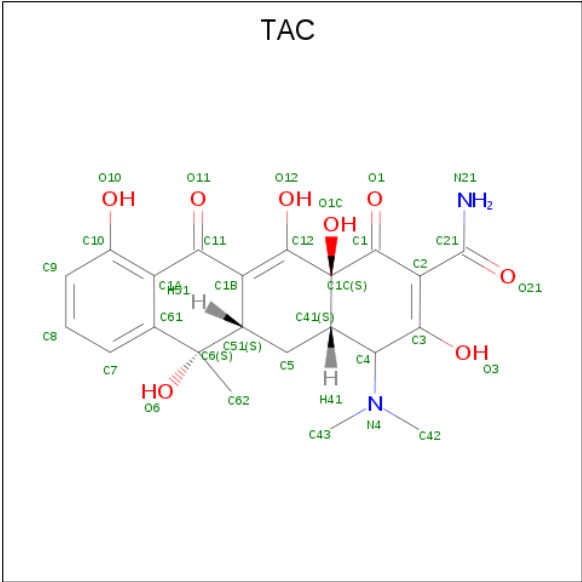
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	CH	1	Total 1	Mg 1	0	0
54	DZ	2	Total 2	Mg 2	0	0
54	B8	1	Total 1	Mg 1	0	0
54	BE	5	Total 5	Mg 5	0	0
54	DU	1	Total 1	Mg 1	0	0
54	B1	2	Total 2	Mg 2	0	0
54	BP	1	Total 1	Mg 1	0	0
54	AS	1	Total 1	Mg 1	0	0
54	B5	2	Total 2	Mg 2	0	0
54	BB	17	Total 17	Mg 17	0	0
54	AJ	1	Total 1	Mg 1	0	0
54	BF	2	Total 2	Mg 2	0	0
54	DR	1	Total 1	Mg 1	0	0
54	B2	1	Total 1	Mg 1	0	0
54	AA	232	Total 232	Mg 232	0	0
54	AR	1	Total 1	Mg 1	0	0
54	B6	1	Total 1	Mg 1	0	0
54	CG	2	Total 2	Mg 2	0	0
54	BU	2	Total 2	Mg 2	0	0
54	A1	1	Total 1	Mg 1	0	0
54	DD	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	CC	8	Total 8	Mg 8	0	0
54	DE	3	Total 3	Mg 3	0	0
54	B3	2	Total 2	Mg 2	0	0
54	DA	525	Total 525	Mg 525	0	0
54	B7	3	Total 3	Mg 3	0	0
54	AG	2	Total 2	Mg 2	0	0
54	BO	3	Total 3	Mg 3	0	0
54	AQ	2	Total 2	Mg 2	0	0
54	D1	1	Total 1	Mg 1	0	0
54	AH	2	Total 2	Mg 2	0	0
54	BZ	1	Total 1	Mg 1	0	0
54	AC	9	Total 9	Mg 9	0	0
54	D5	1	Total 1	Mg 1	0	0
54	DP	1	Total 1	Mg 1	0	0
54	CS	1	Total 1	Mg 1	0	0
54	DB	14	Total 14	Mg 14	0	0

- Molecule 55 is TETRACYCLINE (three-letter code: TAC) (formula: $C_{22}H_{24}N_2O_8$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
55	AA	1	Total	C	H	N	O	0	0
			33	22	1	2	8		
55	CA	1	Total	C		N	O	0	0
			32	22		2	8		

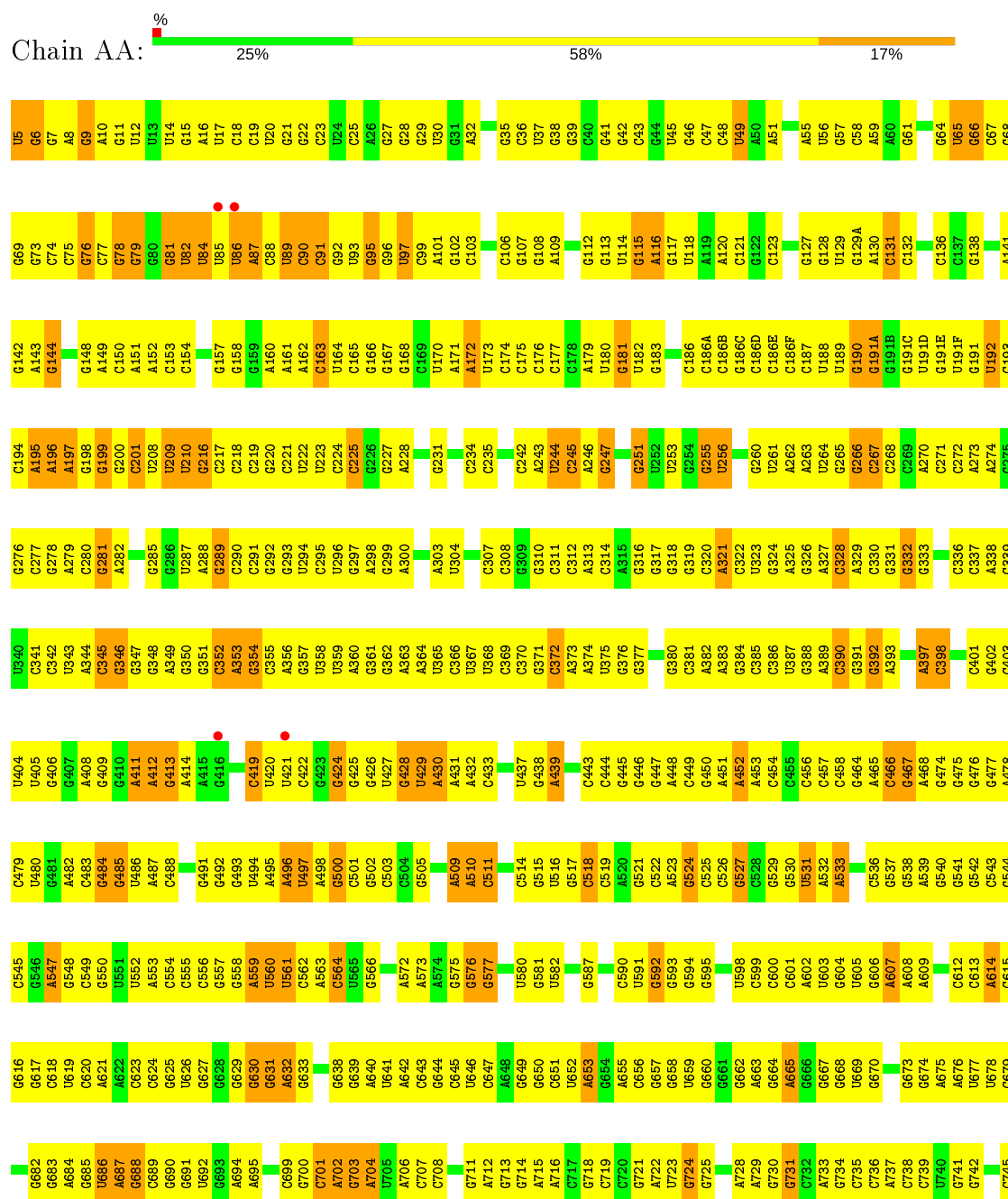
- Molecule 56 is ZINC ION (three-letter code: ZN) (formula: Zn).

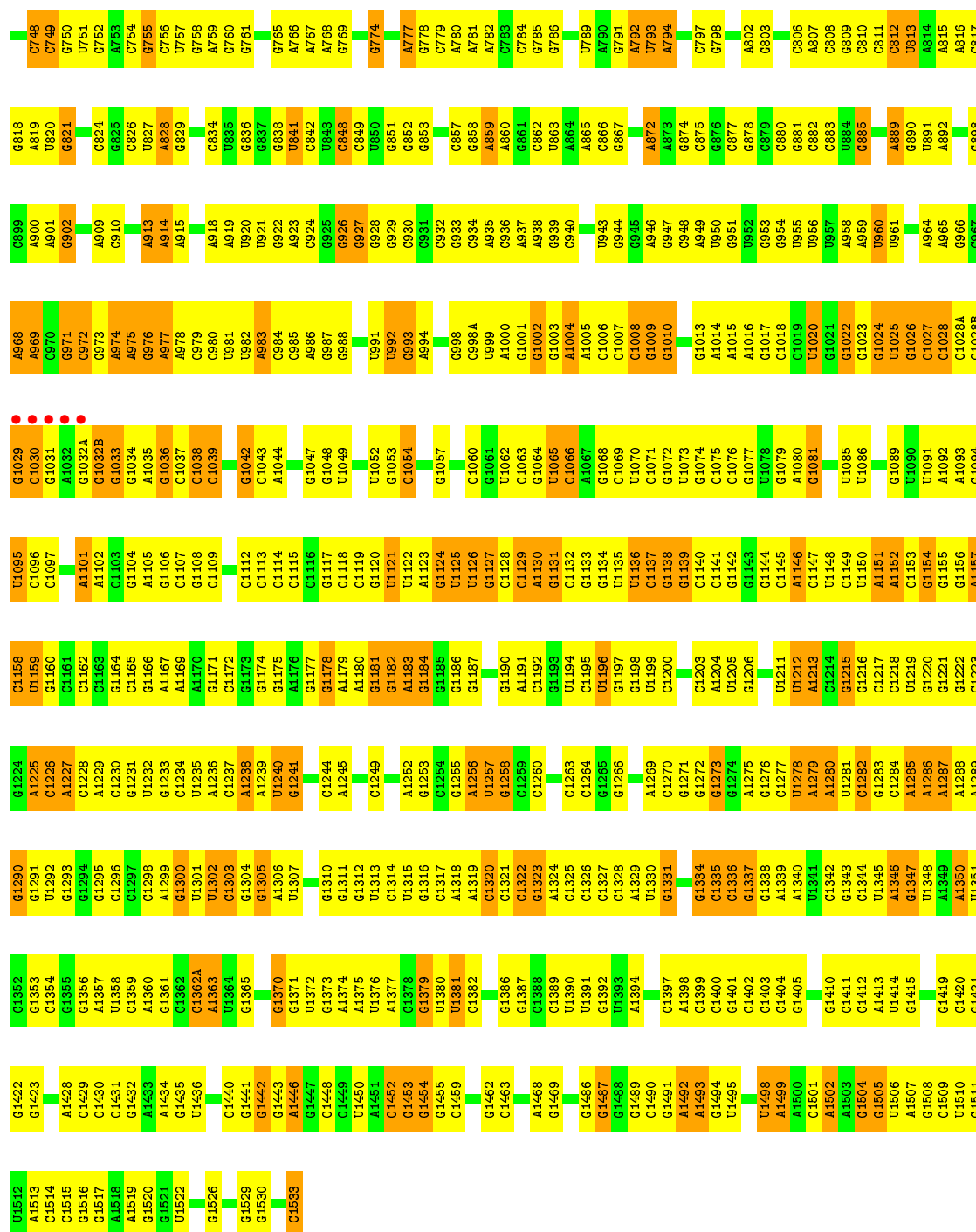
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	AG	1	Total	Zn	0	0
			1	1		
56	AQ	1	Total	Zn	0	0
			1	1		
56	CQ	1	Total	Zn	0	0
			1	1		
56	CG	1	Total	Zn	0	0
			1	1		

3 Residue-property plots

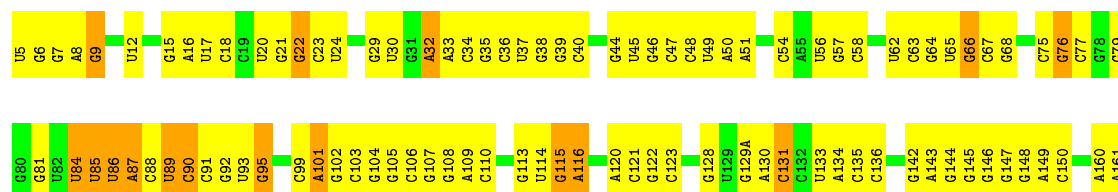
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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

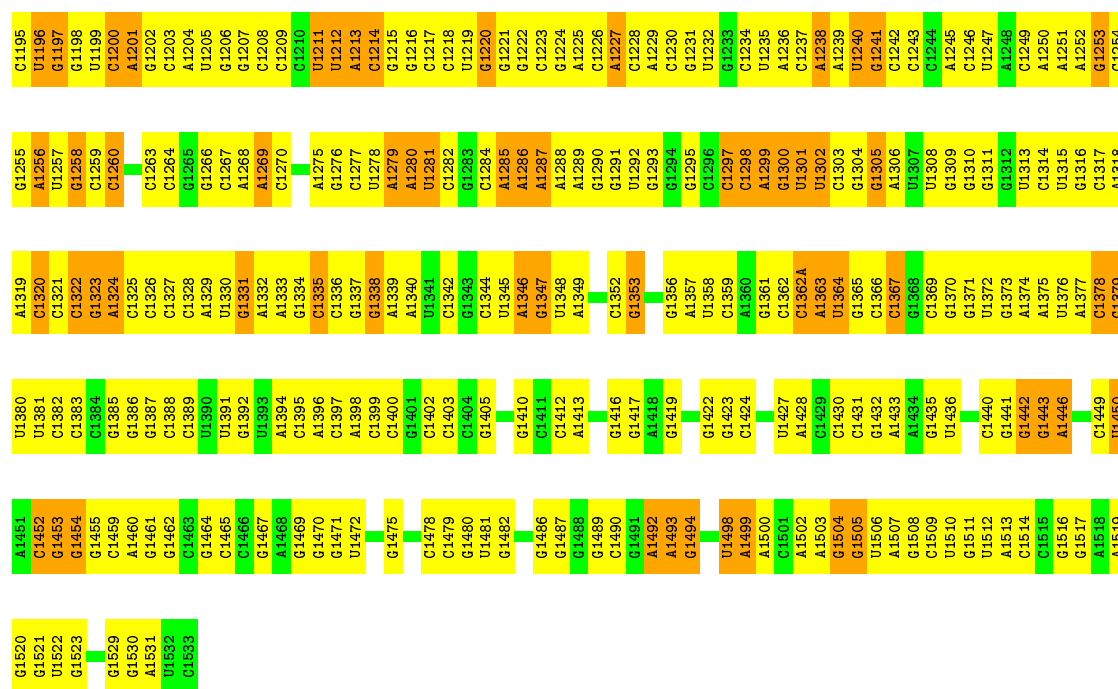




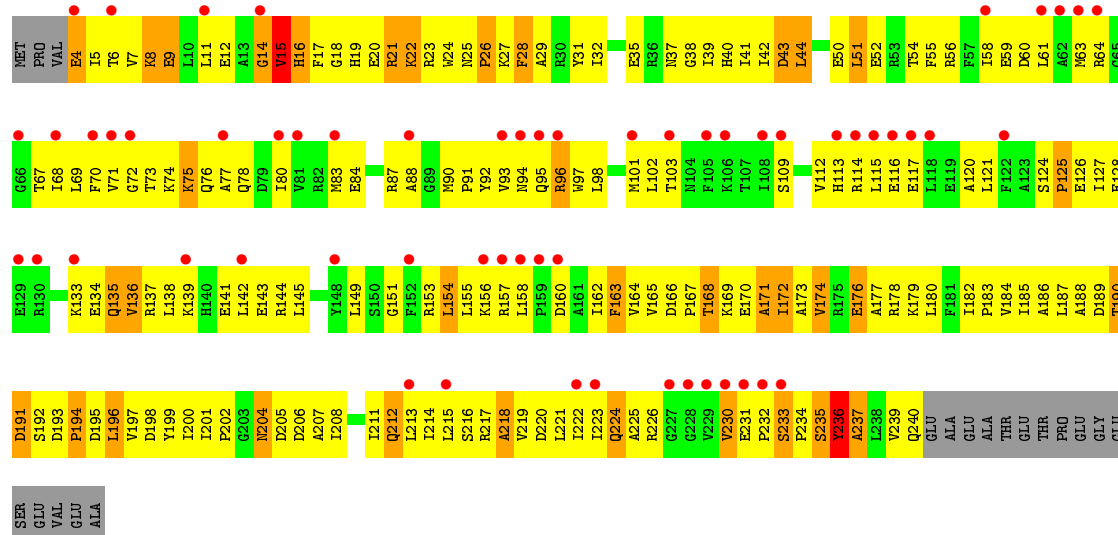
Molecule 1: 16S ribosomal RNA



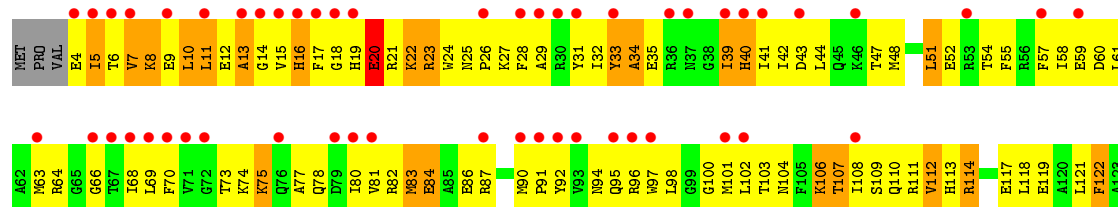
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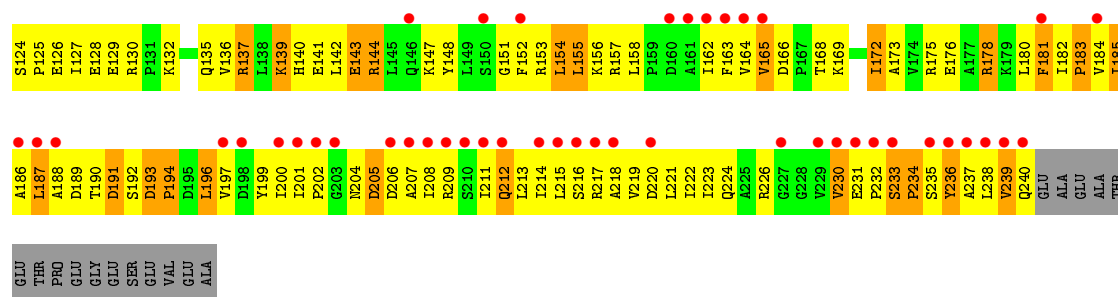


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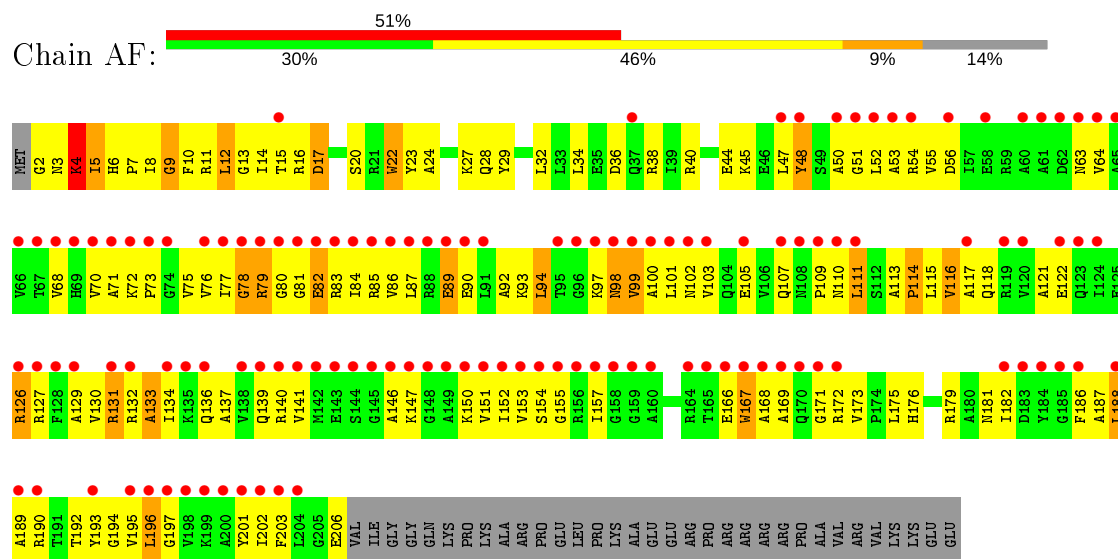


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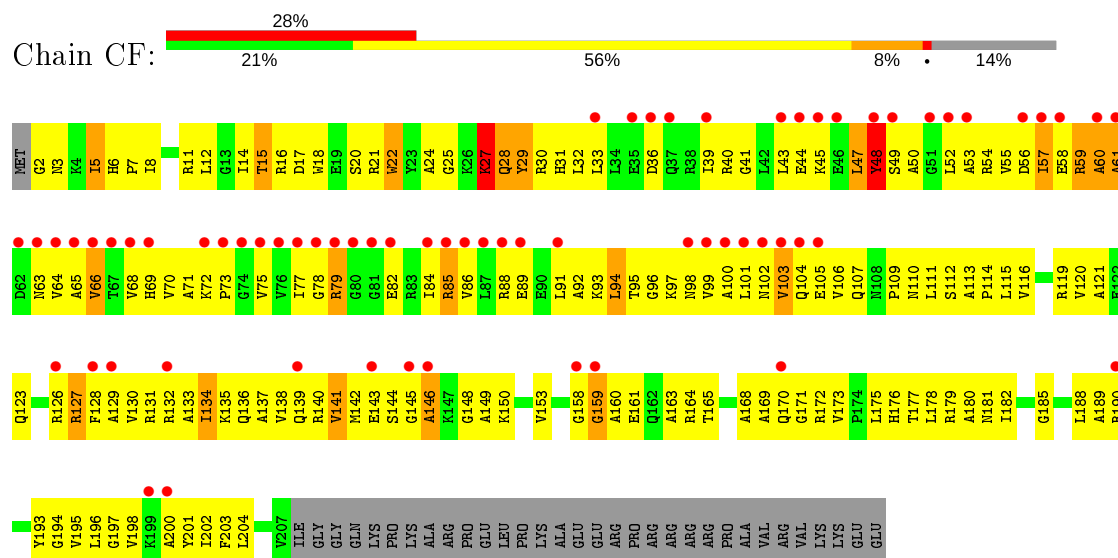




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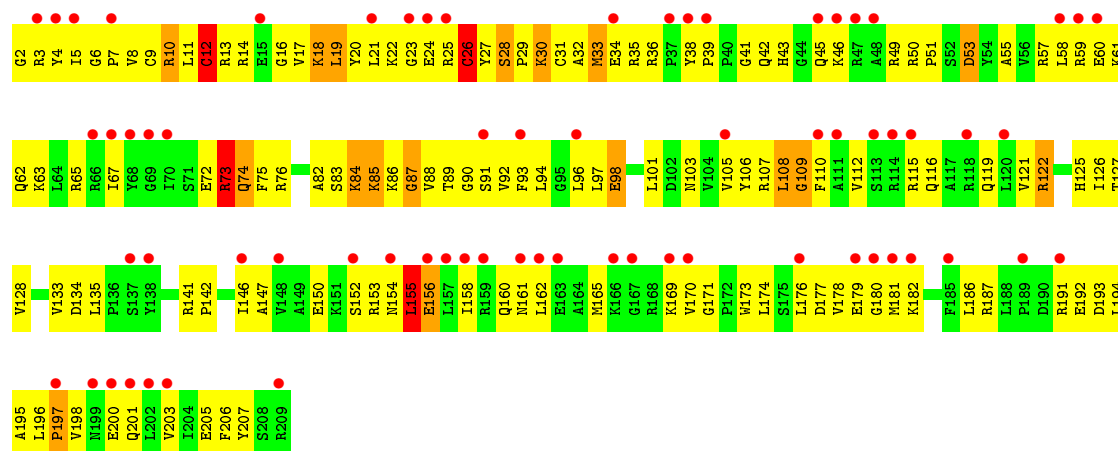


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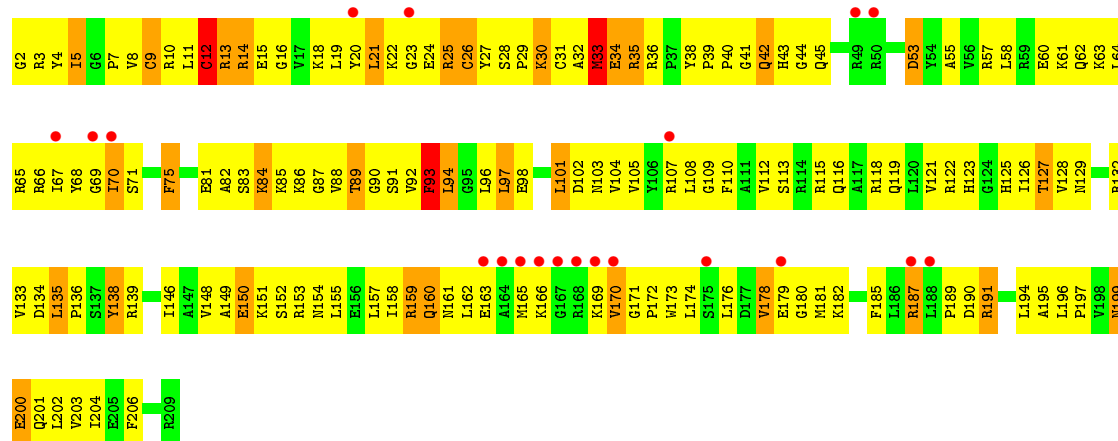


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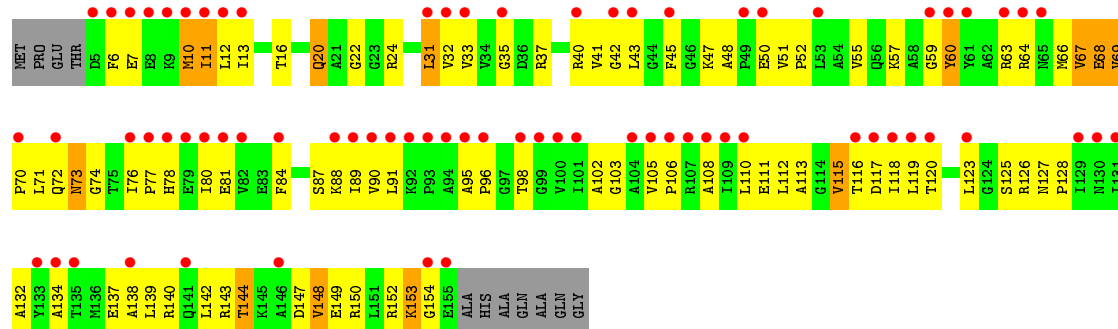




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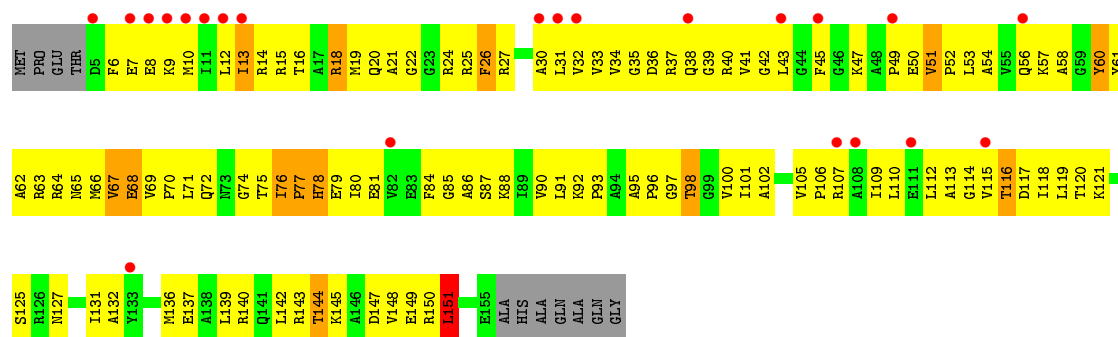


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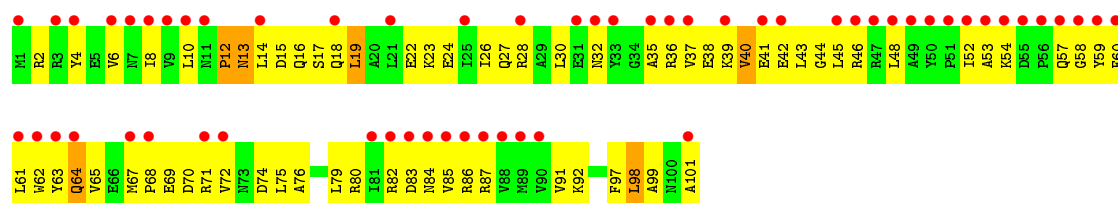


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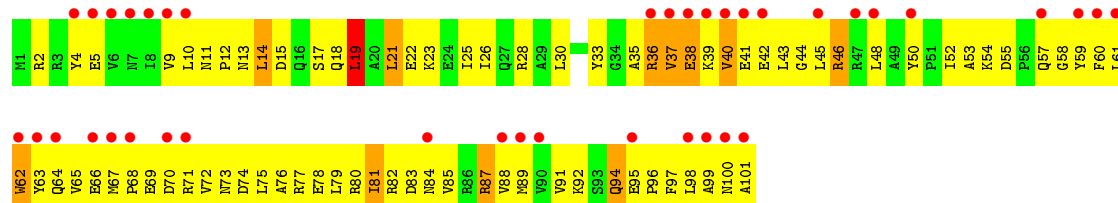




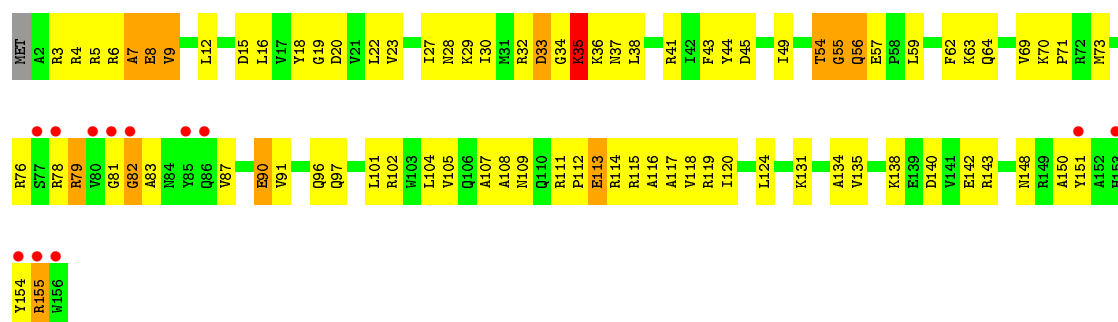
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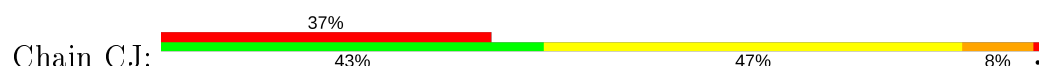
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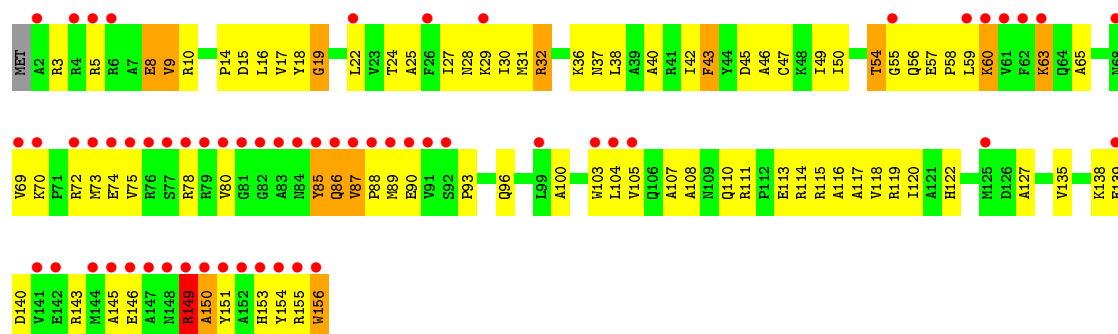


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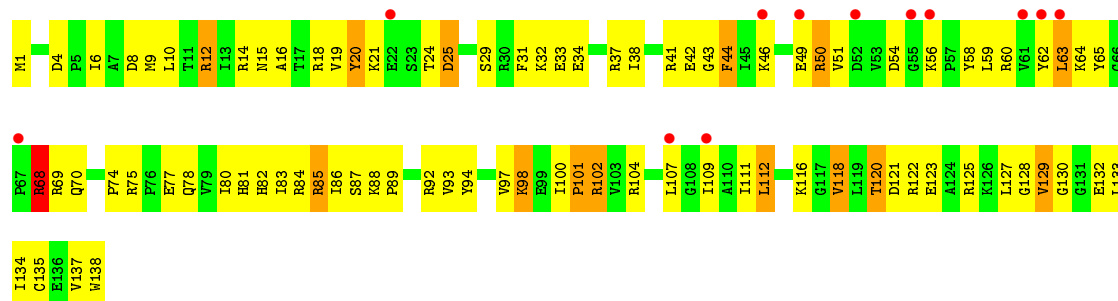


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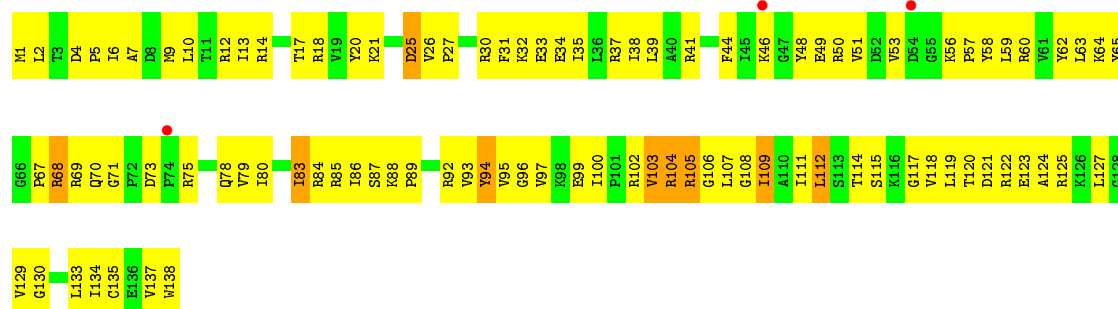




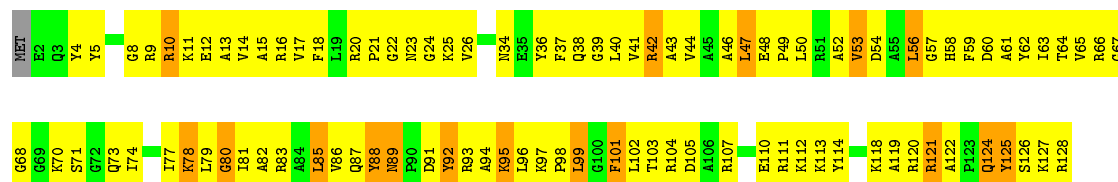
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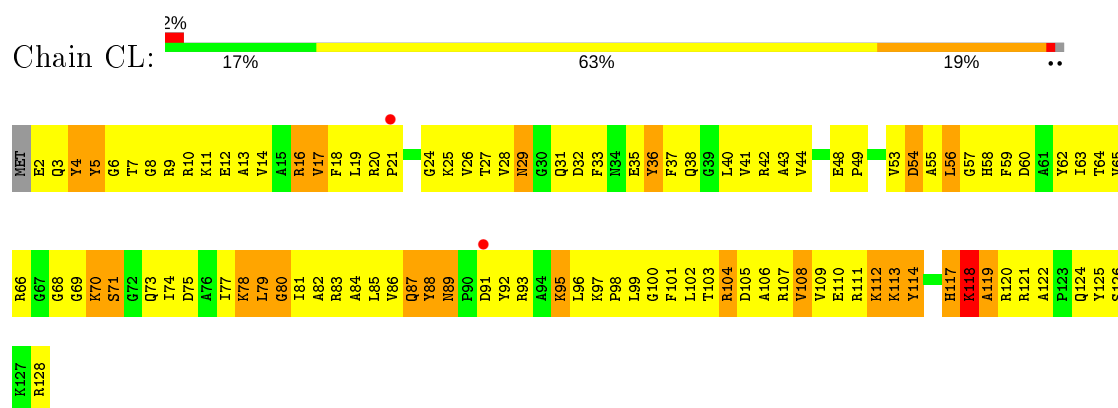
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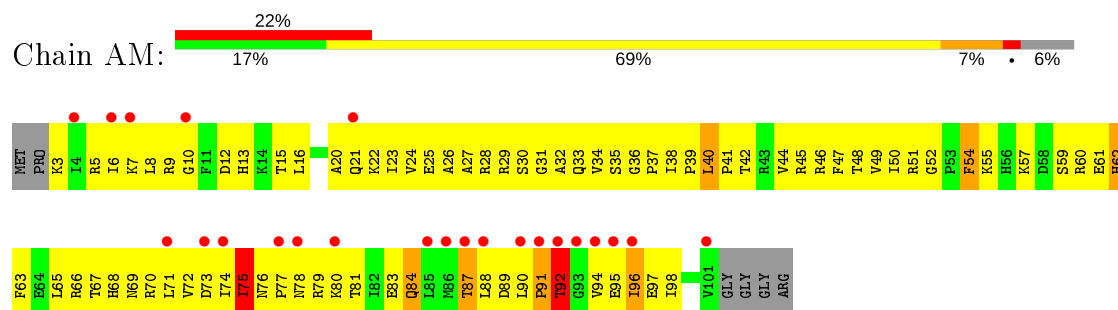
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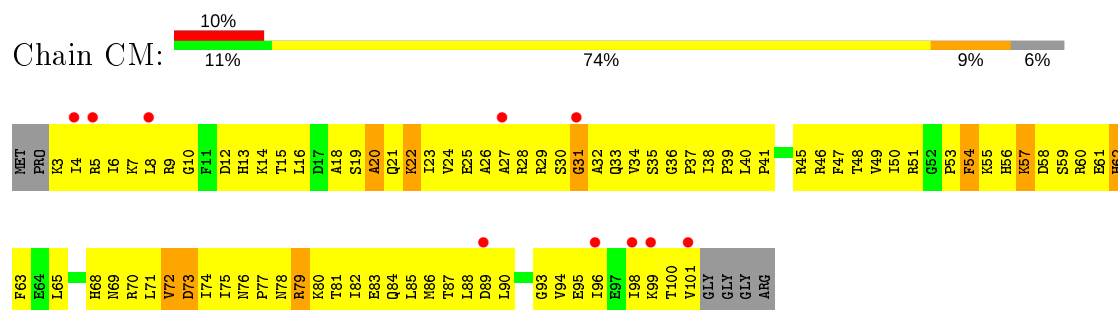
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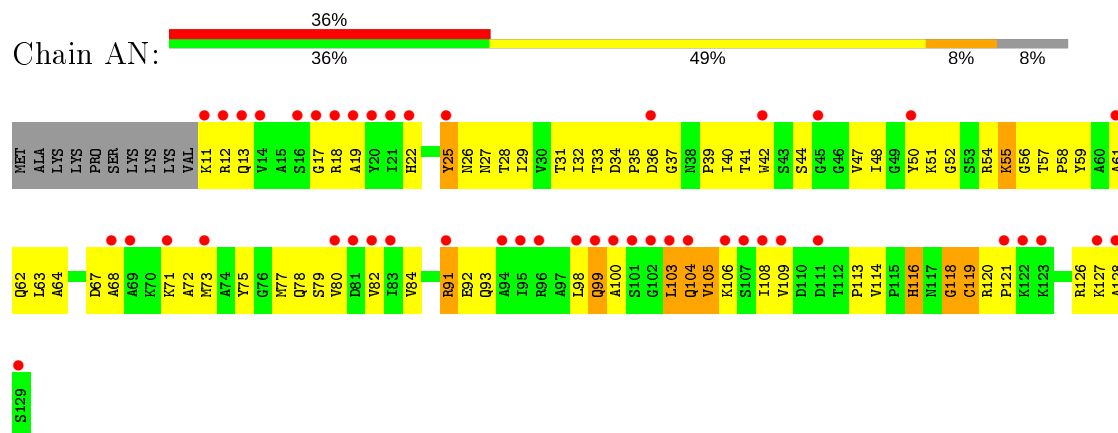
• Molecule 10: 30S RIBOSOMAL PROTEIN S10



• Molecule 10: 30S RIBOSOMAL PROTEIN S10



• Molecule 11: 30S RIBOSOMAL PROTEIN S11



• Molecule 11: 30S RIBOSOMAL PROTEIN S11

ALA
PRO
ARG
LYS

• Molecule 14: 30S RIBOSOMAL PROTEIN S14



MET A2 R3 R4 A5 L6 I7 E8 K9 K10 K11 R12 R13 T13 P14 K15 K16 F16 K17 V18 Y21 Y22 R23 C24 V25 V26 C27 G28 R29 S32 V33 Y34 R35 F36 F37 G38 L39 C40 R41 I42 C43 R44 R45 H49 Q52 L53 P54 G55 V56 R57 K58 A59 S60 W61

• Molecule 14: 30S RIBOSOMAL PROTEIN S14



MET A2 R3 R4 A5 L6 I7 E8 K9 K10 K11 R12 R13 T13 P14 K15 K16 F16 K17 V18 Y21 Y22 R23 C24 V25 V26 C27 G28 R29 S32 V33 Y34 R35 F36 F37 G38 L39 C40 R41 I42 C43 R44 R45 H49 Q52 L53 P54 G55 V56 R57 K58 A59 S60 W61

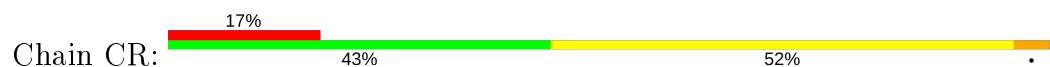
• Molecule 15: 30S RIBOSOMAL PROTEIN S15



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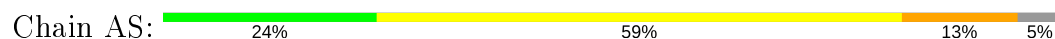
• Molecule 15: 30S RIBOSOMAL PROTEIN S15



MET F2 I3 T4 E6 E7 K8 V11 V12 F15 A16 A17 F18 F19 D20 D21 T22 G23 D24 T25 E26 V27 Q28 V29 A30 L31 L32 T33 I34 R35 R36 R37 R38 L39 H42 L43 K47 K48 H51 S52 H53 H54 G55 L56 L57 H58 H59 V60 V61 Q62 Q63 R64 R65 R66 L67 R68 R69 L70 Q71

R72 E73 D74 E75 E76 E77 Y78 L81 R82 R83 R84 R85 R86 R87 R88 R89

• Molecule 16: 30S RIBOSOMAL PROTEIN S16

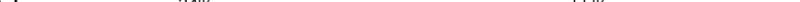


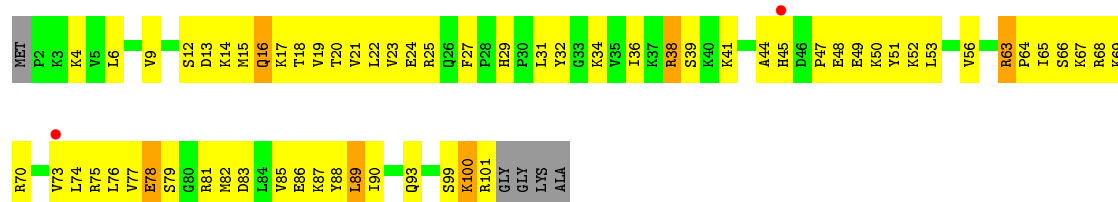
K1 V2 K3 T4 R5 L6 A7 F9 G10 N14 P15 H16 I17 R18 R19 V20 V21 T22 D23 D24 A25 R26 K27 R28 D29 G30 R31 Y32 I33 E34 R35 I36 G37 Y38 Y39 D40 P41 R42 R43 T44 T45 P46 D47 W48 L49 K50 V51 D52 V53 E54 R55 A56 R57 L60 S61 V62 L63

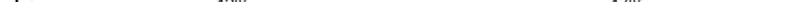
A64 Q65 P66 T67 D68 T69 A70 R71 R72 L73 L74 A77 G78 G79 F80 R81 Q82 E83 A84 ARG GLU GLY ALA

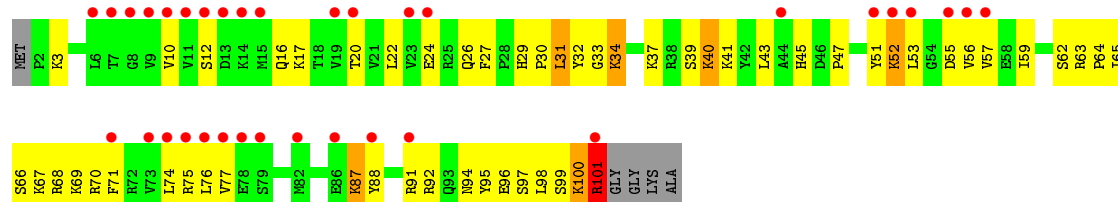
• Molecule 16: 30S RIBOSOMAL PROTEIN S16

D68	M1
T69	V2
A70	K3
R71	I4
R72	B5
L73	L6
	A7
Q76	R8
A77	F9
G78	G10
V79	S11
F80	K12
B81	H13
Q82	M14
E83	P15
A84	H16
ARG	V17
GLU	R18
GLY	
ALA	V21
	T22
	D23
	A24
	R25
	K27
	R28
	D29
	G30
	I33
	G37
	D40
	P41
	R42
	T45
	P46
	D47
	H48
	L49
	K50
	V51
	D52
	V53
	E54
	R55
	A56
	R57
	Y58
	S61
	V62
	G63
	A64
	D65
	P66
	T67

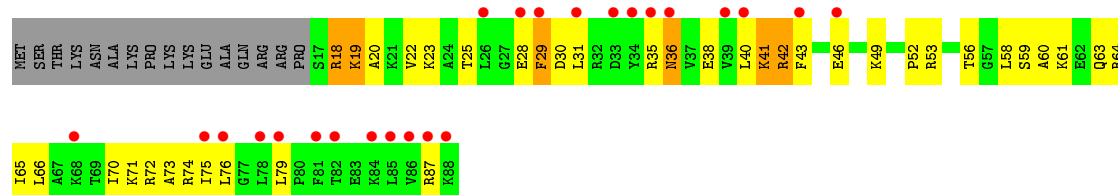
Chain AT: 

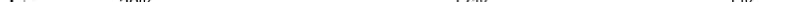


Chain CT: 



Chain AU: 27% 38% 38% 7% 18%

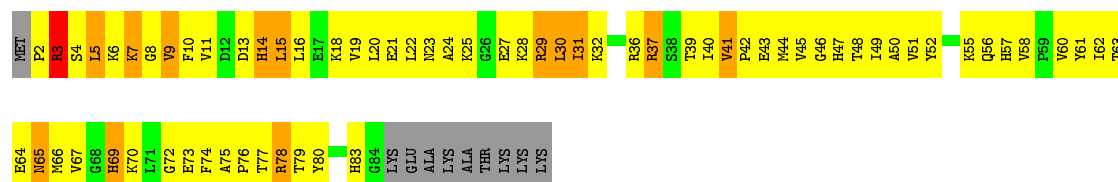


Chain CU: 




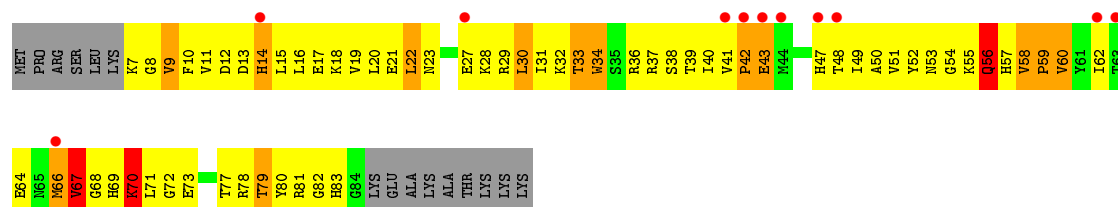
- Molecule 19: 30S RIBOSOMAL PROTEIN S19

Chain AV: 



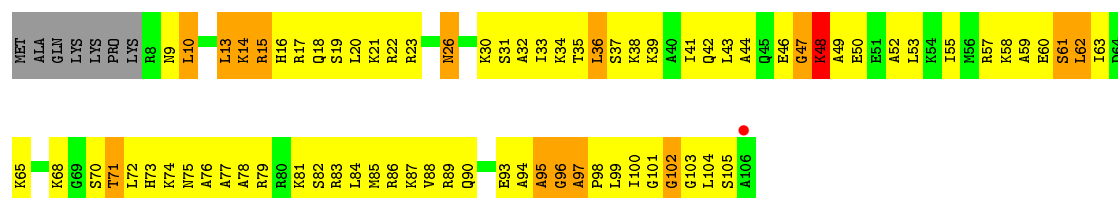
- Molecule 19: 30S RIBOSOMAL PROTEIN S19

Chain CV: 



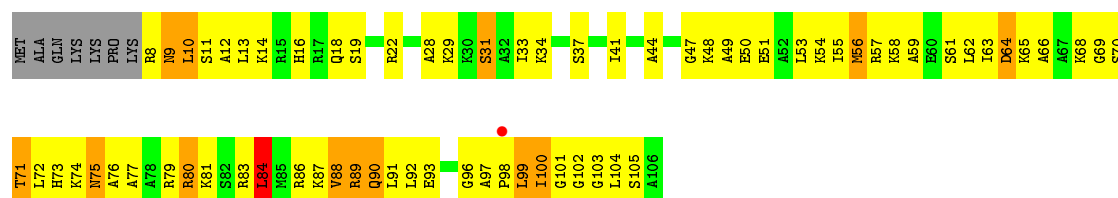
- Molecule 20: 30S RIBOSOMAL PROTEIN S20

Chain AW: 



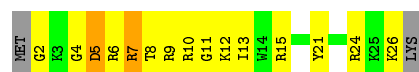
- Molecule 20: 30S RIBOSOMAL PROTEIN S20

Chain CW: 



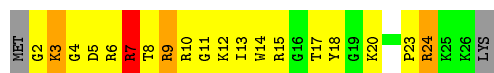
- Molecule 21: 30S RIBOSOMAL PROTEIN THX

Chain AX: 



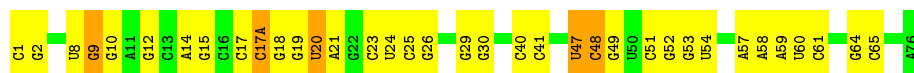
- Molecule 21: 30S RIBOSOMAL PROTEIN THX

Chain CX:  22% 56% 11% 7%




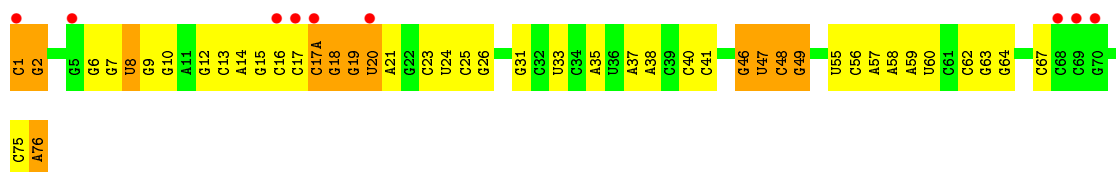
- Molecule 22: TRNA-FMET

Chain AC:  53% 40% 6%



- Molecule 22: TRNA-FMET

Chain CC:  12% 42% 43% 16%



- Molecule 23: MRNA

Chain A1:  50% 50%

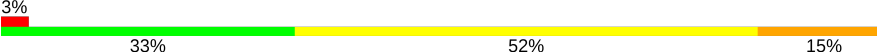


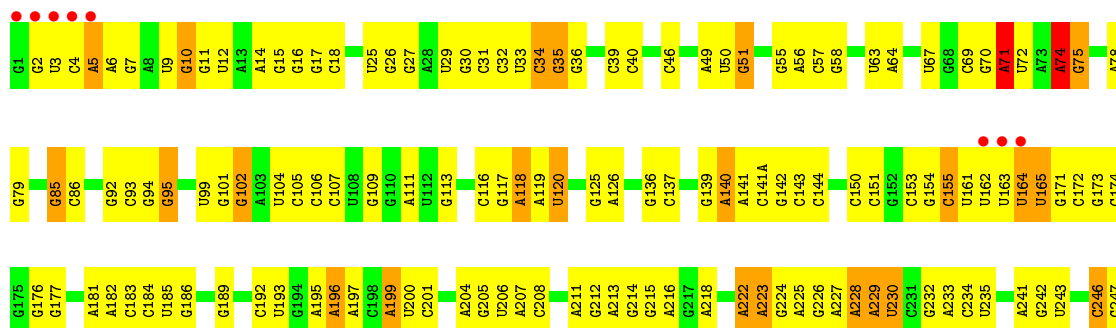
- Molecule 23: MRNA

Chain C1:  50% 50%



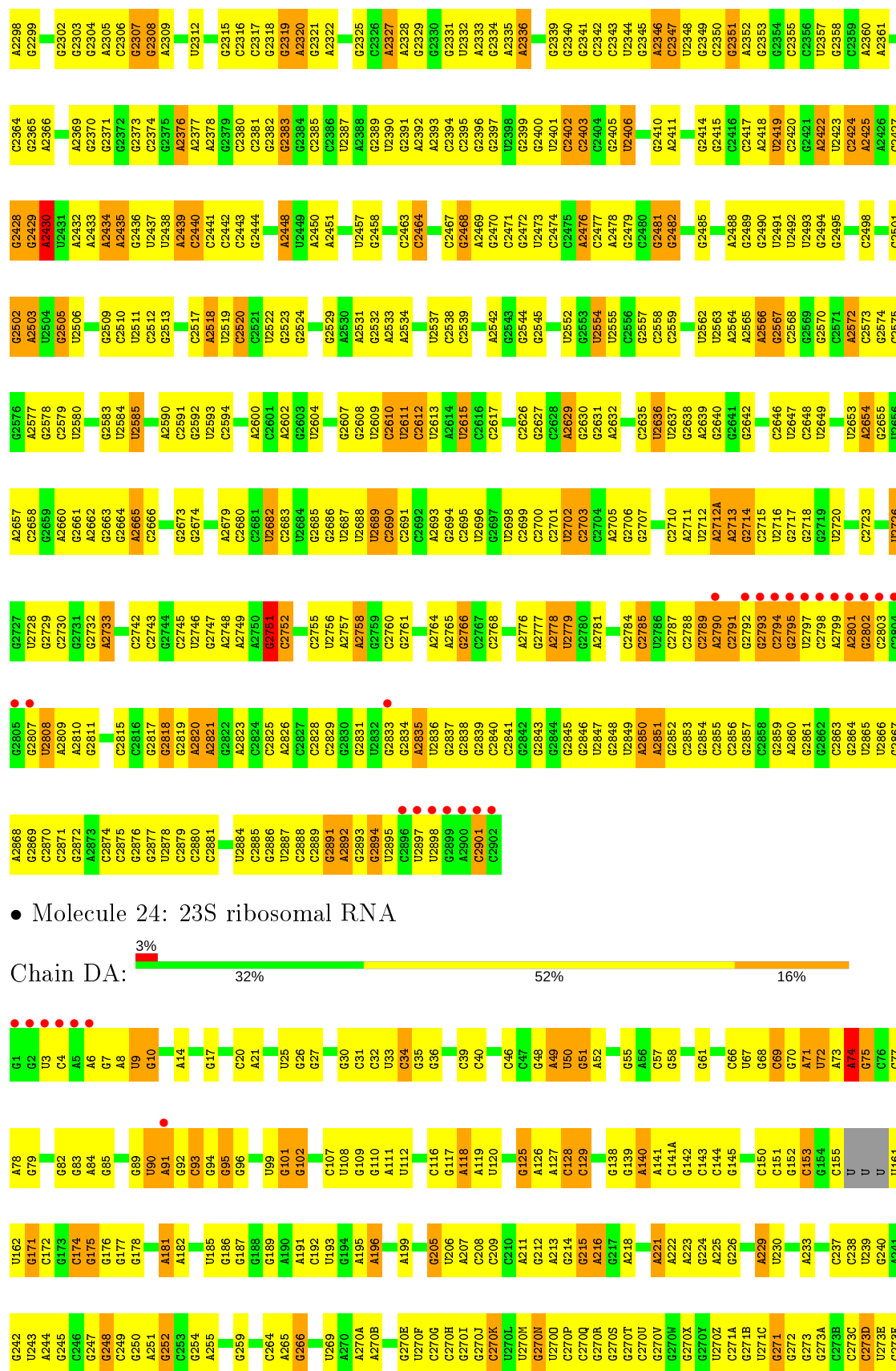
- Molecule 24: 23S ribosomal RNA

Chain BA:  3% 33% 52% 15%



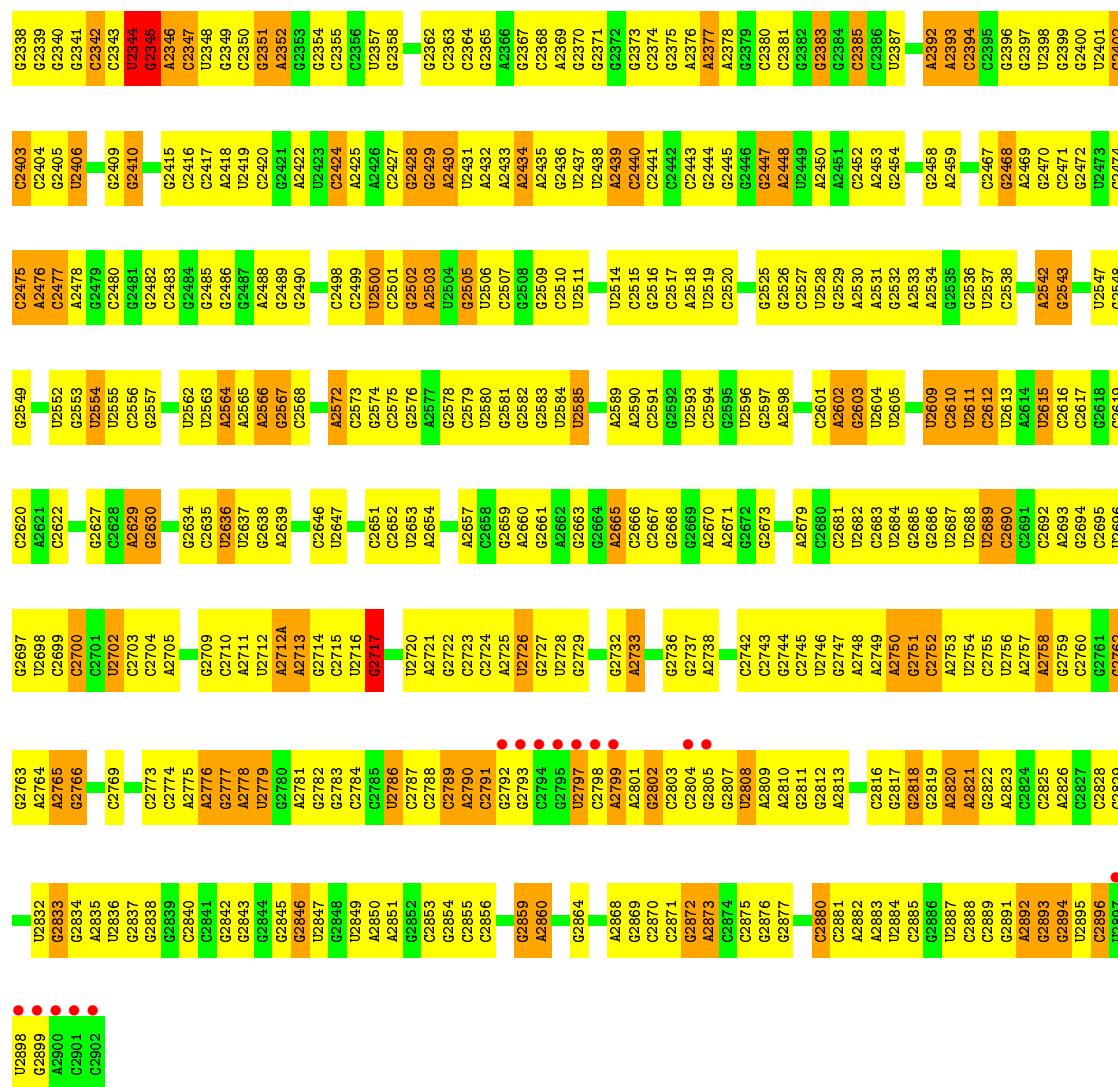
G1195	A1129	U1065	G997	G926	G859	G792	G728	G654Q	U606	A529	U459	G370	C296	G248
G1201	U1130	U1066	C998	G928	U860	A793	G729	G654P	U607	G530	A460	G371	C297	C249
G1202	G1132	A1067	U999	G929	A863	G794	C730	C654Q	A608	C531	C462	A371	G298	C250
G1203	U1133	G1068	A1000	U930	C865	C795	G733	G654R		A532	G463		G299	A251
G1204	C1135	A1069	A1001	G931	C865	C796	G734	G654T	G611	G534	U383	U384	A300	G252
G1205	G1136	A1070	G1002	G932	C866	C797	A735	A654U	G612	U534	U464	U385	G301	C253
G1206	G1137	G1071	G1003	A933	A866	G798	C736	A654V	U613	C535	C465	C386	C302	G254
G1207	G1138	C1072	C1004	G938	C867	G799	C737	A654W	G614	C537	A466	G387	U303	
G1208	G1139	A1073	C1005		U868	G801	G738	G656	G615	G539	G467	U388	U304	G259
G1209	C1140	G1074	G1006	A941	G869	A802	G739	G656	A616	G540	G468	U389	U305	G260
G1210	U1141	C1075		U942	G873	G805	U740	G658	G617	C541	G469	G307	U306	G261
G1211	U1142	A1076	A1009	U943	G874	C806	U741	C659	G618		A470	A394	G308	A265
G1212	A1142A	U1077	A1010	U944	G875	C806	G742	G660	G618A	G545	A471	U395	G309	G266
G1213	A1143	C1079	G1011	G945	C876	U807	G743	G661	G619	C546	A472	U396	G310	
	G1144	A1080	C1012	G946	U877	G808	G744	G662	G620	A547	G473	G396	A311	U270F
G1216	C1145	U1081	C1013	G947	A878	G809	G745	G663	A621	A548	U475		A314	C270G
	C1146	U1082	G1014		G879	U810	A746		G622		G476	C404	G315	C270H
A1220	C1147	U1083		G950	G880	U811	U747	U667	G625	G552	A477	G406	G270I	G270J
C1221	A1148	A1084	C1018	C951	G881	C812	G748		U626	U553	A478		G320	C270K
C1222	G1149	A1085	U1019	G952	G882	U813	C749	C671	A627	U554	A479	G411	G321	G270L
G1223	A1086	A1020	A953	G953	G883	C814	A750	C672	G628	G556	A480	A412	G322	U270M
G1224	G1087	A1021	G954	G954	C884	C815	A751	C673	G629	U557	G481	C413	G323	G270N
G1225	C1152	A1088	G955	C955	C885	C816	A752	G674	G630	G558	A482	C414	G324	
G1226	C1153	G1089	G956	G956	C886	C817	C753	A675	G631	G559	A483	A415	A324	U270O
A1227	G1154	U1090	A957	A957	A887	G818	C754	A676	A632		C484	C416	G325	C270P
G1228	A1155	G1091	U958	U958	C888	A819	C755		A633	G563		C417	G326	C270Q
		C1092	A959	A959	C889	A820	C756		G634	C564	G488		G329	G270R
C1236	G1161	U1093	A960	A960	A821	G880	C757		C635	C565	A491	U421	C420	G270S
A1237	C1162	U1094	G961	G961	U822		G760		G636	U566	A492	A422	A330	G270T
G1238	G1163	A1095	G962	G962	C893		A761	C683	A637		C493	A423	C270U	C270V
G1239	G1164	A1096	U963		C894		U762	C684	G638	U569	C494	G424	C335	G270W
U1240	U1165	U1097		G968	U895		G763	C685	U639	G570	G495	G425	C336	G270X
A1241	C1166	A1098	G1034	U969	A896		A764	C686	C640	A571		G426	C337	G270Y
A1242	U1167	G1099	U1035	G970	C897		G765	C687	G641	A572			G338	U270Z
G1243	G1036	C970	G1036	C970	C898		C766	U688	G642	G573	G500	U427	U339	C271A
G1244	U1010	G1037	G1037	C971	A899		U767	A643	A644	C574	A501	A428	A340	G271B
G1245	G1170	C1102	C1038	G972	A900		G768		A645	A575	A502		G341	G271C
A1246	G1171	A1103	G1039	A973	A901		G769	C692	C646	G579	U503	U431	G342	G271D
G1247	G1173	C1104		G974	C902		G770	C693	A646	C580	U504		G343	G271E
G1248	U1105	G1104	G1044	C975	C903		C771	U694	G647	C581	G505	G438	G344	G272
U1249	U1106	A1045	A1045	G975	C904		U773		G651	G582	A507	G440		G273
G1250	G1107	G1046	G1046	C976	U905		A774	C698			G508	U441	G352	G273A
C1251	U1108	U1047	G1047	G977	G906		G775	A705	A653	A586	C509	G442		U273B
G1252	C1109	C1109	A1048	G978	U907		C776	A706	A654	C587	U510	A443	G355	U273C
A1253	G1179	G1110	C1049	G979	C908		G777		A654A	U588	U511	C444	G356	C273F
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G1256	C1181	G1112	G1051		A910		U779	G713	G654C	A590	A513		A359	A275
C1257	A1182	U1113		A983	A911				G654D	C591	A514	U448	G359	A276
G1258	G1183	G1114		A984	C912			G717	G654E	G592		A449	G360	C277
C1259	G1115	C1116		C985			A782	A718	C654F	G593	A515	A450	U362	A278
G1260	G1056	G986	C915	G986	C916		A783	A719	G654G	G594	C517	G451	G363	C279
C1261	A1057	G987	G916	G987	A849		A784		A654H	U594		G452	A363A	C285
A1262	U1058	A988	A917	A988	C850		G785	C721	G654I	C601	C523	G453	G363B	C286
U1263	C1123	G1059	U851	G989	U851		C786	A722	C654J	G602	U524	G454	G363C	C287
G1264	C1124	G919			G919		U787	G723	C654K	G603		A455	G363D	C288
A1265	G1125	U1061		G993	G920		A788	U724	C654L	G604		A456	G363E	A289
G1266	A1126	G1062		C994	G920		A789	G725	G654M	A603		C457	U363F	C290
U1267	G1192	C995		C994	C924		C790	G726	G654N	G605			A363F	
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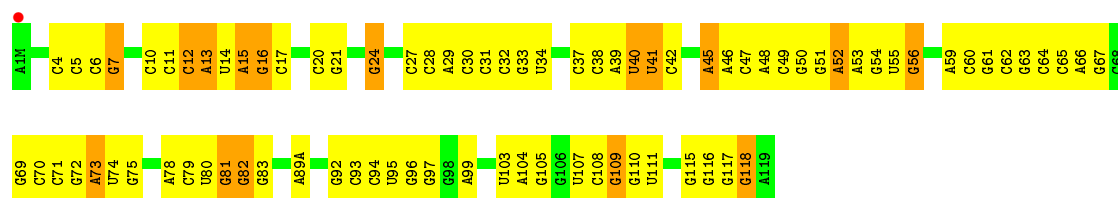


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• Molecule 25: 5S RIBOSOMAL RNA

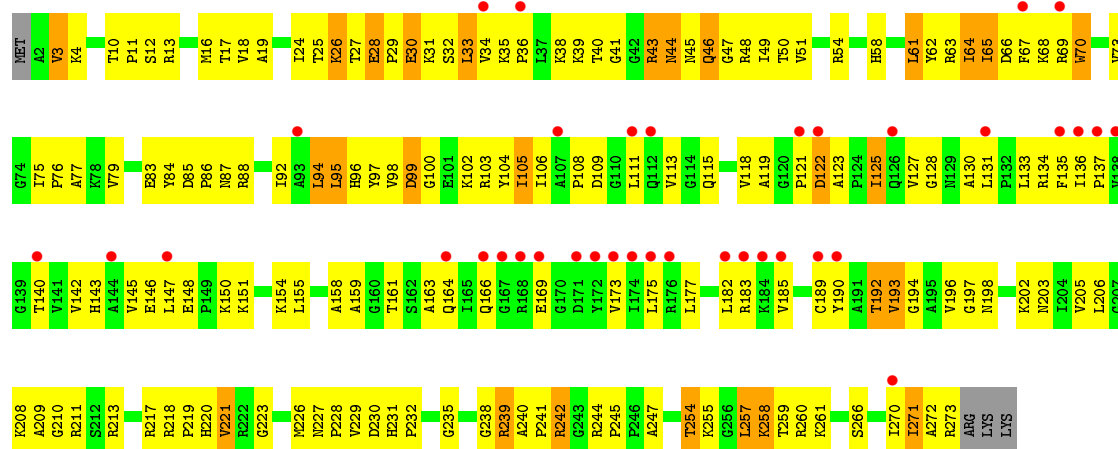


• Molecule 25: 5S RIBOSOMAL RNA

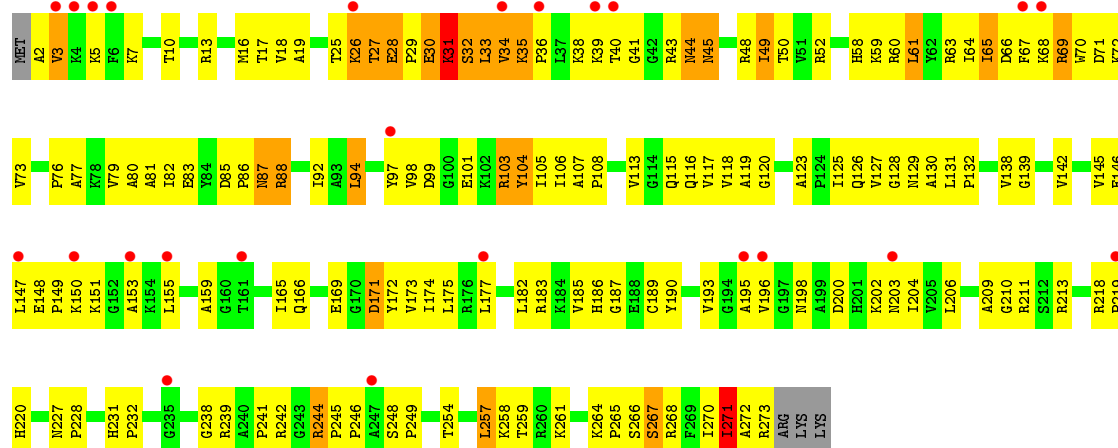
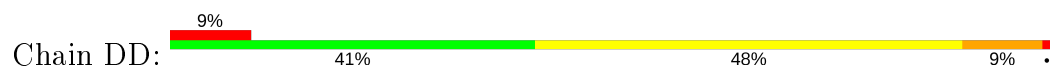




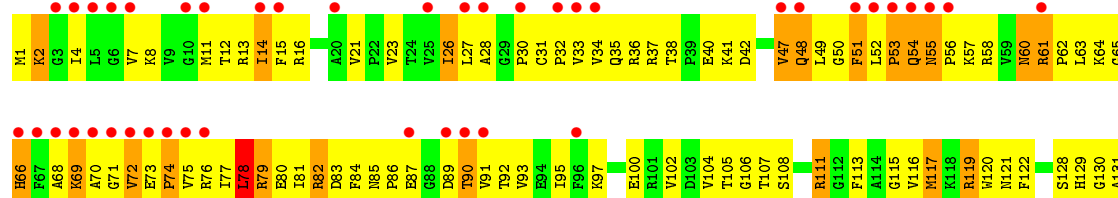
• Molecule 26: 50S ribosomal protein L2



• Molecule 26: 50S ribosomal protein L2

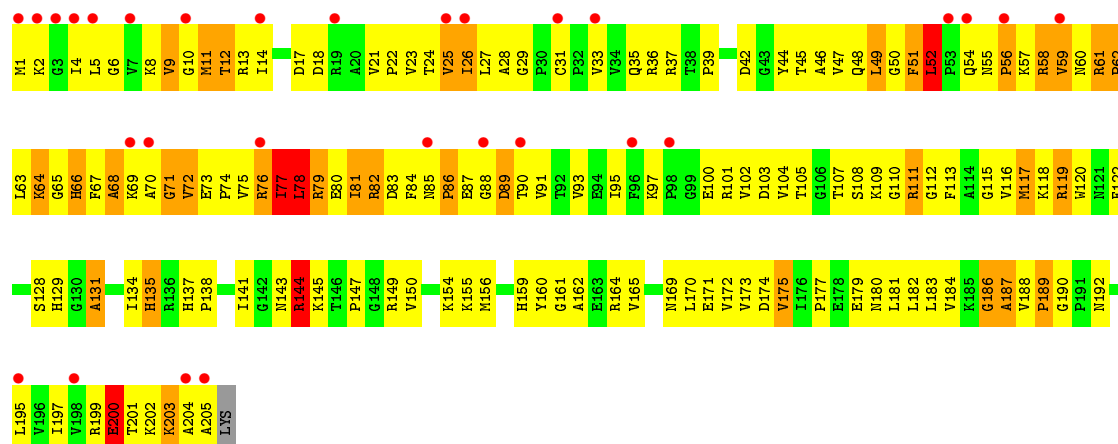


• Molecule 27: 50S ribosomal protein L3

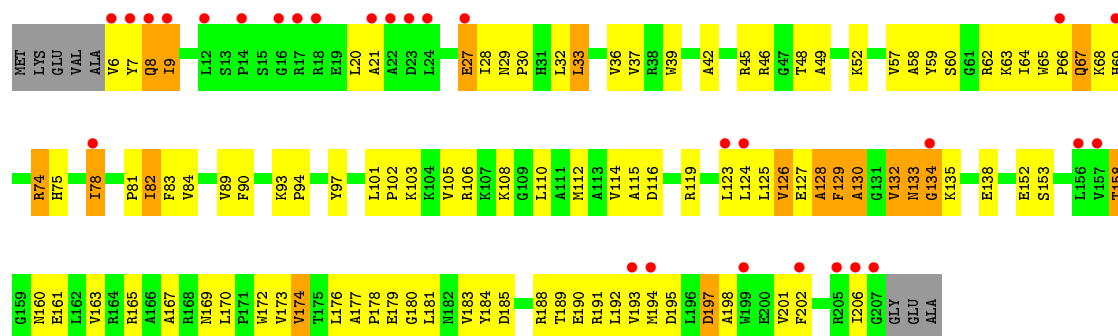




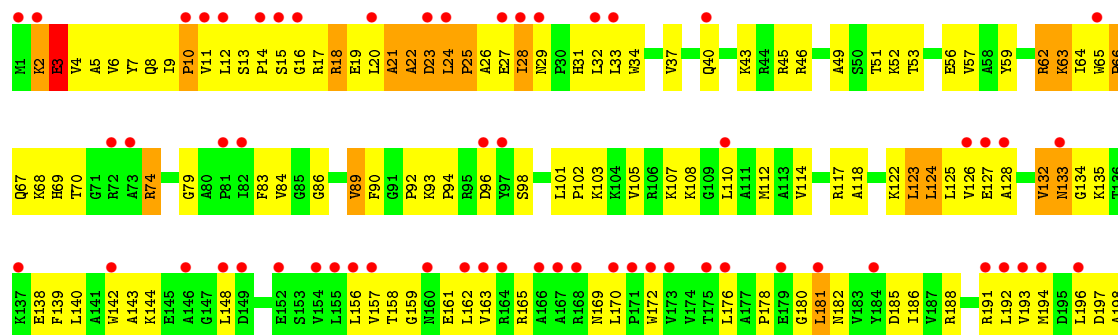
• Molecule 27: 50S ribosomal protein L3

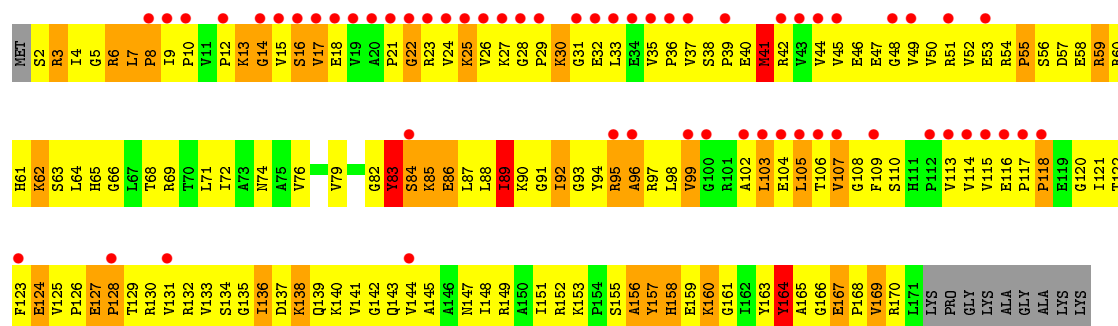


• Molecule 28: 50S ribosomal protein L4

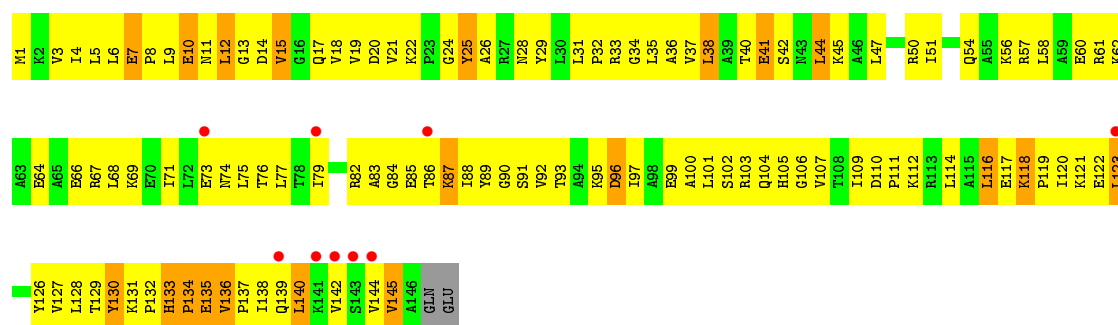


• Molecule 28: 50S ribosomal protein L4

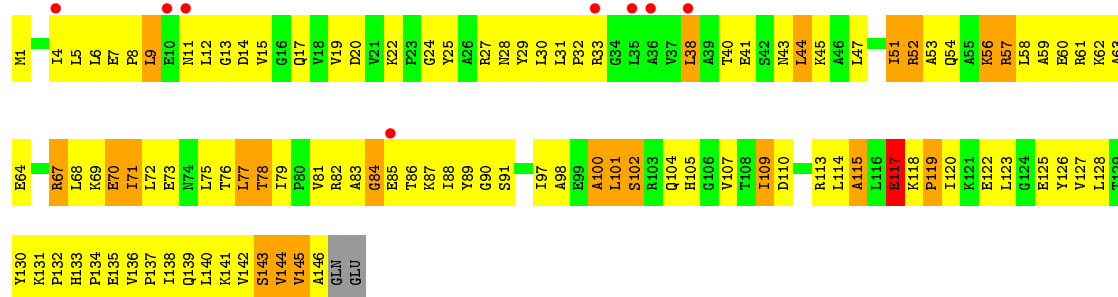




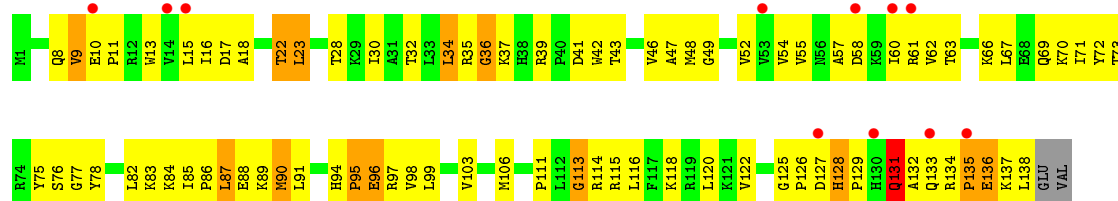
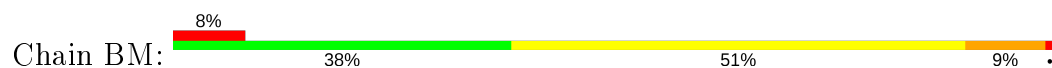
• Molecule 31: 50S ribosomal protein L9



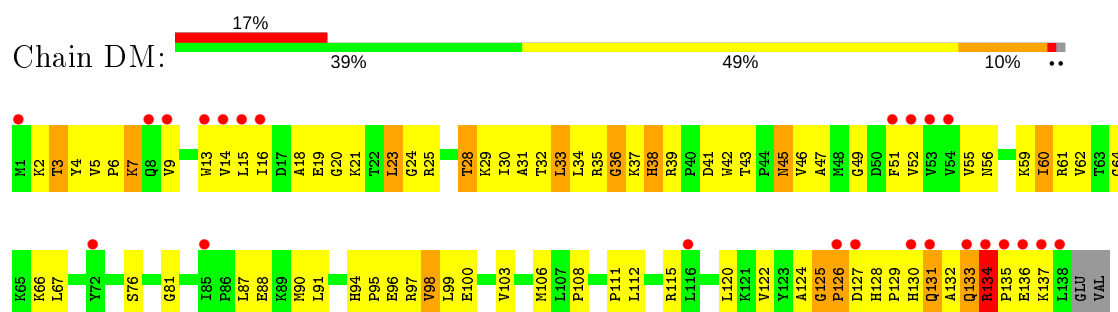
• Molecule 31: 50S ribosomal protein L9



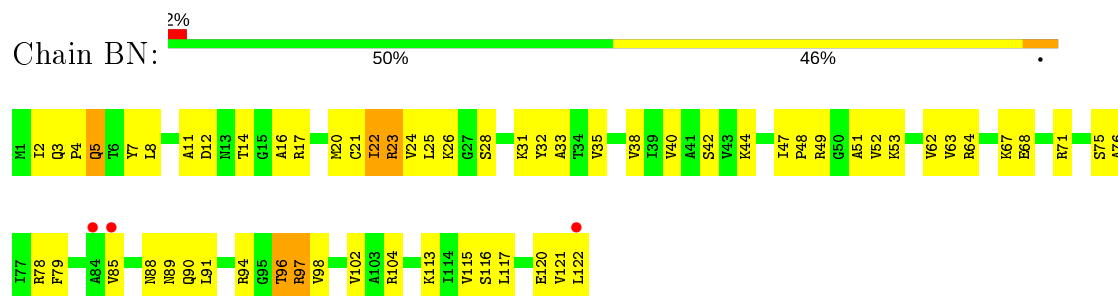
• Molecule 32: 50S ribosomal protein L13



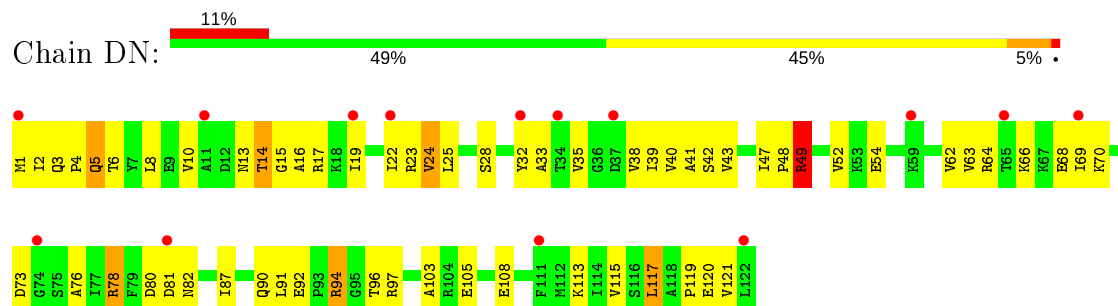
• Molecule 32: 50S ribosomal protein L13



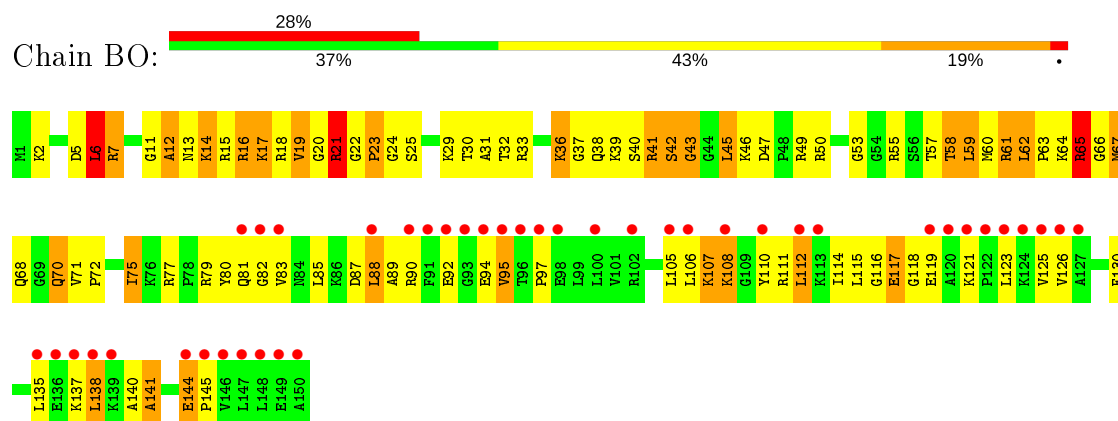
- Molecule 33: 50S ribosomal protein L14



- Molecule 33: 50S ribosomal protein L14

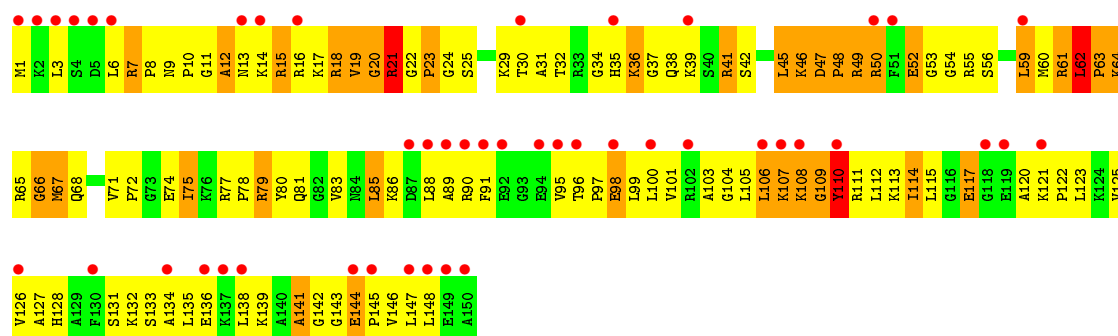


- Molecule 34: 50S ribosomal protein L15

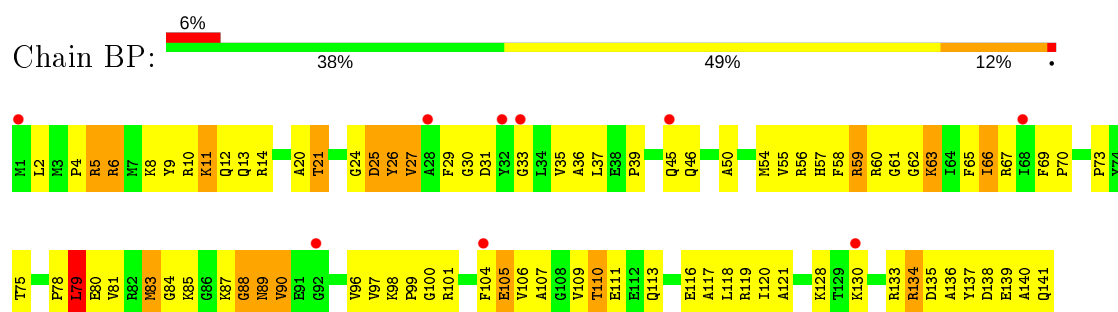


- Molecule 34: 50S ribosomal protein L15

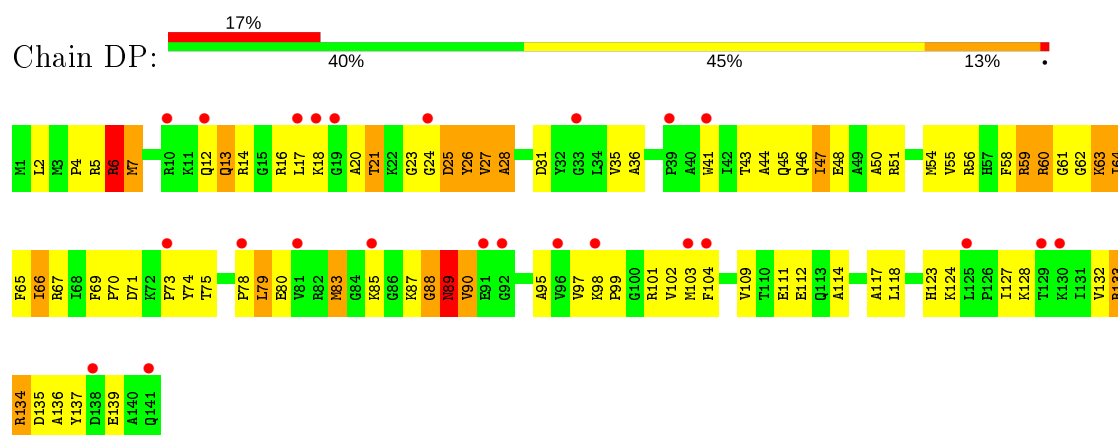




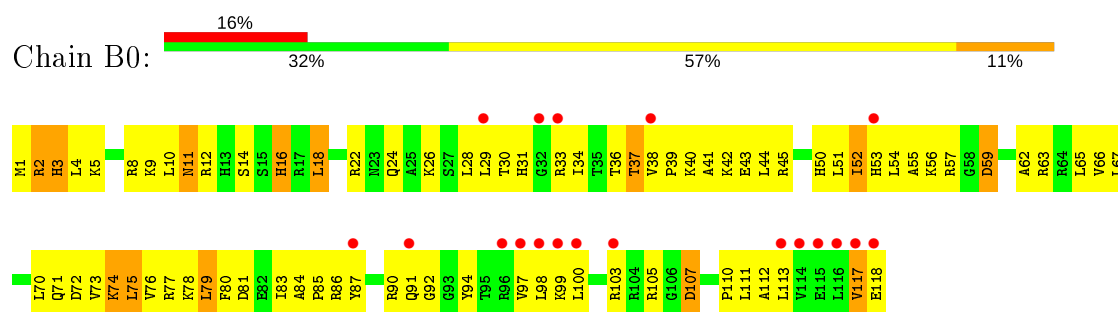
• Molecule 35: 50S ribosomal protein L16



• Molecule 35: 50S ribosomal protein L16

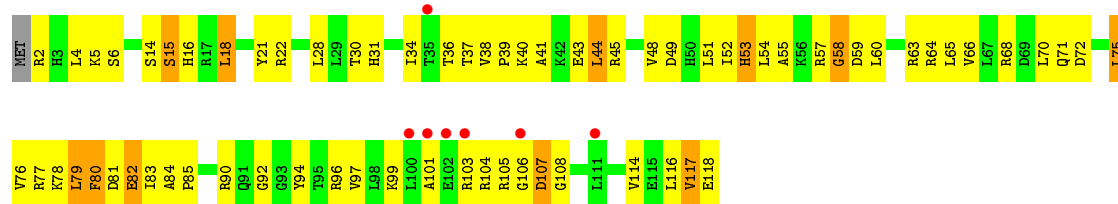


• Molecule 36: 50S ribosomal protein L17

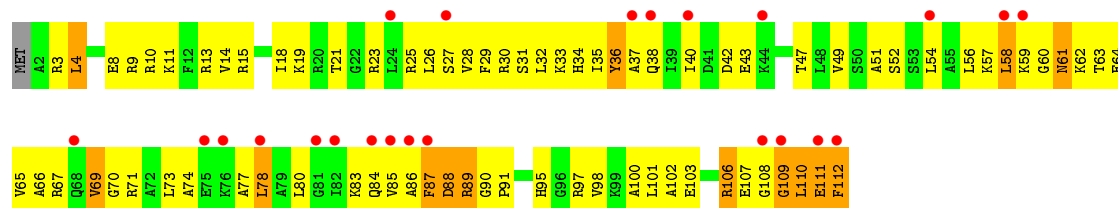


• Molecule 36: 50S ribosomal protein L17

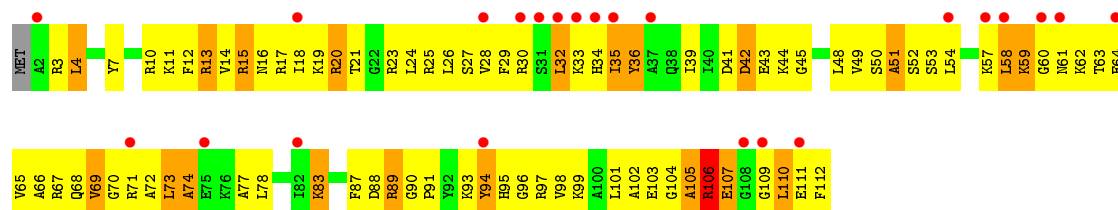




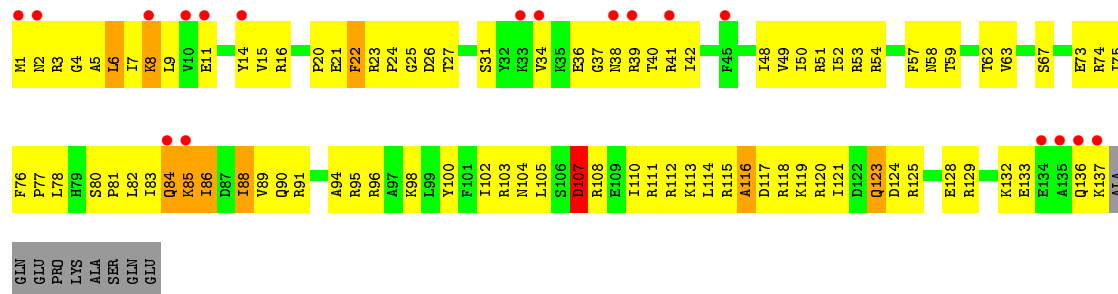
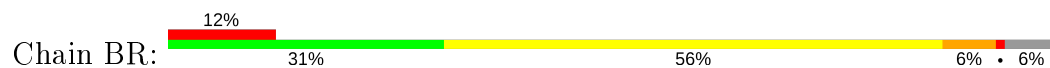
• Molecule 37: 50S ribosomal protein L18



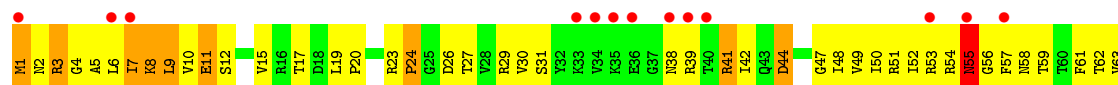
• Molecule 37: 50S ribosomal protein L18

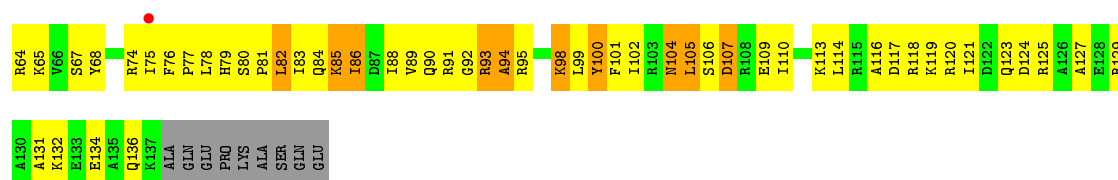


• Molecule 38: 50S ribosomal protein L19

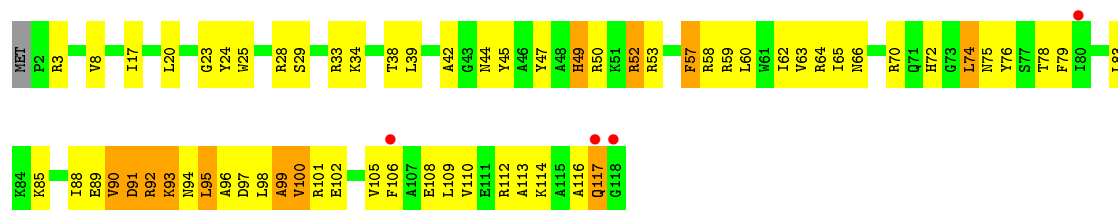


• Molecule 38: 50S ribosomal protein L19

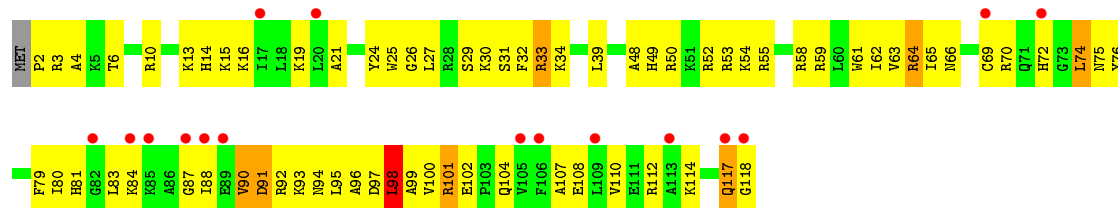




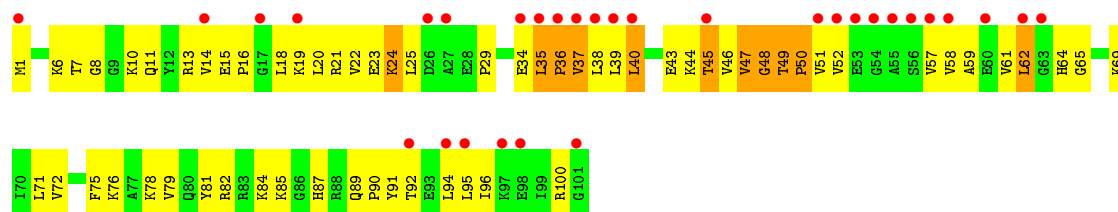
• Molecule 39: 50S ribosomal protein L20



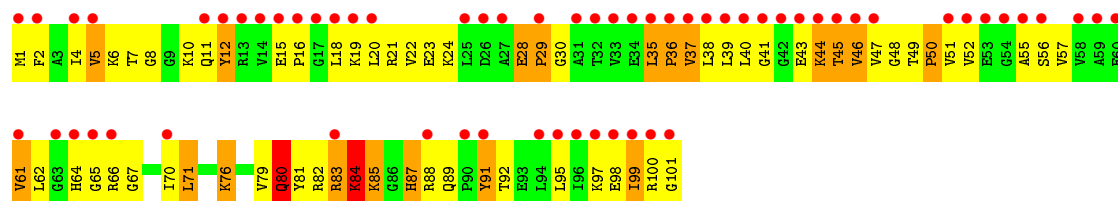
• Molecule 39: 50S ribosomal protein L20



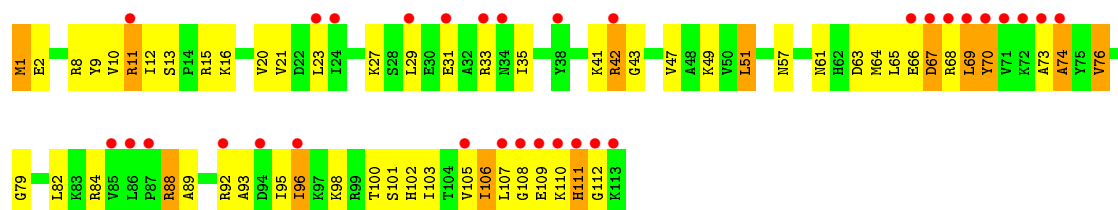
• Molecule 40: 50S ribosomal protein L21



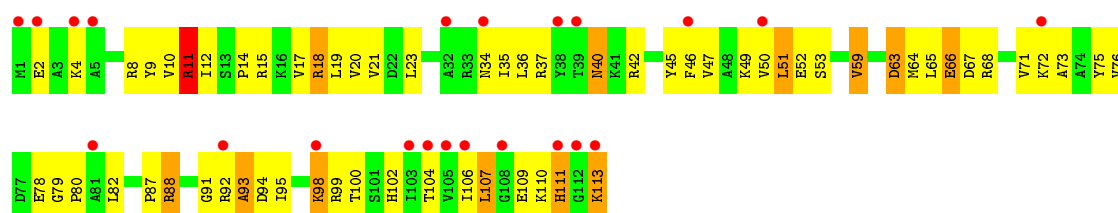
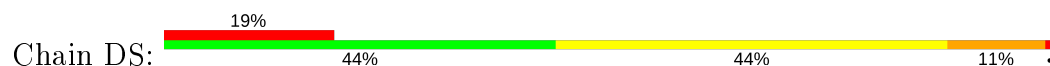
• Molecule 40: 50S ribosomal protein L21



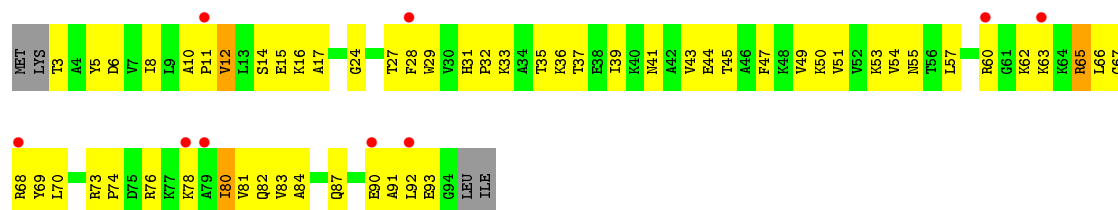
- Molecule 41: 50S ribosomal protein L22



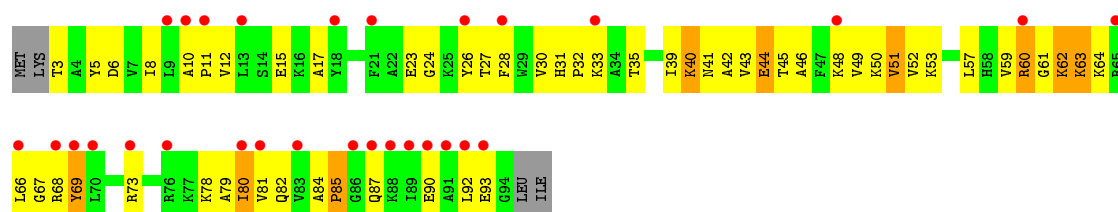
- Molecule 41: 50S ribosomal protein L22



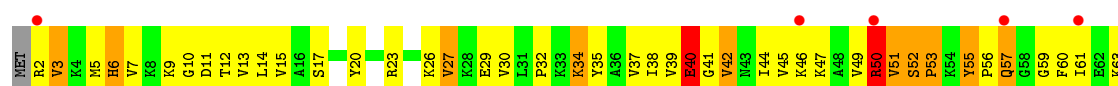
- Molecule 42: 50S ribosomal protein L23

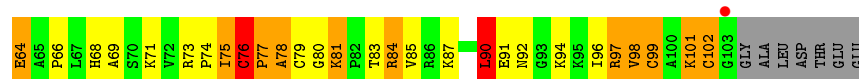


- Molecule 42: 50S ribosomal protein L23

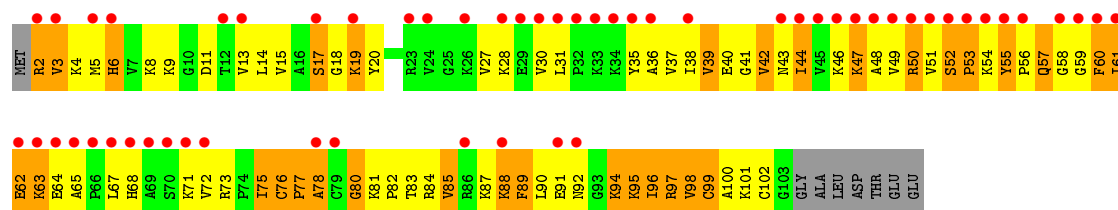
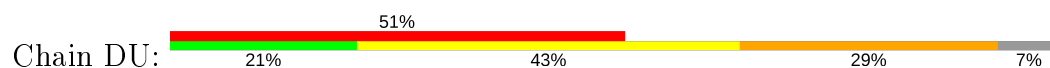


- Molecule 43: 50S ribosomal protein L24

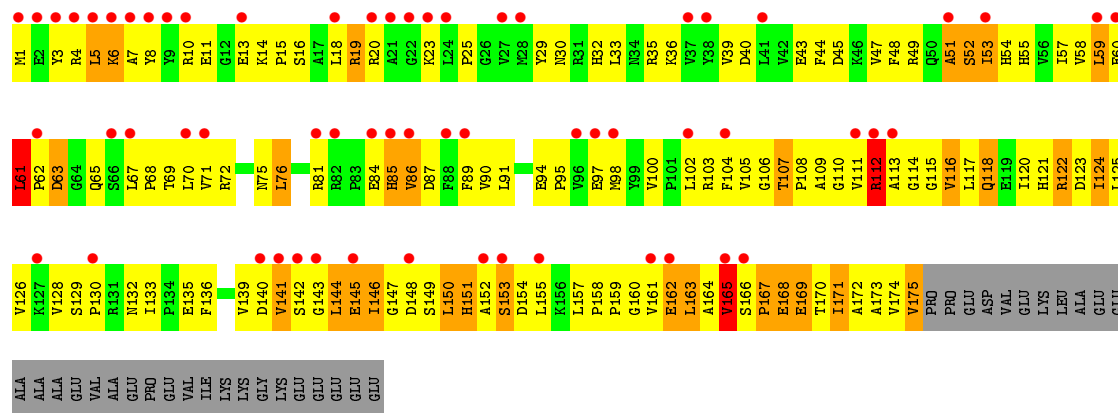
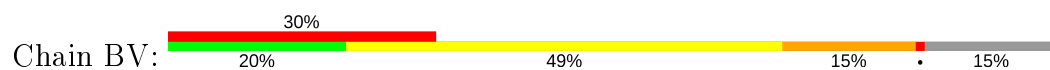




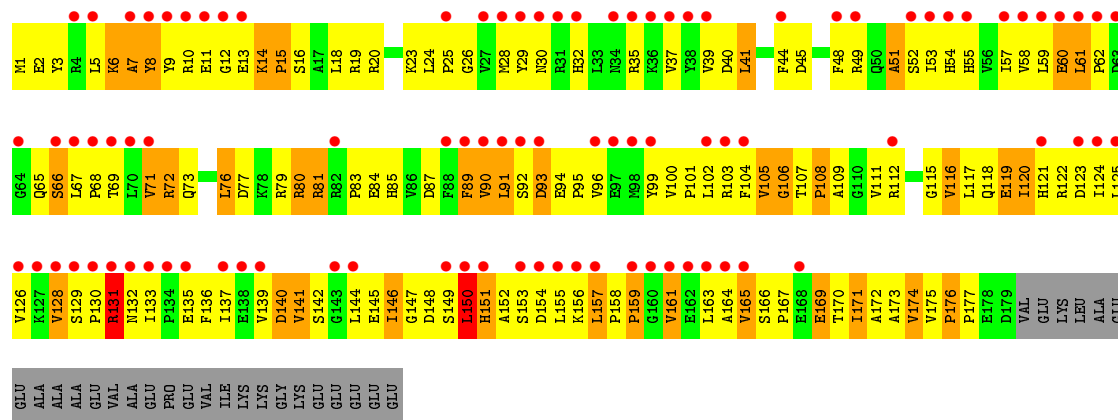
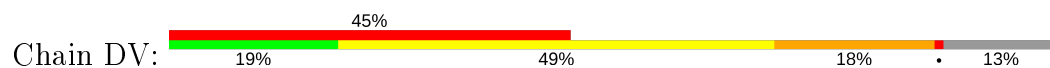
- Molecule 43: 50S ribosomal protein L24



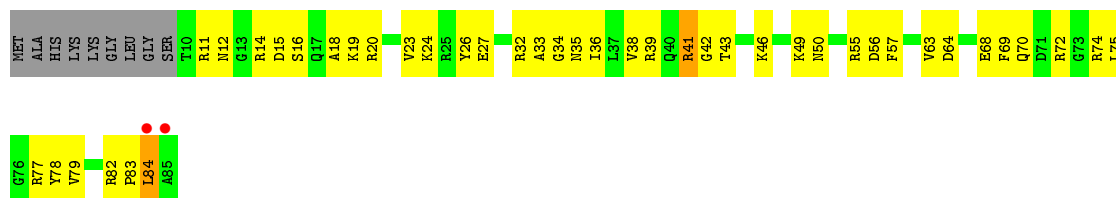
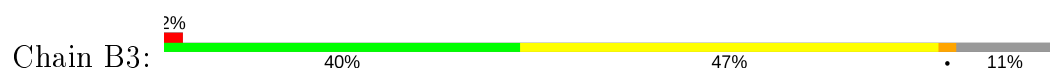
- Molecule 44: 50S ribosomal protein L25



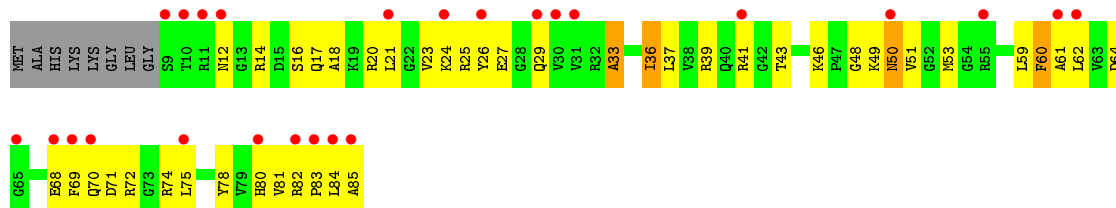
- Molecule 44: 50S ribosomal protein L25



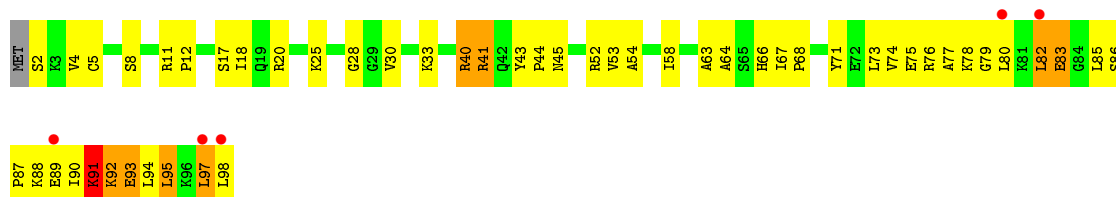
- Molecule 45: 50S ribosomal protein L27



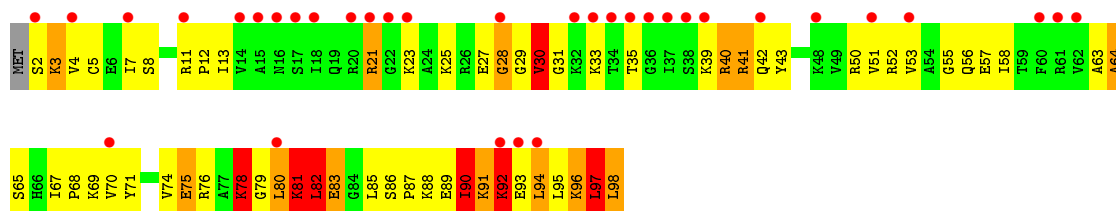
- Molecule 45: 50S ribosomal protein L27



- Molecule 46: 50S ribosomal protein L28

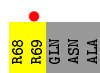


- Molecule 46: 50S ribosomal protein L28

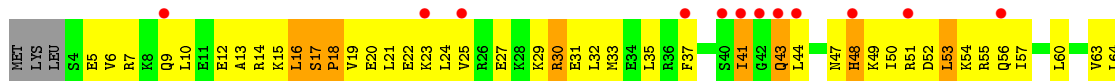


- Molecule 47: 50S ribosomal protein L29





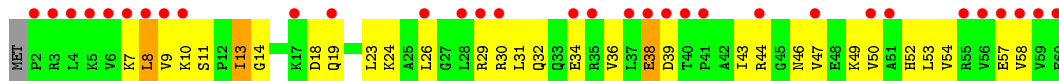
- Molecule 47: 50S ribosomal protein L29



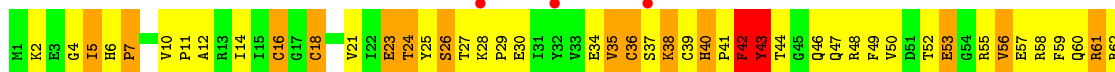
- Molecule 48: 50S ribosomal protein L30



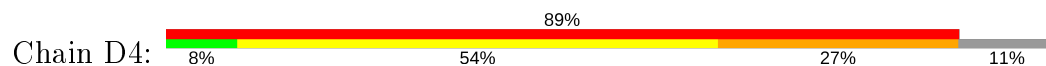
- Molecule 48: 50S ribosomal protein L30



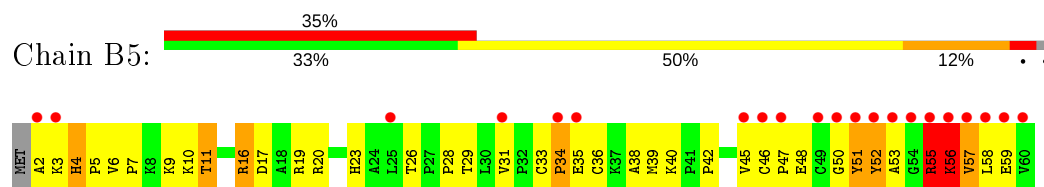
- Molecule 49: 50S ribosomal protein L31



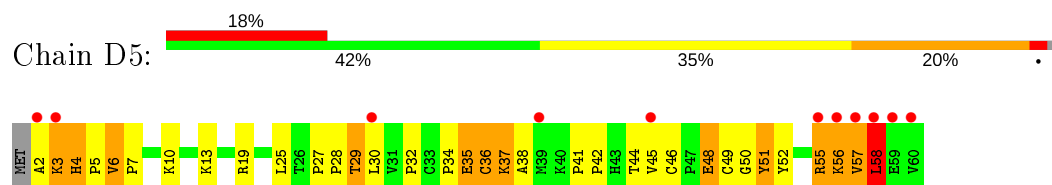
- Molecule 49: 50S ribosomal protein L31



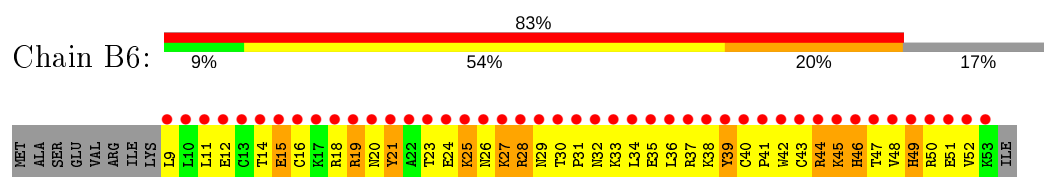
- Molecule 50: 50S ribosomal protein L32



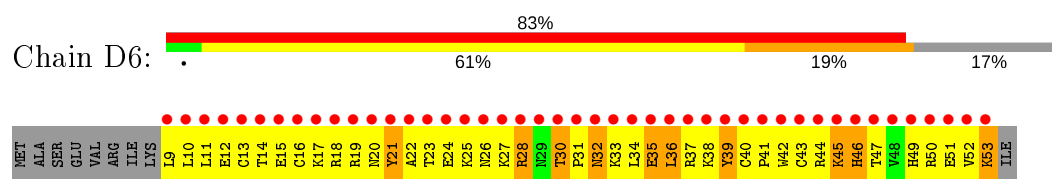
- Molecule 50: 50S ribosomal protein L32



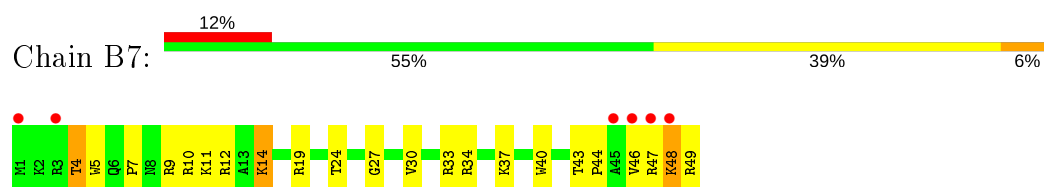
- Molecule 51: 50S ribosomal protein L33



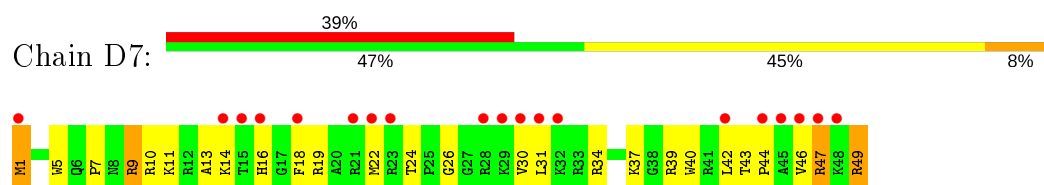
- Molecule 51: 50S ribosomal protein L33



- Molecule 52: 50S ribosomal protein L34

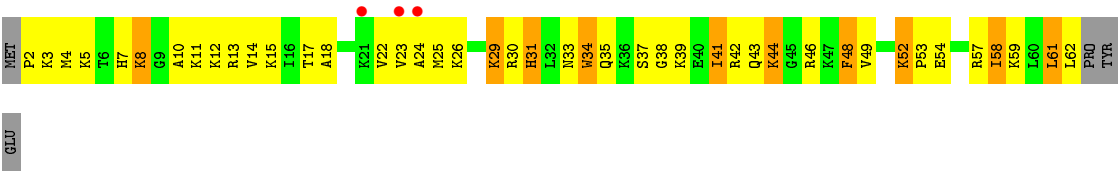


- Molecule 52: 50S ribosomal protein L34

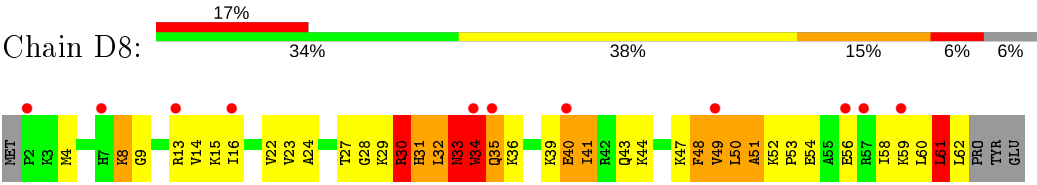


- Molecule 53: 50S ribosomal protein L35





• Molecule 53: 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	209.27Å 448.54Å 615.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	173.07 – 3.30 224.27 – 3.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (173.07-3.30) 93.5 (224.27-3.30)	Depositor EDS
R_{merge}	0.42	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 3.33Å)	Xtriage
Refinement program	PHENIX dev_987	Depositor
R, R_{free}	0.202 , 0.254 0.197 , 0.255	Depositor DCC
R_{free} test set	2000 reflections (0.23%)	wwPDB-VP
Wilson B-factor (Å ²)	101.3	Xtriage
Anisotropy	0.267	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 83.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	292440	wwPDB-VP
Average B, all atoms (Å ²)	135.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.59% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.31	2/36234 (0.0%)	0.62	7/56554 (0.0%)
1	CA	0.30	0/36237	0.60	4/56558 (0.0%)
2	AE	0.28	0/1959	0.47	0/2642
2	CE	0.25	0/1959	0.43	0/2642
3	AF	0.25	0/1629	0.41	0/2195
3	CF	0.26	0/1636	0.42	0/2205
4	AG	0.40	2/1733 (0.1%)	0.49	0/2318
4	CG	0.36	1/1733 (0.1%)	0.50	1/2318 (0.0%)
5	AH	0.29	0/1171	0.46	0/1576
5	CH	0.28	0/1171	0.47	0/1576
6	AI	0.28	0/856	0.43	0/1154
6	CI	0.27	0/856	0.43	0/1154
7	AJ	0.28	0/1276	0.42	0/1709
7	CJ	0.32	0/1276	0.45	0/1709
8	AK	0.28	0/1136	0.46	0/1527
8	CK	0.68	4/1136 (0.4%)	0.57	1/1527 (0.1%)
9	AL	0.39	1/1029 (0.1%)	0.49	0/1379
9	CL	0.31	0/1029	0.46	0/1379
10	AM	0.25	0/814	0.44	0/1095
10	CM	0.28	0/814	0.47	0/1095
11	AN	0.27	0/900	0.46	0/1213
11	CN	0.25	0/900	0.43	0/1213
12	AO	0.29	0/991	0.47	0/1327
12	CO	0.31	0/991	0.47	0/1327
13	AP	0.30	0/938	0.47	0/1258
13	CP	0.26	0/943	0.44	0/1265
14	AQ	0.31	0/501	0.45	0/664
14	CQ	0.31	0/501	0.54	1/664 (0.2%)
15	AR	0.27	0/745	0.42	0/992
15	CR	0.26	0/745	0.38	0/992
16	AS	0.32	0/721	0.47	0/970
16	CS	0.27	0/721	0.44	0/970

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AT	0.30	0/847	0.44	0/1131
17	CT	0.33	0/847	0.53	1/1131 (0.1%)
18	AU	0.26	0/596	0.44	0/790
18	CU	0.28	0/596	0.45	0/790
19	AV	0.34	0/680	0.58	0/915
19	CV	0.35	0/638	0.58	0/860
20	AW	0.41	0/765	0.54	0/1007
20	CW	0.27	0/765	0.44	0/1007
21	AX	0.28	0/221	0.43	0/288
21	CX	0.41	0/221	0.61	0/288
22	AC	0.47	2/1832 (0.1%)	0.82	5/2855 (0.2%)
22	CC	0.45	2/1832 (0.1%)	0.80	5/2855 (0.2%)
23	A1	0.33	0/94	0.62	0/144
23	C1	0.40	0/94	0.67	0/144
24	BA	0.43	1/70233 (0.0%)	0.77	36/109643 (0.0%)
24	DA	0.39	4/70167 (0.0%)	0.73	38/109541 (0.0%)
25	BB	0.37	0/2928	0.73	1/4568 (0.0%)
25	DB	0.34	0/2928	0.62	0/4568
26	BD	0.39	0/2165	0.57	0/2919
26	DD	0.59	5/2165 (0.2%)	0.55	0/2919
27	BE	0.32	0/1601	0.52	0/2160
27	DE	0.32	0/1601	0.55	0/2160
28	BF	0.32	0/1620	0.49	0/2194
28	DF	0.29	0/1662	0.49	0/2249
29	BG	0.30	0/1499	0.48	0/2016
29	DG	0.27	0/1499	0.46	0/2016
30	BH	0.38	0/1332	0.63	2/1802 (0.1%)
30	DH	0.25	0/1332	0.52	2/1802 (0.1%)
31	BK	0.28	0/1151	0.47	0/1558
31	DK	0.27	0/1151	0.48	0/1558
32	BM	0.28	0/1131	0.50	0/1525
32	DM	0.28	0/1131	0.46	0/1525
33	BN	0.30	0/943	0.48	0/1269
33	DN	0.30	0/943	0.47	0/1269
34	BO	0.39	0/1162	0.64	0/1544
34	DO	0.38	0/1162	0.57	0/1544
35	BP	0.35	0/1143	0.53	0/1527
35	DP	0.41	2/1143 (0.2%)	0.82	3/1527 (0.2%)
36	B0	0.35	0/982	0.53	1/1312 (0.1%)
36	D0	0.30	0/974	0.50	0/1302
37	BQ	0.32	0/892	0.54	0/1187
37	DQ	0.39	0/892	0.51	0/1187
38	BR	0.31	0/1155	0.47	0/1542

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DR	0.34	0/1155	0.51	0/1542
39	B1	0.36	0/982	0.52	0/1306
39	D1	0.31	0/982	0.46	0/1306
40	B2	0.32	0/790	0.52	0/1057
40	D2	0.35	0/790	0.53	0/1057
41	BS	0.31	0/911	0.50	0/1220
41	DS	0.30	0/911	0.50	0/1220
42	BT	0.42	0/739	0.52	0/993
42	DT	0.36	0/739	0.50	0/993
43	BU	0.37	0/798	0.51	0/1064
43	DU	0.33	0/798	0.50	0/1064
44	BV	0.32	0/1427	0.50	0/1935
44	DV	0.27	0/1460	0.45	0/1982
45	B3	0.33	0/615	0.50	0/819
45	D3	0.32	0/621	0.48	0/827
46	BZ	0.37	0/770	0.56	0/1022
46	DZ	0.33	0/770	0.55	0/1022
47	BW	0.39	0/560	0.55	0/741
47	DW	0.29	0/583	0.48	0/771
48	BX	0.31	0/474	0.48	0/635
48	DX	0.26	0/474	0.45	0/635
49	B4	0.81	3/545 (0.6%)	0.65	2/733 (0.3%)
49	D4	0.44	1/527 (0.2%)	0.55	0/709
50	B5	0.33	0/473	0.54	0/639
50	D5	0.29	0/473	0.47	0/639
51	B6	0.44	0/396	0.70	2/529 (0.4%)
51	D6	0.44	0/396	0.62	0/529
52	B7	0.43	0/438	0.68	0/575
52	D7	0.31	0/438	0.53	0/575
53	B8	0.40	0/494	0.58	0/649
53	D8	0.49	0/494	0.84	3/649 (0.5%)
All	All	0.37	30/316019 (0.0%)	0.66	115/472742 (0.0%)

The worst 5 of 30 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	DA	2377	A	N9-C4	20.50	1.50	1.37
26	DD	104	TYR	CD1-CE1	13.75	1.59	1.39
8	CK	94	TYR	CD2-CE2	-13.18	1.19	1.39
49	B4	16	CYS	CB-SG	-12.84	1.60	1.82
26	DD	104	TYR	CD2-CE2	12.77	1.58	1.39

The worst 5 of 115 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	DA	2377	A	C2-N3-C4	28.76	124.98	110.60
24	BA	2751	G	N1-C6-O6	20.94	132.47	119.90
24	DA	2377	A	C8-N9-C4	-20.26	97.69	105.80
35	DP	6	ARG	NE-CZ-NH1	19.44	130.02	120.30
22	CC	17(A)	C	N3-C4-C5	-18.15	114.64	121.90

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32369	0	16335	1780	1
1	CA	32372	0	16338	2038	3
2	AE	1924	0	1975	321	0
2	CE	1924	0	1975	349	0
3	AF	1605	0	1668	210	0
3	CF	1612	0	1677	235	0
4	AG	1703	0	1764	273	0
4	CG	1703	0	1763	334	0
5	AH	1155	0	1213	125	0
5	CH	1155	0	1212	196	0
6	AI	843	0	857	100	0
6	CI	843	0	857	107	0
7	AJ	1257	0	1296	153	0
7	CJ	1257	0	1296	176	0
8	AK	1116	0	1177	120	0
8	CK	1116	0	1176	177	0
9	AL	1010	0	1037	267	0
9	CL	1010	0	1037	291	0
10	AM	801	0	849	149	0
10	CM	801	0	849	238	1
11	AN	885	0	904	79	0
11	CN	885	0	904	87	0
12	AO	975	0	1062	108	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	CO	975	0	1062	91	0
13	AP	928	0	987	157	0
13	CP	933	0	992	195	0
14	AQ	492	0	529	74	0
14	CQ	492	0	530	133	0
15	AR	734	0	771	54	0
15	CR	734	0	771	76	0
16	AS	705	0	725	116	0
16	CS	705	0	725	94	0
17	AT	834	0	904	96	0
17	CT	834	0	904	88	0
18	AU	591	0	662	60	0
18	CU	591	0	662	69	0
19	AV	665	0	686	181	0
19	CV	624	0	636	250	0
20	AW	763	0	861	140	0
20	CW	763	0	861	87	0
21	AX	217	0	234	26	0
21	CX	217	0	234	60	0
22	AC	1640	0	836	47	0
22	CC	1640	0	836	67	0
23	A1	85	0	43	1	0
23	C1	85	0	43	5	0
24	BA	62707	0	31611	2736	0
24	DA	62647	0	31583	2861	2
25	BB	2617	0	1328	127	0
25	DB	2617	0	1328	167	0
26	BD	2115	0	2195	286	0
26	DD	2115	0	2192	237	0
27	BE	1568	0	1634	180	0
27	DE	1568	0	1634	297	0
28	BF	1585	0	1632	147	0
28	DF	1627	0	1680	173	0
29	BG	1474	0	1535	213	0
29	DG	1474	0	1535	220	0
30	BH	1307	0	1382	220	0
30	DH	1307	0	1382	277	0
31	BK	1136	0	1223	174	1
31	DK	1136	0	1223	158	0
32	BM	1104	0	1180	105	0
32	DM	1104	0	1180	132	0
33	BN	933	0	996	66	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	DN	933	0	996	84	0
34	BO	1145	0	1228	187	0
34	DO	1145	0	1228	239	0
35	BP	1122	0	1179	127	0
35	DP	1122	0	1178	151	0
36	B0	968	0	1033	102	0
36	D0	960	0	1021	95	0
37	BQ	882	0	943	149	0
37	DQ	882	0	943	207	0
38	BR	1141	0	1202	135	0
38	DR	1141	0	1202	123	0
39	B1	964	0	1022	114	0
39	D1	964	0	1021	140	0
40	B2	779	0	852	103	0
40	D2	779	0	851	175	0
41	BS	900	0	964	66	0
41	DS	900	0	964	75	0
42	BT	725	0	778	72	0
42	DT	725	0	778	86	0
43	BU	785	0	878	136	0
43	DU	785	0	878	153	0
44	BV	1397	0	1430	209	0
44	DV	1428	0	1454	255	0
45	B3	607	0	628	43	0
45	D3	613	0	633	59	0
46	BZ	763	0	848	91	0
46	DZ	763	0	848	93	0
47	BW	558	0	610	62	0
47	DW	581	0	629	71	0
48	BX	469	0	518	31	0
48	DX	469	0	518	39	0
49	B4	533	0	522	132	0
49	D4	515	0	510	157	0
50	B5	459	0	480	67	0
50	D5	459	0	476	46	0
51	B6	389	0	404	142	0
51	D6	389	0	404	166	0
52	B7	430	0	480	55	0
52	D7	430	0	479	73	0
53	B8	488	0	560	110	0
53	D8	488	0	559	138	0
54	A1	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	AA	232	0	0	0	0
54	AC	9	0	0	0	0
54	AG	2	0	0	0	0
54	AH	2	0	0	0	0
54	AJ	1	0	0	0	0
54	AQ	2	0	0	0	0
54	AR	1	0	0	0	0
54	AS	1	0	0	0	0
54	B1	2	0	0	0	0
54	B2	1	0	0	0	0
54	B3	2	0	0	0	0
54	B5	2	0	0	0	0
54	B6	1	0	0	0	0
54	B7	3	0	0	0	0
54	B8	1	0	0	0	0
54	BA	627	0	0	0	0
54	BB	17	0	0	0	0
54	BE	5	0	0	0	0
54	BF	2	0	0	0	0
54	BO	3	0	0	0	0
54	BP	1	0	0	0	0
54	BU	2	0	0	0	0
54	BZ	1	0	0	0	0
54	CA	204	0	0	0	0
54	CC	8	0	0	0	0
54	CG	2	0	0	0	0
54	CH	1	0	0	0	0
54	CS	1	0	0	0	0
54	D1	1	0	0	0	0
54	D5	1	0	0	0	0
54	DA	525	0	0	0	0
54	DB	14	0	0	0	0
54	DD	1	0	0	0	0
54	DE	3	0	0	0	0
54	DP	1	0	0	0	0
54	DR	1	0	0	0	0
54	DU	1	0	0	0	0
54	DZ	2	0	0	0	0
55	AA	32	1	21	4	0
55	CA	32	0	22	3	0
56	AG	1	0	0	0	0
56	AQ	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	CG	1	0	0	2	0
56	CQ	1	0	0	0	0
All	All	292439	1	197340	20528	4

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 43.

The worst 5 of 20528 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)
24:DA:1600:C:C2'	52:D7:49:ARG:HE	0.98	1.56
4:CG:31:CYS:SG	4:CG:33:MET:HE2	1.43	1.53
1:CA:598:U:O3'	8:CK:94:TYR:CE2	1.65	1.48
19:CV:70:LYS:CE	19:CV:73:GLU:HG3	1.44	1.48
24:DA:1600:C:H2'	52:D7:49:ARG:NE	1.12	1.43

All (4) 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)
31:BK:89:TYR:O	1:CA:357:G:O2'[4_555]	2.01	0.19
1:CA:86:U:O2'	24:DA:276:A:OP2[3_545]	2.09	0.11
1:AA:1175:G:O2'	10:CM:80:LYS:NZ[4_555]	2.18	0.02
1:CA:84:U:O2'	24:DA:273:G:OP1[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%)	162 (69%)	47 (20%)	26 (11%)	0 2
2	CE	235/256 (92%)	166 (71%)	44 (19%)	25 (11%)	0 3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	AF	203/239 (85%)	150 (74%)	36 (18%)	17 (8%)	1	5
3	CF	204/239 (85%)	138 (68%)	51 (25%)	15 (7%)	1	7
4	AG	206/208 (99%)	157 (76%)	35 (17%)	14 (7%)	1	8
4	CG	206/208 (99%)	140 (68%)	44 (21%)	22 (11%)	0	3
5	AH	149/162 (92%)	127 (85%)	17 (11%)	5 (3%)	3	22
5	CH	149/162 (92%)	112 (75%)	31 (21%)	6 (4%)	3	18
6	AI	99/101 (98%)	81 (82%)	14 (14%)	4 (4%)	3	18
6	CI	99/101 (98%)	82 (83%)	11 (11%)	6 (6%)	1	10
7	AJ	153/156 (98%)	126 (82%)	17 (11%)	10 (6%)	1	9
7	CJ	153/156 (98%)	112 (73%)	33 (22%)	8 (5%)	2	13
8	AK	136/138 (99%)	103 (76%)	27 (20%)	6 (4%)	2	16
8	CK	136/138 (99%)	114 (84%)	15 (11%)	7 (5%)	2	13
9	AL	125/128 (98%)	93 (74%)	26 (21%)	6 (5%)	2	14
9	CL	125/128 (98%)	93 (74%)	21 (17%)	11 (9%)	1	5
10	AM	97/105 (92%)	75 (77%)	17 (18%)	5 (5%)	2	13
10	CM	97/105 (92%)	69 (71%)	23 (24%)	5 (5%)	2	13
11	AN	117/129 (91%)	88 (75%)	20 (17%)	9 (8%)	1	6
11	CN	117/129 (91%)	94 (80%)	17 (14%)	6 (5%)	2	13
12	AO	123/128 (96%)	96 (78%)	17 (14%)	10 (8%)	1	6
12	CO	123/128 (96%)	91 (74%)	23 (19%)	9 (7%)	1	7
13	AP	114/126 (90%)	87 (76%)	15 (13%)	12 (10%)	0	3
13	CP	115/126 (91%)	82 (71%)	19 (16%)	14 (12%)	0	1
14	AQ	58/61 (95%)	43 (74%)	11 (19%)	4 (7%)	1	8
14	CQ	58/61 (95%)	40 (69%)	12 (21%)	6 (10%)	0	3
15	AR	86/89 (97%)	71 (83%)	9 (10%)	6 (7%)	1	7
15	CR	86/89 (97%)	72 (84%)	13 (15%)	1 (1%)	13	42
16	AS	82/88 (93%)	61 (74%)	18 (22%)	3 (4%)	3	20
16	CS	82/88 (93%)	59 (72%)	17 (21%)	6 (7%)	1	7
17	AT	98/105 (93%)	78 (80%)	16 (16%)	4 (4%)	3	17
17	CT	98/105 (93%)	76 (78%)	15 (15%)	7 (7%)	1	7
18	AU	70/88 (80%)	58 (83%)	7 (10%)	5 (7%)	1	7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	CU	70/88 (80%)	53 (76%)	13 (19%)	4 (6%)	1	11
19	AV	81/93 (87%)	53 (65%)	19 (24%)	9 (11%)	0	2
19	CV	76/93 (82%)	48 (63%)	19 (25%)	9 (12%)	0	2
20	AW	97/106 (92%)	67 (69%)	17 (18%)	13 (13%)	0	1
20	CW	97/106 (92%)	64 (66%)	22 (23%)	11 (11%)	0	2
21	AX	23/27 (85%)	17 (74%)	4 (17%)	2 (9%)	1	5
21	CX	23/27 (85%)	14 (61%)	5 (22%)	4 (17%)	0	1
26	BD	270/276 (98%)	227 (84%)	31 (12%)	12 (4%)	2	16
26	DD	270/276 (98%)	223 (83%)	35 (13%)	12 (4%)	2	16
27	BE	203/206 (98%)	151 (74%)	35 (17%)	17 (8%)	1	5
27	DE	203/206 (98%)	133 (66%)	40 (20%)	30 (15%)	0	1
28	BF	200/210 (95%)	171 (86%)	21 (10%)	8 (4%)	3	18
28	DF	206/210 (98%)	155 (75%)	33 (16%)	18 (9%)	1	5
29	BG	179/182 (98%)	132 (74%)	32 (18%)	15 (8%)	1	5
29	DG	179/182 (98%)	128 (72%)	35 (20%)	16 (9%)	1	4
30	BH	168/180 (93%)	107 (64%)	30 (18%)	31 (18%)	0	1
30	DH	168/180 (93%)	103 (61%)	30 (18%)	35 (21%)	0	0
31	BK	144/148 (97%)	102 (71%)	28 (19%)	14 (10%)	0	3
31	DK	144/148 (97%)	98 (68%)	31 (22%)	15 (10%)	0	3
32	BM	136/140 (97%)	101 (74%)	24 (18%)	11 (8%)	1	6
32	DM	136/140 (97%)	103 (76%)	22 (16%)	11 (8%)	1	6
33	BN	120/122 (98%)	106 (88%)	12 (10%)	2 (2%)	9	35
33	DN	120/122 (98%)	107 (89%)	10 (8%)	3 (2%)	5	27
34	BO	148/150 (99%)	99 (67%)	27 (18%)	22 (15%)	0	1
34	DO	148/150 (99%)	85 (57%)	31 (21%)	32 (22%)	0	0
35	BP	139/141 (99%)	104 (75%)	21 (15%)	14 (10%)	0	3
35	DP	139/141 (99%)	100 (72%)	24 (17%)	15 (11%)	0	2
36	B0	116/118 (98%)	91 (78%)	14 (12%)	11 (10%)	0	4
36	D0	115/118 (98%)	85 (74%)	21 (18%)	9 (8%)	1	6
37	BQ	109/112 (97%)	82 (75%)	15 (14%)	12 (11%)	0	2
37	DQ	109/112 (97%)	74 (68%)	22 (20%)	13 (12%)	0	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	BR	135/146 (92%)	101 (75%)	25 (18%)	9 (7%)	1	8
38	DR	135/146 (92%)	105 (78%)	19 (14%)	11 (8%)	1	6
39	B1	115/118 (98%)	92 (80%)	17 (15%)	6 (5%)	2	13
39	D1	115/118 (98%)	89 (77%)	20 (17%)	6 (5%)	2	13
40	B2	99/101 (98%)	74 (75%)	17 (17%)	8 (8%)	1	6
40	D2	99/101 (98%)	68 (69%)	16 (16%)	15 (15%)	0	1
41	BS	111/113 (98%)	91 (82%)	14 (13%)	6 (5%)	2	12
41	DS	111/113 (98%)	86 (78%)	17 (15%)	8 (7%)	1	7
42	BT	90/96 (94%)	75 (83%)	13 (14%)	2 (2%)	6	30
42	DT	90/96 (94%)	67 (74%)	13 (14%)	10 (11%)	0	2
43	BU	100/110 (91%)	64 (64%)	18 (18%)	18 (18%)	0	1
43	DU	100/110 (91%)	57 (57%)	18 (18%)	25 (25%)	0	0
44	BV	173/206 (84%)	105 (61%)	47 (27%)	21 (12%)	0	2
44	DV	177/206 (86%)	110 (62%)	37 (21%)	30 (17%)	0	1
45	B3	74/85 (87%)	57 (77%)	15 (20%)	2 (3%)	5	26
45	D3	75/85 (88%)	63 (84%)	9 (12%)	3 (4%)	3	18
46	BZ	95/98 (97%)	72 (76%)	17 (18%)	6 (6%)	1	9
46	DZ	95/98 (97%)	69 (73%)	12 (13%)	14 (15%)	0	1
47	BW	64/72 (89%)	54 (84%)	5 (8%)	5 (8%)	1	6
47	DW	67/72 (93%)	51 (76%)	9 (13%)	7 (10%)	0	3
48	BX	57/60 (95%)	51 (90%)	5 (9%)	1 (2%)	8	35
48	DX	57/60 (95%)	46 (81%)	9 (16%)	2 (4%)	3	21
49	B4	64/71 (90%)	33 (52%)	21 (33%)	10 (16%)	0	1
49	D4	61/71 (86%)	22 (36%)	23 (38%)	16 (26%)	0	0
50	B5	57/60 (95%)	42 (74%)	10 (18%)	5 (9%)	1	5
50	D5	57/60 (95%)	41 (72%)	6 (10%)	10 (18%)	0	1
51	B6	43/54 (80%)	24 (56%)	12 (28%)	7 (16%)	0	1
51	D6	43/54 (80%)	24 (56%)	13 (30%)	6 (14%)	0	1
52	B7	47/49 (96%)	42 (89%)	4 (8%)	1 (2%)	7	31
52	D7	47/49 (96%)	42 (89%)	5 (11%)	0	100	100
53	B8	59/65 (91%)	44 (75%)	10 (17%)	5 (8%)	1	5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
53	D8	59/65 (91%)	38 (64%)	8 (14%)	13 (22%)	0	0
All	All	11341/12044 (94%)	8378 (74%)	1945 (17%)	1018 (9%)	1	4

5 of 1018 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AE	135	GLN
2	AE	136	VAL
2	AE	194	PRO
2	AE	195	ASP
2	AE	214	ILE

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%)	182 (89%)	23 (11%)	6	23
2	CE	205/220 (93%)	176 (86%)	29 (14%)	3	16
3	AF	159/188 (85%)	147 (92%)	12 (8%)	13	39
3	CF	160/188 (85%)	146 (91%)	14 (9%)	10	33
4	AG	180/180 (100%)	166 (92%)	14 (8%)	12	38
4	CG	180/180 (100%)	161 (89%)	19 (11%)	6	25
5	AH	116/123 (94%)	105 (90%)	11 (10%)	8	29
5	CH	116/123 (94%)	104 (90%)	12 (10%)	7	26
6	AI	90/90 (100%)	85 (94%)	5 (6%)	21	52
6	CI	90/90 (100%)	81 (90%)	9 (10%)	7	27
7	AJ	126/127 (99%)	118 (94%)	8 (6%)	18	47
7	CJ	126/127 (99%)	116 (92%)	10 (8%)	12	37
8	AK	119/119 (100%)	108 (91%)	11 (9%)	9	31
8	CK	119/119 (100%)	108 (91%)	11 (9%)	9	31
9	AL	98/99 (99%)	86 (88%)	12 (12%)	5	20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	CL	98/99 (99%)	79 (81%)	19 (19%)	1	5
10	AM	89/92 (97%)	82 (92%)	7 (8%)	12	37
10	CM	89/92 (97%)	82 (92%)	7 (8%)	12	37
11	AN	90/99 (91%)	86 (96%)	4 (4%)	28	59
11	CN	90/99 (91%)	85 (94%)	5 (6%)	21	52
12	AO	104/107 (97%)	97 (93%)	7 (7%)	16	45
12	CO	104/107 (97%)	97 (93%)	7 (7%)	16	45
13	AP	94/101 (93%)	89 (95%)	5 (5%)	22	53
13	CP	94/101 (93%)	78 (83%)	16 (17%)	2	9
14	AQ	49/50 (98%)	44 (90%)	5 (10%)	7	27
14	CQ	49/50 (98%)	45 (92%)	4 (8%)	11	36
15	AR	79/80 (99%)	73 (92%)	6 (8%)	13	39
15	CR	79/80 (99%)	76 (96%)	3 (4%)	33	62
16	AS	72/74 (97%)	62 (86%)	10 (14%)	3	16
16	CS	72/74 (97%)	68 (94%)	4 (6%)	21	52
17	AT	95/97 (98%)	90 (95%)	5 (5%)	22	53
17	CT	95/97 (98%)	92 (97%)	3 (3%)	39	67
18	AU	63/77 (82%)	60 (95%)	3 (5%)	25	56
18	CU	63/77 (82%)	59 (94%)	4 (6%)	18	47
19	AV	72/80 (90%)	63 (88%)	9 (12%)	4	19
19	CV	67/80 (84%)	56 (84%)	11 (16%)	2	10
20	AW	76/82 (93%)	70 (92%)	6 (8%)	12	37
20	CW	76/82 (93%)	69 (91%)	7 (9%)	9	31
21	AX	20/22 (91%)	20 (100%)	0	100	100
21	CX	20/22 (91%)	18 (90%)	2 (10%)	7	27
26	BD	214/218 (98%)	192 (90%)	22 (10%)	7	26
26	DD	214/218 (98%)	197 (92%)	17 (8%)	12	37
27	BE	165/166 (99%)	149 (90%)	16 (10%)	8	29
27	DE	165/166 (99%)	150 (91%)	15 (9%)	9	31
28	BF	161/166 (97%)	150 (93%)	11 (7%)	16	44
28	DF	165/166 (99%)	156 (94%)	9 (6%)	21	52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	BG	155/156 (99%)	145 (94%)	10 (6%)	17	46
29	DG	155/156 (99%)	141 (91%)	14 (9%)	9	32
30	BH	142/148 (96%)	119 (84%)	23 (16%)	2	10
30	DH	142/148 (96%)	128 (90%)	14 (10%)	8	28
31	BK	122/124 (98%)	110 (90%)	12 (10%)	8	29
31	DK	122/124 (98%)	109 (89%)	13 (11%)	6	25
32	BM	117/119 (98%)	113 (97%)	4 (3%)	37	65
32	DM	117/119 (98%)	109 (93%)	8 (7%)	16	44
33	BN	100/100 (100%)	95 (95%)	5 (5%)	24	55
33	DN	100/100 (100%)	95 (95%)	5 (5%)	24	55
34	BO	116/116 (100%)	101 (87%)	15 (13%)	4	18
34	DO	116/116 (100%)	102 (88%)	14 (12%)	5	20
35	BP	111/111 (100%)	102 (92%)	9 (8%)	11	36
35	DP	111/111 (100%)	102 (92%)	9 (8%)	11	36
36	B0	101/101 (100%)	94 (93%)	7 (7%)	15	44
36	D0	100/101 (99%)	95 (95%)	5 (5%)	24	55
37	BQ	87/88 (99%)	82 (94%)	5 (6%)	20	51
37	DQ	87/88 (99%)	78 (90%)	9 (10%)	7	26
38	BR	120/127 (94%)	111 (92%)	9 (8%)	13	39
38	DR	120/127 (94%)	107 (89%)	13 (11%)	6	24
39	B1	93/94 (99%)	87 (94%)	6 (6%)	17	46
39	D1	93/94 (99%)	88 (95%)	5 (5%)	22	53
40	B2	82/82 (100%)	75 (92%)	7 (8%)	10	35
40	D2	82/82 (100%)	71 (87%)	11 (13%)	4	16
41	BS	92/92 (100%)	82 (89%)	10 (11%)	6	24
41	DS	92/92 (100%)	82 (89%)	10 (11%)	6	24
42	BT	74/78 (95%)	69 (93%)	5 (7%)	16	44
42	DT	74/78 (95%)	69 (93%)	5 (7%)	16	44
43	BU	85/91 (93%)	70 (82%)	15 (18%)	2	8
43	DU	85/91 (93%)	73 (86%)	12 (14%)	3	16
44	BV	154/179 (86%)	135 (88%)	19 (12%)	4	20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
44	DV	158/179 (88%)	144 (91%)	14 (9%)	9	32
45	B3	61/67 (91%)	58 (95%)	3 (5%)	25	56
45	D3	62/67 (92%)	57 (92%)	5 (8%)	11	36
46	BZ	82/83 (99%)	77 (94%)	5 (6%)	18	48
46	DZ	82/83 (99%)	65 (79%)	17 (21%)	1	4
47	BW	62/67 (92%)	55 (89%)	7 (11%)	6	22
47	DW	64/67 (96%)	62 (97%)	2 (3%)	40	67
48	BX	51/52 (98%)	47 (92%)	4 (8%)	12	38
48	DX	51/52 (98%)	48 (94%)	3 (6%)	19	49
49	B4	59/63 (94%)	51 (86%)	8 (14%)	3	16
49	D4	57/63 (90%)	51 (90%)	6 (10%)	7	25
50	B5	51/52 (98%)	44 (86%)	7 (14%)	3	16
50	D5	51/52 (98%)	44 (86%)	7 (14%)	3	16
51	B6	44/52 (85%)	40 (91%)	4 (9%)	9	31
51	D6	44/52 (85%)	38 (86%)	6 (14%)	3	16
52	B7	42/42 (100%)	38 (90%)	4 (10%)	8	29
52	D7	42/42 (100%)	36 (86%)	6 (14%)	3	15
53	B8	51/55 (93%)	43 (84%)	8 (16%)	2	12
53	D8	51/55 (93%)	45 (88%)	6 (12%)	5	21
All	All	9584/9992 (96%)	8705 (91%)	879 (9%)	9	31

5 of 879 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
49	B4	53	GLU
5	CH	78	HIS
44	DV	72	ARG
51	B6	44	ARG
2	CE	187	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 125 such sidechains are listed below:

Mol	Chain	Res	Type
2	CE	25	ASN

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Mol	Chain	Res	Type
8	CK	82	HIS
43	DU	6	HIS
2	CE	94	ASN
4	CG	43	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1506/1506 (100%)	279 (18%)	29 (1%)
1	CA	1505/1506 (99%)	284 (18%)	32 (2%)
22	AC	76/77 (98%)	5 (6%)	1 (1%)
22	CC	77/77 (100%)	9 (11%)	2 (2%)
23	A1	3/4 (75%)	1 (33%)	0
23	C1	3/4 (75%)	0	0
24	BA	2911/2912 (99%)	552 (18%)	37 (1%)
24	DA	2908/2912 (99%)	571 (19%)	43 (1%)
25	BB	121/122 (99%)	21 (17%)	0
25	DB	121/122 (99%)	25 (20%)	0
All	All	9231/9242 (99%)	1747 (18%)	144 (1%)

5 of 1747 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	6	G
1	AA	9	G
1	AA	32	A
1	AA	39	G
1	AA	47	C

5 of 144 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
24	BA	2689	U
1	CA	560	U
24	DA	2439	A
1	CA	89	U
1	CA	328	C

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 1693 ligands modelled in this entry, 1691 are monoatomic - leaving 2 for Mogul analysis.

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	$\# Z > 2$
55	TAC	CA	1805	54	33,35,35	1.49	5 (15%)	42,58,58	1.61	7 (16%)
55	TAC	AA	1833	54	33,35,35	1.53	5 (15%)	42,58,58	1.60	6 (14%)

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
55	TAC	CA	1805	54	-	8/8/74/74	0/4/4/4
55	TAC	AA	1833	54	-	4/8/74/74	0/4/4/4

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	AA	1833	TAC	C1A-C10	4.93	1.49	1.41
55	CA	1805	TAC	C1A-C10	4.61	1.48	1.41
55	AA	1833	TAC	C1A-C61	3.96	1.49	1.41
55	CA	1805	TAC	C1A-C61	3.72	1.48	1.41
55	CA	1805	TAC	C6-C61	-3.56	1.50	1.53

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	AA	1833	TAC	C41-C1C-C1	-5.06	105.24	111.05
55	CA	1805	TAC	C41-C1C-C1	-4.84	105.49	111.05
55	AA	1833	TAC	O12-C12-C1C	4.60	120.03	113.37
55	CA	1805	TAC	O12-C12-C1C	4.22	119.48	113.37
55	AA	1833	TAC	O12-C12-C1B	-4.04	118.37	123.90

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

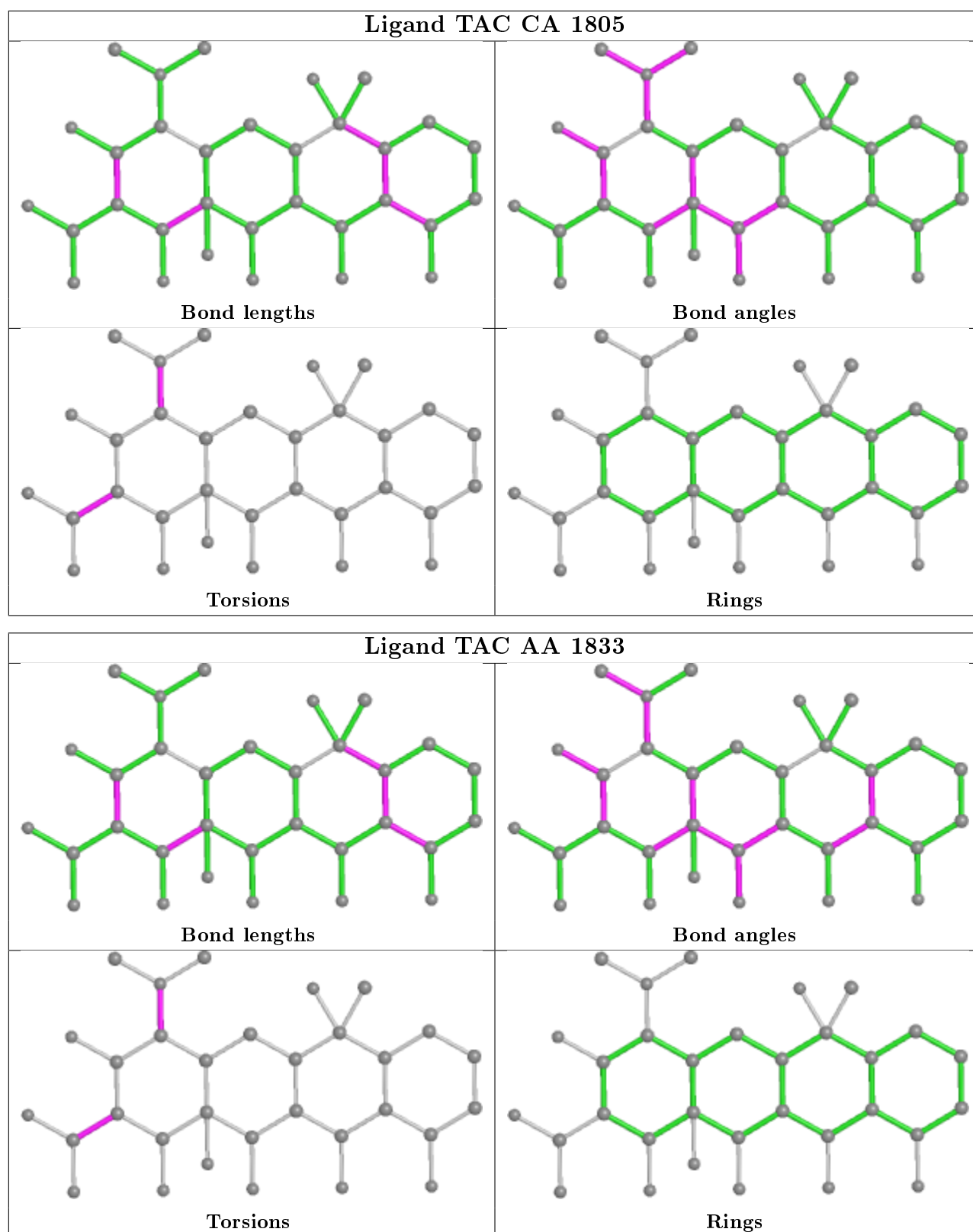
Mol	Chain	Res	Type	Atoms
55	CA	1805	TAC	C1-C2-C21-O21
55	CA	1805	TAC	C1-C2-C21-N21
55	CA	1805	TAC	C3-C2-C21-O21
55	CA	1805	TAC	C3-C2-C21-N21
55	CA	1805	TAC	C3-C4-N4-C42

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
55	CA	1805	TAC	3	0
55	AA	1833	TAC	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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	1506/1506 (100%)	-0.58	9 (0%) 89 90	89, 141, 216, 277	0
1	CA	1506/1506 (100%)	-0.67	8 (0%) 91 91	103, 152, 218, 275	0
2	AE	237/256 (92%)	1.01	59 (24%) 0 0	139, 172, 204, 216	0
2	CE	237/256 (92%)	1.81	97 (40%) 0 0	160, 191, 219, 228	0
3	AF	205/239 (85%)	2.59	123 (60%) 0 0	116, 151, 183, 201	0
3	CF	206/239 (86%)	1.43	67 (32%) 0 0	148, 179, 201, 211	0
4	AG	208/208 (100%)	1.43	68 (32%) 0 0	112, 149, 172, 183	0
4	CG	208/208 (100%)	0.41	20 (9%) 8 8	128, 153, 171, 180	0
5	AH	151/162 (93%)	2.15	73 (48%) 0 0	111, 139, 161, 195	0
5	CH	151/162 (93%)	0.67	22 (14%) 2 2	129, 154, 177, 196	0
6	AI	101/101 (100%)	2.63	58 (57%) 0 0	116, 141, 162, 167	0
6	CI	101/101 (100%)	1.68	39 (38%) 0 0	128, 149, 163, 178	0
7	AJ	155/156 (99%)	-0.05	12 (7%) 13 12	129, 151, 187, 211	0
7	CJ	155/156 (99%)	1.95	58 (37%) 0 0	146, 167, 195, 204	0
8	AK	138/138 (100%)	0.39	12 (8%) 10 10	118, 148, 162, 170	0
8	CK	138/138 (100%)	0.19	3 (2%) 62 60	131, 159, 174, 180	0
9	AL	127/128 (99%)	-0.74	0 100 100	119, 169, 186, 192	0
9	CL	127/128 (99%)	-0.29	2 (1%) 72 70	133, 185, 199, 208	0
10	AM	99/105 (94%)	0.72	23 (23%) 0 1	119, 170, 197, 210	0
10	CM	99/105 (94%)	0.07	10 (10%) 7 6	149, 191, 204, 209	0
11	AN	119/129 (92%)	2.04	47 (39%) 0 0	115, 137, 170, 198	0
11	CN	119/129 (92%)	2.01	57 (47%) 0 0	124, 149, 178, 196	0
12	AO	125/128 (97%)	1.58	43 (34%) 0 0	106, 128, 150, 192	0
12	CO	125/128 (97%)	0.23	3 (2%) 59 56	111, 134, 159, 205	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AP	116/126 (92%)	-0.71	0 100 100	103, 153, 174, 184	0
13	CP	117/126 (92%)	0.31	16 (13%) 3 2	143, 179, 196, 205	0
14	AQ	60/61 (98%)	-0.19	1 (1%) 70 68	123, 143, 159, 161	0
14	CQ	60/61 (98%)	-0.19	3 (5%) 28 27	148, 176, 188, 191	0
15	AR	88/89 (98%)	-0.06	1 (1%) 80 81	109, 136, 155, 162	0
15	CR	88/89 (98%)	0.88	15 (17%) 1 1	121, 151, 168, 172	0
16	AS	84/88 (95%)	-0.95	0 100 100	135, 156, 179, 198	0
16	CS	84/88 (95%)	-0.69	0 100 100	121, 143, 167, 203	0
17	AT	100/105 (95%)	-0.04	2 (2%) 65 64	123, 147, 162, 173	0
17	CT	100/105 (95%)	1.27	34 (34%) 0 0	122, 145, 159, 182	0
18	AU	72/88 (81%)	1.19	24 (33%) 0 0	118, 142, 168, 195	0
18	CU	72/88 (81%)	1.99	31 (43%) 0 0	134, 157, 181, 199	0
19	AV	83/93 (89%)	-0.33	0 100 100	133, 158, 180, 191	0
19	CV	78/93 (83%)	0.48	11 (14%) 2 2	169, 195, 210, 221	0
20	AW	99/106 (93%)	-0.44	1 (1%) 82 82	137, 159, 187, 196	0
20	CW	99/106 (93%)	-0.30	1 (1%) 82 82	112, 142, 177, 194	0
21	AX	25/27 (92%)	-0.75	0 100 100	120, 150, 170, 187	0
21	CX	25/27 (92%)	-0.98	0 100 100	144, 171, 192, 209	0
22	AC	77/77 (100%)	-0.37	0 100 100	102, 125, 153, 175	0
22	CC	77/77 (100%)	0.19	9 (11%) 4 4	106, 145, 175, 205	0
23	A1	4/4 (100%)	-0.39	0 100 100	106, 109, 114, 165	0
23	C1	4/4 (100%)	-0.26	0 100 100	127, 131, 143, 184	0
24	BA	2912/2912 (100%)	-0.18	77 (2%) 56 53	68, 102, 240, 278	0
24	DA	2909/2912 (99%)	-0.26	101 (3%) 44 42	79, 114, 258, 279	0
25	BB	122/122 (100%)	-0.57	1 (0%) 86 86	92, 122, 145, 211	0
25	DB	122/122 (100%)	-0.16	9 (7%) 14 14	115, 152, 178, 226	0
26	BD	272/276 (98%)	0.66	37 (13%) 3 2	69, 96, 117, 140	0
26	DD	272/276 (98%)	0.70	24 (8%) 10 10	72, 106, 130, 155	0
27	BE	205/206 (99%)	1.25	53 (25%) 0 0	73, 117, 163, 177	0
27	DE	205/206 (99%)	0.71	29 (14%) 2 2	79, 122, 168, 196	0
28	BF	202/210 (96%)	0.61	29 (14%) 2 2	74, 108, 149, 175	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	DF	208/210 (99%)	1.58	66 (31%) 0 0	82, 125, 187, 213	0
29	BG	181/182 (99%)	0.04	8 (4%) 34 33	105, 127, 167, 186	0
29	DG	181/182 (99%)	3.57	138 (76%) 0 0	136, 166, 194, 204	0
30	BH	170/180 (94%)	-0.12	5 (2%) 51 50	103, 135, 159, 175	0
30	DH	170/180 (94%)	1.65	59 (34%) 0 0	154, 222, 249, 262	0
31	BK	146/148 (98%)	-0.09	9 (6%) 20 20	103, 151, 170, 179	0
31	DK	146/148 (98%)	-0.20	8 (5%) 25 23	111, 159, 178, 185	0
32	BM	138/140 (98%)	0.54	11 (7%) 12 11	90, 115, 153, 183	0
32	DM	138/140 (98%)	0.91	24 (17%) 1 1	93, 129, 168, 189	0
33	BN	122/122 (100%)	0.06	3 (2%) 57 54	83, 111, 132, 139	0
33	DN	122/122 (100%)	0.77	14 (11%) 4 4	86, 116, 130, 140	0
34	BO	150/150 (100%)	1.08	42 (28%) 0 0	70, 113, 143, 207	0
34	DO	150/150 (100%)	1.51	46 (30%) 0 0	85, 129, 167, 206	0
35	BP	141/141 (100%)	0.34	9 (6%) 19 19	85, 107, 132, 163	0
35	DP	141/141 (100%)	0.93	24 (17%) 1 1	95, 126, 152, 177	0
36	B0	118/118 (100%)	0.96	19 (16%) 1 2	90, 110, 131, 148	0
36	D0	117/118 (99%)	0.20	7 (5%) 21 21	88, 111, 135, 146	0
37	BQ	111/112 (99%)	0.93	23 (20%) 1 1	90, 119, 148, 164	0
37	DQ	111/112 (99%)	0.98	23 (20%) 1 1	114, 146, 168, 190	0
38	BR	137/146 (93%)	0.48	18 (13%) 3 3	104, 125, 173, 202	0
38	DR	137/146 (93%)	0.61	14 (10%) 6 6	103, 121, 177, 212	0
39	B1	117/118 (99%)	0.04	4 (3%) 45 43	77, 106, 141, 168	0
39	D1	117/118 (99%)	0.76	16 (13%) 3 2	90, 122, 155, 178	0
40	B2	101/101 (100%)	1.23	31 (30%) 0 0	79, 122, 154, 181	0
40	D2	101/101 (100%)	2.78	62 (61%) 0 0	95, 149, 165, 181	0
41	BS	113/113 (100%)	1.54	32 (28%) 0 0	81, 102, 141, 191	0
41	DS	113/113 (100%)	1.18	22 (19%) 1 1	83, 107, 140, 194	0
42	BT	92/96 (95%)	0.73	9 (9%) 7 7	81, 98, 126, 145	0
42	DT	92/96 (95%)	1.32	29 (31%) 0 0	96, 117, 140, 159	0
43	BU	102/110 (92%)	0.32	6 (5%) 22 22	95, 123, 171, 190	0
43	DU	102/110 (92%)	2.70	56 (54%) 0 0	104, 142, 195, 212	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	BV	175/206 (84%)	1.84	61 (34%) 0 0	104, 142, 218, 229	0
44	DV	179/206 (86%)	2.09	93 (51%) 0 0	132, 174, 237, 251	0
45	B3	76/85 (89%)	0.21	2 (2%) 56 53	85, 101, 121, 163	0
45	D3	77/85 (90%)	1.90	25 (32%) 0 0	98, 117, 141, 175	0
46	BZ	97/98 (98%)	0.36	5 (5%) 27 25	83, 106, 149, 195	0
46	DZ	97/98 (98%)	1.54	34 (35%) 0 0	87, 116, 159, 191	0
47	BW	66/72 (91%)	0.63	5 (7%) 13 13	80, 108, 133, 171	0
47	DW	69/72 (95%)	1.29	16 (23%) 0 1	106, 138, 163, 196	0
48	BX	59/60 (98%)	1.29	13 (22%) 0 1	85, 106, 148, 160	0
48	DX	59/60 (98%)	2.22	32 (54%) 0 0	97, 126, 159, 194	0
49	B4	66/71 (92%)	0.19	3 (4%) 33 32	127, 176, 209, 219	0
49	D4	63/71 (88%)	7.92	63 (100%) 0 0	181, 212, 226, 235	0
50	B5	59/60 (98%)	2.43	21 (35%) 0 0	78, 115, 194, 210	0
50	D5	59/60 (98%)	1.34	11 (18%) 1 1	87, 114, 191, 218	0
51	B6	45/54 (83%)	8.93	45 (100%) 0 0	149, 184, 197, 201	0
51	D6	45/54 (83%)	12.81	45 (100%) 0 0	158, 195, 212, 215	0
52	B7	49/49 (100%)	0.50	6 (12%) 4 3	73, 83, 124, 154	0
52	D7	49/49 (100%)	2.03	19 (38%) 0 0	78, 91, 134, 156	0
53	B8	61/65 (93%)	0.23	3 (4%) 29 27	81, 96, 116, 145	0
53	D8	61/65 (93%)	1.28	11 (18%) 1 1	94, 109, 131, 161	0
All	All	20772/21286 (97%)	0.42	2772 (13%) 3 3	68, 133, 207, 279	0

The worst 5 of 2772 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
51	D6	13	CYS	29.8
51	D6	22	ALA	26.4
51	D6	52	VAL	23.5
51	D6	49	HIS	23.3
50	D5	59	GLU	23.2

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
54	MG	CA	1644	1/1	-0.07	0.46	133,133,133,133	0
54	MG	CA	1738	1/1	-0.03	0.23	114,114,114,114	0
54	MG	AA	1726	1/1	-0.01	0.28	132,132,132,132	0
54	MG	BA	3395	1/1	0.00	0.56	105,105,105,105	0
54	MG	AA	1734	1/1	0.04	0.36	146,146,146,146	0
54	MG	AC	102	1/1	0.04	0.30	123,123,123,123	0
54	MG	DA	3296	1/1	0.04	0.34	114,114,114,114	0
54	MG	BA	3447	1/1	0.12	0.32	116,116,116,116	0
54	MG	BA	3339	1/1	0.12	0.31	115,115,115,115	0
54	MG	AA	1730	1/1	0.14	2.08	116,116,116,116	0
54	MG	BB	211	1/1	0.23	0.42	102,102,102,102	0
54	MG	CA	1650	1/1	0.24	0.80	151,151,151,151	0
54	MG	BA	3411	1/1	0.24	0.46	110,110,110,110	0
54	MG	BA	3237	1/1	0.24	0.38	117,117,117,117	0
54	MG	DA	3041	1/1	0.24	0.26	142,142,142,142	0
54	MG	CA	1605	1/1	0.27	0.36	131,131,131,131	0
54	MG	BA	3093	1/1	0.29	0.31	154,154,154,154	0
54	MG	DB	207	1/1	0.30	0.16	114,114,114,114	0
54	MG	BA	3429	1/1	0.30	0.54	129,129,129,129	0
54	MG	AA	1776	1/1	0.35	0.21	116,116,116,116	0
54	MG	BA	3095	1/1	0.36	0.42	92,92,92,92	0
54	MG	DA	3038	1/1	0.36	0.27	122,122,122,122	0
54	MG	DA	3158	1/1	0.37	0.61	113,113,113,113	0
54	MG	BA	3536	1/1	0.37	0.40	96,96,96,96	0
54	MG	DA	3163	1/1	0.38	0.14	120,120,120,120	0
54	MG	DA	3081	1/1	0.38	0.39	116,116,116,116	0
54	MG	BA	3551	1/1	0.39	0.34	105,105,105,105	0
54	MG	DA	3279	1/1	0.39	0.24	125,125,125,125	0
54	MG	AA	1683	1/1	0.40	0.41	116,116,116,116	0
54	MG	CA	1793	1/1	0.40	0.37	115,115,115,115	0
54	MG	BA	3100	1/1	0.40	0.39	100,100,100,100	0
54	MG	DA	3333	1/1	0.41	0.46	128,128,128,128	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	BE	304	1/1	0.41	0.68	112,112,112,112	0
54	MG	AA	1686	1/1	0.42	0.20	120,120,120,120	0
54	MG	BA	3527	1/1	0.42	0.42	109,109,109,109	0
54	MG	DA	3386	1/1	0.42	0.35	102,102,102,102	0
54	MG	DA	3074	1/1	0.42	0.43	109,109,109,109	0
54	MG	CA	1631	1/1	0.42	0.26	134,134,134,134	0
54	MG	DB	206	1/1	0.43	0.37	142,142,142,142	0
54	MG	BA	3052	1/1	0.43	0.25	107,107,107,107	0
54	MG	DA	3293	1/1	0.44	1.77	112,112,112,112	0
54	MG	CA	1602	1/1	0.45	0.56	115,115,115,115	0
54	MG	DA	3367	1/1	0.45	1.02	125,125,125,125	0
54	MG	AA	1810	1/1	0.45	0.58	126,126,126,126	0
54	MG	AA	1769	1/1	0.46	0.23	124,124,124,124	0
54	MG	DA	3032	1/1	0.47	0.38	127,127,127,127	0
54	MG	B6	101	1/1	0.47	0.64	128,128,128,128	0
54	MG	DA	3011	1/1	0.48	0.26	128,128,128,128	0
54	MG	BA	3472	1/1	0.48	0.29	114,114,114,114	0
54	MG	DA	3016	1/1	0.48	0.37	123,123,123,123	0
54	MG	DA	3002	1/1	0.48	0.41	109,109,109,109	0
54	MG	BA	3084	1/1	0.49	0.80	110,110,110,110	0
54	MG	AA	1763	1/1	0.49	0.36	110,110,110,110	0
54	MG	CA	1727	1/1	0.50	0.18	113,113,113,113	0
54	MG	BA	3521	1/1	0.51	0.22	123,123,123,123	0
54	MG	CA	1747	1/1	0.51	0.53	122,122,122,122	0
54	MG	BA	3285	1/1	0.52	0.51	114,114,114,114	0
54	MG	AA	1816	1/1	0.52	0.28	115,115,115,115	0
54	MG	BA	3618	1/1	0.53	0.74	107,107,107,107	0
54	MG	BA	3455	1/1	0.53	0.52	107,107,107,107	0
54	MG	CA	1766	1/1	0.53	0.28	107,107,107,107	0
54	MG	CA	1713	1/1	0.53	0.12	137,137,137,137	0
54	MG	BA	3509	1/1	0.53	0.42	104,104,104,104	0
54	MG	AA	1790	1/1	0.53	0.50	115,115,115,115	0
54	MG	AA	1625	1/1	0.54	0.26	110,110,110,110	0
54	MG	BA	3505	1/1	0.54	0.48	108,108,108,108	0
54	MG	DA	3478	1/1	0.54	0.42	114,114,114,114	0
54	MG	AA	1696	1/1	0.54	0.23	104,104,104,104	0
54	MG	BA	3191	1/1	0.54	0.67	111,111,111,111	0
54	MG	DA	3396	1/1	0.55	0.21	95,95,95,95	0
54	MG	CA	1711	1/1	0.55	0.24	119,119,119,119	0
54	MG	AA	1671	1/1	0.55	0.27	110,110,110,110	0
54	MG	BA	3116	1/1	0.56	0.27	137,137,137,137	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	AA	1685	1/1	0.56	0.38	95,95,95,95	0
54	MG	BA	3506	1/1	0.56	0.22	92,92,92,92	0
54	MG	DA	3523	1/1	0.56	0.43	100,100,100,100	0
54	MG	AA	1690	1/1	0.56	0.26	128,128,128,128	0
54	MG	BA	3446	1/1	0.56	0.52	127,127,127,127	0
54	MG	AA	1802	1/1	0.56	0.29	136,136,136,136	0
54	MG	DA	3104	1/1	0.56	0.48	107,107,107,107	0
54	MG	BA	3367	1/1	0.56	0.20	124,124,124,124	0
54	MG	BA	3612	1/1	0.57	0.41	99,99,99,99	0
54	MG	BO	202	1/1	0.57	0.29	98,98,98,98	0
54	MG	BA	3096	1/1	0.57	0.52	129,129,129,129	0
54	MG	BA	3493	1/1	0.58	0.41	116,116,116,116	0
54	MG	DA	3178	1/1	0.58	0.26	100,100,100,100	0
54	MG	AA	1710	1/1	0.58	0.28	116,116,116,116	0
54	MG	BA	3324	1/1	0.58	0.33	101,101,101,101	0
54	MG	CA	1642	1/1	0.58	0.14	105,105,105,105	0
54	MG	CA	1626	1/1	0.58	0.19	117,117,117,117	0
54	MG	DA	3424	1/1	0.58	0.60	115,115,115,115	0
54	MG	BA	3470	1/1	0.59	0.37	117,117,117,117	0
54	MG	AC	108	1/1	0.59	2.21	112,112,112,112	0
54	MG	AA	1628	1/1	0.59	0.36	142,142,142,142	0
54	MG	BA	3384	1/1	0.59	0.23	107,107,107,107	0
54	MG	CA	1799	1/1	0.59	0.21	150,150,150,150	0
54	MG	BA	3403	1/1	0.59	0.36	114,114,114,114	0
54	MG	CA	1787	1/1	0.59	0.25	129,129,129,129	0
54	MG	BA	3539	1/1	0.59	0.49	99,99,99,99	0
54	MG	DA	3295	1/1	0.59	0.44	105,105,105,105	0
54	MG	CA	1773	1/1	0.59	0.21	114,114,114,114	0
54	MG	DA	3412	1/1	0.59	0.15	110,110,110,110	0
54	MG	AA	1751	1/1	0.59	0.56	102,102,102,102	0
54	MG	BA	3530	1/1	0.60	0.40	110,110,110,110	0
54	MG	BA	3075	1/1	0.60	0.53	97,97,97,97	0
54	MG	AA	1758	1/1	0.60	0.28	111,111,111,111	0
54	MG	AA	1820	1/1	0.60	1.32	130,130,130,130	0
54	MG	DA	3164	1/1	0.60	0.39	136,136,136,136	0
54	MG	DA	3485	1/1	0.60	0.19	104,104,104,104	0
54	MG	DA	3449	1/1	0.60	0.39	106,106,106,106	0
54	MG	BA	3543	1/1	0.60	0.30	90,90,90,90	0
54	MG	CA	1662	1/1	0.60	0.34	120,120,120,120	0
54	MG	BA	3370	1/1	0.60	0.41	111,111,111,111	0
54	MG	DA	3087	1/1	0.60	0.14	111,111,111,111	0
54	MG	BA	3457	1/1	0.61	0.31	112,112,112,112	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	DA	3374	1/1	0.61	0.20	106,106,106,106	0
54	MG	DA	3397	1/1	0.61	0.24	96,96,96,96	0
54	MG	CA	1684	1/1	0.61	0.25	115,115,115,115	0
54	MG	DA	3419	1/1	0.61	0.27	100,100,100,100	0
54	MG	BA	3149	1/1	0.61	0.29	110,110,110,110	0
54	MG	AA	1738	1/1	0.61	0.32	117,117,117,117	0
54	MG	AA	1693	1/1	0.61	0.37	123,123,123,123	0
54	MG	BB	214	1/1	0.61	0.44	108,108,108,108	0
54	MG	AS	101	1/1	0.61	0.30	106,106,106,106	0
54	MG	BA	3230	1/1	0.62	0.34	97,97,97,97	0
54	MG	BA	3119	1/1	0.62	0.41	78,78,78,78	0
54	MG	BA	3424	1/1	0.62	0.58	111,111,111,111	0
54	MG	BA	3291	1/1	0.62	0.40	99,99,99,99	0
54	MG	BA	3154	1/1	0.62	0.38	104,104,104,104	0
54	MG	AA	1687	1/1	0.62	0.40	99,99,99,99	0
54	MG	DA	3487	1/1	0.62	0.27	108,108,108,108	0
54	MG	DA	3341	1/1	0.62	0.38	107,107,107,107	0
54	MG	BA	3319	1/1	0.63	0.56	129,129,129,129	0
54	MG	AA	1749	1/1	0.63	0.23	112,112,112,112	0
54	MG	BA	3481	1/1	0.63	0.37	99,99,99,99	0
54	MG	CA	1792	1/1	0.63	0.14	160,160,160,160	0
54	MG	AA	1752	1/1	0.63	0.50	121,121,121,121	0
54	MG	BA	3480	1/1	0.63	0.17	187,187,187,187	0
54	MG	DA	3450	1/1	0.64	0.29	130,130,130,130	0
54	MG	BA	3365	1/1	0.64	0.57	104,104,104,104	0
54	MG	DA	3402	1/1	0.64	0.36	105,105,105,105	0
54	MG	BA	3245	1/1	0.64	0.48	120,120,120,120	0
54	MG	DA	3455	1/1	0.64	0.25	147,147,147,147	0
54	MG	AA	1672	1/1	0.64	0.26	112,112,112,112	0
54	MG	DA	3486	1/1	0.64	1.05	112,112,112,112	0
54	MG	DA	3017	1/1	0.64	0.27	111,111,111,111	0
54	MG	DA	3377	1/1	0.64	0.36	102,102,102,102	0
54	MG	BA	3124	1/1	0.64	0.30	110,110,110,110	0
54	MG	BA	3102	1/1	0.64	0.26	98,98,98,98	0
54	MG	DA	3371	1/1	0.64	0.30	111,111,111,111	0
54	MG	AA	1807	1/1	0.64	0.24	101,101,101,101	0
54	MG	DA	3093	1/1	0.64	0.21	106,106,106,106	0
54	MG	DA	3463	1/1	0.64	0.36	109,109,109,109	0
54	MG	AQ	102	1/1	0.65	0.34	118,118,118,118	0
54	MG	AA	1636	1/1	0.65	0.32	92,92,92,92	0
54	MG	CA	1765	1/1	0.65	0.25	126,126,126,126	0
54	MG	BA	3617	1/1	0.65	0.38	134,134,134,134	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	AA	1724	1/1	0.65	0.42	115,115,115,115	0
54	MG	DA	3430	1/1	0.65	0.21	105,105,105,105	0
54	MG	DA	3517	1/1	0.65	0.32	106,106,106,106	0
54	MG	DA	3256	1/1	0.65	1.67	103,103,103,103	0
54	MG	DA	3304	1/1	0.65	0.24	83,83,83,83	0
54	MG	BA	3448	1/1	0.65	0.25	95,95,95,95	0
54	MG	AA	1676	1/1	0.65	0.45	132,132,132,132	0
54	MG	DA	3162	1/1	0.65	0.38	108,108,108,108	0
54	MG	BA	3056	1/1	0.65	0.53	101,101,101,101	0
54	MG	DA	3051	1/1	0.65	0.28	81,81,81,81	0
54	MG	DA	3098	1/1	0.66	0.16	139,139,139,139	0
54	MG	BA	3314	1/1	0.66	0.17	104,104,104,104	0
54	MG	DA	3252	1/1	0.66	0.22	108,108,108,108	0
54	MG	CA	1751	1/1	0.66	0.59	118,118,118,118	0
54	MG	DA	3177	1/1	0.66	0.25	99,99,99,99	0
54	MG	DA	3343	1/1	0.66	0.34	95,95,95,95	0
54	MG	BB	206	1/1	0.67	0.27	97,97,97,97	0
54	MG	DA	3410	1/1	0.67	0.44	118,118,118,118	0
54	MG	BA	3437	1/1	0.67	0.27	81,81,81,81	0
54	MG	DA	3280	1/1	0.67	0.21	94,94,94,94	0
54	MG	BA	3443	1/1	0.67	0.45	124,124,124,124	0
54	MG	AA	1745	1/1	0.67	0.26	128,128,128,128	0
54	MG	AA	1787	1/1	0.67	0.18	115,115,115,115	0
54	MG	CA	1745	1/1	0.67	0.24	132,132,132,132	0
54	MG	AA	1719	1/1	0.67	0.26	110,110,110,110	0
54	MG	AA	1611	1/1	0.67	0.17	138,138,138,138	0
54	MG	DA	3398	1/1	0.67	0.29	130,130,130,130	0
54	MG	AA	1688	1/1	0.67	0.10	146,146,146,146	0
54	MG	BA	3369	1/1	0.67	0.44	94,94,94,94	0
54	MG	CA	1731	1/1	0.68	0.51	110,110,110,110	0
54	MG	CA	1749	1/1	0.68	0.20	120,120,120,120	0
54	MG	CA	1716	1/1	0.68	0.47	126,126,126,126	0
54	MG	BA	3188	1/1	0.68	0.61	120,120,120,120	0
54	MG	DA	3321	1/1	0.68	0.19	89,89,89,89	0
54	MG	DA	3407	1/1	0.68	0.21	114,114,114,114	0
54	MG	BA	3566	1/1	0.68	0.40	100,100,100,100	0
54	MG	BA	3122	1/1	0.68	0.26	114,114,114,114	0
54	MG	DA	3359	1/1	0.68	0.30	102,102,102,102	0
54	MG	BA	3477	1/1	0.68	0.38	93,93,93,93	0
54	MG	CA	1663	1/1	0.68	0.13	105,105,105,105	0
54	MG	BA	3066	1/1	0.68	0.38	97,97,97,97	0
54	MG	BA	3398	1/1	0.68	0.60	105,105,105,105	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	BA	3374	1/1	0.68	0.16	104,104,104,104	0
54	MG	CA	1700	1/1	0.68	0.34	92,92,92,92	0
54	MG	DA	3310	1/1	0.68	0.50	111,111,111,111	0
54	MG	BA	3212	1/1	0.68	0.47	124,124,124,124	0
54	MG	AG	301	1/1	0.68	0.14	114,114,114,114	0
54	MG	BA	3278	1/1	0.69	0.34	101,101,101,101	0
54	MG	AA	1773	1/1	0.69	0.54	137,137,137,137	0
54	MG	CA	1622	1/1	0.69	0.47	122,122,122,122	0
54	MG	AA	1750	1/1	0.69	0.61	110,110,110,110	0
54	MG	BA	3357	1/1	0.69	0.78	119,119,119,119	0
54	MG	DA	3080	1/1	0.69	0.20	114,114,114,114	0
54	MG	BA	3329	1/1	0.69	0.45	106,106,106,106	0
54	MG	BA	3576	1/1	0.69	0.41	120,120,120,120	0
54	MG	AA	1670	1/1	0.69	0.28	83,83,83,83	0
54	MG	DE	302	1/1	0.69	0.27	97,97,97,97	0
54	MG	DA	3018	1/1	0.69	0.45	83,83,83,83	0
54	MG	BA	3442	1/1	0.69	0.49	112,112,112,112	0
54	MG	BA	3069	1/1	0.70	0.54	115,115,115,115	0
54	MG	AA	1772	1/1	0.70	0.32	155,155,155,155	0
54	MG	CG	301	1/1	0.70	0.37	115,115,115,115	0
54	MG	BA	3494	1/1	0.70	0.23	97,97,97,97	0
54	MG	AA	1809	1/1	0.70	0.43	108,108,108,108	0
54	MG	BA	3407	1/1	0.70	0.42	105,105,105,105	0
54	MG	DA	3427	1/1	0.70	0.27	114,114,114,114	0
54	MG	CA	1698	1/1	0.70	0.23	96,96,96,96	0
54	MG	BA	3564	1/1	0.70	0.58	116,116,116,116	0
54	MG	CA	1630	1/1	0.70	0.42	120,120,120,120	0
54	MG	AA	1778	1/1	0.70	0.21	136,136,136,136	0
54	MG	BA	3537	1/1	0.71	0.38	124,124,124,124	0
54	MG	CA	1604	1/1	0.71	0.47	105,105,105,105	0
54	MG	DA	3149	1/1	0.71	0.15	112,112,112,112	0
54	MG	DA	3239	1/1	0.71	0.67	105,105,105,105	0
54	MG	BA	3137	1/1	0.71	0.25	105,105,105,105	0
54	MG	CA	1616	1/1	0.71	0.28	108,108,108,108	0
54	MG	DA	3468	1/1	0.71	0.29	126,126,126,126	0
54	MG	DA	3022	1/1	0.71	0.22	86,86,86,86	0
54	MG	DA	3475	1/1	0.72	0.32	121,121,121,121	0
54	MG	DA	3085	1/1	0.72	0.37	113,113,113,113	0
54	MG	BA	3535	1/1	0.72	0.45	116,116,116,116	0
54	MG	BA	3383	1/1	0.72	0.38	95,95,95,95	0
54	MG	DA	3421	1/1	0.72	0.24	141,141,141,141	0
54	MG	DA	3481	1/1	0.72	0.38	101,101,101,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	CA	1794	1/1	0.72	0.42	109,109,109,109	0
54	MG	BA	3205	1/1	0.72	0.27	88,88,88,88	0
54	MG	DB	208	1/1	0.72	0.11	105,105,105,105	0
54	MG	BA	3214	1/1	0.72	0.74	93,93,93,93	0
54	MG	CA	1688	1/1	0.72	0.38	101,101,101,101	0
54	MG	DA	3004	1/1	0.72	0.34	120,120,120,120	0
54	MG	CA	1784	1/1	0.72	0.18	94,94,94,94	0
54	MG	BA	3615	1/1	0.73	0.21	92,92,92,92	0
54	MG	AA	1829	1/1	0.73	0.27	112,112,112,112	0
54	MG	AA	1765	1/1	0.73	0.15	137,137,137,137	0
54	MG	BA	3235	1/1	0.73	0.37	128,128,128,128	0
54	MG	DD	301	1/1	0.73	0.39	119,119,119,119	0
54	MG	DA	3352	1/1	0.73	0.35	81,81,81,81	0
54	MG	CA	1723	1/1	0.73	0.46	111,111,111,111	0
54	MG	CA	1756	1/1	0.73	0.33	111,111,111,111	0
54	MG	BA	3300	1/1	0.73	0.34	102,102,102,102	0
54	MG	BA	3440	1/1	0.73	0.33	79,79,79,79	0
54	MG	DA	3461	1/1	0.73	0.18	102,102,102,102	0
54	MG	DB	209	1/1	0.73	0.28	131,131,131,131	0
54	MG	BA	3292	1/1	0.73	0.48	113,113,113,113	0
54	MG	BA	3465	1/1	0.73	0.64	107,107,107,107	0
54	MG	BA	3228	1/1	0.73	0.54	85,85,85,85	0
54	MG	DA	3453	1/1	0.73	0.23	104,104,104,104	0
54	MG	BA	3269	1/1	0.73	0.23	85,85,85,85	0
54	MG	DA	3272	1/1	0.74	0.24	92,92,92,92	0
54	MG	BA	3459	1/1	0.74	0.37	91,91,91,91	0
54	MG	DA	3434	1/1	0.74	0.36	110,110,110,110	0
54	MG	DA	3320	1/1	0.74	0.70	110,110,110,110	0
54	MG	DB	210	1/1	0.74	0.20	73,73,73,73	0
54	MG	CA	1695	1/1	0.74	0.44	111,111,111,111	0
54	MG	CA	1774	1/1	0.74	0.33	110,110,110,110	0
54	MG	BA	3496	1/1	0.74	0.47	108,108,108,108	0
54	MG	BA	3275	1/1	0.74	0.52	111,111,111,111	0
54	MG	DA	3482	1/1	0.74	0.14	120,120,120,120	0
54	MG	CC	108	1/1	0.74	0.33	129,129,129,129	0
54	MG	BA	3541	1/1	0.74	0.51	120,120,120,120	0
54	MG	BA	3562	1/1	0.74	0.33	97,97,97,97	0
54	MG	BA	3548	1/1	0.74	0.36	96,96,96,96	0
54	MG	DA	3168	1/1	0.74	0.16	95,95,95,95	0
54	MG	BA	3196	1/1	0.74	0.28	109,109,109,109	0
54	MG	DA	3195	1/1	0.74	0.22	104,104,104,104	0
54	MG	BA	3484	1/1	0.74	0.33	116,116,116,116	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	DA	3203	1/1	0.74	0.26	90,90,90,90	0
54	MG	AA	1674	1/1	0.75	0.47	119,119,119,119	0
54	MG	DA	3474	1/1	0.75	0.34	107,107,107,107	0
54	MG	BA	3071	1/1	0.75	0.29	103,103,103,103	0
54	MG	BA	3534	1/1	0.75	0.41	95,95,95,95	0
54	MG	CA	1707	1/1	0.75	0.45	109,109,109,109	0
54	MG	DA	3318	1/1	0.75	0.43	91,91,91,91	0
54	MG	AA	1643	1/1	0.75	0.12	112,112,112,112	0
54	MG	DA	3125	1/1	0.75	0.18	105,105,105,105	0
54	MG	BA	3485	1/1	0.75	0.25	90,90,90,90	0
54	MG	BA	3127	1/1	0.75	0.26	109,109,109,109	0
54	MG	AA	1782	1/1	0.75	0.14	168,168,168,168	0
54	MG	CA	1803	1/1	0.75	0.37	123,123,123,123	0
54	MG	AA	1805	1/1	0.75	0.80	108,108,108,108	0
54	MG	AA	1796	1/1	0.75	0.26	109,109,109,109	0
54	MG	AA	1801	1/1	0.75	0.21	97,97,97,97	0
54	MG	BA	3376	1/1	0.75	0.52	96,96,96,96	0
54	MG	BA	3458	1/1	0.75	0.47	96,96,96,96	0
54	MG	CA	1638	1/1	0.75	0.28	128,128,128,128	0
54	MG	BA	3320	1/1	0.75	0.35	104,104,104,104	0
54	MG	CA	1755	1/1	0.75	0.17	97,97,97,97	0
54	MG	CA	1679	1/1	0.75	0.15	94,94,94,94	0
54	MG	DA	3512	1/1	0.75	0.39	81,81,81,81	0
54	MG	DA	3324	1/1	0.75	0.23	109,109,109,109	0
54	MG	DA	3027	1/1	0.75	0.11	115,115,115,115	0
54	MG	CA	1601	1/1	0.75	0.20	108,108,108,108	0
54	MG	BA	3396	1/1	0.75	0.49	101,101,101,101	0
54	MG	BA	3368	1/1	0.75	0.43	93,93,93,93	0
54	MG	CA	1778	1/1	0.76	0.43	118,118,118,118	0
54	MG	BA	3452	1/1	0.76	0.29	131,131,131,131	0
54	MG	BA	3513	1/1	0.76	0.20	112,112,112,112	0
54	MG	DB	204	1/1	0.76	0.13	111,111,111,111	0
54	MG	CA	1728	1/1	0.76	0.26	144,144,144,144	0
54	MG	BA	3204	1/1	0.76	0.50	98,98,98,98	0
54	MG	CA	1712	1/1	0.76	0.23	105,105,105,105	0
54	MG	DA	3519	1/1	0.76	0.21	94,94,94,94	0
54	MG	CA	1753	1/1	0.76	0.20	95,95,95,95	0
54	MG	BA	3296	1/1	0.76	0.45	93,93,93,93	0
54	MG	BA	3090	1/1	0.76	0.18	78,78,78,78	0
54	MG	DA	3348	1/1	0.76	0.18	108,108,108,108	0
54	MG	DA	3460	1/1	0.76	0.19	96,96,96,96	0
54	MG	DA	3464	1/1	0.76	0.20	101,101,101,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	BA	3379	1/1	0.76	0.37	106,106,106,106	0
54	MG	BA	3340	1/1	0.76	0.62	95,95,95,95	0
54	MG	DA	3042	1/1	0.76	0.23	111,111,111,111	0
54	MG	BA	3251	1/1	0.76	0.56	109,109,109,109	0
54	MG	DA	3260	1/1	0.76	0.38	128,128,128,128	0
54	MG	CA	1761	1/1	0.76	0.20	170,170,170,170	0
54	MG	DA	3037	1/1	0.76	1.07	117,117,117,117	0
54	MG	AH	202	1/1	0.77	0.13	108,108,108,108	0
54	MG	BA	3414	1/1	0.77	0.20	98,98,98,98	0
54	MG	DA	3385	1/1	0.77	0.19	95,95,95,95	0
54	MG	BB	207	1/1	0.77	0.34	131,131,131,131	0
54	MG	AA	1748	1/1	0.77	0.66	130,130,130,130	0
54	MG	BA	3132	1/1	0.77	0.34	127,127,127,127	0
54	MG	AA	1770	1/1	0.77	0.53	98,98,98,98	0
54	MG	CA	1608	1/1	0.77	0.21	103,103,103,103	0
54	MG	AA	1692	1/1	0.77	0.24	108,108,108,108	0
54	MG	DA	3416	1/1	0.77	0.32	100,100,100,100	0
54	MG	DA	3370	1/1	0.77	0.16	96,96,96,96	0
54	MG	BA	3390	1/1	0.77	0.26	81,81,81,81	0
54	MG	BA	3265	1/1	0.77	0.28	96,96,96,96	0
54	MG	DA	3103	1/1	0.77	0.12	117,117,117,117	0
54	MG	BA	3110	1/1	0.77	0.35	92,92,92,92	0
54	MG	DZ	101	1/1	0.78	0.26	113,113,113,113	0
54	MG	DA	3366	1/1	0.78	0.37	103,103,103,103	0
54	MG	BA	3183	1/1	0.78	0.20	110,110,110,110	0
54	MG	BA	3598	1/1	0.78	0.36	84,84,84,84	0
54	MG	BA	3360	1/1	0.78	0.29	110,110,110,110	0
54	MG	AA	1699	1/1	0.78	0.20	122,122,122,122	0
54	MG	DA	3417	1/1	0.78	0.17	110,110,110,110	0
54	MG	AA	1694	1/1	0.78	0.79	105,105,105,105	0
54	MG	CA	1705	1/1	0.78	0.49	114,114,114,114	0
54	MG	BA	3393	1/1	0.78	0.20	108,108,108,108	0
54	MG	BA	3421	1/1	0.78	0.86	106,106,106,106	0
54	MG	BA	3431	1/1	0.78	0.41	96,96,96,96	0
54	MG	BA	3450	1/1	0.78	0.32	99,99,99,99	0
54	MG	BA	3354	1/1	0.78	0.39	113,113,113,113	0
54	MG	DA	3172	1/1	0.78	0.64	110,110,110,110	0
54	MG	DA	3301	1/1	0.78	1.06	124,124,124,124	0
54	MG	BA	3565	1/1	0.78	0.22	86,86,86,86	0
54	MG	BA	3489	1/1	0.78	0.29	104,104,104,104	0
54	MG	DA	3291	1/1	0.78	0.41	85,85,85,85	0
54	MG	BA	3400	1/1	0.78	0.25	101,101,101,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
54	MG	CC	106	1/1	0.78	0.17	112,112,112,112	0
54	MG	DA	3362	1/1	0.78	0.17	120,120,120,120	0
54	MG	AA	1664	1/1	0.78	0.30	96,96,96,96	0
54	MG	AA	1662	1/1	0.79	1.48	111,111,111,111	0
54	MG	AA	1786	1/1	0.79	0.29	131,131,131,131	0
54	MG	CA	1750	1/1	0.79	0.47	122,122,122,122	0
54	MG	BA	3361	1/1	0.79	0.57	123,123,123,123	0
54	MG	DA	3207	1/1	0.79	0.22	86,86,86,86	0
54	MG	DA	3045	1/1	0.79	0.17	67,67,67,67	0
54	MG	AA	1680	1/1	0.79	0.39	104,104,104,104	0
54	MG	CA	1699	1/1	0.79	0.24	81,81,81,81	0
54	MG	DA	3372	1/1	0.79	0.24	101,101,101,101	0
54	MG	BA	3011	1/1	0.79	0.36	72,72,72,72	0
54	MG	DA	3096	1/1	0.79	0.25	125,125,125,125	0
54	MG	AA	1740	1/1	0.79	0.38	75,75,75,75	0
54	MG	CA	1781	1/1	0.79	0.24	126,126,126,126	0
54	MG	AA	1812	1/1	0.79	0.22	124,124,124,124	0
54	MG	DA	3123	1/1	0.79	0.16	106,106,106,106	0
54	MG	BA	3532	1/1	0.79	0.33	100,100,100,100	0
54	MG	DA	3437	1/1	0.79	0.22	96,96,96,96	0
54	MG	AA	1649	1/1	0.79	0.15	90,90,90,90	0
54	MG	AA	1811	1/1	0.79	0.14	154,154,154,154	0
54	MG	BA	3449	1/1	0.79	0.48	118,118,118,118	0
54	MG	DA	3354	1/1	0.79	0.70	105,105,105,105	0
54	MG	BA	3401	1/1	0.79	0.36	91,91,91,91	0
54	MG	DA	3135	1/1	0.79	0.44	99,99,99,99	0
54	MG	DB	214	1/1	0.79	0.09	118,118,118,118	0
54	MG	BA	3626	1/1	0.79	0.47	103,103,103,103	0
54	MG	AA	1722	1/1	0.79	0.14	109,109,109,109	0
54	MG	CA	1666	1/1	0.79	0.35	120,120,120,120	0
54	MG	BA	3526	1/1	0.79	0.51	115,115,115,115	0
54	MG	BA	3554	1/1	0.80	0.30	99,99,99,99	0
54	MG	DA	3250	1/1	0.80	0.87	105,105,105,105	0
54	MG	CA	1790	1/1	0.80	0.41	118,118,118,118	0
54	MG	DA	3441	1/1	0.80	0.19	116,116,116,116	0
54	MG	DA	3522	1/1	0.80	0.23	113,113,113,113	0
54	MG	BF	301	1/1	0.80	0.86	100,100,100,100	0
54	MG	AA	1741	1/1	0.80	0.24	130,130,130,130	0
54	MG	BA	3242	1/1	0.80	0.52	115,115,115,115	0
54	MG	BA	3540	1/1	0.80	0.47	122,122,122,122	0
54	MG	DA	3339	1/1	0.80	0.40	152,152,152,152	0
54	MG	BA	3538	1/1	0.80	0.67	111,111,111,111	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	CA	1758	1/1	0.80	0.47	110,110,110,110	0
54	MG	DA	3428	1/1	0.80	0.15	89,89,89,89	0
54	MG	BA	3406	1/1	0.80	0.51	86,86,86,86	0
54	MG	AA	1759	1/1	0.80	0.32	87,87,87,87	0
54	MG	AA	1618	1/1	0.80	0.23	98,98,98,98	0
54	MG	DA	3033	1/1	0.80	0.20	89,89,89,89	0
54	MG	DA	3265	1/1	0.80	0.37	115,115,115,115	0
54	MG	DA	3400	1/1	0.80	0.29	105,105,105,105	0
54	MG	BA	3595	1/1	0.80	0.36	105,105,105,105	0
54	MG	AA	1658	1/1	0.80	0.22	79,79,79,79	0
54	MG	DA	3425	1/1	0.80	0.23	122,122,122,122	0
54	MG	DA	3346	1/1	0.80	0.24	93,93,93,93	0
54	MG	DA	3008	1/1	0.80	0.47	93,93,93,93	0
54	MG	CA	1633	1/1	0.81	0.39	107,107,107,107	0
54	MG	AA	1825	1/1	0.81	0.27	93,93,93,93	0
54	MG	DA	3518	1/1	0.81	0.50	94,94,94,94	0
54	MG	BA	3404	1/1	0.81	0.29	93,93,93,93	0
54	MG	DR	201	1/1	0.81	0.67	86,86,86,86	0
54	MG	BA	3160	1/1	0.81	0.55	109,109,109,109	0
54	MG	DA	3233	1/1	0.81	0.29	79,79,79,79	0
54	MG	BB	201	1/1	0.81	0.37	99,99,99,99	0
54	MG	DA	3435	1/1	0.81	0.23	99,99,99,99	0
54	MG	AA	1754	1/1	0.81	0.15	85,85,85,85	0
54	MG	DA	3024	1/1	0.81	0.11	112,112,112,112	0
54	MG	AA	1708	1/1	0.81	0.33	104,104,104,104	0
54	MG	AA	1669	1/1	0.81	0.23	79,79,79,79	0
54	MG	DA	3071	1/1	0.81	0.67	123,123,123,123	0
54	MG	BA	3303	1/1	0.81	0.12	119,119,119,119	0
54	MG	BA	3185	1/1	0.81	0.93	112,112,112,112	0
54	MG	CA	1627	1/1	0.81	0.47	112,112,112,112	0
54	MG	DA	3235	1/1	0.81	0.26	89,89,89,89	0
54	MG	AA	1789	1/1	0.81	0.24	79,79,79,79	0
54	MG	DU	201	1/1	0.81	0.17	103,103,103,103	0
54	MG	AA	1634	1/1	0.81	0.31	97,97,97,97	0
54	MG	CA	1681	1/1	0.81	0.28	96,96,96,96	0
54	MG	DA	3088	1/1	0.81	0.13	99,99,99,99	0
54	MG	BA	3380	1/1	0.81	0.26	91,91,91,91	0
54	MG	DA	3148	1/1	0.81	0.22	70,70,70,70	0
54	MG	BE	305	1/1	0.81	0.43	111,111,111,111	0
54	MG	CA	1645	1/1	0.81	0.12	103,103,103,103	0
54	MG	BA	3441	1/1	0.81	0.23	95,95,95,95	0
54	MG	DA	3509	1/1	0.81	0.17	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	DA	3057	1/1	0.81	0.16	104,104,104,104	0
54	MG	CA	1609	1/1	0.81	0.33	119,119,119,119	0
54	MG	DA	3048	1/1	0.81	0.17	84,84,84,84	0
54	MG	CA	1636	1/1	0.81	0.22	91,91,91,91	0
54	MG	BE	303	1/1	0.81	0.28	72,72,72,72	0
54	MG	CA	1611	1/1	0.81	0.42	114,114,114,114	0
54	MG	BA	3460	1/1	0.81	0.22	90,90,90,90	0
54	MG	BA	3561	1/1	0.81	0.24	86,86,86,86	0
54	MG	BA	3355	1/1	0.81	0.52	90,90,90,90	0
54	MG	DA	3300	1/1	0.81	0.47	107,107,107,107	0
54	MG	DA	3029	1/1	0.81	0.25	87,87,87,87	0
54	MG	BA	3522	1/1	0.81	0.12	106,106,106,106	0
54	MG	CA	1772	1/1	0.81	0.23	109,109,109,109	0
54	MG	AA	1684	1/1	0.81	0.39	123,123,123,123	0
54	MG	BA	3169	1/1	0.81	0.36	104,104,104,104	0
54	MG	BA	3345	1/1	0.81	0.16	95,95,95,95	0
54	MG	DA	3067	1/1	0.81	0.18	97,97,97,97	0
54	MG	BA	3091	1/1	0.81	0.30	103,103,103,103	0
54	MG	AA	1792	1/1	0.82	0.47	93,93,93,93	0
54	MG	AC	107	1/1	0.82	0.20	111,111,111,111	0
54	MG	CA	1693	1/1	0.82	0.42	117,117,117,117	0
54	MG	DA	3044	1/1	0.82	0.11	96,96,96,96	0
54	MG	BA	3392	1/1	0.82	0.35	110,110,110,110	0
54	MG	BA	3323	1/1	0.82	0.40	116,116,116,116	0
54	MG	BA	3428	1/1	0.82	0.38	80,80,80,80	0
54	MG	BA	3092	1/1	0.82	0.44	111,111,111,111	0
54	MG	BA	3286	1/1	0.82	0.22	98,98,98,98	0
54	MG	AA	1675	1/1	0.82	0.12	93,93,93,93	0
54	MG	BA	3482	1/1	0.82	0.40	88,88,88,88	0
54	MG	DA	3436	1/1	0.82	0.14	120,120,120,120	0
54	MG	AA	1668	1/1	0.82	0.24	105,105,105,105	0
54	MG	AA	1727	1/1	0.82	0.12	110,110,110,110	0
54	MG	DA	3368	1/1	0.82	0.87	95,95,95,95	0
54	MG	AA	1652	1/1	0.82	0.35	91,91,91,91	0
54	MG	AA	1704	1/1	0.82	0.41	112,112,112,112	0
54	MG	CA	1706	1/1	0.82	0.32	126,126,126,126	0
54	MG	AA	1828	1/1	0.82	0.34	94,94,94,94	0
54	MG	BA	3088	1/1	0.82	0.40	97,97,97,97	0
54	MG	BA	3177	1/1	0.82	1.63	101,101,101,101	0
54	MG	B3	101	1/1	0.82	0.34	77,77,77,77	0
54	MG	DA	3465	1/1	0.82	0.53	111,111,111,111	0
54	MG	DA	3012	1/1	0.82	0.71	129,129,129,129	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	DA	3444	1/1	0.82	0.29	100,100,100,100	0
54	MG	DB	213	1/1	0.82	0.14	91,91,91,91	0
54	MG	DA	3040	1/1	0.82	0.14	98,98,98,98	0
54	MG	BA	3351	1/1	0.82	0.55	84,84,84,84	0
54	MG	AA	1766	1/1	0.82	0.11	94,94,94,94	0
54	MG	BA	3571	1/1	0.82	0.43	85,85,85,85	0
54	MG	DA	3305	1/1	0.82	0.35	91,91,91,91	0
54	MG	BA	3129	1/1	0.82	0.16	92,92,92,92	0
54	MG	DA	3525	1/1	0.82	0.35	103,103,103,103	0
54	MG	DA	3454	1/1	0.82	0.17	94,94,94,94	0
54	MG	AA	1728	1/1	0.82	0.14	85,85,85,85	0
54	MG	AA	1689	1/1	0.82	0.22	153,153,153,153	0
54	MG	BA	3289	1/1	0.82	0.25	83,83,83,83	0
54	MG	CC	104	1/1	0.82	0.37	95,95,95,95	0
54	MG	CC	107	1/1	0.82	0.92	120,120,120,120	0
54	MG	CA	1647	1/1	0.82	0.31	83,83,83,83	0
54	MG	CA	1754	1/1	0.82	0.44	97,97,97,97	0
54	MG	DA	3355	1/1	0.82	0.15	89,89,89,89	0
54	MG	DA	3299	1/1	0.82	1.67	105,105,105,105	0
54	MG	CA	1694	1/1	0.82	0.23	108,108,108,108	0
54	MG	BA	3486	1/1	0.82	0.22	108,108,108,108	0
54	MG	BA	3619	1/1	0.82	0.23	88,88,88,88	0
54	MG	AA	1815	1/1	0.82	0.49	88,88,88,88	0
54	MG	BA	3312	1/1	0.82	0.43	98,98,98,98	0
54	MG	AA	1715	1/1	0.82	0.31	115,115,115,115	0
54	MG	DA	3484	1/1	0.82	0.18	81,81,81,81	0
54	MG	CA	1717	1/1	0.82	0.25	135,135,135,135	0
54	MG	DA	3332	1/1	0.82	0.25	120,120,120,120	0
54	MG	CA	1687	1/1	0.83	0.41	106,106,106,106	0
54	MG	DA	3513	1/1	0.83	0.28	95,95,95,95	0
54	MG	DA	3456	1/1	0.83	0.26	138,138,138,138	0
54	MG	AQ	101	1/1	0.83	0.34	84,84,84,84	0
54	MG	DA	3283	1/1	0.83	0.22	114,114,114,114	0
54	MG	DA	3106	1/1	0.83	1.48	122,122,122,122	0
54	MG	BA	3625	1/1	0.83	0.32	99,99,99,99	0
54	MG	DB	211	1/1	0.83	0.26	107,107,107,107	0
54	MG	AA	1647	1/1	0.83	0.35	96,96,96,96	0
54	MG	CA	1718	1/1	0.83	0.60	114,114,114,114	0
54	MG	DA	3307	1/1	0.83	0.51	102,102,102,102	0
54	MG	DA	3191	1/1	0.83	0.27	103,103,103,103	0
54	MG	BA	3528	1/1	0.83	0.56	104,104,104,104	0
54	MG	BA	3107	1/1	0.83	0.52	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	BA	3287	1/1	0.83	0.25	95,95,95,95	0
54	MG	BA	3233	1/1	0.83	0.29	106,106,106,106	0
54	MG	DA	3422	1/1	0.83	0.28	93,93,93,93	0
54	MG	BA	3413	1/1	0.83	0.39	120,120,120,120	0
54	MG	CC	101	1/1	0.83	0.29	130,130,130,130	0
54	MG	DA	3092	1/1	0.83	0.31	80,80,80,80	0
54	MG	DA	3157	1/1	0.83	0.18	90,90,90,90	0
54	MG	BA	3568	1/1	0.83	0.91	105,105,105,105	0
54	MG	BA	3236	1/1	0.83	0.35	97,97,97,97	0
54	MG	AA	1735	1/1	0.83	0.45	91,91,91,91	0
54	MG	CA	1762	1/1	0.83	0.38	116,116,116,116	0
54	MG	BA	3467	1/1	0.83	0.20	102,102,102,102	0
54	MG	BA	3334	1/1	0.83	0.20	115,115,115,115	0
54	MG	DA	3399	1/1	0.83	0.36	126,126,126,126	0
54	MG	BB	212	1/1	0.83	0.42	103,103,103,103	0
54	MG	BA	3294	1/1	0.83	0.49	79,79,79,79	0
54	MG	AA	1723	1/1	0.83	0.28	92,92,92,92	0
54	MG	DA	3144	1/1	0.83	0.43	85,85,85,85	0
54	MG	BA	3085	1/1	0.83	0.48	95,95,95,95	0
54	MG	AA	1637	1/1	0.83	0.55	115,115,115,115	0
54	MG	BA	3560	1/1	0.83	0.51	91,91,91,91	0
54	MG	CA	1757	1/1	0.83	0.11	149,149,149,149	0
54	MG	BA	3150	1/1	0.83	0.17	90,90,90,90	0
54	MG	BA	3207	1/1	0.83	0.78	116,116,116,116	0
54	MG	BA	3108	1/1	0.83	0.46	82,82,82,82	0
54	MG	B7	101	1/1	0.83	0.38	67,67,67,67	0
54	MG	BA	3301	1/1	0.84	0.25	85,85,85,85	0
54	MG	BB	204	1/1	0.84	0.48	86,86,86,86	0
54	MG	BA	3302	1/1	0.84	0.34	101,101,101,101	0
54	MG	DA	3351	1/1	0.84	0.37	90,90,90,90	0
54	MG	CA	1710	1/1	0.84	0.36	104,104,104,104	0
54	MG	BA	3453	1/1	0.84	0.40	85,85,85,85	0
54	MG	AA	1701	1/1	0.84	0.40	115,115,115,115	0
54	MG	BA	3070	1/1	0.84	0.37	119,119,119,119	0
54	MG	CA	1685	1/1	0.84	0.11	121,121,121,121	0
54	MG	BA	3332	1/1	0.84	0.34	83,83,83,83	0
54	MG	AA	1803	1/1	0.84	0.17	133,133,133,133	0
54	MG	AA	1725	1/1	0.84	0.32	111,111,111,111	0
54	MG	BA	3250	1/1	0.84	0.41	87,87,87,87	0
54	MG	CC	103	1/1	0.84	0.16	150,150,150,150	0
54	MG	CA	1701	1/1	0.84	0.55	92,92,92,92	0
54	MG	BA	3307	1/1	0.84	0.18	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	BA	3231	1/1	0.84	0.47	93,93,93,93	0
54	MG	CA	1776	1/1	0.84	0.40	125,125,125,125	0
54	MG	BA	3249	1/1	0.84	0.32	84,84,84,84	0
54	MG	BA	3344	1/1	0.84	0.23	93,93,93,93	0
54	MG	BA	3112	1/1	0.84	0.31	97,97,97,97	0
54	MG	BA	3310	1/1	0.84	0.28	103,103,103,103	0
54	MG	BA	3247	1/1	0.84	0.45	80,80,80,80	0
54	MG	BA	3388	1/1	0.84	0.53	100,100,100,100	0
54	MG	DA	3183	1/1	0.84	0.37	92,92,92,92	0
54	MG	BA	3606	1/1	0.84	0.36	84,84,84,84	0
54	MG	DA	3215	1/1	0.84	0.21	80,80,80,80	0
54	MG	BA	3514	1/1	0.84	0.54	90,90,90,90	0
54	MG	BA	3490	1/1	0.84	0.41	100,100,100,100	0
54	MG	CA	1618	1/1	0.84	0.56	123,123,123,123	0
54	MG	DA	3391	1/1	0.84	0.14	94,94,94,94	0
54	MG	AA	1651	1/1	0.84	0.19	108,108,108,108	0
54	MG	AA	1764	1/1	0.84	0.11	118,118,118,118	0
54	MG	DA	3483	1/1	0.84	0.27	88,88,88,88	0
54	MG	BA	3600	1/1	0.84	0.54	97,97,97,97	0
54	MG	AA	1832	1/1	0.84	0.23	102,102,102,102	0
54	MG	BA	3389	1/1	0.84	0.25	102,102,102,102	0
54	MG	AA	1617	1/1	0.84	0.37	91,91,91,91	0
54	MG	DA	3520	1/1	0.84	0.16	100,100,100,100	0
54	MG	DA	3315	1/1	0.84	0.19	125,125,125,125	0
54	MG	BA	3097	1/1	0.84	0.40	83,83,83,83	0
54	MG	BA	3217	1/1	0.84	0.19	92,92,92,92	0
54	MG	AA	1757	1/1	0.84	0.11	118,118,118,118	0
54	MG	CA	1775	1/1	0.84	0.14	90,90,90,90	0
54	MG	BA	3525	1/1	0.85	0.26	96,96,96,96	0
54	MG	DA	3046	1/1	0.85	0.13	82,82,82,82	0
54	MG	AA	1721	1/1	0.85	0.23	115,115,115,115	0
54	MG	BA	3503	1/1	0.85	0.19	105,105,105,105	0
54	MG	BA	3046	1/1	0.85	0.42	86,86,86,86	0
54	MG	BA	3607	1/1	0.85	0.30	94,94,94,94	0
54	MG	CA	1789	1/1	0.85	0.26	121,121,121,121	0
54	MG	BA	3086	1/1	0.85	0.27	88,88,88,88	0
54	MG	B2	201	1/1	0.85	0.12	90,90,90,90	0
54	MG	DA	3095	1/1	0.85	0.09	121,121,121,121	0
54	MG	BA	3511	1/1	0.85	0.25	80,80,80,80	0
54	MG	DA	3028	1/1	0.85	0.32	122,122,122,122	0
54	MG	DA	3129	1/1	0.85	0.21	115,115,115,115	0
54	MG	DA	3173	1/1	0.85	0.15	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	CA	1796	1/1	0.85	0.24	115,115,115,115	0
54	MG	AA	1623	1/1	0.85	0.34	81,81,81,81	0
54	MG	CA	1613	1/1	0.85	0.37	94,94,94,94	0
54	MG	BA	3311	1/1	0.85	0.25	100,100,100,100	0
54	MG	BA	3279	1/1	0.85	0.46	74,74,74,74	0
54	MG	BA	3034	1/1	0.85	0.37	69,69,69,69	0
54	MG	AA	1743	1/1	0.85	0.21	136,136,136,136	0
54	MG	AA	1779	1/1	0.85	0.43	88,88,88,88	0
54	MG	DP	201	1/1	0.85	0.24	102,102,102,102	0
54	MG	BB	208	1/1	0.85	0.41	90,90,90,90	0
54	MG	CA	1752	1/1	0.85	0.37	106,106,106,106	0
54	MG	DA	3209	1/1	0.85	0.23	100,100,100,100	0
54	MG	AA	1709	1/1	0.85	0.07	155,155,155,155	0
54	MG	DA	3100	1/1	0.85	0.36	100,100,100,100	0
54	MG	BA	3189	1/1	0.85	0.25	88,88,88,88	0
54	MG	BA	3415	1/1	0.85	0.53	90,90,90,90	0
54	MG	DA	3205	1/1	0.85	0.18	106,106,106,106	0
54	MG	DA	3292	1/1	0.85	0.16	129,129,129,129	0
54	MG	BA	3611	1/1	0.85	0.38	101,101,101,101	0
54	MG	DA	3021	1/1	0.85	0.14	77,77,77,77	0
54	MG	BA	3412	1/1	0.85	0.28	94,94,94,94	0
54	MG	BA	3336	1/1	0.85	0.30	109,109,109,109	0
54	MG	CA	1763	1/1	0.85	0.28	94,94,94,94	0
54	MG	BA	3432	1/1	0.85	0.18	126,126,126,126	0
54	MG	BA	3504	1/1	0.85	0.40	88,88,88,88	0
54	MG	AC	109	1/1	0.85	0.23	105,105,105,105	0
54	MG	AA	1716	1/1	0.85	0.45	107,107,107,107	0
54	MG	AA	1795	1/1	0.85	0.12	102,102,102,102	0
54	MG	BA	3475	1/1	0.85	0.07	270,270,270,270	0
54	MG	AA	1831	1/1	0.85	0.17	124,124,124,124	0
54	MG	BA	3246	1/1	0.86	0.39	78,78,78,78	0
54	MG	BA	3156	1/1	0.86	0.78	108,108,108,108	0
54	MG	AA	1733	1/1	0.86	0.22	120,120,120,120	0
54	MG	BA	3508	1/1	0.86	0.45	85,85,85,85	0
54	MG	AA	1793	1/1	0.86	0.37	103,103,103,103	0
54	MG	BA	3358	1/1	0.86	0.41	108,108,108,108	0
54	MG	CA	1725	1/1	0.86	0.35	106,106,106,106	0
54	MG	BE	302	1/1	0.86	0.79	104,104,104,104	0
54	MG	BA	3348	1/1	0.86	0.39	90,90,90,90	0
54	MG	BA	3077	1/1	0.86	0.34	77,77,77,77	0
54	MG	DA	3405	1/1	0.86	0.27	121,121,121,121	0
54	MG	AA	1729	1/1	0.86	0.39	108,108,108,108	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	DA	3089	1/1	0.86	0.19	117,117,117,117	0
54	MG	CA	1676	1/1	0.86	0.32	102,102,102,102	0
54	MG	BA	3342	1/1	0.86	0.52	95,95,95,95	0
54	MG	DA	3472	1/1	0.86	0.56	102,102,102,102	0
54	MG	BA	3094	1/1	0.86	0.43	97,97,97,97	0
54	MG	CA	1641	1/1	0.86	0.20	135,135,135,135	0
54	MG	BA	3466	1/1	0.86	0.32	92,92,92,92	0
54	MG	CA	1702	1/1	0.86	0.25	156,156,156,156	0
54	MG	AJ	201	1/1	0.86	0.52	108,108,108,108	0
54	MG	DA	3240	1/1	0.86	0.21	89,89,89,89	0
54	MG	AR	101	1/1	0.86	0.39	98,98,98,98	0
54	MG	BA	3483	1/1	0.86	0.18	89,89,89,89	0
54	MG	BA	3451	1/1	0.86	0.24	102,102,102,102	0
54	MG	CS	101	1/1	0.86	0.44	115,115,115,115	0
54	MG	CA	1770	1/1	0.86	0.12	106,106,106,106	0
54	MG	DA	3196	1/1	0.86	0.17	101,101,101,101	0
54	MG	BA	3377	1/1	0.86	0.13	109,109,109,109	0
54	MG	BA	3282	1/1	0.86	0.53	107,107,107,107	0
54	MG	DA	3492	1/1	0.86	0.17	111,111,111,111	0
54	MG	AA	1691	1/1	0.86	0.36	105,105,105,105	0
54	MG	BA	3194	1/1	0.86	0.26	113,113,113,113	0
54	MG	BA	3439	1/1	0.86	0.41	109,109,109,109	0
54	MG	BA	3559	1/1	0.86	0.67	105,105,105,105	0
54	MG	DA	3390	1/1	0.86	0.21	144,144,144,144	0
54	MG	DA	3392	1/1	0.86	1.13	97,97,97,97	0
54	MG	BA	3385	1/1	0.86	0.43	72,72,72,72	0
54	MG	AA	1614	1/1	0.86	0.37	114,114,114,114	0
54	MG	CA	1704	1/1	0.86	0.57	95,95,95,95	0
54	MG	DA	3247	1/1	0.86	0.21	89,89,89,89	0
54	MG	BA	3399	1/1	0.86	0.27	90,90,90,90	0
54	MG	DA	3253	1/1	0.86	0.15	103,103,103,103	0
54	MG	BA	3043	1/1	0.86	0.33	83,83,83,83	0
54	MG	DA	3452	1/1	0.86	0.70	91,91,91,91	0
54	MG	BA	3507	1/1	0.87	0.57	127,127,127,127	0
54	MG	DA	3314	1/1	0.87	0.21	83,83,83,83	0
54	MG	BA	3271	1/1	0.87	0.37	96,96,96,96	0
54	MG	AA	1718	1/1	0.87	0.33	124,124,124,124	0
54	MG	BA	3024	1/1	0.87	0.20	81,81,81,81	0
54	MG	BA	3317	1/1	0.87	0.39	99,99,99,99	0
54	MG	BA	3337	1/1	0.87	0.13	75,75,75,75	0
54	MG	DA	3349	1/1	0.87	0.20	88,88,88,88	0
54	MG	BA	3306	1/1	0.87	0.28	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	DA	3285	1/1	0.87	0.12	67,67,67,67	0
54	MG	AA	1678	1/1	0.87	0.40	108,108,108,108	0
54	MG	BA	3155	1/1	0.87	0.30	113,113,113,113	0
54	MG	DA	3394	1/1	0.87	1.01	106,106,106,106	0
54	MG	BA	3241	1/1	0.87	0.37	91,91,91,91	0
54	MG	BA	3558	1/1	0.87	0.37	118,118,118,118	0
54	MG	B3	102	1/1	0.87	0.42	93,93,93,93	0
54	MG	DA	3451	1/1	0.87	0.21	90,90,90,90	0
54	MG	BA	3135	1/1	0.87	0.17	90,90,90,90	0
54	MG	BA	3372	1/1	0.87	0.66	99,99,99,99	0
54	MG	CA	1786	1/1	0.87	0.07	192,192,192,192	0
54	MG	CA	1632	1/1	0.87	0.43	111,111,111,111	0
54	MG	BA	3563	1/1	0.87	0.41	96,96,96,96	0
54	MG	B8	101	1/1	0.87	0.29	101,101,101,101	0
54	MG	BA	3378	1/1	0.87	0.30	129,129,129,129	0
54	MG	BA	3418	1/1	0.87	0.29	98,98,98,98	0
54	MG	BA	3321	1/1	0.87	0.23	71,71,71,71	0
54	MG	DA	3415	1/1	0.87	0.11	84,84,84,84	0
54	MG	DA	3447	1/1	0.87	0.12	87,87,87,87	0
54	MG	BA	3498	1/1	0.87	0.54	107,107,107,107	0
54	MG	CA	1769	1/1	0.87	0.17	136,136,136,136	0
54	MG	BP	201	1/1	0.87	1.34	115,115,115,115	0
54	MG	AA	1824	1/1	0.87	0.13	120,120,120,120	0
54	MG	DA	3335	1/1	0.87	0.21	78,78,78,78	0
54	MG	BA	3622	1/1	0.87	0.17	120,120,120,120	0
54	MG	AA	1639	1/1	0.87	0.42	91,91,91,91	0
54	MG	DA	3395	1/1	0.87	0.27	87,87,87,87	0
54	MG	DA	3432	1/1	0.87	0.42	91,91,91,91	0
54	MG	AA	1622	1/1	0.87	0.40	96,96,96,96	0
54	MG	DA	3151	1/1	0.87	0.25	113,113,113,113	0
54	MG	BA	3206	1/1	0.87	0.30	99,99,99,99	0
54	MG	CA	1683	1/1	0.87	0.21	113,113,113,113	0
54	MG	AA	1794	1/1	0.87	0.17	116,116,116,116	0
54	MG	BA	3624	1/1	0.87	0.50	92,92,92,92	0
54	MG	BA	3454	1/1	0.87	0.29	103,103,103,103	0
54	MG	CA	1780	1/1	0.87	0.10	137,137,137,137	0
54	MG	CA	1736	1/1	0.87	0.53	85,85,85,85	0
54	MG	AC	105	1/1	0.87	0.08	107,107,107,107	0
54	MG	BA	3082	1/1	0.87	0.38	109,109,109,109	0
54	MG	AA	1641	1/1	0.87	0.17	90,90,90,90	0
54	MG	CA	1658	1/1	0.87	0.45	120,120,120,120	0
54	MG	BA	3405	1/1	0.87	0.25	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	DA	3031	1/1	0.87	0.56	70,70,70,70	0
54	MG	CA	1628	1/1	0.87	0.04	149,149,149,149	0
54	MG	BA	3073	1/1	0.87	0.93	108,108,108,108	0
54	MG	AA	1771	1/1	0.87	0.20	117,117,117,117	0
54	MG	DA	3387	1/1	0.87	0.24	106,106,106,106	0
54	MG	BA	3552	1/1	0.87	0.17	98,98,98,98	0
54	MG	DA	3322	1/1	0.87	0.26	110,110,110,110	0
54	MG	BA	3419	1/1	0.87	0.19	129,129,129,129	0
54	MG	CA	1779	1/1	0.87	0.22	112,112,112,112	0
54	MG	DA	3248	1/1	0.88	0.40	112,112,112,112	0
54	MG	DA	3330	1/1	0.88	0.20	82,82,82,82	0
54	MG	BA	3148	1/1	0.88	0.20	59,59,59,59	0
54	MG	DA	3329	1/1	0.88	0.28	110,110,110,110	0
54	MG	BA	3519	1/1	0.88	0.40	75,75,75,75	0
54	MG	AA	1642	1/1	0.88	0.15	103,103,103,103	0
54	MG	AA	1813	1/1	0.88	0.15	131,131,131,131	0
54	MG	CA	1740	1/1	0.88	0.17	109,109,109,109	0
54	MG	BA	3001	1/1	0.88	0.44	53,53,53,53	0
54	MG	BA	3166	1/1	0.88	0.24	86,86,86,86	0
54	MG	BA	3079	1/1	0.88	0.51	99,99,99,99	0
54	MG	CA	1680	1/1	0.88	0.26	94,94,94,94	0
54	MG	DA	3479	1/1	0.88	0.31	106,106,106,106	0
54	MG	BA	3283	1/1	0.88	0.19	108,108,108,108	0
54	MG	DA	3480	1/1	0.88	0.20	84,84,84,84	0
54	MG	DA	3010	1/1	0.88	0.20	103,103,103,103	0
54	MG	AA	1712	1/1	0.88	0.32	97,97,97,97	0
54	MG	BA	3030	1/1	0.88	0.29	66,66,66,66	0
54	MG	AA	1830	1/1	0.88	0.09	135,135,135,135	0
54	MG	DA	3516	1/1	0.88	0.17	92,92,92,92	0
54	MG	DA	3273	1/1	0.88	0.31	83,83,83,83	0
54	MG	BA	3208	1/1	0.88	0.37	91,91,91,91	0
54	MG	BA	3410	1/1	0.88	0.25	120,120,120,120	0
54	MG	DA	3382	1/1	0.88	0.37	80,80,80,80	0
54	MG	DA	3411	1/1	0.88	0.17	68,68,68,68	0
54	MG	CA	1612	1/1	0.88	0.12	122,122,122,122	0
54	MG	CA	1798	1/1	0.88	0.34	84,84,84,84	0
54	MG	AA	1784	1/1	0.88	0.37	91,91,91,91	0
54	MG	DA	3194	1/1	0.88	0.23	91,91,91,91	0
54	MG	BA	3614	1/1	0.88	1.59	109,109,109,109	0
54	MG	AA	1791	1/1	0.88	0.25	104,104,104,104	0
54	MG	AA	1800	1/1	0.88	0.41	92,92,92,92	0
54	MG	DA	3345	1/1	0.88	0.35	107,107,107,107	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	AA	1629	1/1	0.88	0.09	186,186,186,186	0
54	MG	DA	3423	1/1	0.88	0.12	123,123,123,123	0
54	MG	AA	1753	1/1	0.88	0.09	143,143,143,143	0
54	MG	CA	1804	1/1	0.88	0.23	119,119,119,119	0
54	MG	BA	3518	1/1	0.88	0.19	86,86,86,86	0
54	MG	DA	3381	1/1	0.88	0.24	97,97,97,97	0
54	MG	BA	3464	1/1	0.88	0.42	80,80,80,80	0
54	MG	BA	3153	1/1	0.88	0.31	89,89,89,89	0
54	MG	DA	3047	1/1	0.88	0.08	124,124,124,124	0
54	MG	DA	3007	1/1	0.88	0.23	116,116,116,116	0
54	MG	BA	3134	1/1	0.88	0.39	130,130,130,130	0
54	MG	DA	3443	1/1	0.88	0.14	103,103,103,103	0
54	MG	BA	3567	1/1	0.88	0.54	114,114,114,114	0
54	MG	AA	1775	1/1	0.88	0.28	80,80,80,80	0
54	MG	DA	3113	1/1	0.88	0.27	105,105,105,105	0
54	MG	DA	3365	1/1	0.88	0.17	100,100,100,100	0
54	MG	AA	1711	1/1	0.88	0.28	118,118,118,118	0
54	MG	BA	3014	1/1	0.89	0.37	68,68,68,68	0
54	MG	CA	1797	1/1	0.89	0.15	127,127,127,127	0
54	MG	BA	3255	1/1	0.89	0.53	110,110,110,110	0
54	MG	AA	1612	1/1	0.89	0.22	135,135,135,135	0
54	MG	AC	104	1/1	0.89	0.27	107,107,107,107	0
54	MG	CA	1724	1/1	0.89	0.14	98,98,98,98	0
54	MG	DA	3446	1/1	0.89	0.24	92,92,92,92	0
54	MG	CA	1696	1/1	0.89	0.34	98,98,98,98	0
54	MG	CH	201	1/1	0.89	0.30	114,114,114,114	0
54	MG	CA	1672	1/1	0.89	0.22	101,101,101,101	0
54	MG	BA	3557	1/1	0.89	0.14	92,92,92,92	0
54	MG	BA	3547	1/1	0.89	0.33	108,108,108,108	0
54	MG	DA	3034	1/1	0.89	0.17	91,91,91,91	0
54	MG	DA	3161	1/1	0.89	0.25	77,77,77,77	0
54	MG	BA	3545	1/1	0.89	0.23	108,108,108,108	0
54	MG	CA	1659	1/1	0.89	0.13	158,158,158,158	0
54	MG	BA	3299	1/1	0.89	0.50	78,78,78,78	0
54	MG	DA	3198	1/1	0.89	0.26	95,95,95,95	0
54	MG	DA	3338	1/1	0.89	0.35	95,95,95,95	0
55	TAC	CA	1805	32/32	0.89	0.11	126,153,170,174	0
54	MG	BA	3359	1/1	0.89	0.15	92,92,92,92	0
54	MG	BA	3553	1/1	0.89	0.48	99,99,99,99	0
54	MG	BA	3594	1/1	0.89	0.69	94,94,94,94	0
54	MG	DA	3462	1/1	0.89	0.13	102,102,102,102	0
54	MG	B7	102	1/1	0.89	0.29	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	AA	1732	1/1	0.89	0.39	112,112,112,112	0
54	MG	BA	3353	1/1	0.89	0.37	93,93,93,93	0
54	MG	DA	3086	1/1	0.89	0.11	84,84,84,84	0
54	MG	DA	3083	1/1	0.89	0.49	117,117,117,117	0
54	MG	CA	1621	1/1	0.89	0.31	84,84,84,84	0
54	MG	BA	3510	1/1	0.89	0.45	118,118,118,118	0
54	MG	AA	1742	1/1	0.89	0.24	108,108,108,108	0
54	MG	B1	202	1/1	0.89	0.28	100,100,100,100	0
54	MG	BA	3575	1/1	0.89	0.13	109,109,109,109	0
54	MG	DA	3101	1/1	0.89	0.40	94,94,94,94	0
54	MG	CA	1671	1/1	0.89	0.38	75,75,75,75	0
54	MG	CA	1748	1/1	0.89	0.12	81,81,81,81	0
54	MG	CA	1664	1/1	0.89	0.30	110,110,110,110	0
54	MG	BA	3517	1/1	0.89	0.20	121,121,121,121	0
54	MG	BA	3468	1/1	0.89	0.17	84,84,84,84	0
54	MG	DA	3378	1/1	0.89	0.23	100,100,100,100	0
54	MG	DA	3289	1/1	0.89	0.21	83,83,83,83	0
54	MG	DA	3138	1/1	0.89	0.20	79,79,79,79	0
54	MG	BA	3325	1/1	0.89	0.14	89,89,89,89	0
54	MG	BA	3546	1/1	0.89	0.26	97,97,97,97	0
54	MG	DA	3313	1/1	0.89	0.29	122,122,122,122	0
54	MG	BA	3266	1/1	0.89	0.30	77,77,77,77	0
54	MG	BA	3488	1/1	0.89	0.51	109,109,109,109	0
54	MG	BA	3397	1/1	0.89	0.39	92,92,92,92	0
54	MG	DA	3066	1/1	0.89	0.22	79,79,79,79	0
54	MG	BA	3461	1/1	0.89	0.27	79,79,79,79	0
54	MG	BA	3608	1/1	0.89	0.16	108,108,108,108	0
54	MG	BA	3010	1/1	0.89	0.23	128,128,128,128	0
54	MG	CA	1619	1/1	0.89	0.15	111,111,111,111	0
54	MG	DA	3258	1/1	0.89	0.24	98,98,98,98	0
54	MG	CA	1764	1/1	0.89	0.31	110,110,110,110	0
54	MG	DA	3069	1/1	0.90	0.29	101,101,101,101	0
54	MG	BA	3425	1/1	0.90	0.10	137,137,137,137	0
54	MG	DE	301	1/1	0.90	0.17	73,73,73,73	0
54	MG	BB	213	1/1	0.90	0.41	72,72,72,72	0
54	MG	AA	1645	1/1	0.90	0.26	93,93,93,93	0
54	MG	BA	3190	1/1	0.90	0.34	93,93,93,93	0
54	MG	CA	1735	1/1	0.90	0.10	103,103,103,103	0
54	MG	DA	3325	1/1	0.90	0.39	74,74,74,74	0
54	MG	BA	3152	1/1	0.90	0.55	90,90,90,90	0
54	MG	AA	1821	1/1	0.90	0.16	110,110,110,110	0
54	MG	DA	3068	1/1	0.90	0.40	122,122,122,122	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	BA	3515	1/1	0.90	0.52	112,112,112,112	0
54	MG	BA	3422	1/1	0.90	0.18	120,120,120,120	0
54	MG	DA	3380	1/1	0.90	0.32	94,94,94,94	0
54	MG	DA	3431	1/1	0.90	0.56	101,101,101,101	0
54	MG	BA	3373	1/1	0.90	0.11	131,131,131,131	0
54	MG	DA	3360	1/1	0.90	0.25	85,85,85,85	0
54	MG	DA	3200	1/1	0.90	0.14	112,112,112,112	0
54	MG	BA	3182	1/1	0.90	0.23	101,101,101,101	0
54	MG	AA	1739	1/1	0.90	0.54	99,99,99,99	0
54	MG	DA	3469	1/1	0.90	0.20	107,107,107,107	0
54	MG	CA	1667	1/1	0.90	0.23	139,139,139,139	0
54	MG	BA	3478	1/1	0.90	0.13	155,155,155,155	0
54	MG	BA	3248	1/1	0.90	0.41	74,74,74,74	0
54	MG	BA	3570	1/1	0.90	0.22	82,82,82,82	0
54	MG	BA	3326	1/1	0.90	0.36	89,89,89,89	0
54	MG	BB	205	1/1	0.90	0.46	93,93,93,93	0
54	MG	DA	3401	1/1	0.90	0.26	103,103,103,103	0
54	MG	CA	1610	1/1	0.90	0.18	147,147,147,147	0
54	MG	DA	3369	1/1	0.90	0.36	76,76,76,76	0
54	MG	BA	3140	1/1	0.90	0.33	84,84,84,84	0
54	MG	DA	3466	1/1	0.90	0.24	94,94,94,94	0
54	MG	BA	3063	1/1	0.90	0.21	121,121,121,121	0
54	MG	DA	3121	1/1	0.90	0.17	68,68,68,68	0
54	MG	BA	3178	1/1	0.90	0.48	78,78,78,78	0
54	MG	DA	3511	1/1	0.90	0.78	111,111,111,111	0
54	MG	DA	3445	1/1	0.90	0.31	89,89,89,89	0
54	MG	BA	3544	1/1	0.90	0.37	77,77,77,77	0
54	MG	DA	3269	1/1	0.90	0.20	78,78,78,78	0
54	MG	BA	3371	1/1	0.90	0.41	81,81,81,81	0
54	MG	AA	1707	1/1	0.90	0.13	94,94,94,94	0
54	MG	CA	1682	1/1	0.90	0.26	101,101,101,101	0
54	MG	BA	3322	1/1	0.90	0.27	78,78,78,78	0
54	MG	BA	3167	1/1	0.90	0.37	95,95,95,95	0
54	MG	BB	209	1/1	0.90	0.26	116,116,116,116	0
54	MG	BA	3139	1/1	0.90	0.31	66,66,66,66	0
54	MG	BA	3497	1/1	0.90	0.39	78,78,78,78	0
54	MG	CA	1760	1/1	0.90	0.21	135,135,135,135	0
54	MG	DA	3058	1/1	0.90	0.56	109,109,109,109	0
54	MG	DA	3438	1/1	0.90	0.21	134,134,134,134	0
54	MG	DA	3471	1/1	0.90	0.16	102,102,102,102	0
54	MG	BA	3161	1/1	0.90	0.16	101,101,101,101	0
54	MG	CA	1785	1/1	0.90	0.28	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	DA	3060	1/1	0.90	0.15	101,101,101,101	0
54	MG	DA	3036	1/1	0.90	0.23	108,108,108,108	0
54	MG	BA	3318	1/1	0.90	0.30	88,88,88,88	0
54	MG	BA	3343	1/1	0.90	0.23	86,86,86,86	0
54	MG	BA	3226	1/1	0.90	0.45	87,87,87,87	0
54	MG	DA	3255	1/1	0.90	0.14	87,87,87,87	0
54	MG	BA	3133	1/1	0.90	0.40	92,92,92,92	0
54	MG	DA	3176	1/1	0.90	0.21	112,112,112,112	0
54	MG	BA	3469	1/1	0.90	0.52	125,125,125,125	0
54	MG	DA	3212	1/1	0.90	0.32	59,59,59,59	0
54	MG	BA	3456	1/1	0.90	0.29	108,108,108,108	0
54	MG	AG	302	1/1	0.90	0.32	162,162,162,162	0
54	MG	BA	3234	1/1	0.90	0.48	84,84,84,84	0
54	MG	AA	1646	1/1	0.90	0.07	150,150,150,150	0
54	MG	CA	1620	1/1	0.90	0.24	73,73,73,73	0
54	MG	AA	1797	1/1	0.90	0.33	82,82,82,82	0
54	MG	AC	106	1/1	0.91	0.19	119,119,119,119	0
54	MG	DA	3180	1/1	0.91	0.31	82,82,82,82	0
54	MG	D1	201	1/1	0.91	0.19	87,87,87,87	0
54	MG	DA	3257	1/1	0.91	0.32	88,88,88,88	0
54	MG	DA	3131	1/1	0.91	0.17	94,94,94,94	0
54	MG	AA	1631	1/1	0.91	0.45	96,96,96,96	0
54	MG	AA	1744	1/1	0.91	0.20	180,180,180,180	0
54	MG	BA	3309	1/1	0.91	0.36	84,84,84,84	0
54	MG	AA	1705	1/1	0.91	0.28	98,98,98,98	0
54	MG	DA	3404	1/1	0.91	0.14	66,66,66,66	0
54	MG	BA	3550	1/1	0.91	0.31	99,99,99,99	0
54	MG	BA	3060	1/1	0.91	0.26	105,105,105,105	0
54	MG	DA	3234	1/1	0.91	0.30	92,92,92,92	0
54	MG	CA	1615	1/1	0.91	0.25	106,106,106,106	0
54	MG	DA	3155	1/1	0.91	0.13	80,80,80,80	0
54	MG	DA	3336	1/1	0.91	0.16	115,115,115,115	0
54	MG	BB	210	1/1	0.91	0.40	78,78,78,78	0
54	MG	BA	3131	1/1	0.91	0.23	101,101,101,101	0
54	MG	BA	3211	1/1	0.91	0.41	77,77,77,77	0
54	MG	DB	212	1/1	0.91	0.65	102,102,102,102	0
54	MG	BA	3216	1/1	0.91	0.19	95,95,95,95	0
54	MG	AA	1747	1/1	0.91	0.11	159,159,159,159	0
54	MG	AA	1761	1/1	0.91	0.08	152,152,152,152	0
54	MG	DA	3141	1/1	0.91	0.22	85,85,85,85	0
54	MG	AA	1826	1/1	0.91	0.14	94,94,94,94	0
54	MG	DA	3175	1/1	0.91	0.16	101,101,101,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	BA	3572	1/1	0.91	0.17	113,113,113,113	0
54	MG	BA	3261	1/1	0.91	0.14	90,90,90,90	0
54	MG	CA	1637	1/1	0.91	0.19	121,121,121,121	0
54	MG	AA	1621	1/1	0.91	0.44	147,147,147,147	0
54	MG	DA	3052	1/1	0.91	0.35	120,120,120,120	0
54	MG	BA	3597	1/1	0.91	0.27	69,69,69,69	0
54	MG	CA	1730	1/1	0.91	0.41	121,121,121,121	0
54	MG	BA	3164	1/1	0.91	0.43	80,80,80,80	0
54	MG	DA	3311	1/1	0.91	0.16	92,92,92,92	0
54	MG	DB	203	1/1	0.91	0.21	95,95,95,95	0
54	MG	BA	3627	1/1	0.91	0.44	89,89,89,89	0
54	MG	BA	3031	1/1	0.91	0.33	63,63,63,63	0
54	MG	DA	3323	1/1	0.91	0.12	79,79,79,79	0
54	MG	DA	3470	1/1	0.91	0.25	124,124,124,124	0
54	MG	DA	3245	1/1	0.91	0.35	83,83,83,83	0
54	MG	AA	1654	1/1	0.91	0.41	113,113,113,113	0
54	MG	DA	3142	1/1	0.91	0.13	99,99,99,99	0
54	MG	DA	3521	1/1	0.91	0.08	111,111,111,111	0
54	MG	BA	3256	1/1	0.91	0.28	68,68,68,68	0
54	MG	BA	3333	1/1	0.91	0.42	99,99,99,99	0
54	MG	DA	3347	1/1	0.91	0.35	116,116,116,116	0
54	MG	BA	3436	1/1	0.91	0.26	118,118,118,118	0
54	MG	CA	1768	1/1	0.91	0.11	106,106,106,106	0
54	MG	CA	1726	1/1	0.91	0.27	111,111,111,111	0
54	MG	AA	1819	1/1	0.91	0.23	81,81,81,81	0
54	MG	BA	3523	1/1	0.91	0.20	64,64,64,64	0
54	MG	DA	3303	1/1	0.91	0.36	140,140,140,140	0
54	MG	BA	3599	1/1	0.91	0.38	115,115,115,115	0
54	MG	CA	1729	1/1	0.91	0.33	115,115,115,115	0
54	MG	BA	3616	1/1	0.91	0.39	92,92,92,92	0
54	MG	BA	3298	1/1	0.91	0.34	73,73,73,73	0
54	MG	BA	3573	1/1	0.91	0.37	96,96,96,96	0
54	MG	DA	3488	1/1	0.91	0.52	105,105,105,105	0
54	MG	DA	3376	1/1	0.91	0.28	87,87,87,87	0
54	MG	BA	3474	1/1	0.91	0.31	102,102,102,102	0
54	MG	DA	3510	1/1	0.91	0.20	77,77,77,77	0
55	TAC	AA	1833	32/32	0.91	0.18	99,129,142,143	0
54	MG	BA	3445	1/1	0.91	0.17	156,156,156,156	0
54	MG	CA	1746	1/1	0.92	0.38	92,92,92,92	0
54	MG	AA	1788	1/1	0.92	0.29	124,124,124,124	0
54	MG	DA	3459	1/1	0.92	0.24	108,108,108,108	0
54	MG	DA	3208	1/1	0.92	0.24	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	DA	3025	1/1	0.92	0.35	88,88,88,88	0
54	MG	BA	3048	1/1	0.92	0.13	70,70,70,70	0
54	MG	BA	3065	1/1	0.92	0.17	135,135,135,135	0
54	MG	CA	1668	1/1	0.92	0.35	145,145,145,145	0
54	MG	B5	102	1/1	0.92	0.11	92,92,92,92	0
54	MG	BA	3586	1/1	0.92	0.39	62,62,62,62	0
54	MG	DA	3489	1/1	0.92	0.24	98,98,98,98	0
54	MG	BA	3293	1/1	0.92	0.39	77,77,77,77	0
54	MG	AA	1756	1/1	0.92	0.25	86,86,86,86	0
54	MG	DA	3429	1/1	0.92	0.24	97,97,97,97	0
54	MG	DA	3458	1/1	0.92	0.09	115,115,115,115	0
54	MG	DB	201	1/1	0.92	0.14	88,88,88,88	0
54	MG	DA	3026	1/1	0.92	0.13	122,122,122,122	0
54	MG	BA	3426	1/1	0.92	0.34	77,77,77,77	0
54	MG	CA	1741	1/1	0.92	0.20	136,136,136,136	0
54	MG	AA	1630	1/1	0.92	0.26	105,105,105,105	0
54	MG	CA	1634	1/1	0.92	0.14	110,110,110,110	0
54	MG	BA	3290	1/1	0.92	0.26	78,78,78,78	0
54	MG	BA	3492	1/1	0.92	0.42	76,76,76,76	0
54	MG	BA	3430	1/1	0.92	0.13	87,87,87,87	0
54	MG	BA	3533	1/1	0.92	0.62	106,106,106,106	0
54	MG	BA	3111	1/1	0.92	0.18	68,68,68,68	0
54	MG	BA	3277	1/1	0.92	0.15	97,97,97,97	0
54	MG	AA	1785	1/1	0.92	0.16	131,131,131,131	0
54	MG	BA	3117	1/1	0.92	0.27	102,102,102,102	0
54	MG	DA	3524	1/1	0.92	0.50	86,86,86,86	0
54	MG	DA	3193	1/1	0.92	0.16	69,69,69,69	0
54	MG	BA	3050	1/1	0.92	0.47	75,75,75,75	0
54	MG	CA	1691	1/1	0.92	0.35	95,95,95,95	0
54	MG	BA	3304	1/1	0.92	0.27	90,90,90,90	0
54	MG	BA	3264	1/1	0.92	0.43	75,75,75,75	0
54	MG	AA	1697	1/1	0.92	0.45	143,143,143,143	0
54	MG	CA	1661	1/1	0.92	0.35	98,98,98,98	0
54	MG	BA	3253	1/1	0.92	0.14	89,89,89,89	0
54	MG	BA	3423	1/1	0.92	0.59	89,89,89,89	0
54	MG	BA	3363	1/1	0.92	0.34	73,73,73,73	0
54	MG	DA	3306	1/1	0.92	0.20	92,92,92,92	0
54	MG	CA	1677	1/1	0.92	0.17	114,114,114,114	0
54	MG	DA	3188	1/1	0.92	0.38	69,69,69,69	0
54	MG	DB	205	1/1	0.92	0.18	85,85,85,85	0
54	MG	DA	3373	1/1	0.92	0.21	112,112,112,112	0
54	MG	BA	3288	1/1	0.92	0.61	100,100,100,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	BA	3556	1/1	0.92	0.14	91,91,91,91	0
54	MG	DA	3340	1/1	0.92	0.13	89,89,89,89	0
54	MG	DA	3020	1/1	0.92	0.10	62,62,62,62	0
54	MG	BA	3356	1/1	0.92	0.22	128,128,128,128	0
54	MG	DA	3312	1/1	0.92	0.19	87,87,87,87	0
54	MG	BA	3209	1/1	0.92	0.37	79,79,79,79	0
54	MG	DA	3334	1/1	0.92	0.09	136,136,136,136	0
54	MG	DA	3154	1/1	0.92	0.24	111,111,111,111	0
54	MG	AA	1615	1/1	0.92	0.21	95,95,95,95	0
54	MG	DA	3063	1/1	0.92	0.23	76,76,76,76	0
54	MG	DA	3099	1/1	0.92	0.30	74,74,74,74	0
54	MG	BA	3609	1/1	0.92	0.22	102,102,102,102	0
54	MG	BA	3499	1/1	0.92	0.14	103,103,103,103	0
54	MG	AA	1817	1/1	0.92	0.50	101,101,101,101	0
54	MG	CA	1714	1/1	0.92	0.31	94,94,94,94	0
54	MG	DA	3414	1/1	0.92	0.09	95,95,95,95	0
54	MG	DZ	102	1/1	0.92	0.14	88,88,88,88	0
54	MG	BA	3163	1/1	0.92	0.21	104,104,104,104	0
54	MG	DA	3152	1/1	0.92	0.18	112,112,112,112	0
54	MG	DA	3316	1/1	0.92	0.75	124,124,124,124	0
54	MG	DA	3005	1/1	0.92	0.23	86,86,86,86	0
54	MG	BA	3232	1/1	0.92	0.20	93,93,93,93	0
54	MG	DA	3079	1/1	0.92	0.22	97,97,97,97	0
54	MG	DA	3326	1/1	0.92	0.29	82,82,82,82	0
54	MG	CA	1771	1/1	0.92	0.31	92,92,92,92	0
54	MG	DA	3420	1/1	0.92	0.11	108,108,108,108	0
54	MG	AA	1665	1/1	0.92	0.26	84,84,84,84	0
54	MG	DA	3357	1/1	0.92	0.19	105,105,105,105	0
54	MG	DA	3502	1/1	0.93	0.25	64,64,64,64	0
54	MG	CA	1623	1/1	0.93	0.07	180,180,180,180	0
54	MG	BA	3020	1/1	0.93	0.22	109,109,109,109	0
54	MG	BA	3284	1/1	0.93	0.12	121,121,121,121	0
54	MG	DA	3413	1/1	0.93	0.63	115,115,115,115	0
54	MG	BA	3027	1/1	0.93	0.25	69,69,69,69	0
54	MG	BA	3621	1/1	0.93	0.32	66,66,66,66	0
54	MG	CA	1657	1/1	0.93	0.16	142,142,142,142	0
54	MG	BA	3574	1/1	0.93	0.36	60,60,60,60	0
54	MG	BA	3433	1/1	0.93	0.15	107,107,107,107	0
54	MG	CA	1788	1/1	0.93	0.37	87,87,87,87	0
54	MG	CA	1689	1/1	0.93	0.42	122,122,122,122	0
54	MG	DA	3403	1/1	0.93	0.21	84,84,84,84	0
54	MG	BA	3215	1/1	0.93	0.28	119,119,119,119	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	DA	3156	1/1	0.93	0.82	113,113,113,113	0
54	MG	A1	101	1/1	0.93	0.29	72,72,72,72	0
54	MG	AA	1767	1/1	0.93	0.37	100,100,100,100	0
54	MG	BA	3114	1/1	0.93	0.44	83,83,83,83	0
54	MG	BA	3170	1/1	0.93	0.33	90,90,90,90	0
54	MG	DA	3503	1/1	0.93	0.76	105,105,105,105	0
54	MG	DA	3356	1/1	0.93	0.29	64,64,64,64	0
54	MG	BA	3542	1/1	0.93	0.48	100,100,100,100	0
54	MG	DA	3408	1/1	0.93	0.23	107,107,107,107	0
54	MG	CA	1732	1/1	0.93	0.28	144,144,144,144	0
54	MG	DA	3061	1/1	0.93	0.25	64,64,64,64	0
54	MG	CA	1673	1/1	0.93	0.14	89,89,89,89	0
54	MG	BA	3203	1/1	0.93	0.39	86,86,86,86	0
54	MG	DA	3197	1/1	0.93	0.28	103,103,103,103	0
54	MG	CA	1692	1/1	0.93	0.22	104,104,104,104	0
54	MG	BA	3387	1/1	0.93	0.08	135,135,135,135	0
54	MG	DA	3001	1/1	0.93	0.23	83,83,83,83	0
54	MG	DA	3204	1/1	0.93	0.19	126,126,126,126	0
54	MG	BA	3588	1/1	0.93	0.41	109,109,109,109	0
54	MG	DA	3160	1/1	0.93	0.44	84,84,84,84	0
54	MG	AA	1635	1/1	0.93	0.33	122,122,122,122	0
54	MG	CA	1629	1/1	0.93	0.07	164,164,164,164	0
54	MG	BA	3623	1/1	0.93	0.21	86,86,86,86	0
54	MG	AA	1822	1/1	0.93	0.10	144,144,144,144	0
54	MG	B7	103	1/1	0.93	0.16	88,88,88,88	0
54	MG	BA	3463	1/1	0.93	0.28	77,77,77,77	0
54	MG	CA	1777	1/1	0.93	0.29	133,133,133,133	0
54	MG	DA	3134	1/1	0.93	0.11	105,105,105,105	0
54	MG	BA	3366	1/1	0.93	0.34	95,95,95,95	0
54	MG	BA	3067	1/1	0.93	1.00	108,108,108,108	0
54	MG	BA	3136	1/1	0.93	0.31	62,62,62,62	0
54	MG	BA	3053	1/1	0.93	0.49	92,92,92,92	0
54	MG	AA	1661	1/1	0.93	0.36	94,94,94,94	0
54	MG	BA	3335	1/1	0.93	0.28	96,96,96,96	0
54	MG	BA	3268	1/1	0.93	0.28	87,87,87,87	0
54	MG	BA	3350	1/1	0.93	1.22	115,115,115,115	0
54	MG	CA	1655	1/1	0.93	0.43	125,125,125,125	0
54	MG	BA	3273	1/1	0.93	0.36	70,70,70,70	0
54	MG	BA	3592	1/1	0.93	0.28	112,112,112,112	0
54	MG	DA	3137	1/1	0.93	0.18	74,74,74,74	0
54	MG	DA	3070	1/1	0.93	0.31	76,76,76,76	0
54	MG	DA	3393	1/1	0.93	0.23	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	DA	3409	1/1	0.93	0.33	132,132,132,132	0
54	MG	CA	1708	1/1	0.93	0.26	143,143,143,143	0
54	MG	BB	216	1/1	0.93	0.24	111,111,111,111	0
54	MG	AA	1806	1/1	0.93	0.43	100,100,100,100	0
54	MG	BA	3123	1/1	0.93	0.34	73,73,73,73	0
54	MG	BA	3126	1/1	0.93	0.14	89,89,89,89	0
54	MG	AA	1632	1/1	0.93	0.34	116,116,116,116	0
54	MG	DA	3054	1/1	0.93	0.37	88,88,88,88	0
54	MG	CA	1715	1/1	0.93	0.37	128,128,128,128	0
54	MG	AA	1659	1/1	0.93	0.15	71,71,71,71	0
54	MG	DA	3249	1/1	0.93	0.33	65,65,65,65	0
54	MG	CA	1782	1/1	0.93	0.38	98,98,98,98	0
54	MG	BA	3604	1/1	0.93	0.23	97,97,97,97	0
54	MG	AA	1605	1/1	0.93	0.20	108,108,108,108	0
54	MG	DA	3302	1/1	0.93	0.32	79,79,79,79	0
54	MG	CA	1656	1/1	0.93	0.18	129,129,129,129	0
54	MG	BA	3587	1/1	0.93	0.35	102,102,102,102	0
54	MG	DA	3457	1/1	0.93	0.14	102,102,102,102	0
54	MG	AA	1619	1/1	0.94	0.18	96,96,96,96	0
54	MG	BA	3603	1/1	0.94	1.34	113,113,113,113	0
54	MG	DA	3077	1/1	0.94	0.13	96,96,96,96	0
54	MG	DA	3308	1/1	0.94	0.25	94,94,94,94	0
54	MG	DA	3202	1/1	0.94	0.26	88,88,88,88	0
54	MG	DA	3337	1/1	0.94	0.16	88,88,88,88	0
54	MG	DA	3133	1/1	0.94	0.18	74,74,74,74	0
54	MG	AA	1681	1/1	0.94	0.11	146,146,146,146	0
54	MG	BA	3023	1/1	0.94	0.20	66,66,66,66	0
54	MG	BA	3427	1/1	0.94	0.44	91,91,91,91	0
54	MG	CA	1675	1/1	0.94	0.08	111,111,111,111	0
54	MG	DA	3514	1/1	0.94	0.13	71,71,71,71	0
54	MG	BA	3033	1/1	0.94	0.32	75,75,75,75	0
54	MG	BO	203	1/1	0.94	0.17	70,70,70,70	0
54	MG	AA	1827	1/1	0.94	0.17	82,82,82,82	0
54	MG	DA	3433	1/1	0.94	0.21	66,66,66,66	0
54	MG	BA	3308	1/1	0.94	0.38	110,110,110,110	0
54	MG	DA	3078	1/1	0.94	0.10	97,97,97,97	0
54	MG	BA	3128	1/1	0.94	0.57	99,99,99,99	0
54	MG	CA	1703	1/1	0.94	0.11	93,93,93,93	0
54	MG	CA	1614	1/1	0.94	0.16	121,121,121,121	0
54	MG	AA	1714	1/1	0.94	0.18	115,115,115,115	0
54	MG	BU	202	1/1	0.94	0.20	80,80,80,80	0
54	MG	DA	3107	1/1	0.94	0.23	100,100,100,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	BA	3347	1/1	0.94	0.28	72,72,72,72	0
54	MG	DA	3110	1/1	0.94	0.27	75,75,75,75	0
54	MG	BA	3281	1/1	0.94	0.71	106,106,106,106	0
54	MG	BA	3078	1/1	0.94	0.32	106,106,106,106	0
54	MG	DA	3128	1/1	0.94	0.27	65,65,65,65	0
54	MG	DA	3150	1/1	0.94	0.42	96,96,96,96	0
54	MG	DA	3375	1/1	0.94	0.22	127,127,127,127	0
54	MG	DA	3406	1/1	0.94	0.17	103,103,103,103	0
54	MG	BA	3491	1/1	0.94	0.37	84,84,84,84	0
54	MG	CA	1624	1/1	0.94	0.32	129,129,129,129	0
54	MG	CA	1739	1/1	0.94	0.24	112,112,112,112	0
54	MG	BA	3569	1/1	0.94	0.45	79,79,79,79	0
54	MG	BA	3055	1/1	0.94	0.50	69,69,69,69	0
54	MG	DA	3084	1/1	0.94	0.11	98,98,98,98	0
54	MG	DA	3274	1/1	0.94	0.22	83,83,83,83	0
54	MG	BA	3420	1/1	0.94	0.43	70,70,70,70	0
54	MG	BA	3018	1/1	0.94	0.31	53,53,53,53	0
54	MG	AA	1667	1/1	0.94	0.37	88,88,88,88	0
54	MG	CA	1722	1/1	0.94	0.10	109,109,109,109	0
54	MG	BA	3238	1/1	0.94	0.38	112,112,112,112	0
54	MG	AA	1700	1/1	0.94	0.14	123,123,123,123	0
54	MG	DA	3388	1/1	0.94	0.08	152,152,152,152	0
54	MG	BA	3280	1/1	0.94	0.30	106,106,106,106	0
54	MG	AA	1781	1/1	0.94	0.47	120,120,120,120	0
54	MG	BA	3362	1/1	0.94	0.59	70,70,70,70	0
54	MG	AA	1702	1/1	0.94	0.35	77,77,77,77	0
54	MG	CA	1606	1/1	0.94	0.39	100,100,100,100	0
54	MG	BA	3476	1/1	0.94	0.45	59,59,59,59	0
54	MG	DA	3254	1/1	0.94	0.40	74,74,74,74	0
54	MG	CA	1737	1/1	0.94	0.38	97,97,97,97	0
54	MG	DA	3476	1/1	0.94	0.44	99,99,99,99	0
54	MG	DA	3116	1/1	0.94	0.26	77,77,77,77	0
54	MG	BA	3272	1/1	0.94	0.29	52,52,52,52	0
54	MG	AA	1679	1/1	0.94	0.28	105,105,105,105	0
54	MG	BA	3524	1/1	0.94	0.46	90,90,90,90	0
54	MG	DA	3043	1/1	0.94	0.21	106,106,106,106	0
54	MG	CA	1686	1/1	0.94	0.41	79,79,79,79	0
54	MG	DA	3146	1/1	0.94	0.51	87,87,87,87	0
54	MG	BA	3516	1/1	0.94	0.24	80,80,80,80	0
54	MG	DA	3015	1/1	0.94	0.18	98,98,98,98	0
54	MG	BA	3416	1/1	0.94	0.18	70,70,70,70	0
54	MG	DA	3062	1/1	0.94	0.32	112,112,112,112	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	DA	3284	1/1	0.94	0.28	100,100,100,100	0
54	MG	BA	3605	1/1	0.94	0.17	82,82,82,82	0
54	MG	DA	3251	1/1	0.94	0.16	91,91,91,91	0
54	MG	AC	103	1/1	0.94	0.41	75,75,75,75	0
54	MG	DA	3246	1/1	0.94	0.09	103,103,103,103	0
54	MG	DA	3290	1/1	0.94	0.21	107,107,107,107	0
54	MG	AA	1746	1/1	0.94	0.16	92,92,92,92	0
54	MG	AA	1610	1/1	0.94	0.31	71,71,71,71	0
54	MG	DA	3448	1/1	0.94	0.15	89,89,89,89	0
54	MG	DA	3019	1/1	0.94	0.24	84,84,84,84	0
54	MG	DA	3216	1/1	0.94	0.19	77,77,77,77	0
54	MG	CA	1767	1/1	0.94	0.37	90,90,90,90	0
54	MG	DA	3056	1/1	0.94	0.16	86,86,86,86	0
54	MG	BB	215	1/1	0.94	0.17	129,129,129,129	0
54	MG	DA	3276	1/1	0.94	0.17	97,97,97,97	0
54	MG	DA	3065	1/1	0.94	0.28	103,103,103,103	0
54	MG	BA	3151	1/1	0.94	0.28	103,103,103,103	0
54	MG	DA	3275	1/1	0.94	0.20	93,93,93,93	0
54	MG	AA	1799	1/1	0.94	0.42	79,79,79,79	0
54	MG	BA	3274	1/1	0.94	0.47	93,93,93,93	0
54	MG	DA	3145	1/1	0.94	0.17	110,110,110,110	0
54	MG	DA	3006	1/1	0.94	0.42	69,69,69,69	0
54	MG	CA	1674	1/1	0.94	0.68	117,117,117,117	0
54	MG	BA	3005	1/1	0.94	0.22	61,61,61,61	0
54	MG	BA	3512	1/1	0.94	0.23	97,97,97,97	0
54	MG	DA	3206	1/1	0.94	0.40	58,58,58,58	0
54	MG	BA	3270	1/1	0.94	0.20	87,87,87,87	0
54	MG	DA	3498	1/1	0.94	0.10	106,106,106,106	0
54	MG	AA	1760	1/1	0.94	0.20	122,122,122,122	0
54	MG	AA	1633	1/1	0.94	0.41	80,80,80,80	0
54	MG	AA	1762	1/1	0.94	0.15	124,124,124,124	0
54	MG	BA	3240	1/1	0.95	0.52	93,93,93,93	0
54	MG	DA	3076	1/1	0.95	0.28	75,75,75,75	0
54	MG	AA	1703	1/1	0.95	0.23	87,87,87,87	0
54	MG	DA	3091	1/1	0.95	0.15	87,87,87,87	0
54	MG	DE	303	1/1	0.95	0.19	70,70,70,70	0
54	MG	BA	3199	1/1	0.95	0.08	78,78,78,78	0
54	MG	BA	3179	1/1	0.95	0.66	108,108,108,108	0
54	MG	DA	3350	1/1	0.95	0.30	82,82,82,82	0
54	MG	AA	1814	1/1	0.95	0.11	152,152,152,152	0
54	MG	AA	1804	1/1	0.95	0.11	130,130,130,130	0
54	MG	DA	3319	1/1	0.95	0.17	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	CA	1607	1/1	0.95	0.43	83,83,83,83	0
54	MG	BA	3394	1/1	0.95	0.45	85,85,85,85	0
54	MG	DA	3050	1/1	0.95	0.12	108,108,108,108	0
54	MG	BA	3186	1/1	0.95	0.28	62,62,62,62	0
54	MG	BA	3051	1/1	0.95	0.22	72,72,72,72	0
54	MG	BZ	101	1/1	0.95	0.22	69,69,69,69	0
54	MG	B1	201	1/1	0.95	0.28	61,61,61,61	0
54	MG	BA	3120	1/1	0.95	0.51	97,97,97,97	0
54	MG	AA	1673	1/1	0.95	0.16	133,133,133,133	0
54	MG	AA	1608	1/1	0.95	0.14	111,111,111,111	0
54	MG	BA	3047	1/1	0.95	0.23	64,64,64,64	0
54	MG	DA	3493	1/1	0.95	0.14	64,64,64,64	0
54	MG	DA	3515	1/1	0.95	0.12	94,94,94,94	0
54	MG	BA	3042	1/1	0.95	0.17	94,94,94,94	0
54	MG	AA	1736	1/1	0.95	0.12	122,122,122,122	0
54	MG	DA	3210	1/1	0.95	0.24	63,63,63,63	0
54	MG	DA	3082	1/1	0.95	0.12	99,99,99,99	0
54	MG	BA	3021	1/1	0.95	0.43	72,72,72,72	0
54	MG	BA	3580	1/1	0.95	0.34	64,64,64,64	0
54	MG	CA	1783	1/1	0.95	0.41	97,97,97,97	0
54	MG	BE	301	1/1	0.95	0.29	61,61,61,61	0
54	MG	DA	3294	1/1	0.95	0.33	64,64,64,64	0
54	MG	DA	3112	1/1	0.95	0.26	71,71,71,71	0
54	MG	AA	1655	1/1	0.95	0.46	106,106,106,106	0
54	MG	DA	3426	1/1	0.95	0.15	159,159,159,159	0
54	MG	BA	3402	1/1	0.95	0.18	81,81,81,81	0
54	MG	CA	1665	1/1	0.95	0.46	103,103,103,103	0
56	ZN	CQ	101	1/1	0.95	0.07	188,188,188,188	0
54	MG	DA	3364	1/1	0.95	0.16	112,112,112,112	0
54	MG	CA	1743	1/1	0.95	0.36	117,117,117,117	0
54	MG	DA	3286	1/1	0.95	0.50	115,115,115,115	0
54	MG	CA	1709	1/1	0.95	0.35	110,110,110,110	0
54	MG	BA	3072	1/1	0.95	0.42	87,87,87,87	0
54	MG	AH	201	1/1	0.95	0.15	118,118,118,118	0
54	MG	BA	3025	1/1	0.95	0.38	65,65,65,65	0
54	MG	BA	3596	1/1	0.95	0.38	88,88,88,88	0
54	MG	AA	1607	1/1	0.95	0.39	99,99,99,99	0
54	MG	BA	3381	1/1	0.95	0.53	65,65,65,65	0
54	MG	AA	1626	1/1	0.95	0.22	80,80,80,80	0
54	MG	DA	3353	1/1	0.95	0.43	108,108,108,108	0
54	MG	DA	3490	1/1	0.95	0.09	120,120,120,120	0
54	MG	DA	3140	1/1	0.95	0.14	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	DA	3187	1/1	0.95	0.21	70,70,70,70	0
54	MG	AA	1780	1/1	0.95	0.08	154,154,154,154	0
54	MG	DA	3023	1/1	0.95	0.27	86,86,86,86	0
54	MG	BA	3138	1/1	0.95	0.22	81,81,81,81	0
54	MG	BA	3462	1/1	0.95	0.43	113,113,113,113	0
54	MG	DA	3049	1/1	0.95	0.10	105,105,105,105	0
54	MG	DA	3185	1/1	0.95	0.21	66,66,66,66	0
54	MG	DA	3105	1/1	0.95	0.16	110,110,110,110	0
54	MG	BA	3145	1/1	0.95	0.40	83,83,83,83	0
54	MG	DA	3282	1/1	0.95	0.18	88,88,88,88	0
54	MG	DA	3342	1/1	0.95	0.26	114,114,114,114	0
54	MG	AA	1648	1/1	0.95	0.28	123,123,123,123	0
54	MG	BA	3409	1/1	0.95	0.44	86,86,86,86	0
54	MG	BU	201	1/1	0.95	0.12	105,105,105,105	0
54	MG	DA	3213	1/1	0.95	0.26	67,67,67,67	0
54	MG	AA	1818	1/1	0.95	0.21	156,156,156,156	0
54	MG	BA	3142	1/1	0.95	0.47	48,48,48,48	0
54	MG	DA	3009	1/1	0.95	0.30	74,74,74,74	0
54	MG	CA	1720	1/1	0.95	0.30	98,98,98,98	0
54	MG	DA	3186	1/1	0.95	0.15	60,60,60,60	0
54	MG	BA	3435	1/1	0.95	0.10	109,109,109,109	0
54	MG	CG	302	1/1	0.95	0.40	180,180,180,180	0
54	MG	BA	3202	1/1	0.95	0.27	65,65,65,65	0
54	MG	DA	3090	1/1	0.95	0.24	90,90,90,90	0
54	MG	BA	3391	1/1	0.95	0.22	103,103,103,103	0
54	MG	DA	3467	1/1	0.95	0.10	159,159,159,159	0
54	MG	DA	3165	1/1	0.95	0.20	59,59,59,59	0
54	MG	BA	3364	1/1	0.95	0.25	137,137,137,137	0
54	MG	DA	3384	1/1	0.95	0.09	77,77,77,77	0
54	MG	DA	3288	1/1	0.95	0.24	95,95,95,95	0
56	ZN	CG	303	1/1	0.95	0.18	161,161,161,161	0
54	MG	DA	3035	1/1	0.95	0.13	93,93,93,93	0
54	MG	DA	3136	1/1	0.95	0.26	64,64,64,64	0
54	MG	DA	3227	1/1	0.95	0.23	83,83,83,83	0
54	MG	DA	3389	1/1	0.95	0.19	94,94,94,94	0
54	MG	CA	1625	1/1	0.95	0.35	142,142,142,142	0
54	MG	CA	1670	1/1	0.95	0.22	91,91,91,91	0
54	MG	DA	3192	1/1	0.95	0.22	64,64,64,64	0
54	MG	DA	3190	1/1	0.95	0.38	80,80,80,80	0
54	MG	DA	3442	1/1	0.95	0.13	112,112,112,112	0
54	MG	BA	3064	1/1	0.95	0.24	113,113,113,113	0
54	MG	BA	3106	1/1	0.95	0.27	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	BA	3529	1/1	0.95	0.29	89,89,89,89	0
54	MG	BA	3316	1/1	0.95	0.30	82,82,82,82	0
54	MG	BA	3032	1/1	0.95	0.29	69,69,69,69	0
54	MG	DA	3271	1/1	0.95	0.26	62,62,62,62	0
54	MG	BA	3115	1/1	0.95	0.37	68,68,68,68	0
54	MG	DA	3259	1/1	0.95	0.38	76,76,76,76	0
54	MG	BA	3019	1/1	0.95	0.29	49,49,49,49	0
54	MG	BA	3444	1/1	0.95	0.07	186,186,186,186	0
54	MG	BA	3313	1/1	0.96	0.26	61,61,61,61	0
54	MG	AA	1755	1/1	0.96	0.20	143,143,143,143	0
54	MG	DA	3309	1/1	0.96	0.07	145,145,145,145	0
54	MG	CA	1654	1/1	0.96	0.18	128,128,128,128	0
54	MG	CA	1697	1/1	0.96	0.17	185,185,185,185	0
54	MG	CA	1800	1/1	0.96	0.12	145,145,145,145	0
54	MG	BA	3555	1/1	0.96	0.20	67,67,67,67	0
54	MG	CA	1652	1/1	0.96	0.41	120,120,120,120	0
54	MG	DA	3115	1/1	0.96	0.23	75,75,75,75	0
54	MG	BA	3438	1/1	0.96	0.43	62,62,62,62	0
54	MG	DA	3317	1/1	0.96	0.46	131,131,131,131	0
54	MG	AA	1613	1/1	0.96	0.17	144,144,144,144	0
54	MG	AA	1660	1/1	0.96	0.14	126,126,126,126	0
54	MG	BA	3579	1/1	0.96	0.45	85,85,85,85	0
54	MG	AC	101	1/1	0.96	0.16	78,78,78,78	0
54	MG	BA	3223	1/1	0.96	0.46	84,84,84,84	0
54	MG	BB	202	1/1	0.96	0.24	92,92,92,92	0
54	MG	AA	1808	1/1	0.96	0.15	139,139,139,139	0
54	MG	DA	3064	1/1	0.96	0.28	79,79,79,79	0
54	MG	DA	3130	1/1	0.96	0.32	92,92,92,92	0
54	MG	CA	1660	1/1	0.96	0.14	118,118,118,118	0
54	MG	BA	3044	1/1	0.96	0.16	58,58,58,58	0
54	MG	BA	3037	1/1	0.96	0.44	71,71,71,71	0
54	MG	BA	3165	1/1	0.96	0.17	119,119,119,119	0
54	MG	DA	3119	1/1	0.96	0.32	65,65,65,65	0
54	MG	DA	3379	1/1	0.96	0.46	64,64,64,64	0
54	MG	BA	3352	1/1	0.96	0.35	87,87,87,87	0
54	MG	BA	3341	1/1	0.96	0.36	71,71,71,71	0
54	MG	BO	201	1/1	0.96	0.15	90,90,90,90	0
54	MG	CA	1719	1/1	0.96	0.12	116,116,116,116	0
56	ZN	AG	303	1/1	0.96	0.25	153,153,153,153	0
54	MG	DA	3122	1/1	0.96	0.28	67,67,67,67	0
54	MG	BA	3068	1/1	0.96	0.19	71,71,71,71	0
54	MG	DA	3102	1/1	0.96	0.11	150,150,150,150	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	AA	1777	1/1	0.96	0.05	141,141,141,141	0
54	MG	DA	3241	1/1	0.96	0.24	69,69,69,69	0
54	MG	BA	3500	1/1	0.96	0.19	129,129,129,129	0
54	MG	DA	3244	1/1	0.96	0.19	84,84,84,84	0
54	MG	CA	1640	1/1	0.96	0.29	92,92,92,92	0
54	MG	BA	3520	1/1	0.96	0.41	129,129,129,129	0
54	MG	DA	3439	1/1	0.96	0.07	84,84,84,84	0
54	MG	BA	3602	1/1	0.96	0.50	66,66,66,66	0
54	MG	BA	3487	1/1	0.96	0.06	116,116,116,116	0
54	MG	DA	3223	1/1	0.96	0.26	54,54,54,54	0
54	MG	BA	3105	1/1	0.96	0.23	68,68,68,68	0
54	MG	BA	3260	1/1	0.96	0.20	126,126,126,126	0
54	MG	DA	3217	1/1	0.96	0.23	89,89,89,89	0
54	MG	DA	3226	1/1	0.96	0.26	81,81,81,81	0
54	MG	BA	3040	1/1	0.96	0.25	88,88,88,88	0
54	MG	AA	1627	1/1	0.96	0.32	87,87,87,87	0
54	MG	BA	3039	1/1	0.96	0.37	98,98,98,98	0
54	MG	DA	3287	1/1	0.96	0.23	67,67,67,67	0
54	MG	BA	3531	1/1	0.96	0.38	101,101,101,101	0
54	MG	DA	3230	1/1	0.96	0.30	65,65,65,65	0
54	MG	BA	3045	1/1	0.96	0.43	66,66,66,66	0
54	MG	DA	3238	1/1	0.96	0.12	117,117,117,117	0
54	MG	BA	3103	1/1	0.96	0.21	93,93,93,93	0
54	MG	BA	3080	1/1	0.96	0.19	125,125,125,125	0
54	MG	BA	3171	1/1	0.96	0.26	87,87,87,87	0
54	MG	BA	3417	1/1	0.96	0.23	78,78,78,78	0
54	MG	AA	1606	1/1	0.96	0.09	155,155,155,155	0
54	MG	DA	3494	1/1	0.96	0.33	45,45,45,45	0
54	MG	BA	3061	1/1	0.96	0.42	64,64,64,64	0
54	MG	CA	1801	1/1	0.96	0.23	139,139,139,139	0
54	MG	DA	3418	1/1	0.96	0.35	61,61,61,61	0
54	MG	DA	3268	1/1	0.96	0.14	63,63,63,63	0
54	MG	CA	1635	1/1	0.96	0.29	78,78,78,78	0
54	MG	DA	3059	1/1	0.96	0.22	68,68,68,68	0
54	MG	DA	3199	1/1	0.96	0.14	77,77,77,77	0
54	MG	BA	3305	1/1	0.96	0.32	80,80,80,80	0
54	MG	DA	3473	1/1	0.96	0.13	157,157,157,157	0
54	MG	DA	3153	1/1	0.96	0.12	145,145,145,145	0
54	MG	DA	3229	1/1	0.96	0.27	94,94,94,94	0
54	MG	BA	3113	1/1	0.96	0.14	72,72,72,72	0
54	MG	BA	3349	1/1	0.96	0.48	69,69,69,69	0
54	MG	AA	1644	1/1	0.96	0.26	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	DA	3508	1/1	0.96	0.26	68,68,68,68	0
54	MG	DA	3201	1/1	0.96	0.29	73,73,73,73	0
54	MG	BA	3610	1/1	0.96	0.14	85,85,85,85	0
54	MG	BA	3338	1/1	0.96	0.26	103,103,103,103	0
54	MG	BA	3172	1/1	0.96	0.24	93,93,93,93	0
54	MG	CA	1648	1/1	0.96	0.13	96,96,96,96	0
54	MG	BA	3434	1/1	0.96	0.62	107,107,107,107	0
54	MG	BA	3168	1/1	0.96	0.34	52,52,52,52	0
54	MG	BA	3578	1/1	0.96	0.17	88,88,88,88	0
54	MG	AA	1823	1/1	0.96	0.11	138,138,138,138	0
54	MG	BA	3193	1/1	0.96	0.45	76,76,76,76	0
54	MG	CA	1795	1/1	0.96	0.23	112,112,112,112	0
54	MG	BA	3013	1/1	0.96	0.24	63,63,63,63	0
54	MG	CA	1744	1/1	0.96	0.33	97,97,97,97	0
54	MG	AA	1638	1/1	0.96	0.38	104,104,104,104	0
54	MG	DA	3211	1/1	0.96	0.23	71,71,71,71	0
54	MG	BA	3382	1/1	0.96	0.48	78,78,78,78	0
54	MG	DA	3117	1/1	0.96	0.27	72,72,72,72	0
54	MG	BA	3386	1/1	0.96	0.15	117,117,117,117	0
54	MG	AA	1677	1/1	0.96	0.30	125,125,125,125	0
54	MG	DA	3118	1/1	0.96	0.21	61,61,61,61	0
54	MG	DA	3224	1/1	0.96	0.16	61,61,61,61	0
54	MG	DA	3179	1/1	0.96	0.18	85,85,85,85	0
54	MG	CA	1643	1/1	0.96	0.07	148,148,148,148	0
54	MG	BA	3583	1/1	0.96	0.28	59,59,59,59	0
54	MG	BA	3146	1/1	0.96	0.47	82,82,82,82	0
54	MG	BA	3375	1/1	0.96	0.50	80,80,80,80	0
54	MG	AA	1650	1/1	0.96	0.26	85,85,85,85	0
54	MG	DA	3278	1/1	0.97	0.10	80,80,80,80	0
54	MG	DA	3053	1/1	0.97	0.31	100,100,100,100	0
54	MG	DA	3221	1/1	0.97	0.27	61,61,61,61	0
54	MG	AA	1798	1/1	0.97	0.42	100,100,100,100	0
54	MG	BA	3297	1/1	0.97	0.40	78,78,78,78	0
54	MG	BA	3218	1/1	0.97	0.36	75,75,75,75	0
54	MG	DA	3073	1/1	0.97	0.11	102,102,102,102	0
54	MG	BA	3200	1/1	0.97	0.12	149,149,149,149	0
54	MG	CA	1742	1/1	0.97	0.35	98,98,98,98	0
54	MG	DA	3491	1/1	0.97	0.32	65,65,65,65	0
54	MG	BA	3620	1/1	0.97	0.14	72,72,72,72	0
54	MG	AA	1737	1/1	0.97	0.39	132,132,132,132	0
54	MG	DA	3014	1/1	0.97	0.39	69,69,69,69	0
54	MG	BA	3035	1/1	0.97	0.26	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	BA	3257	1/1	0.97	0.30	70,70,70,70	0
54	MG	DA	3328	1/1	0.97	0.04	138,138,138,138	0
54	MG	DA	3383	1/1	0.97	0.37	84,84,84,84	0
54	MG	BA	3295	1/1	0.97	0.43	70,70,70,70	0
54	MG	BA	3012	1/1	0.97	0.21	70,70,70,70	0
54	MG	BA	3016	1/1	0.97	0.06	143,143,143,143	0
54	MG	B5	101	1/1	0.97	0.16	61,61,61,61	0
54	MG	DA	3440	1/1	0.97	0.42	83,83,83,83	0
54	MG	DA	3030	1/1	0.97	0.28	89,89,89,89	0
54	MG	DA	3139	1/1	0.97	0.27	67,67,67,67	0
54	MG	DA	3496	1/1	0.97	0.14	72,72,72,72	0
54	MG	BA	3220	1/1	0.97	0.23	76,76,76,76	0
54	MG	DA	3120	1/1	0.97	0.15	75,75,75,75	0
54	MG	DA	3506	1/1	0.97	0.28	61,61,61,61	0
54	MG	BA	3201	1/1	0.97	0.18	122,122,122,122	0
54	MG	BA	3054	1/1	0.97	0.41	91,91,91,91	0
54	MG	BA	3577	1/1	0.97	0.31	61,61,61,61	0
54	MG	BA	3038	1/1	0.97	0.30	67,67,67,67	0
54	MG	BA	3263	1/1	0.97	0.35	50,50,50,50	0
54	MG	CA	1690	1/1	0.97	0.22	102,102,102,102	0
54	MG	DA	3277	1/1	0.97	0.34	77,77,77,77	0
54	MG	BA	3036	1/1	0.97	0.25	63,63,63,63	0
54	MG	BA	3346	1/1	0.97	0.28	112,112,112,112	0
54	MG	DA	3159	1/1	0.97	0.10	128,128,128,128	0
54	MG	DA	3232	1/1	0.97	0.24	78,78,78,78	0
54	MG	BA	3244	1/1	0.97	0.10	112,112,112,112	0
54	MG	BA	3187	1/1	0.97	0.34	56,56,56,56	0
54	MG	BA	3028	1/1	0.97	0.36	57,57,57,57	0
54	MG	CA	1617	1/1	0.97	0.23	140,140,140,140	0
54	MG	DA	3505	1/1	0.97	0.13	72,72,72,72	0
54	MG	BA	3181	1/1	0.97	0.26	79,79,79,79	0
54	MG	DA	3072	1/1	0.97	0.31	94,94,94,94	0
54	MG	BA	3225	1/1	0.97	0.54	92,92,92,92	0
54	MG	DA	3231	1/1	0.97	0.23	74,74,74,74	0
54	MG	BA	3158	1/1	0.97	0.52	67,67,67,67	0
54	MG	BA	3593	1/1	0.97	0.37	57,57,57,57	0
54	MG	BA	3239	1/1	0.97	0.39	82,82,82,82	0
54	MG	BA	3258	1/1	0.97	0.45	74,74,74,74	0
54	MG	BA	3502	1/1	0.97	0.52	90,90,90,90	0
54	MG	DA	3214	1/1	0.97	0.22	63,63,63,63	0
54	MG	BA	3613	1/1	0.97	0.09	111,111,111,111	0
54	MG	BA	3254	1/1	0.97	0.31	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	BA	3057	1/1	0.97	0.35	93,93,93,93	0
54	MG	DA	3218	1/1	0.97	0.35	77,77,77,77	0
54	MG	DA	3228	1/1	0.97	0.08	80,80,80,80	0
54	MG	BA	3581	1/1	0.97	0.32	82,82,82,82	0
54	MG	DA	3261	1/1	0.97	0.15	78,78,78,78	0
54	MG	DA	3219	1/1	0.97	0.28	71,71,71,71	0
54	MG	DA	3143	1/1	0.97	0.10	117,117,117,117	0
54	MG	CA	1651	1/1	0.97	0.22	116,116,116,116	0
54	MG	BA	3252	1/1	0.97	0.28	70,70,70,70	0
54	MG	BA	3327	1/1	0.97	0.21	117,117,117,117	0
54	MG	BA	3141	1/1	0.97	0.23	63,63,63,63	0
54	MG	BA	3471	1/1	0.97	0.46	91,91,91,91	0
54	MG	BA	3210	1/1	0.97	0.52	78,78,78,78	0
54	MG	DA	3507	1/1	0.97	0.19	79,79,79,79	0
54	MG	AA	1695	1/1	0.97	0.07	152,152,152,152	0
54	MG	AA	1774	1/1	0.97	0.20	72,72,72,72	0
54	MG	BA	3331	1/1	0.97	0.43	74,74,74,74	0
54	MG	BA	3473	1/1	0.97	0.41	82,82,82,82	0
54	MG	CA	1678	1/1	0.97	0.07	140,140,140,140	0
54	MG	AA	1609	1/1	0.97	0.39	87,87,87,87	0
54	MG	DA	3132	1/1	0.97	0.22	78,78,78,78	0
54	MG	DA	3109	1/1	0.97	0.26	63,63,63,63	0
54	MG	BA	3584	1/1	0.97	0.36	100,100,100,100	0
54	MG	DA	3477	1/1	0.97	0.23	93,93,93,93	0
54	MG	AA	1731	1/1	0.97	0.54	90,90,90,90	0
54	MG	DB	202	1/1	0.97	0.11	113,113,113,113	0
54	MG	AA	1713	1/1	0.97	0.14	107,107,107,107	0
54	MG	BA	3590	1/1	0.97	0.52	116,116,116,116	0
54	MG	DA	3236	1/1	0.97	0.28	60,60,60,60	0
54	MG	DA	3108	1/1	0.97	0.26	67,67,67,67	0
54	MG	D5	101	1/1	0.97	0.10	63,63,63,63	0
54	MG	AA	1717	1/1	0.97	0.07	137,137,137,137	0
54	MG	BA	3330	1/1	0.97	0.21	102,102,102,102	0
54	MG	AA	1620	1/1	0.97	0.24	105,105,105,105	0
54	MG	BA	3098	1/1	0.97	0.43	75,75,75,75	0
54	MG	BA	3015	1/1	0.97	0.25	61,61,61,61	0
54	MG	BA	3162	1/1	0.97	0.27	72,72,72,72	0
54	MG	CA	1603	1/1	0.97	0.56	93,93,93,93	0
54	MG	DA	3170	1/1	0.97	0.29	80,80,80,80	0
54	MG	CA	1669	1/1	0.97	0.14	130,130,130,130	0
54	MG	BA	3229	1/1	0.97	0.32	89,89,89,89	0
54	MG	BA	3585	1/1	0.97	0.21	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	DA	3171	1/1	0.97	0.35	87,87,87,87	0
54	MG	DA	3174	1/1	0.97	0.16	81,81,81,81	0
54	MG	CA	1733	1/1	0.97	0.35	124,124,124,124	0
54	MG	BA	3408	1/1	0.97	0.13	109,109,109,109	0
54	MG	AA	1666	1/1	0.97	0.09	123,123,123,123	0
54	MG	CA	1759	1/1	0.97	0.09	157,157,157,157	0
54	MG	AA	1720	1/1	0.97	0.17	101,101,101,101	0
54	MG	BA	3058	1/1	0.97	0.26	103,103,103,103	0
54	MG	BA	3227	1/1	0.97	0.31	82,82,82,82	0
54	MG	BA	3041	1/1	0.97	0.07	142,142,142,142	0
54	MG	CA	1639	1/1	0.98	0.34	129,129,129,129	0
54	MG	DA	3003	1/1	0.98	0.32	130,130,130,130	0
54	MG	CC	105	1/1	0.98	0.21	125,125,125,125	0
54	MG	BA	3101	1/1	0.98	0.42	58,58,58,58	0
54	MG	BA	3017	1/1	0.98	0.27	67,67,67,67	0
54	MG	CA	1653	1/1	0.98	0.28	122,122,122,122	0
54	MG	AA	1706	1/1	0.98	0.06	134,134,134,134	0
54	MG	DA	3097	1/1	0.98	0.39	74,74,74,74	0
54	MG	BA	3074	1/1	0.98	0.12	142,142,142,142	0
54	MG	BA	3121	1/1	0.98	0.29	87,87,87,87	0
54	MG	DA	3297	1/1	0.98	0.14	71,71,71,71	0
54	MG	CA	1734	1/1	0.98	0.09	93,93,93,93	0
54	MG	DA	3225	1/1	0.98	0.12	89,89,89,89	0
54	MG	BA	3157	1/1	0.98	0.36	74,74,74,74	0
54	MG	DA	3298	1/1	0.98	0.07	96,96,96,96	0
54	MG	BA	3130	1/1	0.98	0.09	92,92,92,92	0
54	MG	CC	102	1/1	0.98	0.18	83,83,83,83	0
54	MG	DA	3220	1/1	0.98	0.24	70,70,70,70	0
54	MG	BA	3328	1/1	0.98	0.22	119,119,119,119	0
54	MG	DA	3500	1/1	0.98	0.12	88,88,88,88	0
54	MG	BA	3022	1/1	0.98	0.43	65,65,65,65	0
54	MG	BA	3501	1/1	0.98	0.40	99,99,99,99	0
54	MG	DA	3189	1/1	0.98	0.27	65,65,65,65	0
54	MG	BA	3007	1/1	0.98	0.20	63,63,63,63	0
54	MG	DA	3182	1/1	0.98	0.28	62,62,62,62	0
54	MG	AA	1604	1/1	0.98	0.11	135,135,135,135	0
54	MG	CA	1791	1/1	0.98	0.30	78,78,78,78	0
54	MG	BA	3087	1/1	0.98	0.05	142,142,142,142	0
54	MG	BA	3029	1/1	0.98	0.29	74,74,74,74	0
54	MG	DA	3361	1/1	0.98	0.27	93,93,93,93	0
54	MG	CA	1649	1/1	0.98	0.22	113,113,113,113	0
54	MG	BA	3009	1/1	0.98	0.24	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	DA	3358	1/1	0.98	0.37	73,73,73,73	0
54	MG	BA	3143	1/1	0.98	0.41	52,52,52,52	0
54	MG	BA	3026	1/1	0.98	0.21	66,66,66,66	0
54	MG	BA	3197	1/1	0.98	0.20	66,66,66,66	0
54	MG	BA	3081	1/1	0.98	0.26	88,88,88,88	0
54	MG	BA	3002	1/1	0.98	0.39	63,63,63,63	0
54	MG	BA	3006	1/1	0.98	0.22	50,50,50,50	0
54	MG	BB	203	1/1	0.98	0.41	73,73,73,73	0
54	MG	BA	3224	1/1	0.98	0.31	101,101,101,101	0
54	MG	BA	3059	1/1	0.98	0.09	144,144,144,144	0
54	MG	DA	3363	1/1	0.98	0.05	125,125,125,125	0
54	MG	BA	3589	1/1	0.98	0.31	77,77,77,77	0
56	ZN	AQ	103	1/1	0.98	0.09	186,186,186,186	0
54	MG	DA	3127	1/1	0.98	0.23	66,66,66,66	0
54	MG	BA	3004	1/1	0.98	0.30	79,79,79,79	0
54	MG	AA	1656	1/1	0.98	0.24	71,71,71,71	0
54	MG	BA	3083	1/1	0.98	0.29	108,108,108,108	0
54	MG	AA	1624	1/1	0.98	0.12	98,98,98,98	0
54	MG	AA	1768	1/1	0.98	0.13	126,126,126,126	0
54	MG	DA	3039	1/1	0.98	0.48	116,116,116,116	0
54	MG	AA	1663	1/1	0.98	0.13	76,76,76,76	0
54	MG	DA	3243	1/1	0.98	0.18	86,86,86,86	0
54	MG	BA	3222	1/1	0.98	0.36	57,57,57,57	0
54	MG	DA	3281	1/1	0.98	0.24	74,74,74,74	0
54	MG	DA	3181	1/1	0.98	0.18	74,74,74,74	0
54	MG	AA	1682	1/1	0.98	0.12	113,113,113,113	0
54	MG	DA	3169	1/1	0.98	0.36	76,76,76,76	0
54	MG	DA	3166	1/1	0.98	0.29	65,65,65,65	0
54	MG	BA	3213	1/1	0.98	0.26	69,69,69,69	0
54	MG	DA	3222	1/1	0.98	0.27	62,62,62,62	0
54	MG	BA	3144	1/1	0.98	0.41	73,73,73,73	0
54	MG	BA	3173	1/1	0.98	0.31	62,62,62,62	0
54	MG	BA	3243	1/1	0.98	0.49	122,122,122,122	0
54	MG	DA	3013	1/1	0.98	0.25	69,69,69,69	0
54	MG	BA	3262	1/1	0.98	0.37	63,63,63,63	0
54	MG	BA	3076	1/1	0.98	0.09	74,74,74,74	0
54	MG	BA	3184	1/1	0.98	0.21	70,70,70,70	0
54	MG	DA	3242	1/1	0.98	0.34	64,64,64,64	0
54	MG	BA	3159	1/1	0.98	0.23	101,101,101,101	0
54	MG	CA	1802	1/1	0.98	0.39	136,136,136,136	0
54	MG	BA	3125	1/1	0.98	0.32	88,88,88,88	0
54	MG	BA	3109	1/1	0.98	0.46	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	AA	1698	1/1	0.98	0.33	132,132,132,132	0
54	MG	AA	1653	1/1	0.98	0.21	91,91,91,91	0
54	MG	BA	3276	1/1	0.98	0.27	90,90,90,90	0
54	MG	DA	3501	1/1	0.98	0.24	73,73,73,73	0
54	MG	DA	3126	1/1	0.98	0.09	58,58,58,58	0
54	MG	CA	1646	1/1	0.98	0.22	101,101,101,101	0
54	MG	AA	1602	1/1	0.98	0.24	95,95,95,95	0
54	MG	BA	3003	1/1	0.98	0.30	78,78,78,78	0
54	MG	BA	3259	1/1	0.98	0.29	53,53,53,53	0
54	MG	BA	3315	1/1	0.98	0.34	91,91,91,91	0
54	MG	BA	3601	1/1	0.98	0.49	52,52,52,52	0
54	MG	BA	3174	1/1	0.98	0.18	61,61,61,61	0
54	MG	BA	3180	1/1	0.98	0.53	73,73,73,73	0
54	MG	BA	3062	1/1	0.98	0.27	70,70,70,70	0
54	MG	BF	302	1/1	0.98	0.40	127,127,127,127	0
54	MG	BA	3582	1/1	0.98	0.25	68,68,68,68	0
54	MG	BA	3221	1/1	0.98	0.34	89,89,89,89	0
54	MG	BB	217	1/1	0.98	0.10	132,132,132,132	0
54	MG	DA	3266	1/1	0.99	0.13	110,110,110,110	0
54	MG	DA	3262	1/1	0.99	0.13	112,112,112,112	0
54	MG	BA	3104	1/1	0.99	0.35	70,70,70,70	0
54	MG	DA	3075	1/1	0.99	0.29	105,105,105,105	0
54	MG	AA	1640	1/1	0.99	0.22	82,82,82,82	0
54	MG	BA	3479	1/1	0.99	0.38	72,72,72,72	0
54	MG	AA	1657	1/1	0.99	0.43	63,63,63,63	0
54	MG	AA	1783	1/1	0.99	0.13	125,125,125,125	0
54	MG	BA	3549	1/1	0.99	0.10	140,140,140,140	0
54	MG	DA	3331	1/1	0.99	0.09	116,116,116,116	0
54	MG	DA	3184	1/1	0.99	0.23	68,68,68,68	0
54	MG	DA	3167	1/1	0.99	0.07	75,75,75,75	0
54	MG	AA	1601	1/1	0.99	0.27	80,80,80,80	0
54	MG	DA	3263	1/1	0.99	0.14	129,129,129,129	0
54	MG	BA	3591	1/1	0.99	0.46	57,57,57,57	0
54	MG	BA	3175	1/1	0.99	0.10	80,80,80,80	0
54	MG	DA	3499	1/1	0.99	0.14	103,103,103,103	0
54	MG	BA	3267	1/1	0.99	0.07	126,126,126,126	0
54	MG	BA	3089	1/1	0.99	0.51	77,77,77,77	0
54	MG	BA	3198	1/1	0.99	0.36	70,70,70,70	0
54	MG	DA	3094	1/1	0.99	0.13	85,85,85,85	0
54	MG	DA	3270	1/1	0.99	0.20	63,63,63,63	0
54	MG	DA	3327	1/1	0.99	0.32	70,70,70,70	0
54	MG	BA	3008	1/1	0.99	0.49	58,58,58,58	0

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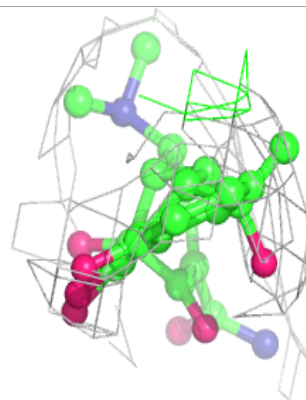
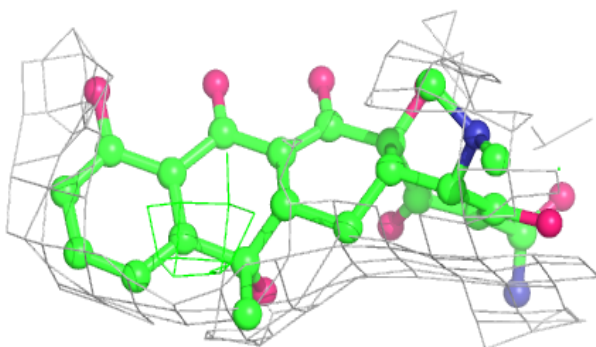
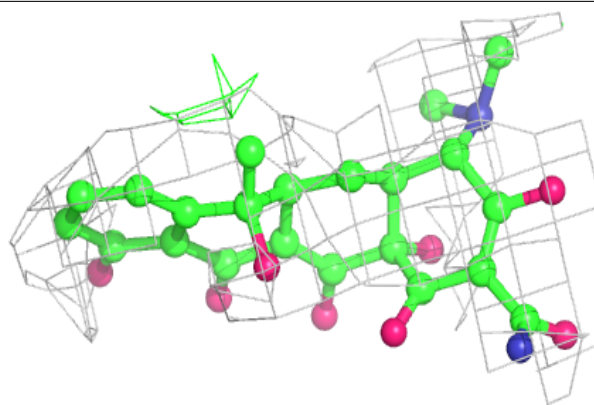
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	DA	3147	1/1	0.99	0.33	82,82,82,82	0
54	MG	DA	3264	1/1	0.99	0.28	80,80,80,80	0
54	MG	DA	3124	1/1	0.99	0.25	69,69,69,69	0
54	MG	BA	3219	1/1	0.99	0.13	123,123,123,123	0
54	MG	BA	3195	1/1	0.99	0.13	82,82,82,82	0
54	MG	AA	1603	1/1	0.99	0.25	109,109,109,109	0
54	MG	DA	3111	1/1	0.99	0.18	64,64,64,64	0
54	MG	DA	3267	1/1	0.99	0.14	79,79,79,79	0
54	MG	DA	3055	1/1	0.99	0.28	59,59,59,59	0
54	MG	DA	3114	1/1	0.99	0.21	82,82,82,82	0
54	MG	BA	3147	1/1	0.99	0.36	64,64,64,64	0
54	MG	DA	3237	1/1	0.99	0.11	63,63,63,63	0
54	MG	BA	3192	1/1	0.99	0.29	67,67,67,67	0
54	MG	CA	1721	1/1	0.99	0.12	128,128,128,128	0
54	MG	DA	3495	1/1	0.99	0.32	78,78,78,78	0
54	MG	DA	3497	1/1	0.99	0.21	50,50,50,50	0
54	MG	BA	3099	1/1	0.99	0.42	74,74,74,74	0
54	MG	BA	3118	1/1	0.99	0.41	90,90,90,90	0
54	MG	DA	3504	1/1	0.99	0.46	67,67,67,67	0
54	MG	BA	3176	1/1	0.99	0.08	89,89,89,89	0
54	MG	BA	3495	1/1	0.99	0.32	73,73,73,73	0
54	MG	DA	3344	1/1	1.00	0.11	124,124,124,124	0
54	MG	AA	1616	1/1	1.00	0.28	158,158,158,158	0
54	MG	BA	3049	1/1	1.00	0.29	88,88,88,88	0

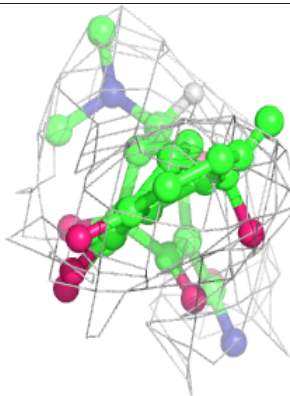
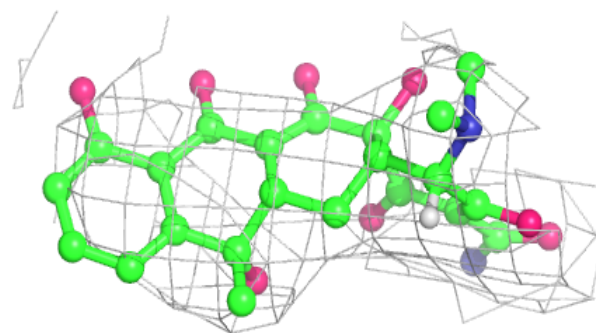
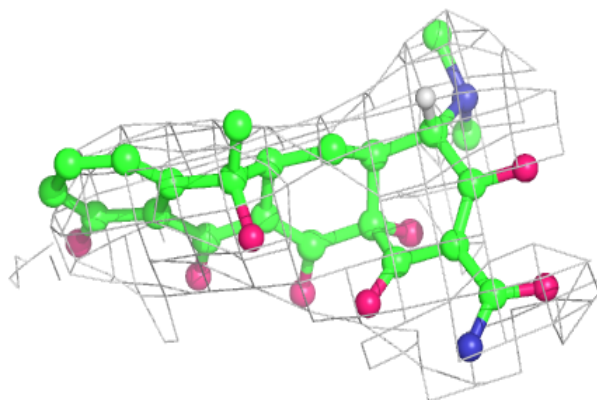
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around TAC CA 1805:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around TAC AA 1833:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.