



wwPDB X-ray Structure Validation Summary Report ⓘ

May 15, 2020 – 02:56 am BST

PDB ID : 4V9B
Title : Crystal Structure of the 70S ribosome with tigecycline.
Authors : Jenner, L.; Yusupov, M.; Yusupova, G.
Deposited on : 2012-07-18
Resolution : 3.10 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

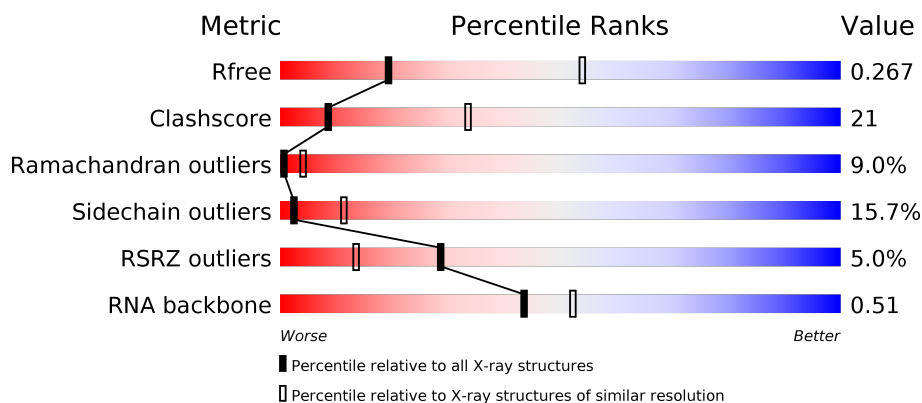
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)
RNA backbone	3102	1116 (3.40-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	
1	CA	1506	
2	AE	256	
2	CE	256	


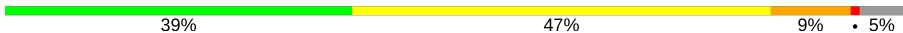
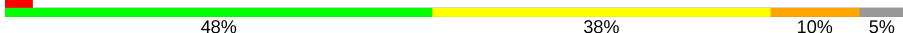



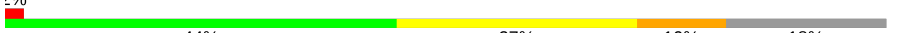




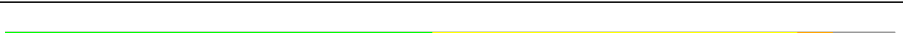


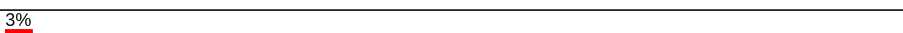




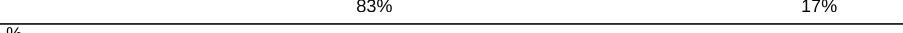

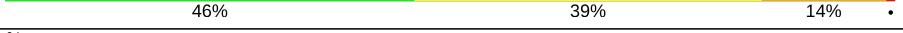



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Mol	Chain	Length	Quality of chain
3	AF	239	
3	CF	239	
4	AG	208	
4	CG	208	
5	AH	162	
5	CH	162	
6	AI	101	
6	CI	101	
7	AJ	156	
7	CJ	156	
8	AK	138	
8	CK	138	
9	AL	128	
9	CL	128	
10	AM	105	
10	CM	105	
11	AN	129	
11	CN	129	
12	AO	128	
12	CO	128	
13	AP	126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




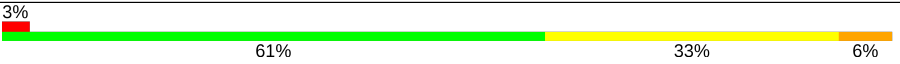
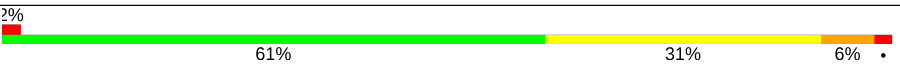

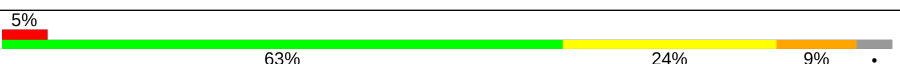
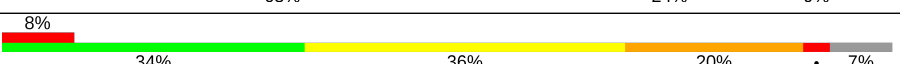
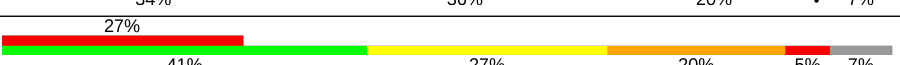
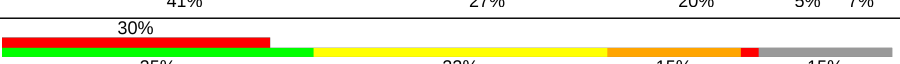
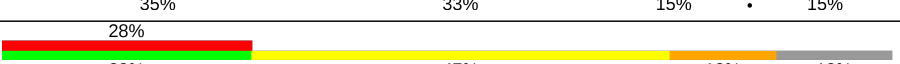
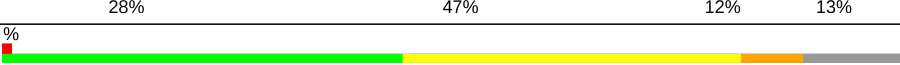





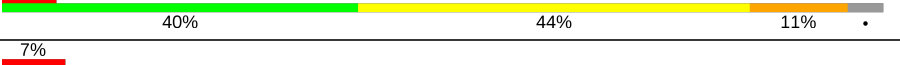
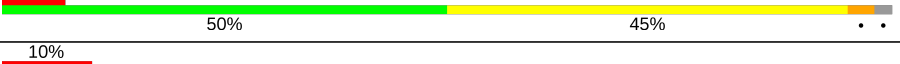


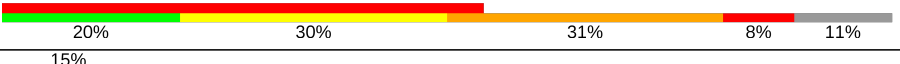
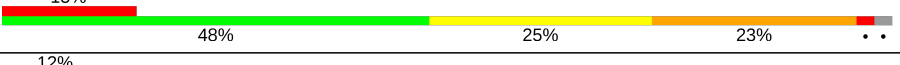


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Mol	Chain	Length	Quality of chain
27	BE	206	
27	DE	206	
28	BF	210	
28	DF	210	
29	BG	182	
29	DG	182	
30	BH	180	
30	DH	180	
31	BK	148	
31	DK	148	
32	BM	140	
32	DM	140	
33	BN	122	
33	DN	122	
34	BO	150	
34	DO	150	
35	BP	141	
35	DP	141	
36	B0	118	
36	D0	118	
37	BQ	112	
37	DQ	112	
38	BR	146	
38	DR	146	
39	B1	118	

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Mol	Chain	Length	Quality of chain
39	D1	118	
40	B2	101	
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	

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Mol	Chain	Length	Quality of chain
52	B7	49	
52	D7	49	
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	1740	-	-	-	X
54	MG	AA	1773	-	-	-	X
54	MG	AA	1782	-	-	-	X
54	MG	AA	1818	-	-	-	X
54	MG	BA	3111	-	-	-	X
54	MG	BA	3180	-	-	-	X
54	MG	BA	3237	-	-	-	X
54	MG	BA	3288	-	-	-	X
54	MG	BA	3300	-	-	-	X
54	MG	BA	3353	-	-	-	X
54	MG	BA	3393	-	-	-	X
54	MG	BA	3423	-	-	-	X
54	MG	BA	3469	-	-	-	X
54	MG	BA	3503	-	-	-	X
54	MG	BA	3509	-	-	-	X
54	MG	BA	3510	-	-	-	X
54	MG	BA	3518	-	-	-	X
54	MG	BA	3522	-	-	-	X
54	MG	BA	3566	-	-	-	X
54	MG	BA	3580	-	-	-	X
54	MG	BA	3588	-	-	-	X
54	MG	BA	3594	-	-	-	X
54	MG	CA	1716	-	-	-	X
54	MG	CA	1785	-	-	-	X
54	MG	DA	3270	-	-	-	X
54	MG	DA	3324	-	-	-	X
54	MG	DA	3329	-	-	-	X
54	MG	DA	3460	-	-	-	X

2 Entry composition

There are 56 unique types of molecules in this entry. The entry contains 295766 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AV	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	AD	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			
22	CD	77	Total	C	N	O	P	0	0	0
			1640	732	298	534	76			

There are 16 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
AD	17A	C	U	CONFLICT	GB AP008226.1
AD	50	U	C	CONFLICT	GB AP008226.1
AD	51	C	G	CONFLICT	GB AP008226.1
AD	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
CD	17A	C	U	CONFLICT	GB AP008226.1
CD	50	U	C	CONFLICT	GB AP008226.1
CD	51	C	G	CONFLICT	GB AP008226.1
CD	63	G	C	CONFLICT	GB AP008226.1

- Molecule 23 is a RNA chain called MRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	A1	6	Total	C	N	O	P	0	0	0
			129	58	24	41	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	C1	6	Total	C	N	O	P	0	0	0
			129	58	24	41	6			

- 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	2906	Total	C	N	O	P	0	0	0
			62587	27857	11709	20116	2905			

There are 14 discrepancies between the modelled and reference sequences:

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

- Molecule 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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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			
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			

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	BA	632	Total 632	Mg 632	0	0
54	CA	199	Total 199	Mg 199	0	0
54	B8	2	Total 2	Mg 2	0	0
54	BE	4	Total 4	Mg 4	0	0
54	DU	2	Total 2	Mg 2	0	0
54	B1	1	Total 1	Mg 1	0	0
54	AN	2	Total 2	Mg 2	0	0
54	CN	1	Total 1	Mg 1	0	0
54	B5	1	Total 1	Mg 1	0	0
54	BB	16	Total 16	Mg 16	0	0
54	D8	1	Total 1	Mg 1	0	0
54	D3	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	236	Total 236	Mg 236	0	0
54	CX	1	Total 1	Mg 1	0	0
54	CG	2	Total 2	Mg 2	0	0

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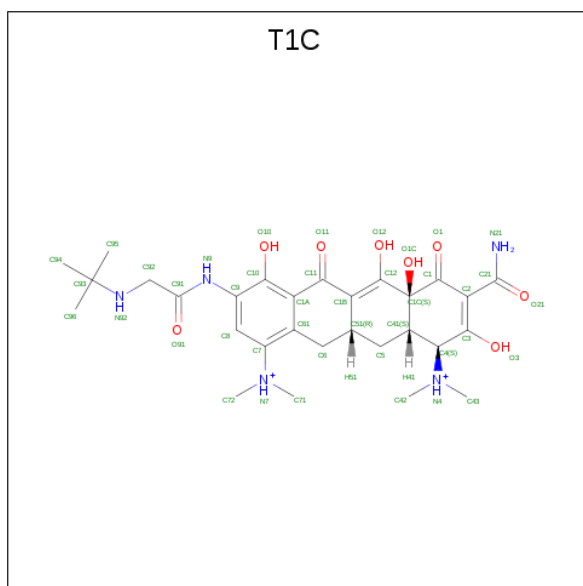
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	BU	2	Total 2	Mg 2	0	0
54	A1	1	Total 1	Mg 1	0	0
54	AD	1	Total 1	Mg 1	0	0
54	CC	9	Total 9	Mg 9	0	0
54	DE	4	Total 4	Mg 4	0	0
54	B3	2	Total 2	Mg 2	0	0
54	DA	523	Total 523	Mg 523	0	0
54	B7	3	Total 3	Mg 3	0	0
54	AG	1	Total 1	Mg 1	0	0
54	BO	2	Total 2	Mg 2	0	0
54	AQ	1	Total 1	Mg 1	0	0
54	D1	1	Total 1	Mg 1	0	0
54	AH	1	Total 1	Mg 1	0	0
54	DP	1	Total 1	Mg 1	0	0
54	AC	8	Total 8	Mg 8	0	0
54	D5	1	Total 1	Mg 1	0	0
54	BD	1	Total 1	Mg 1	0	0
54	AT	1	Total 1	Mg 1	0	0
54	B0	1	Total 1	Mg 1	0	0
54	CS	1	Total 1	Mg 1	0	0
54	CL	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
54	DB	15	Total Mg 15 15	0	0

- Molecule 55 is TIGECYCLINE (three-letter code: T1C) (formula: $C_{29}H_{41}N_5O_8$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
55	AA	1	Total 42	C 29	N 5	O 8	0	0
55	CA	1	Total 42	C 29	N 5	O 8	0	0

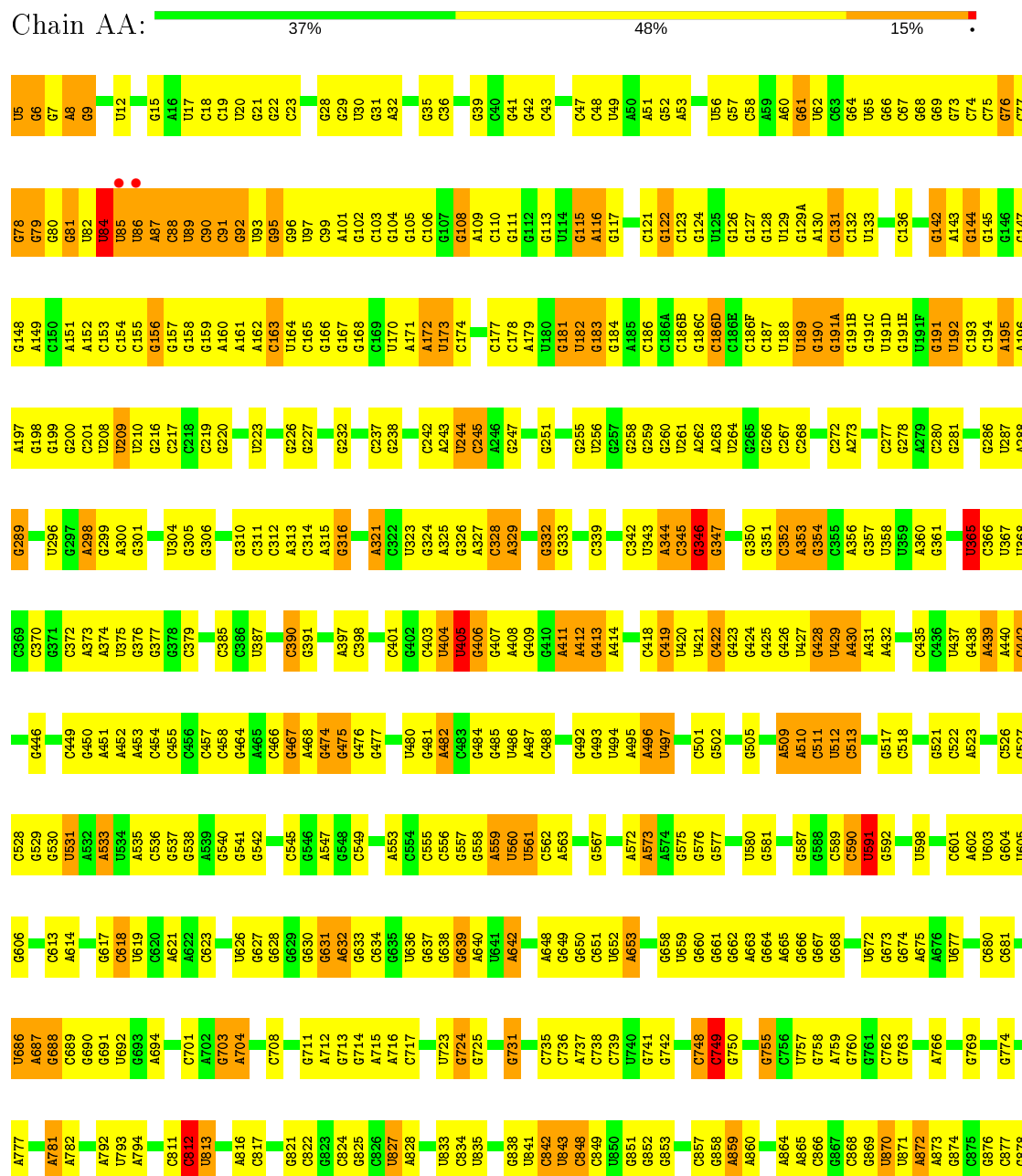
- Molecule 56 is ZINC ION (three-letter code: ZN) (formula: Zn).

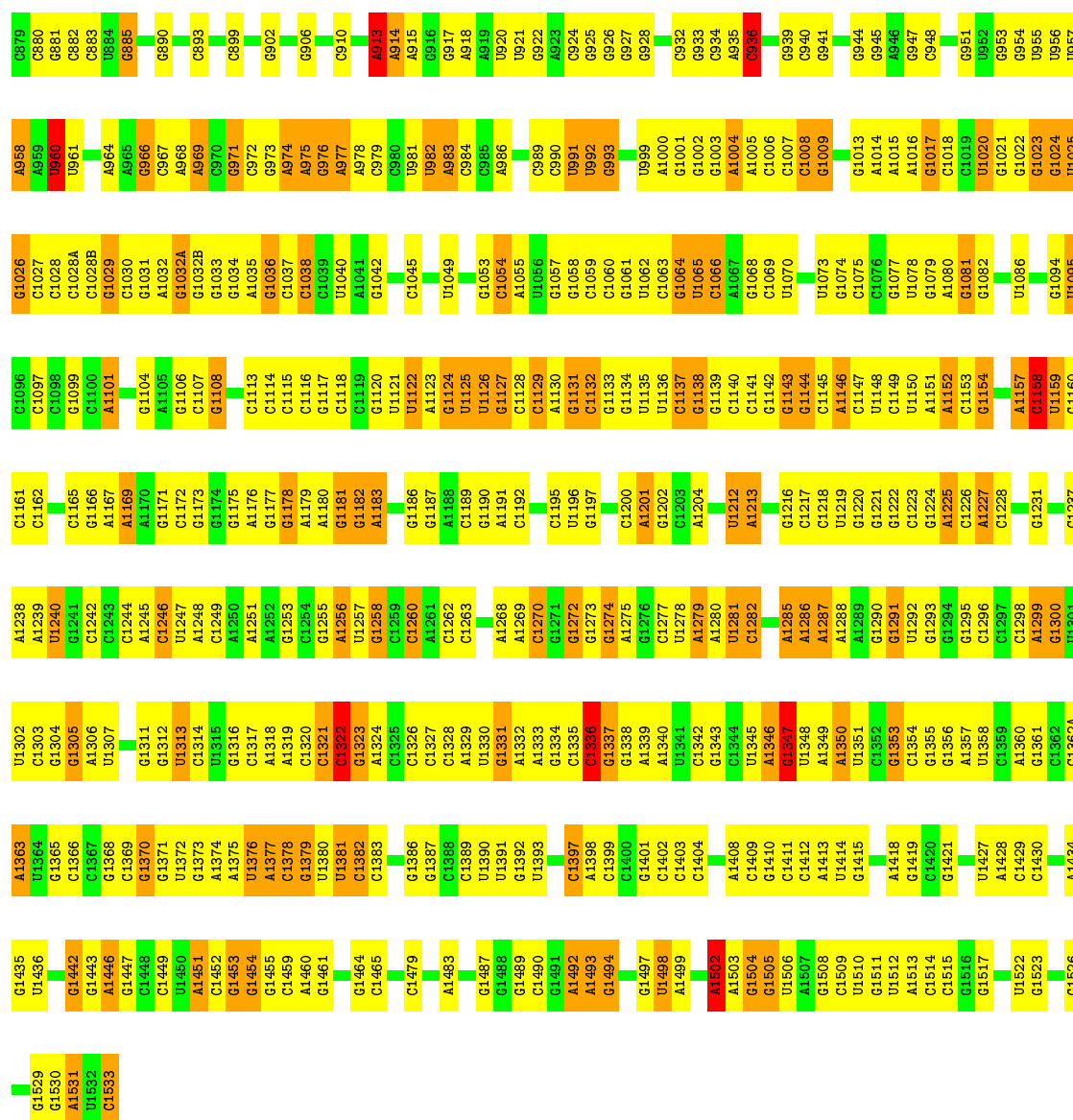
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	AG	1	Total Zn 1 1	0	0
56	AQ	1	Total Zn 1 1	0	0
56	CQ	1	Total Zn 1 1	0	0
56	CG	1	Total Zn 1 1	0	0

3 Residue-property plots

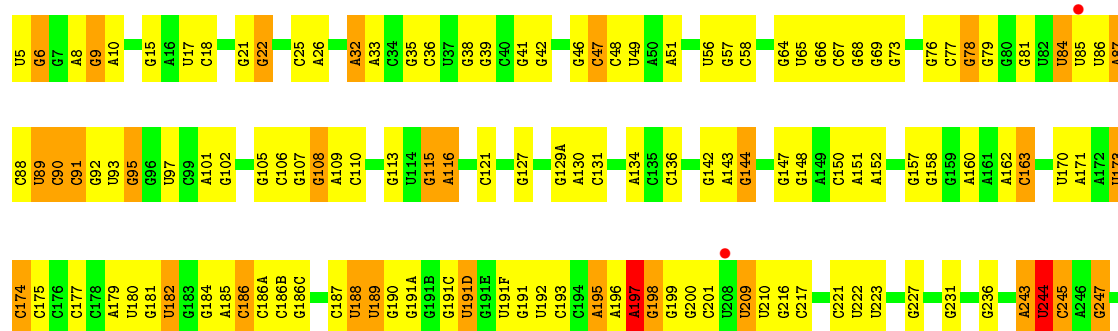
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

• Molecule 1: 16S ribosomal RNA

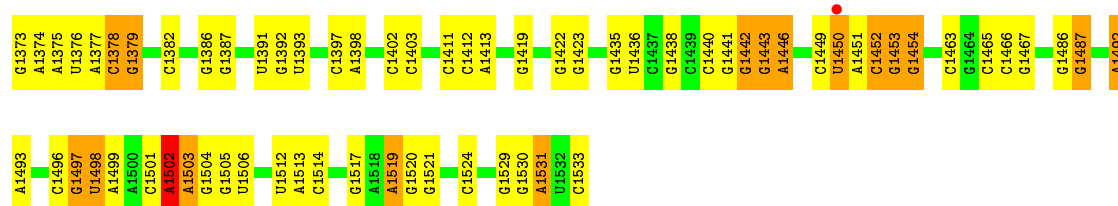




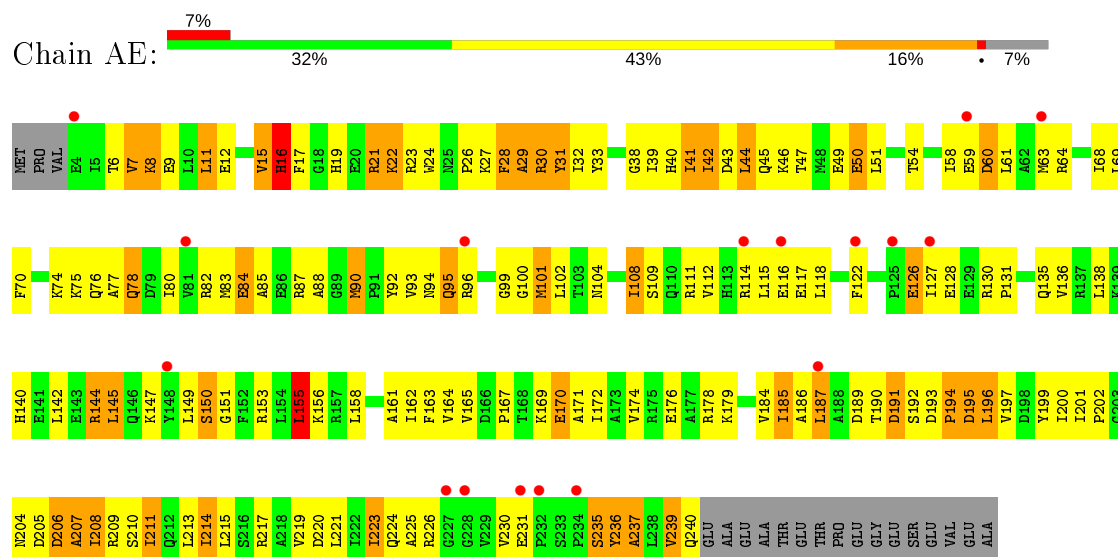
Chain CA: 41% 43% 15%



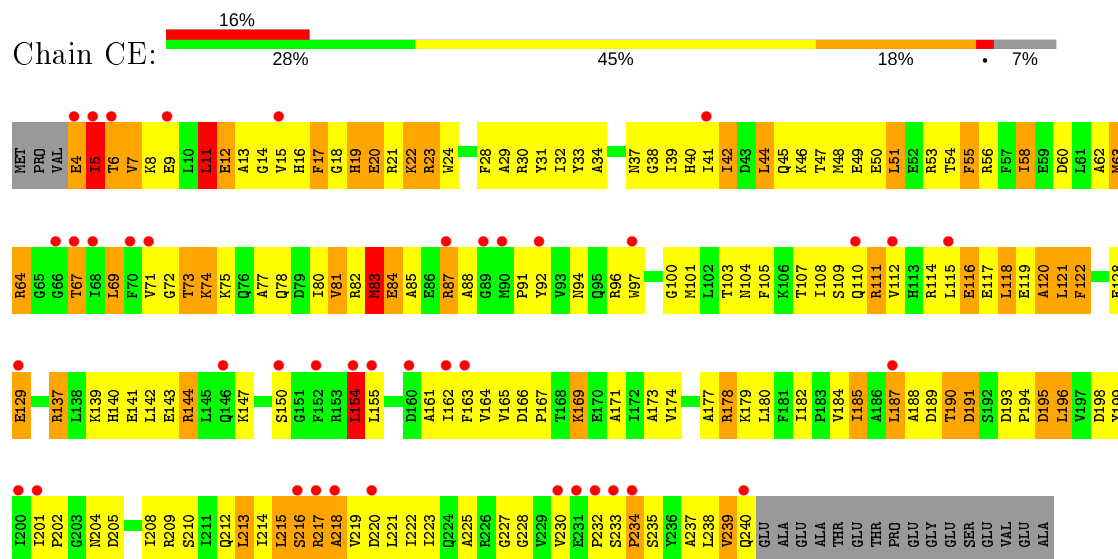




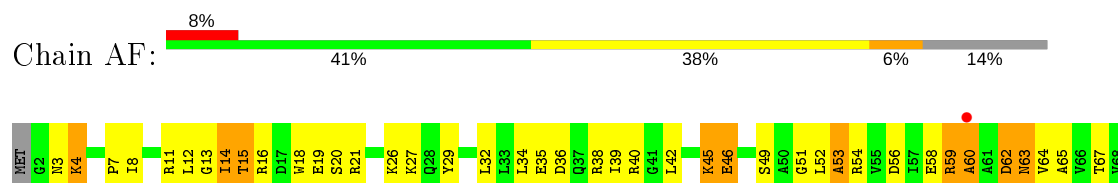
• Molecule 2: 30S RIBOSOMAL PROTEIN S2



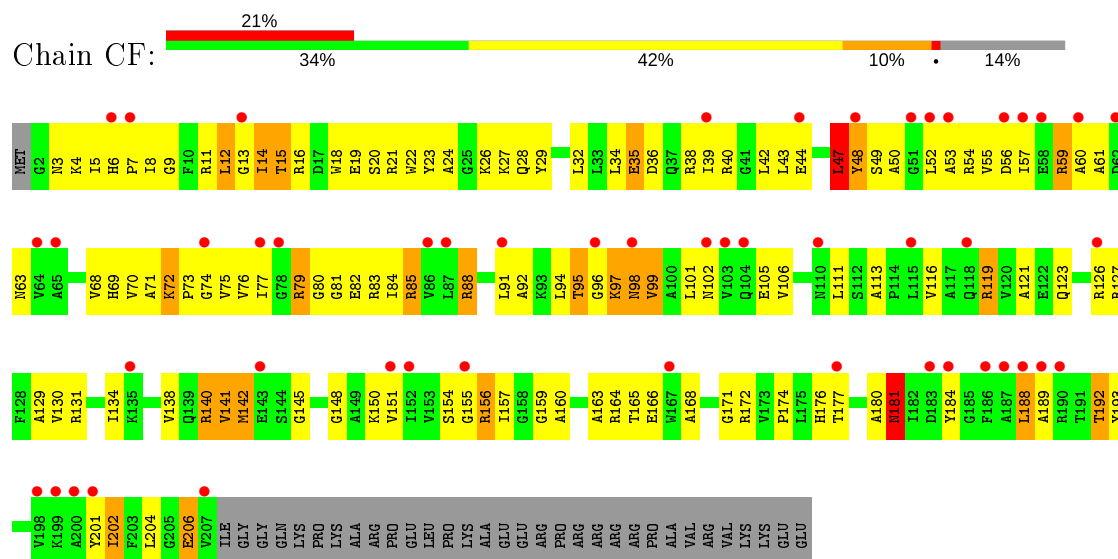
• Molecule 2: 30S RIBOSOMAL PROTEIN S2



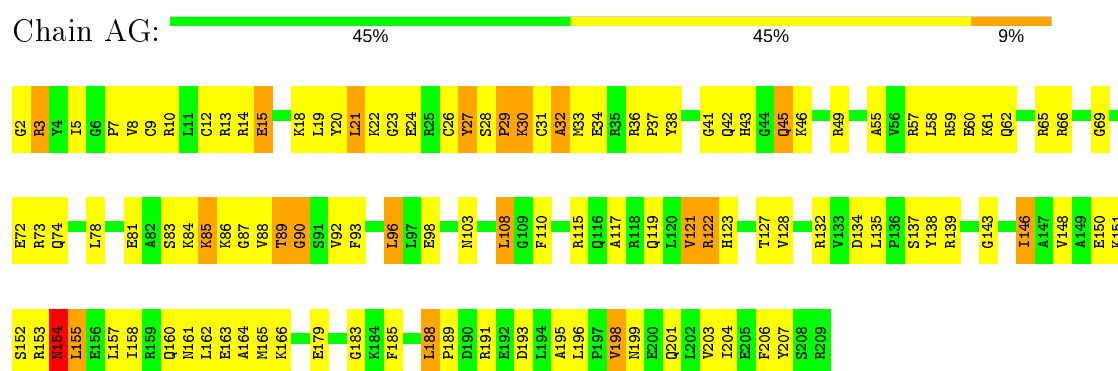
• Molecule 3: 30S RIBOSOMAL PROTEIN S3



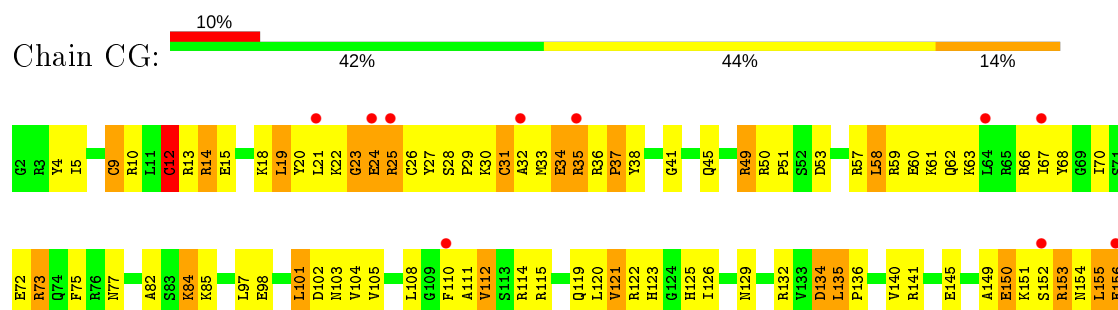
- Molecule 3: 30S RIBOSOMAL PROTEIN S3

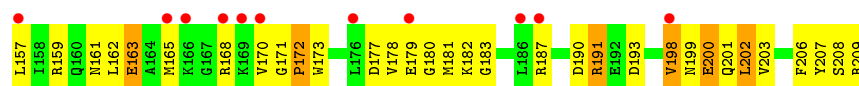


- Molecule 4: 30S RIBOSOMAL PROTEIN S4

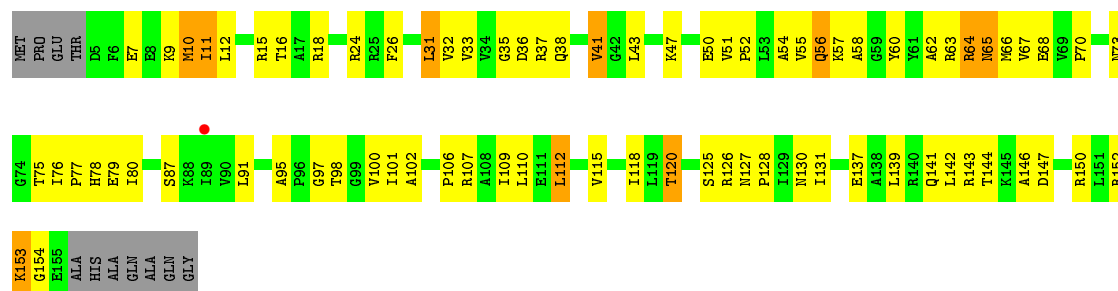


- Molecule 4: 30S RIBOSOMAL PROTEIN S4

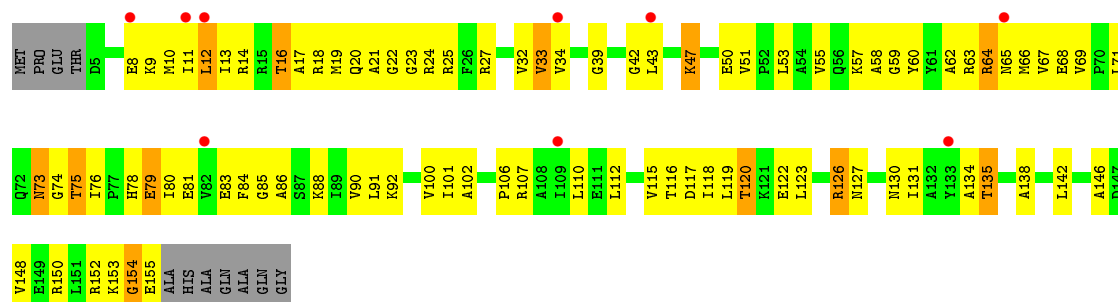
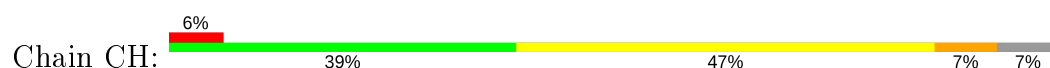




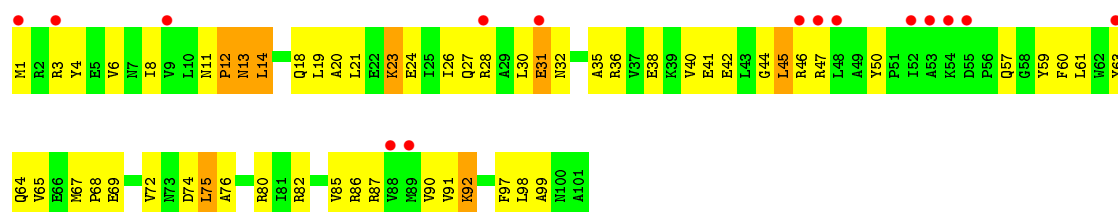
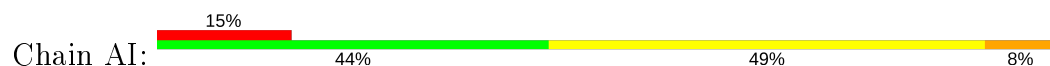
• Molecule 5: 30S RIBOSOMAL PROTEIN S5



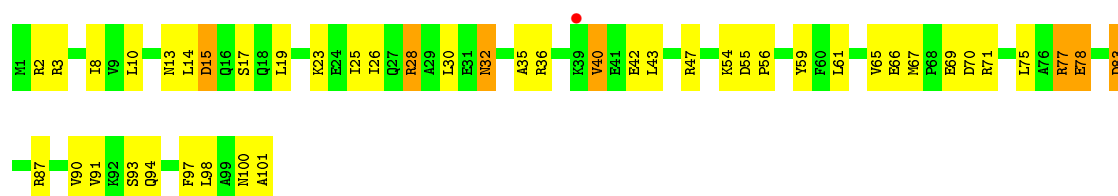
• Molecule 5: 30S RIBOSOMAL PROTEIN S5



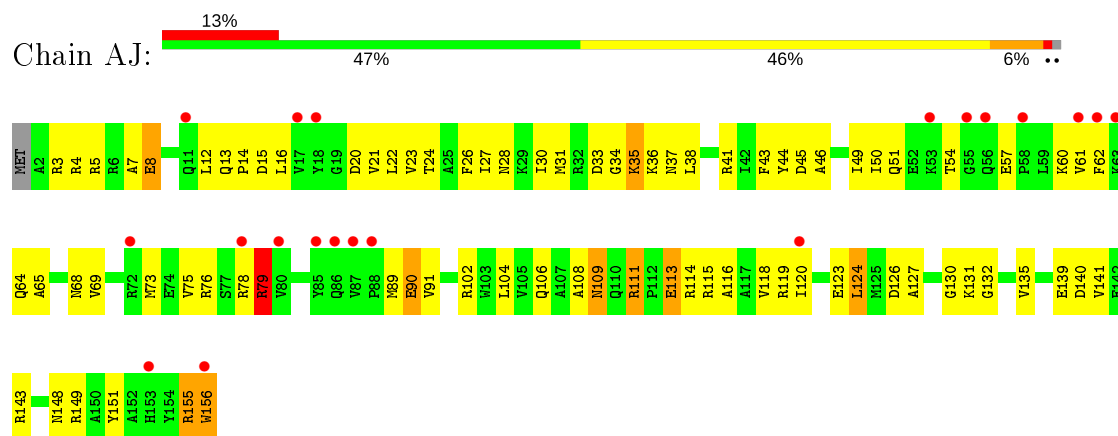
• Molecule 6: 30S RIBOSOMAL PROTEIN S6



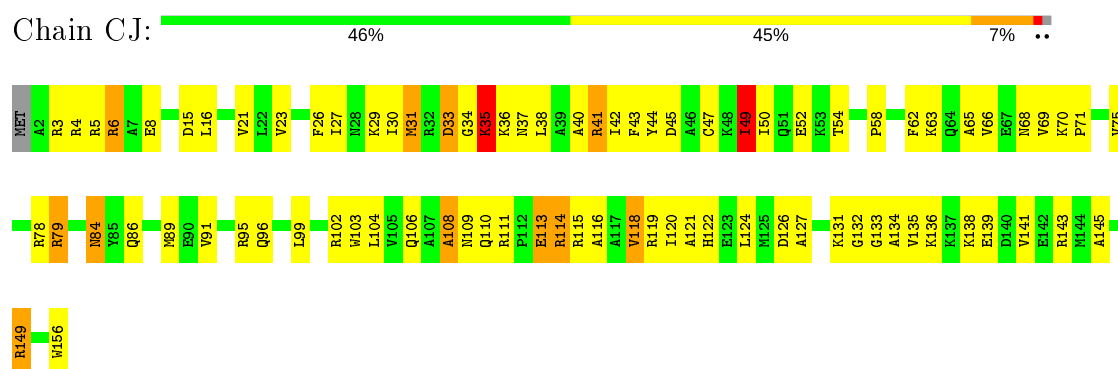
• Molecule 6: 30S RIBOSOMAL PROTEIN S6



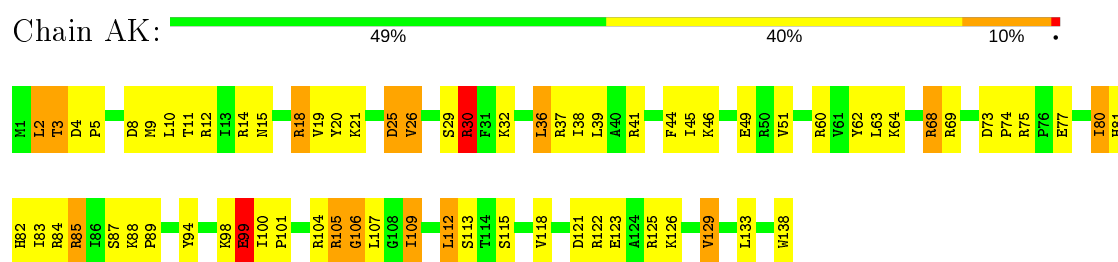
- Molecule 7: 30S RIBOSOMAL PROTEIN S7



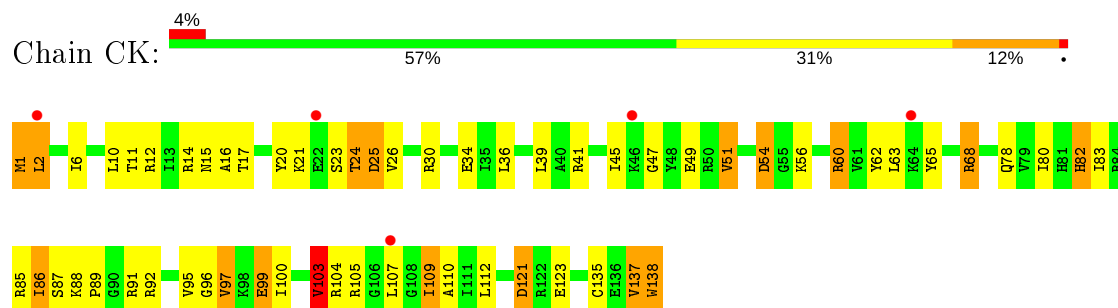
- Molecule 7: 30S RIBOSOMAL PROTEIN S7



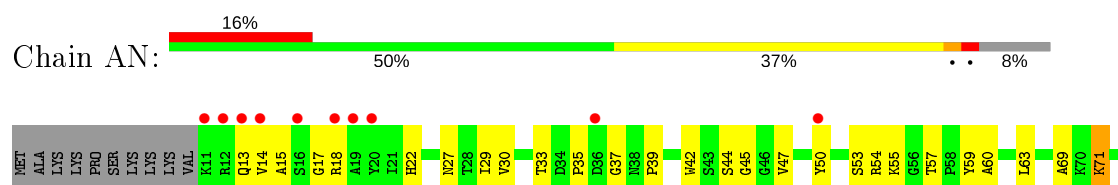
- Molecule 8: 30S RIBOSOMAL PROTEIN S8

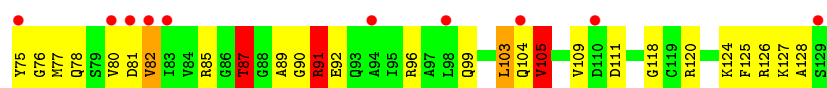


- Molecule 8: 30S RIBOSOMAL PROTEIN S8

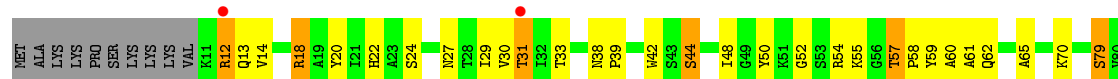


- Molecule 9: 30S RIBOSOMAL PROTEIN S9

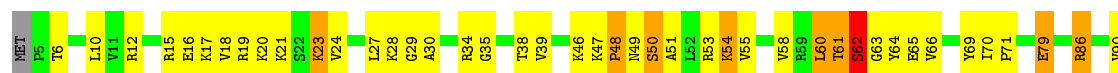




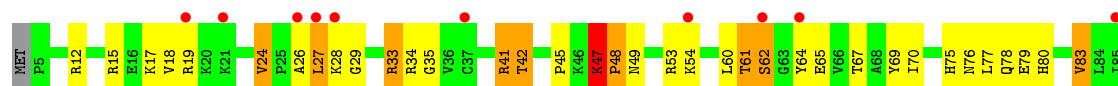
• Molecule 11: 30S RIBOSOMAL PROTEIN S11



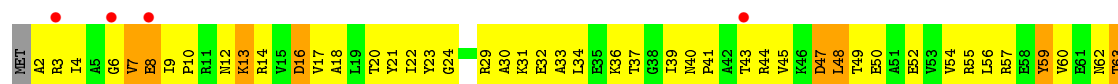
• Molecule 12: 30S RIBOSOMAL PROTEIN S12



• Molecule 12: 30S RIBOSOMAL PROTEIN S12

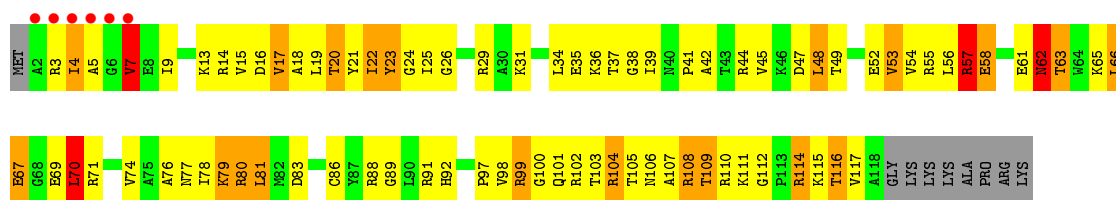


• Molecule 13: 30S RIBOSOMAL PROTEIN S13

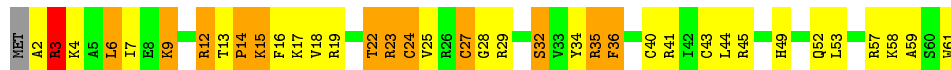
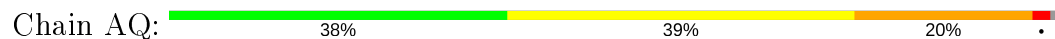


• Molecule 13: 30S RIBOSOMAL PROTEIN S13

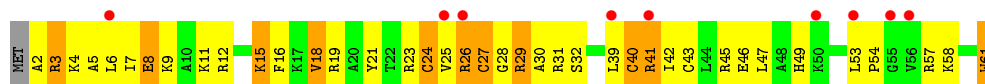




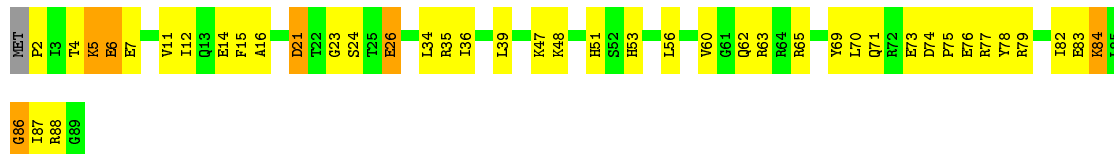
• Molecule 14: 30S RIBOSOMAL PROTEIN S14



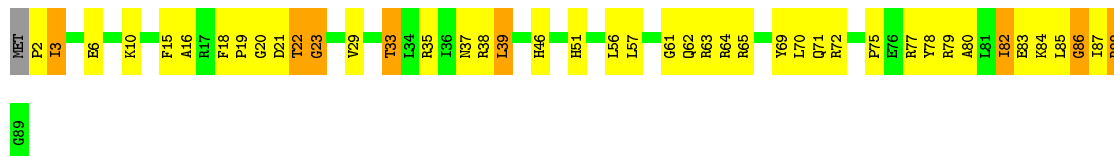
• Molecule 14: 30S RIBOSOMAL PROTEIN S14



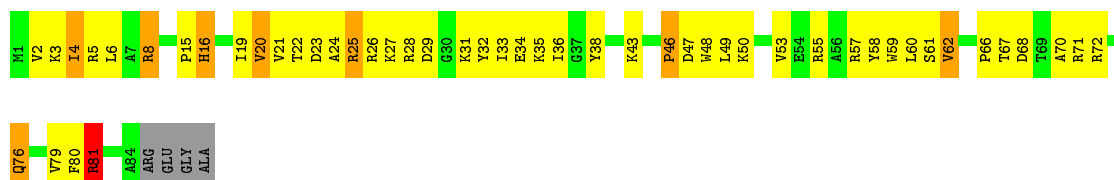
• Molecule 15: 30S RIBOSOMAL PROTEIN S15



• Molecule 15: 30S RIBOSOMAL PROTEIN S15

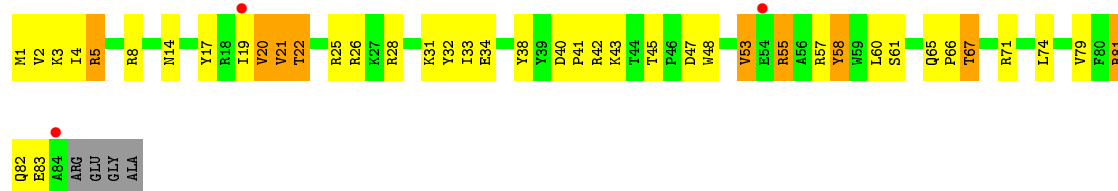


• Molecule 16: 30S RIBOSOMAL PROTEIN S16



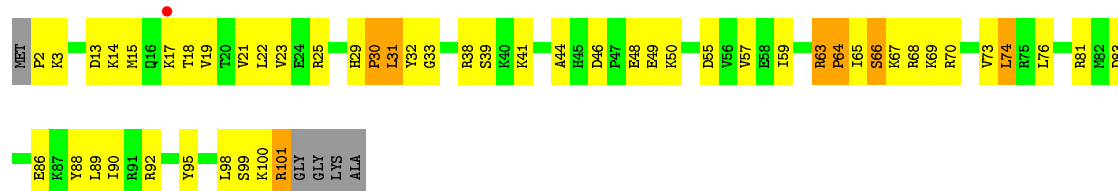
- Molecule 16: 30S RIBOSOMAL PROTEIN S16

Chain CS: 



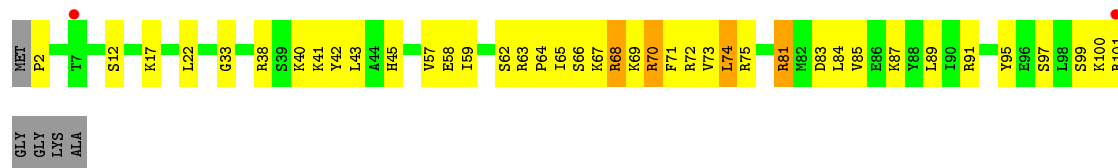
- Molecule 17: 30S RIBOSOMAL PROTEIN S17

Chain AT: 



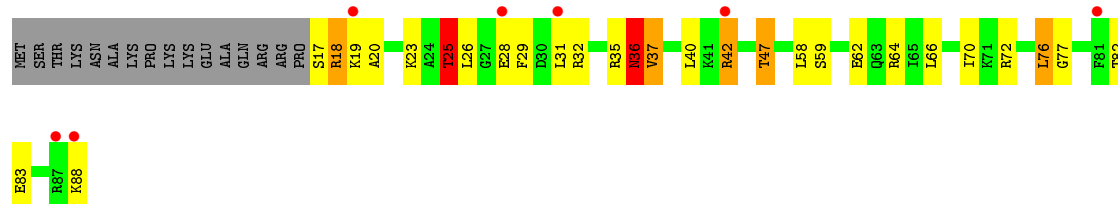
- Molecule 17: 30S RIBOSOMAL PROTEIN S17

Chain CT: 



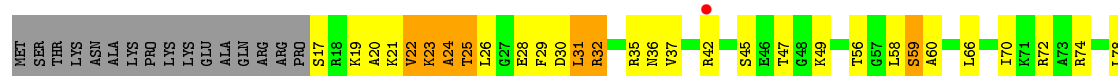
- Molecule 18: 30S RIBOSOMAL PROTEIN S18

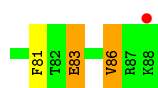
Chain AU: 



- Molecule 18: 30S RIBOSOMAL PROTEIN S18

Chain CU: 

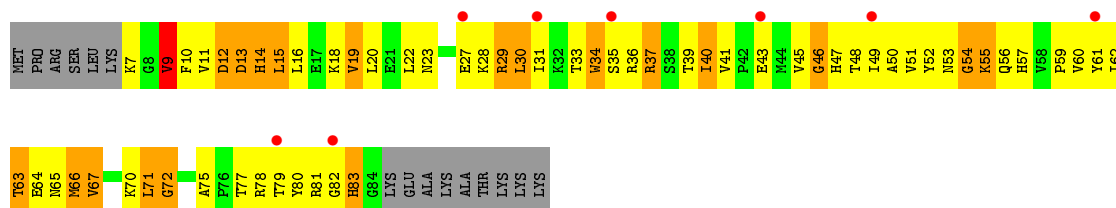
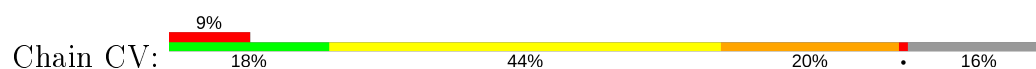




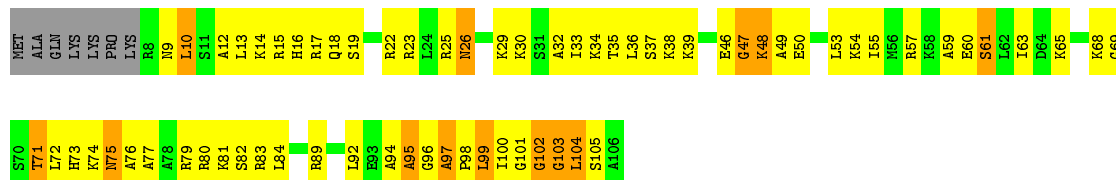
• Molecule 19: 30S RIBOSOMAL PROTEIN S19



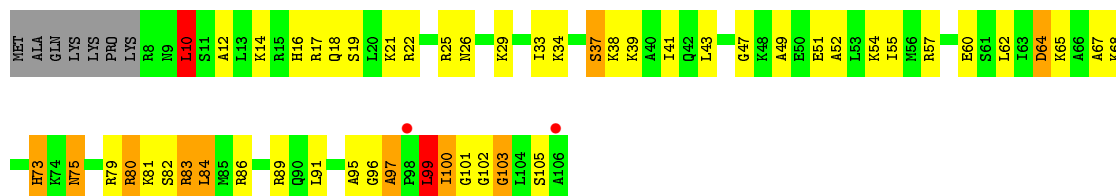
• Molecule 19: 30S RIBOSOMAL PROTEIN S19



• Molecule 20: 30S RIBOSOMAL PROTEIN S20

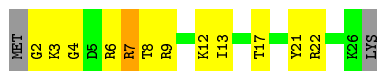


• Molecule 20: 30S RIBOSOMAL PROTEIN S20



• Molecule 21: 30S RIBOSOMAL PROTEIN THX





• Molecule 21: 30S RIBOSOMAL PROTEIN THX

Chain CX: 41% 44% 7% 7%



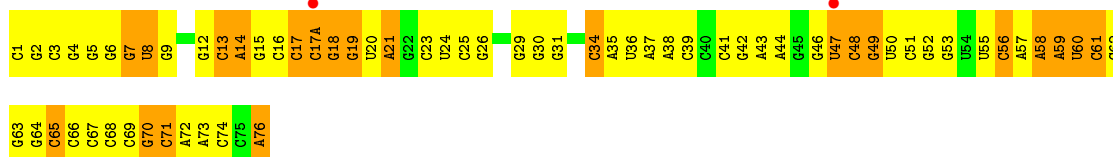
• Molecule 22: TRNA-FMET

Chain AC: 61% 32% 5% •



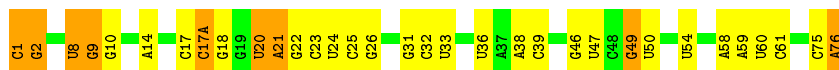
• Molecule 22: TRNA-FMET

Chain AD: 3% 14% 57% 29%



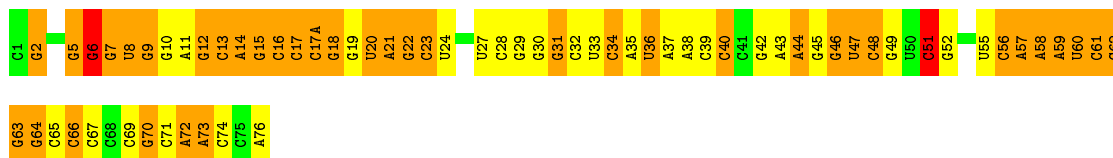
• Molecule 22: TRNA-FMET

Chain CC: 57% 31% 12%



• Molecule 22: TRNA-FMET

Chain CD: 14% 34% 49% •




• Molecule 23: MRNA

Chain A1: 83% 17%



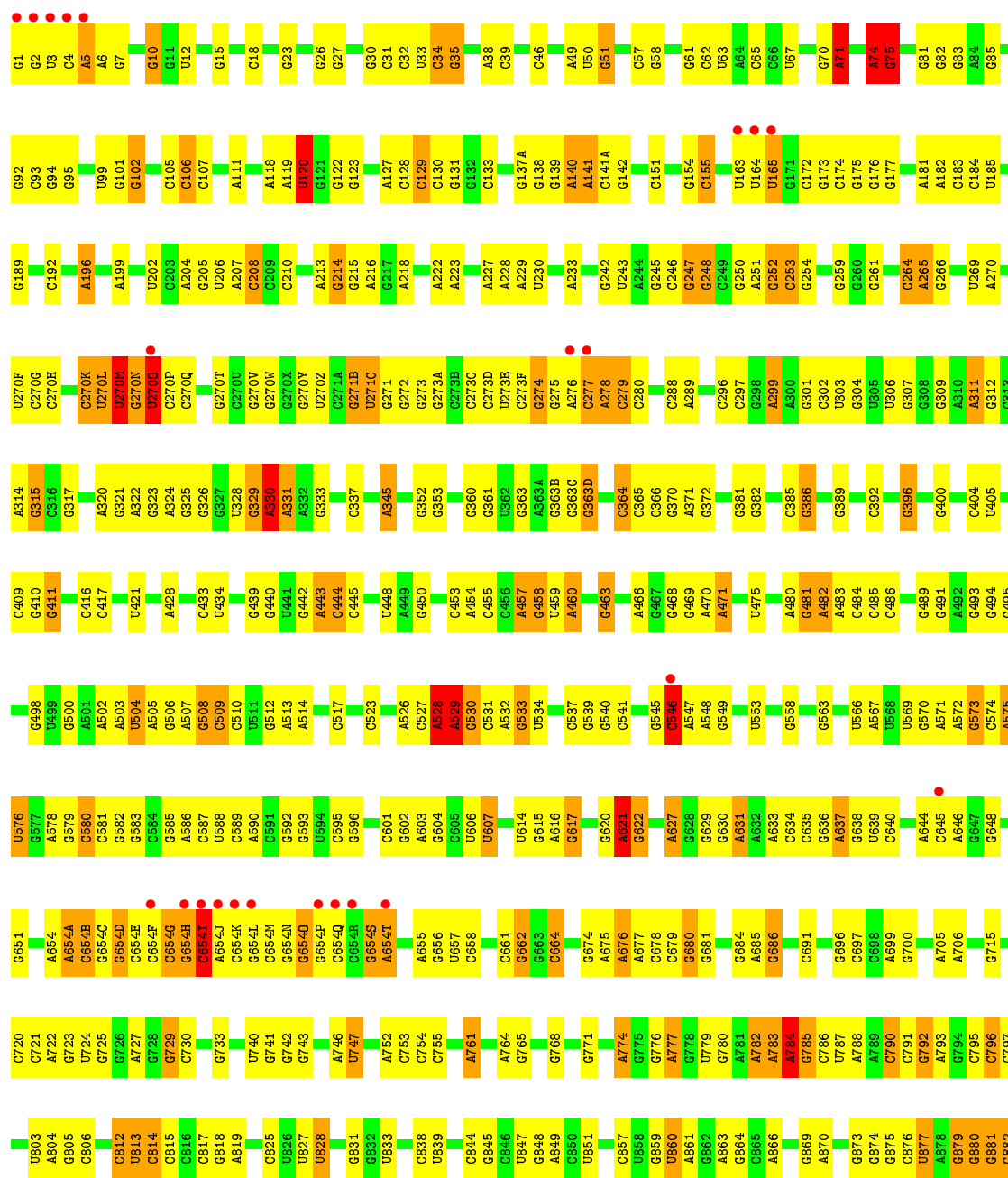
- Molecule 23: MRNA

Chain C1:  83% 17%

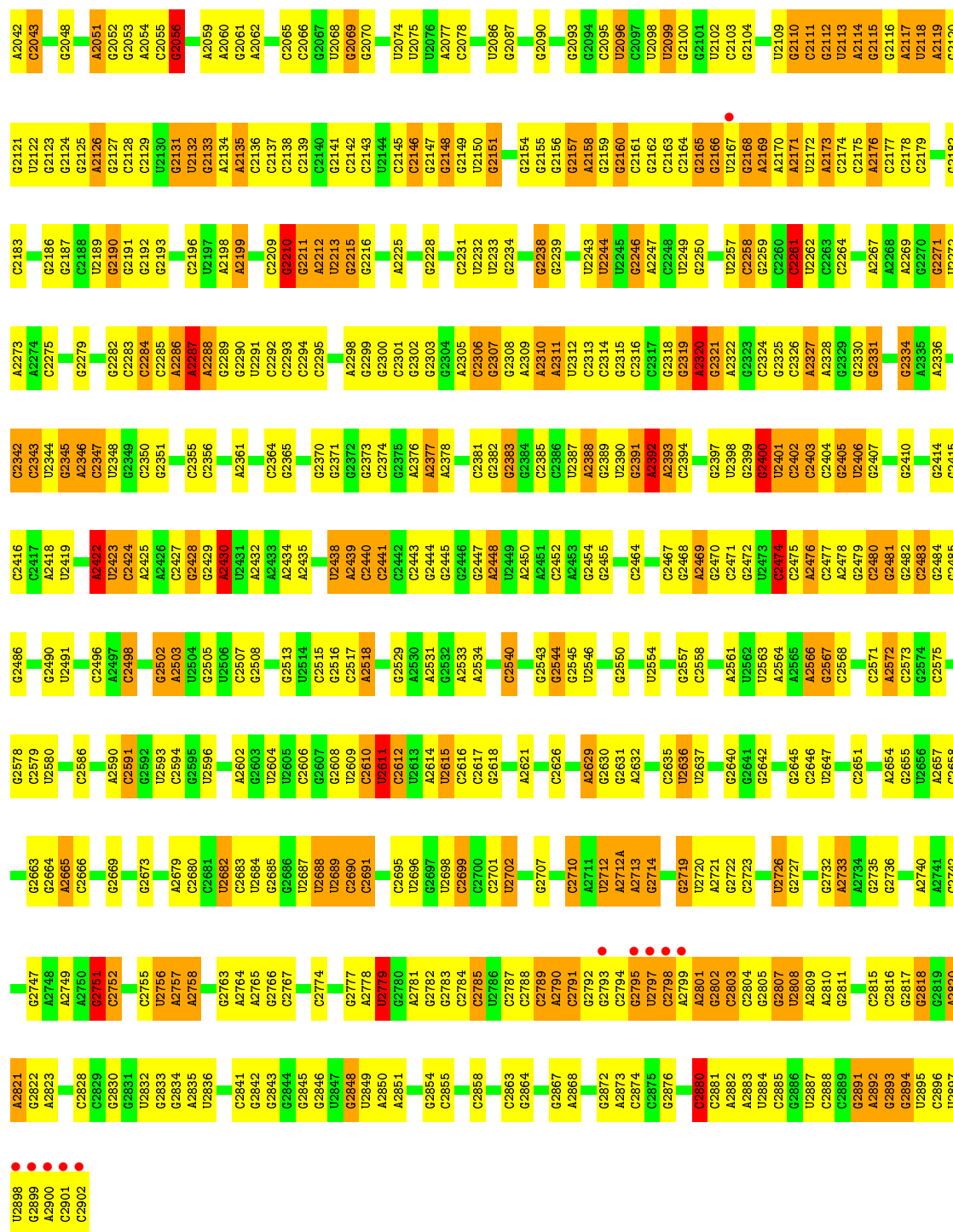


- Molecule 24: 23S ribosomal RNA

Chain BA:  % 45% 40% 13%

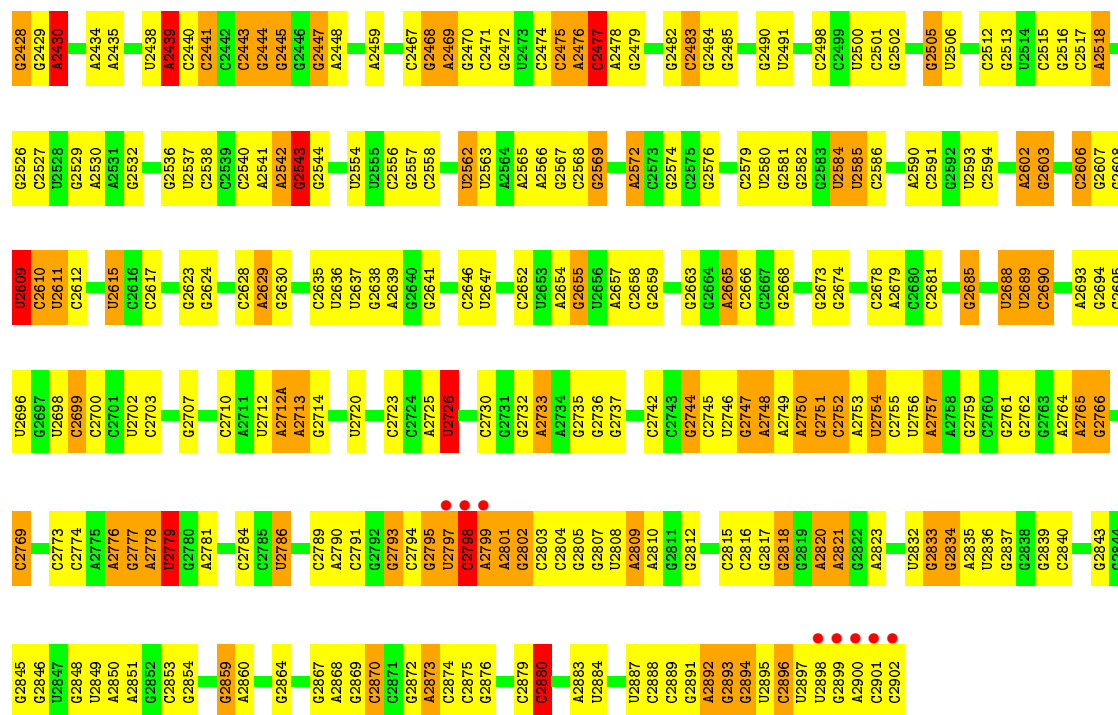




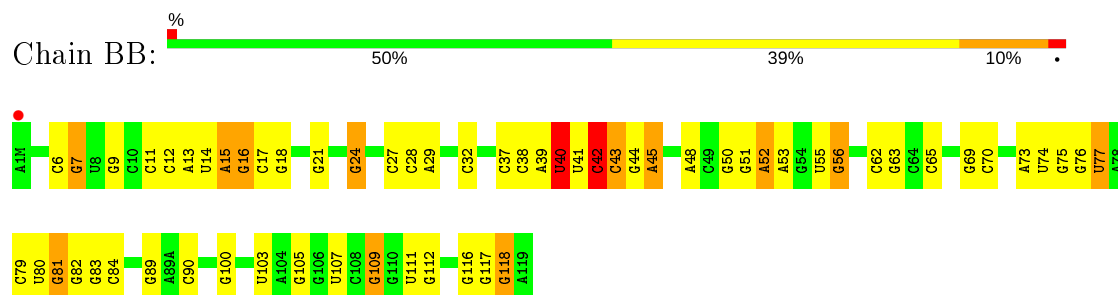


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A142A	G1016	U671	A789	C645	A482	G388	G308	A257	A182	A91
A1443	G1017	A872	C790	A646	A483	G389	G309	G258	C183	G92
C1445	U1018	G673	C791	G647	G390	A310	A310	G259	C184	C93
	U1019	U677	G792	G648	G489	G391	A311		U185	G94
U1082	A1020	A878	A793	G650	G491	C392		A265	U186	G95
U1083	A1021	G879	C796	G651	G492		G315	G266		G96
A1084	U1022	A879	C797	G652	G493	G396	C316		U193	
A1085	G1023	G880	C797	G653	G494	G397	G317	A270B	G194	G102
A1086	G1024	G881	G800	A654	G495	G398	C318	C270C	A103	A103
A1087	G1025	G882	A800	A655	G496	G399	C319	C270D	A196	
A1088	U1026	G883	G801	A656	A502		A320	G270E	U108	U108
A1089	A1027	G884	A802	A657	A503	U403	A321	U270F	G109	
G1089	A1028	G885	U803	G654C	U504	C404	A322	C270G		
U1090	A1029	C986	A804	G654E	U505	U405	A323	C270H	U112	U112
G1091	G1030	A887	G805	G654F	G506	G406	A324	C270I		
C1092	U958	C987	C806	G654G	A507	G407	G325	G270J	G116	G116
C1093	A959	G888	U811	G654H	G508	G408	G326	G270K	U206	U206
U1094	A960	A890	G812	G654I	G509	C409	G327	U270L	A207	A118
A1095	C981	G892	C813	G654J	C510	G410	U328	U270M	C208	A119
A1096	G982	C893	U813	G654K	U511	G411	G329	G270N	U120	U120
U1097	U963	C894	C814	G654L	G512	C414	A331	U270O	G121	G121
A1098	C964	U895	C730	G654M				C270P		
G1099	C965	A896	A734	G654N	A515	A515	A332	G270Q	A126	A126
		C897	A735	G654O	C516	C516	A333	G270R	G214	G214
C1102	G974	C898	A821	G654P	C517	U421		G270S	G128	G128
A1103	C974A	A899	C736	G654Q	C523	A428	C336		C129	C129
C1104	G975	A900	G739	G654R	C527	A429	A340	G270V	G130	G130
U1105	C976	U828	U747	G654S	C527	G430		G270W	A218	A218
G1106	G977	C902	G748	G654T	A528	G430		G270X	G219	G219
		C903	C749		A529		G343	G270Y		C134
C1107	A880	C904	C749		A530	C435	G344		A221	A221
		U905	U833	A655	G531	C436		G271B	G138	G138
G1110	A983	C906	C834	G656	C531	A443	G351	U271C	G139	G139
A1111	A984	U907	A835	U657	C532	C444	G352	G271	A140	A140
C1112	C985	C908	C754	G658	G533		G353	G272	A141	A141
U1113		A909	C755	G659		U443	G354		G141A	G141A
C1052	A910		C756	G660	A536		G355	C273D	G142	G142
C1053	G989	A911	U757	G661	C537	C453		U273E	C143	C143
A1054	A990	C912	U758	G662	G539	U454	U358	G273F	G144	G144
G1055		U913			G540	A455		G274	G145	G145
U1056	G993	C914	U767	G666	C541	C456		A276		A149
A1057	C994	C915	G768	G669	C546	A457	G363	C277		
U1058	C995	G916	G769	A670	A547	G458	A363A	A278	G152	G152
C996	A996	A917	G770		A548	U459	G363B	C279	C153	C153
C997	G997	A918	G771	C673	G549	A460	G363D		G154	G154
C998	C998	G919	A774	G674	U553	G463	U363E	C286	C	C
G1125	A1000	G920	G775	A675	U554	U464	A363F	C287	U	U
A1126	A1001	G921	G776	A676	U555	G465		C288	U	U
		U922		A677	G556	G466	G372	A289	U	U
A1129	U1065	C923	U779	C678	U557	G466		C296		
U1130	U1066		G780	A685	G558	G469	C375	G247	G171	G171
G1131	C1005	A926	A861	G686	G561	A470	G379	C297	C172	C172
	U1006	G928	G862	A687	G562				G173	G173
C1135	A1069	G929	A781	G688	U562	G476		A300	C174	C174
G1136	A1070		A782	G687	G563		U383	G301	G175	G175
A1137	G1071		A783	U688	G564		U384	C302	G252	G252
G1138	C1072		A784	U689	C564		G385		G254	G254
C1139	A1073	G932	A786	G690	C565	A479				
G1140	G1074	G933	C786	C691	U566	A480	G386			
	U1014	C935	U787							

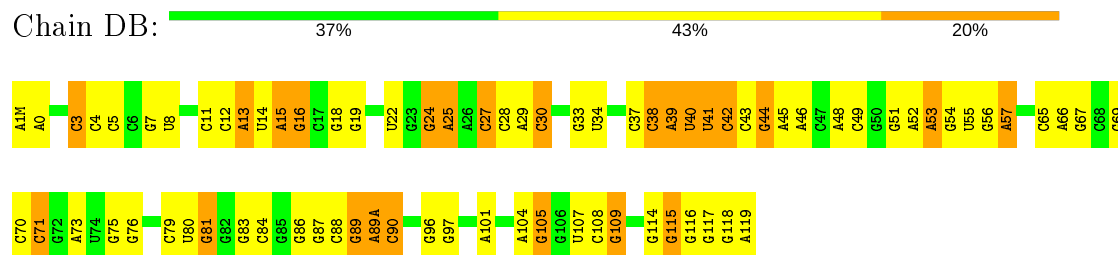




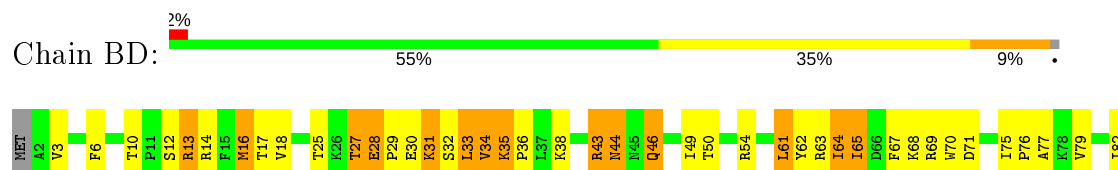
- Molecule 25: 5S RIBOSOMAL RNA

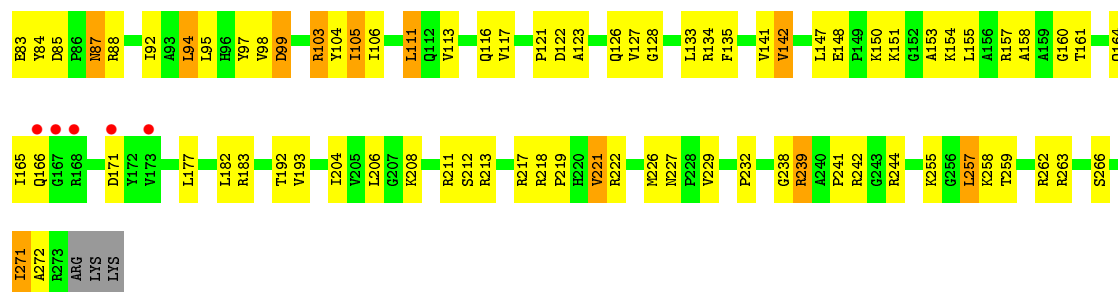


- Molecule 25: 5S RIBOSOMAL RNA

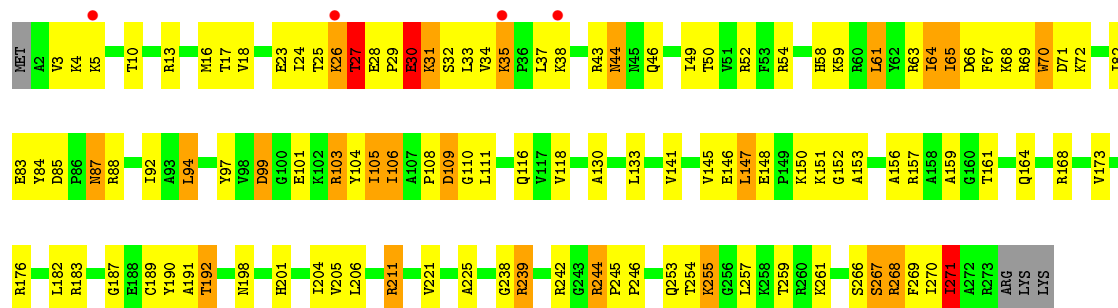


- Molecule 26: 50S ribosomal protein L2

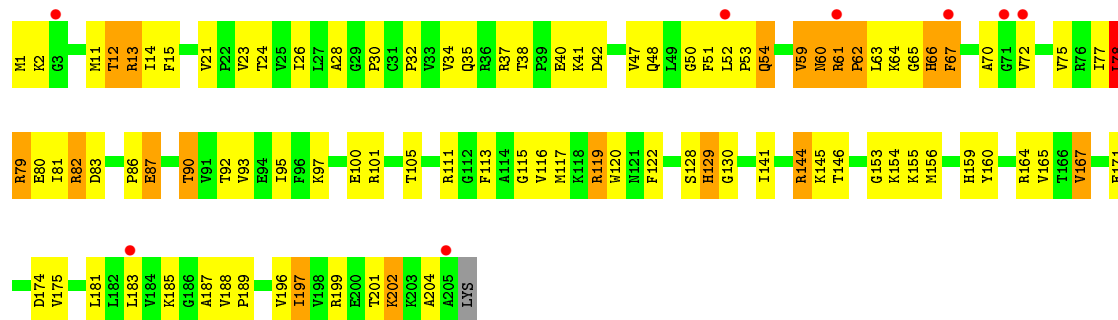




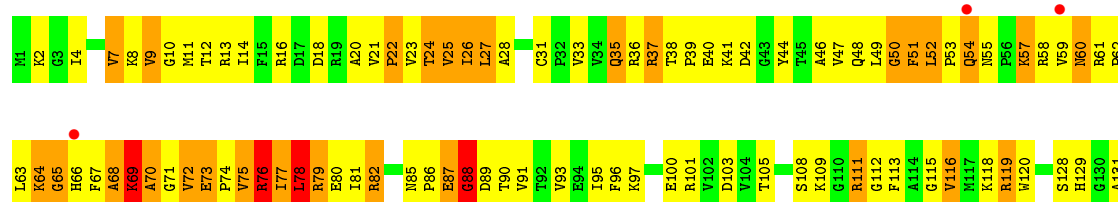
• Molecule 26: 50S ribosomal protein L2



• Molecule 27: 50S ribosomal protein L3

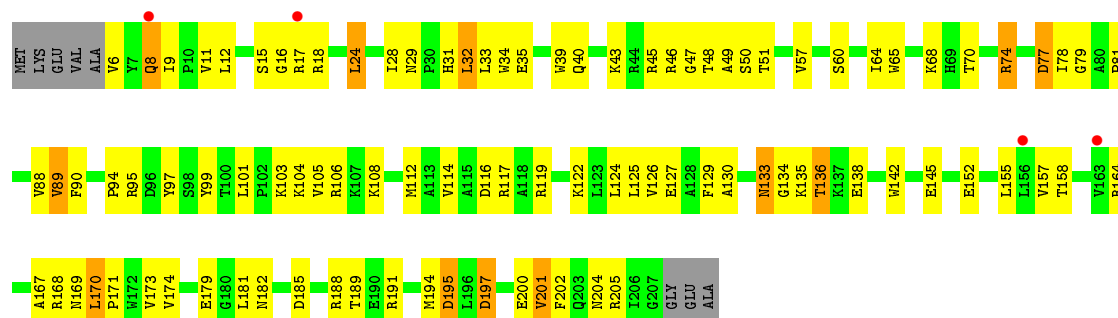


• Molecule 27: 50S ribosomal protein L3

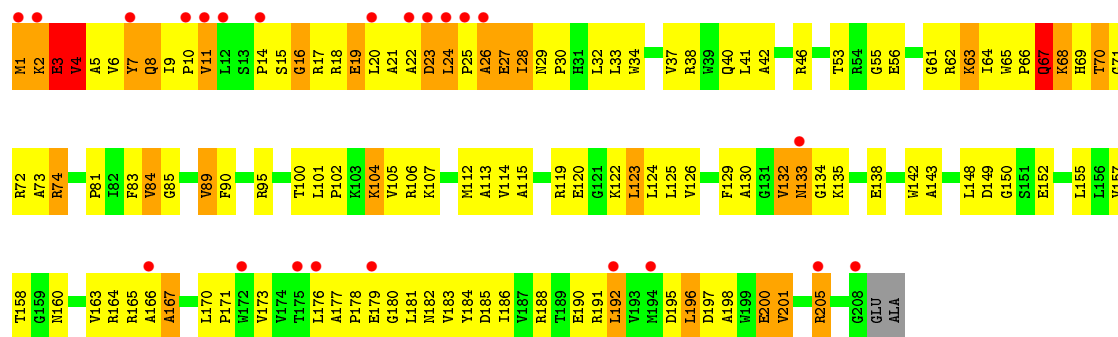




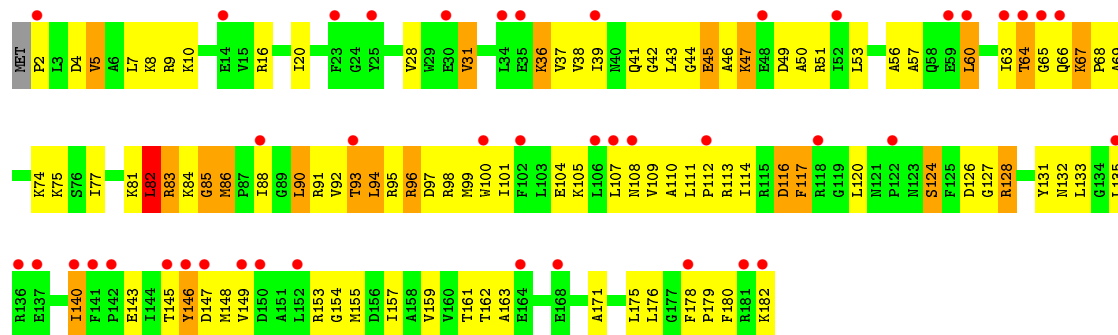
• Molecule 28: 50S ribosomal protein L4



• Molecule 28: 50S ribosomal protein L4

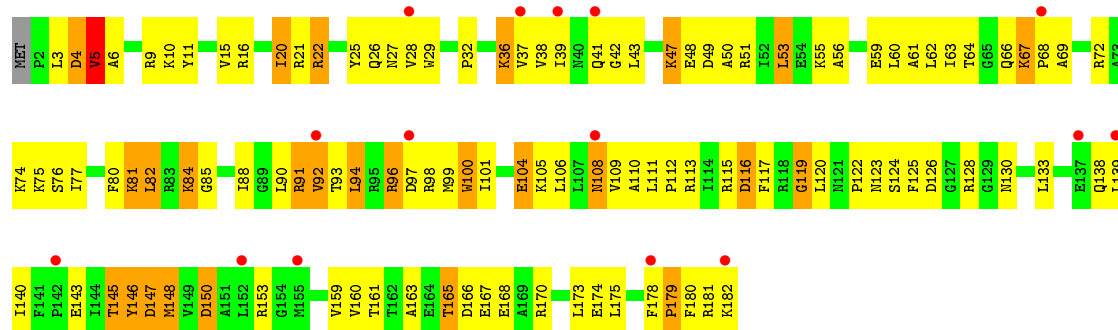


• Molecule 29: 50S ribosomal protein L5

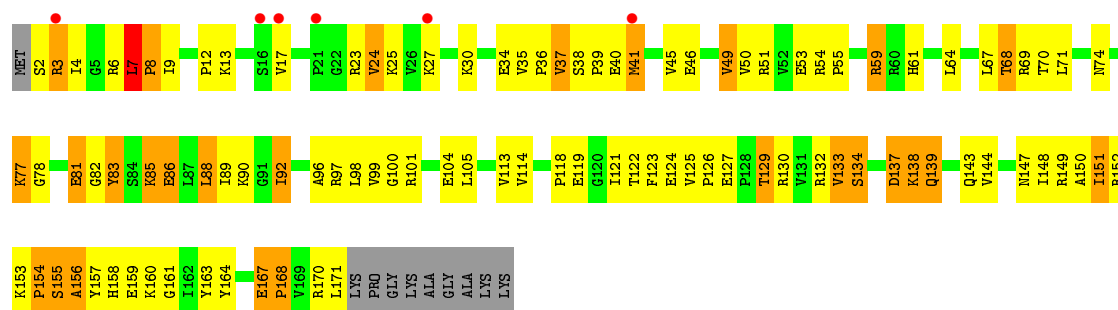


• Molecule 29: 50S ribosomal protein L5

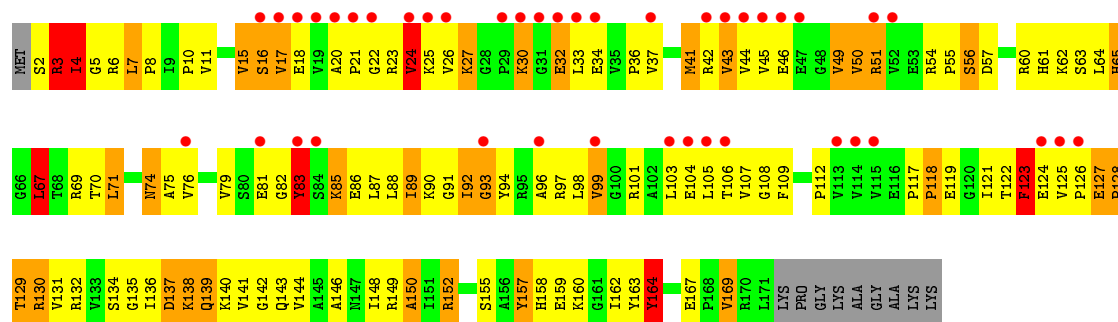




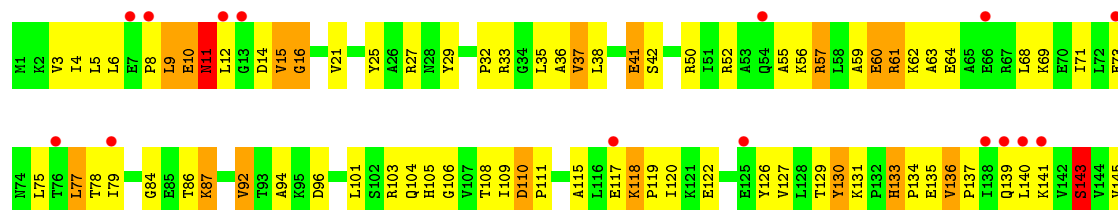
• Molecule 30: 50S ribosomal protein L6



• Molecule 30: 50S ribosomal protein L6



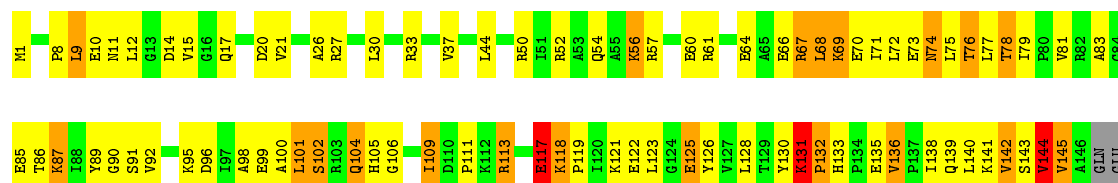
• Molecule 31: 50S ribosomal protein L9





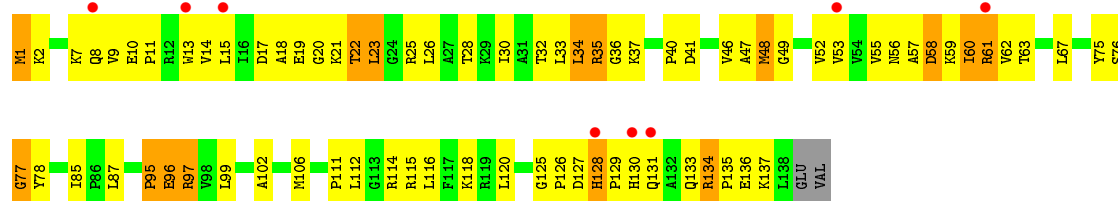
- Molecule 31: 50S ribosomal protein L9

Chain DK: 42% 41% 14% ..



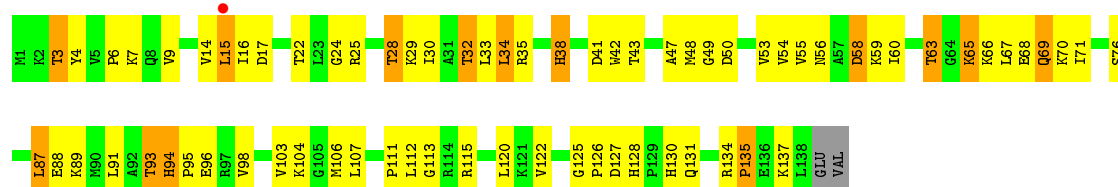
- Molecule 32: 50S ribosomal protein L13

Chain BM: 6% 44% 44% 11% .



- Molecule 32: 50S ribosomal protein L13

Chain DM: 48% 41% 10% .



- Molecule 33: 50S ribosomal protein L14

Chain BN: 71% 24% . .



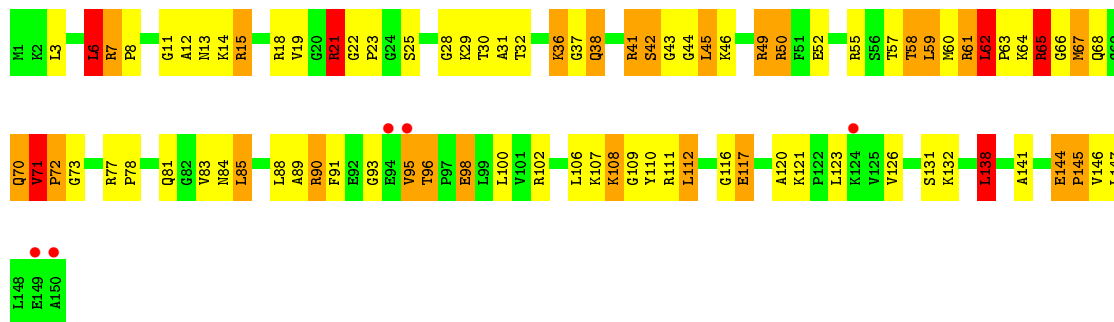
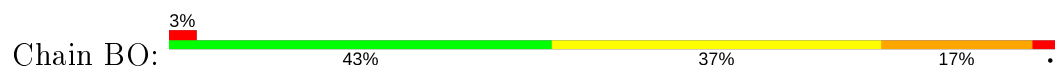
- Molecule 33: 50S ribosomal protein L14

Chain DN: 52% 38% 11%

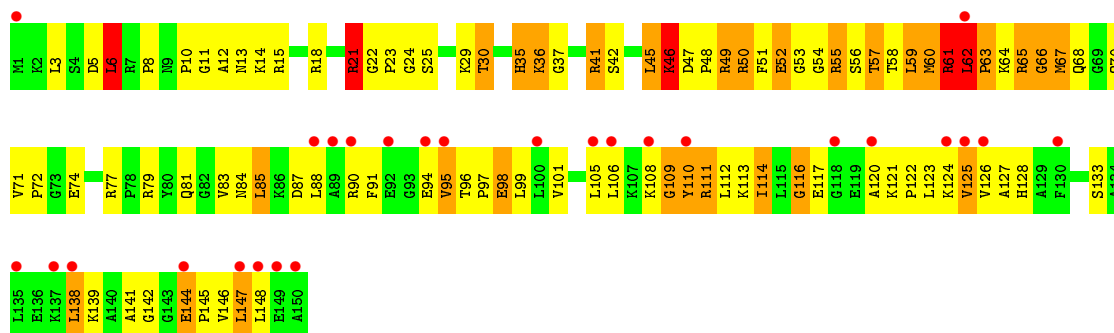




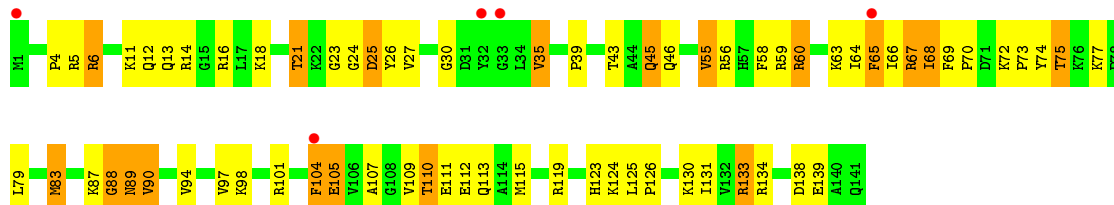
- Molecule 34: 50S ribosomal protein L15



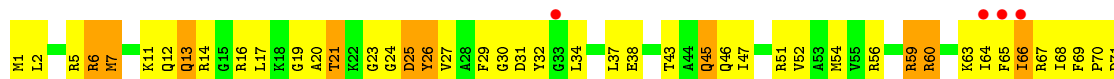
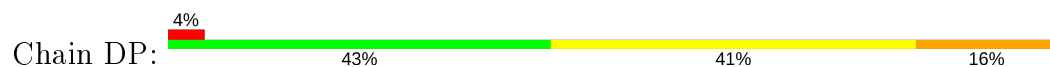
- Molecule 34: 50S ribosomal protein L15



- Molecule 35: 50S ribosomal protein L16



- Molecule 35: 50S ribosomal protein L16

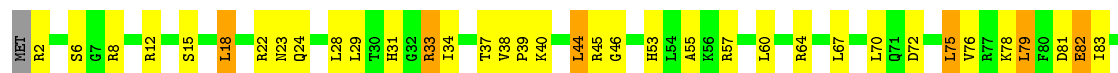




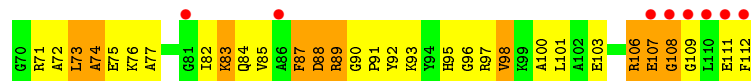
- Molecule 36: 50S ribosomal protein L17



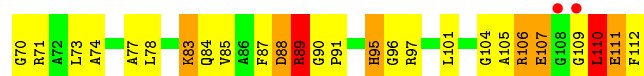
- Molecule 36: 50S ribosomal protein L17



- Molecule 37: 50S ribosomal protein L18

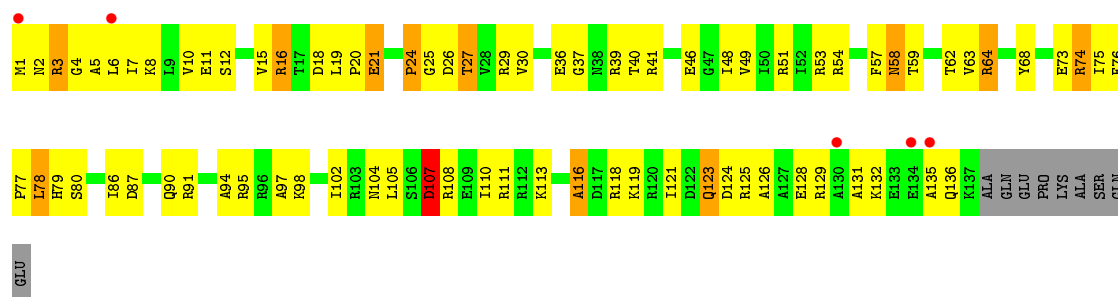


- Molecule 37: 50S ribosomal protein L18

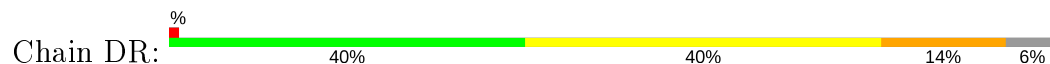


- Molecule 38: 50S ribosomal protein L19

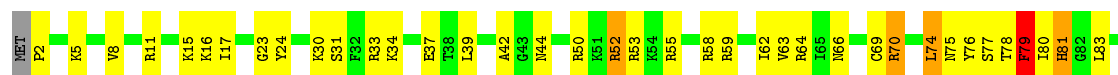




- Molecule 38: 50S ribosomal protein L19



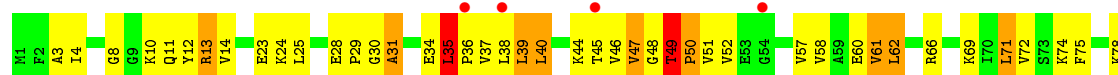
- Molecule 39: 50S ribosomal protein L20



- Molecule 39: 50S ribosomal protein L20

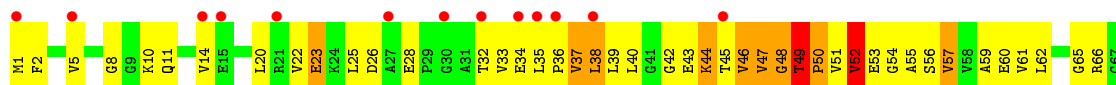


- Molecule 40: 50S ribosomal protein L21





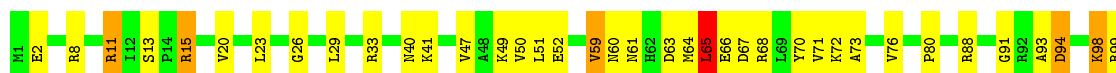
- Molecule 40: 50S ribosomal protein L21



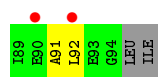
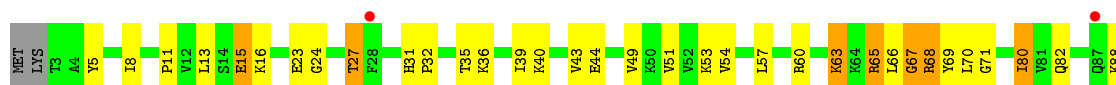
- Molecule 41: 50S ribosomal protein L22



- Molecule 41: 50S ribosomal protein L22

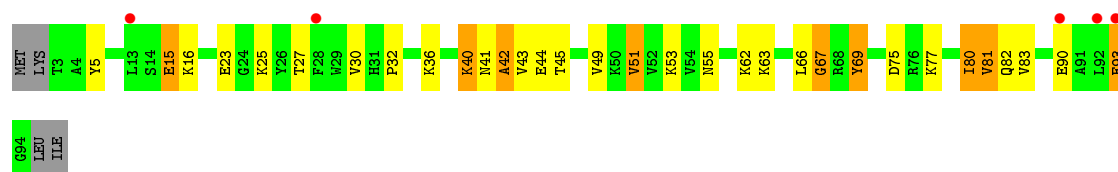


- Molecule 42: 50S ribosomal protein L23

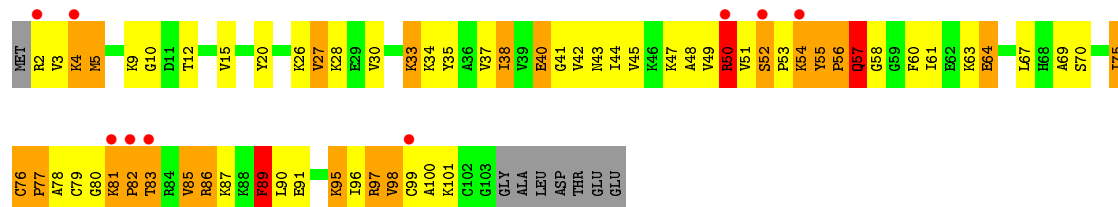


- Molecule 42: 50S ribosomal protein L23

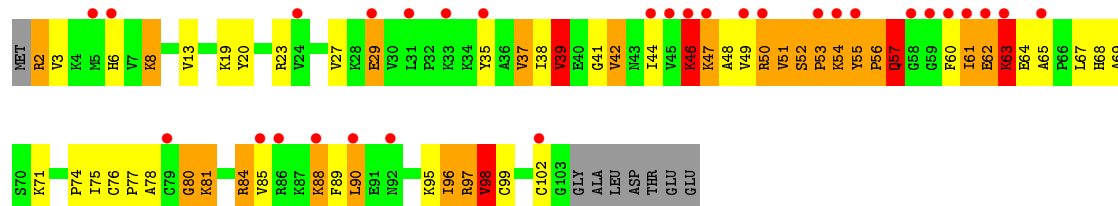
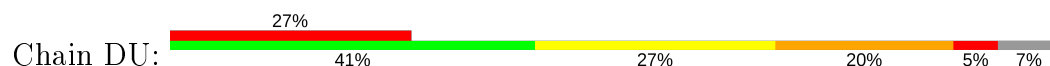




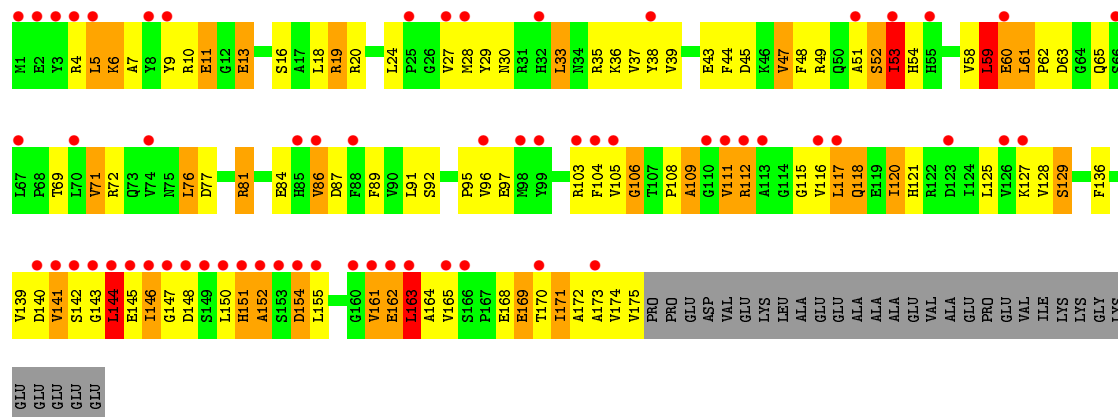
- Molecule 43: 50S ribosomal protein L24



- Molecule 43: 50S ribosomal protein L24

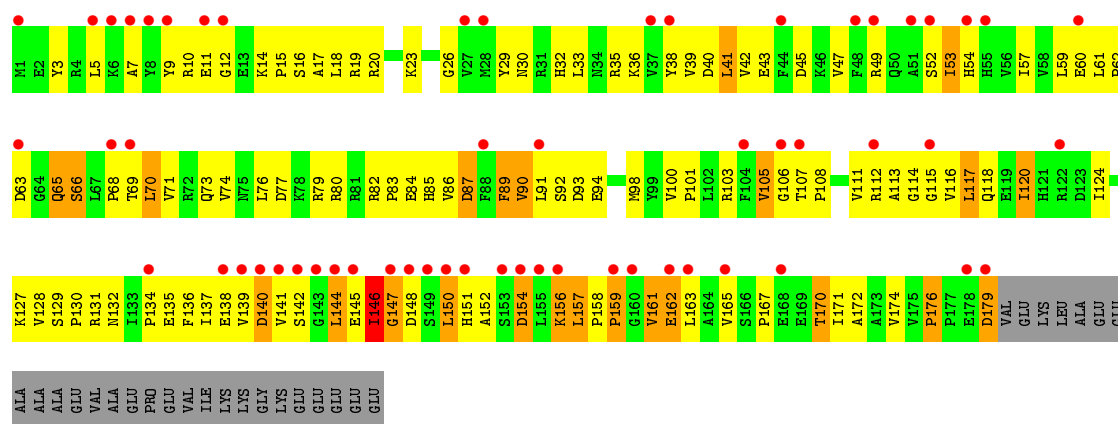


- Molecule 44: 50S ribosomal protein L25

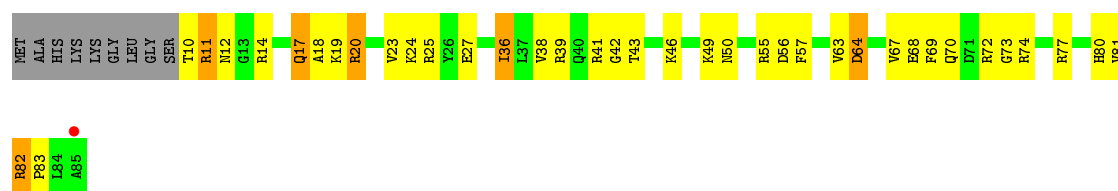


- Molecule 44: 50S ribosomal protein L25

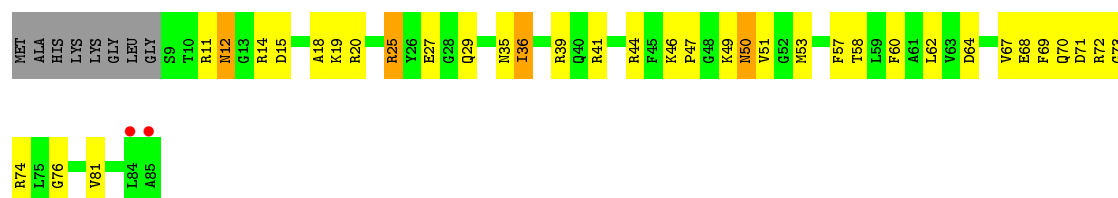




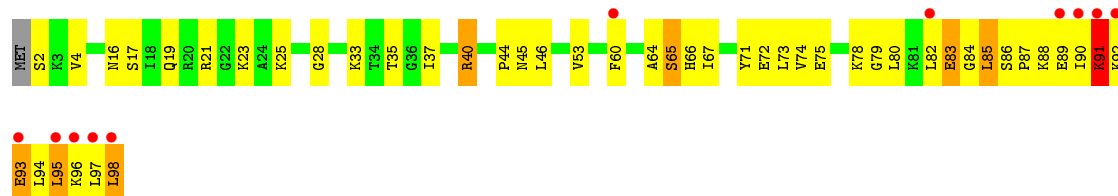
• Molecule 45: 50S ribosomal protein L27



• Molecule 45: 50S ribosomal protein L27

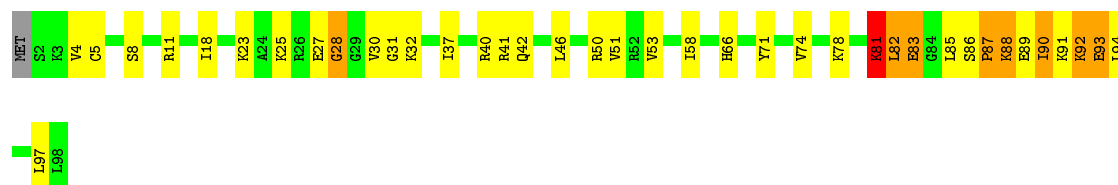


• Molecule 46: 50S ribosomal protein L28



• Molecule 46: 50S ribosomal protein L28

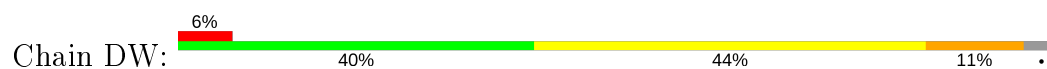




- Molecule 47: 50S ribosomal protein L29



- Molecule 47: 50S ribosomal protein L29



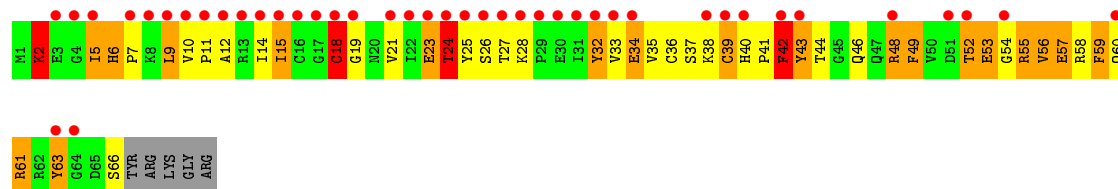
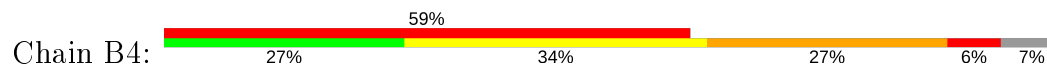
- Molecule 48: 50S ribosomal protein L30



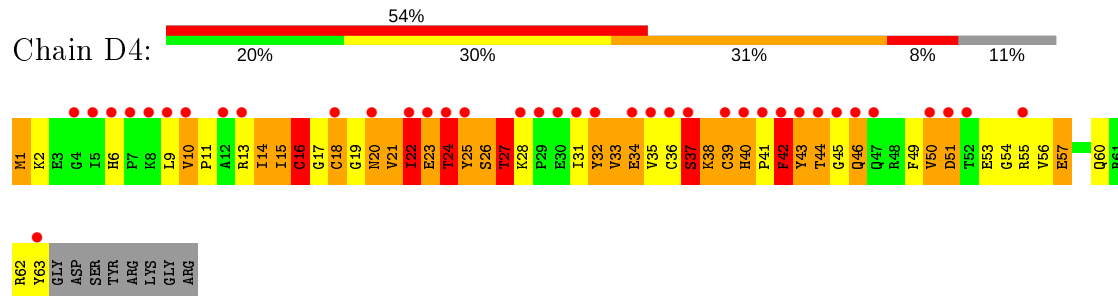
- Molecule 48: 50S ribosomal protein L30



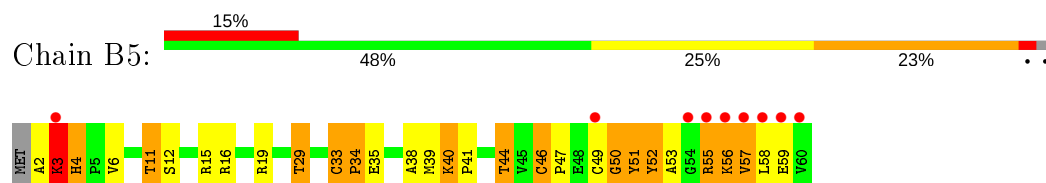
- Molecule 49: 50S ribosomal protein L31



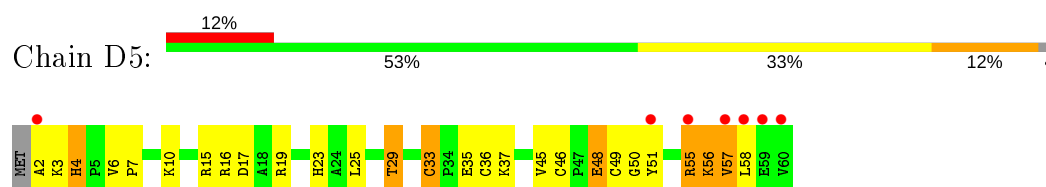
- Molecule 49: 50S ribosomal protein L31



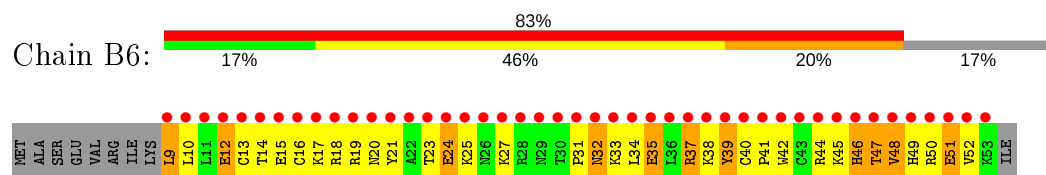
- Molecule 50: 50S ribosomal protein L32



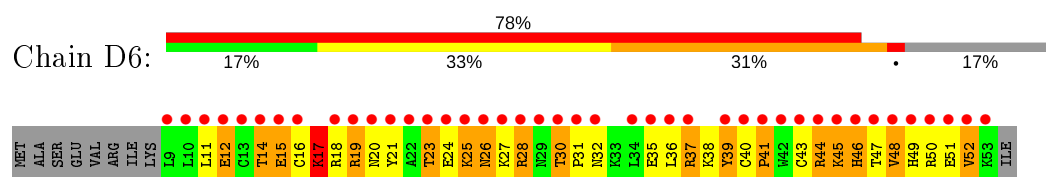
- Molecule 50: 50S ribosomal protein L32



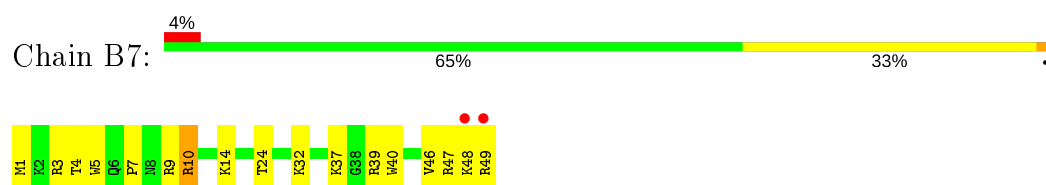
- Molecule 51: 50S ribosomal protein L33



- Molecule 51: 50S ribosomal protein L33

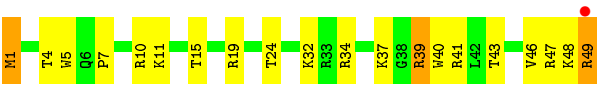


- Molecule 52: 50S ribosomal protein L34

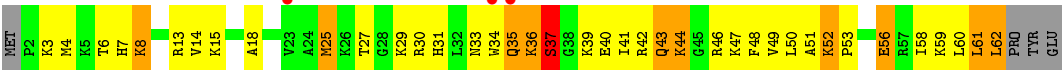


- Molecule 52: 50S ribosomal protein L34





• 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	210.06Å 450.27Å 616.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	153.59 – 3.10 254.47 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (153.59-3.10) 93.4 (254.47-3.10)	Depositor EDS
R_{merge}	0.47	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.89 (at 3.07Å)	Xtriage
Refinement program	PHENIX dev_987	Depositor
R, R_{free}	0.213 , 0.269 0.212 , 0.267	Depositor DCC
R_{free} test set	2000 reflections (0.19%)	wwPDB-VP
Wilson B-factor (Å ²)	83.6	Xtriage
Anisotropy	0.211	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 56.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	295766	wwPDB-VP
Average B, all atoms (Å ²)	111.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.43% 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, T1C

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	0.58	23/36234 (0.1%)	1.04	97/56554 (0.2%)
1	CA	0.50	5/36237 (0.0%)	0.95	67/56558 (0.1%)
2	AE	0.37	0/1959	0.60	1/2642 (0.0%)
2	CE	0.38	0/1959	0.68	4/2642 (0.2%)
3	AF	0.39	0/1629	0.57	0/2195
3	CF	0.37	0/1636	0.56	0/2205
4	AG	0.48	1/1733 (0.1%)	0.66	1/2318 (0.0%)
4	CG	0.45	1/1733 (0.1%)	0.63	1/2318 (0.0%)
5	AH	0.42	0/1171	0.60	0/1576
5	CH	0.38	0/1171	0.57	0/1576
6	AI	0.43	0/856	0.61	0/1154
6	CI	0.37	0/856	0.52	0/1154
7	AJ	0.45	0/1276	0.65	2/1709 (0.1%)
7	CJ	0.39	0/1276	0.59	0/1709
8	AK	0.39	0/1136	0.68	3/1527 (0.2%)
8	CK	0.35	0/1136	0.56	0/1527
9	AL	0.45	0/1029	0.65	0/1379
9	CL	0.41	0/1029	0.62	0/1379
10	AM	0.34	0/814	0.56	0/1095
10	CM	0.38	0/814	0.58	0/1095
11	AN	0.41	0/900	0.58	0/1213
11	CN	0.52	1/900 (0.1%)	0.66	1/1213 (0.1%)
12	AO	0.44	0/991	0.62	0/1327
12	CO	0.42	0/991	0.65	1/1327 (0.1%)
13	AP	0.39	0/938	0.59	0/1258
13	CP	0.35	0/943	0.63	1/1265 (0.1%)
14	AQ	0.45	0/501	0.68	0/664
14	CQ	0.45	0/501	0.64	0/664
15	AR	0.41	0/745	0.57	0/992
15	CR	0.42	0/745	0.54	0/992
16	AS	0.40	0/721	0.79	3/970 (0.3%)
16	CS	0.40	0/721	0.58	0/970

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AT	0.40	0/847	0.57	0/1131
17	CT	0.39	0/847	0.55	0/1131
18	AU	0.41	0/596	0.64	0/790
18	CU	0.41	0/596	0.60	0/790
19	AV	0.46	0/680	0.75	1/915 (0.1%)
19	CV	0.47	0/638	0.78	0/860
20	AW	0.36	0/765	0.59	0/1007
20	CW	0.37	0/765	0.58	0/1007
21	AX	0.37	0/221	0.55	0/288
21	CX	0.36	0/221	0.63	0/288
22	AC	0.66	2/1832 (0.1%)	1.08	8/2855 (0.3%)
22	AD	0.52	2/1832 (0.1%)	1.08	9/2855 (0.3%)
22	CC	0.56	2/1832 (0.1%)	1.00	9/2855 (0.3%)
22	CD	0.54	2/1832 (0.1%)	1.15	11/2855 (0.4%)
23	A1	0.63	0/144	0.84	0/222
23	C1	0.55	0/144	0.86	0/222
24	BA	0.67	14/70233 (0.0%)	1.18	443/109643 (0.4%)
24	DA	0.61	4/70100 (0.0%)	1.09	282/109435 (0.3%)
25	BB	0.63	0/2928	1.12	12/4568 (0.3%)
25	DB	0.55	0/2928	0.99	3/4568 (0.1%)
26	BD	0.54	0/2165	0.73	0/2919
26	DD	0.57	1/2165 (0.0%)	0.70	0/2919
27	BE	0.49	0/1601	0.64	0/2160
27	DE	0.50	0/1601	0.67	1/2160 (0.0%)
28	BF	0.49	0/1620	0.69	0/2194
28	DF	0.44	0/1662	0.64	0/2249
29	BG	0.42	0/1499	0.59	0/2016
29	DG	0.36	0/1499	0.59	0/2016
30	BH	0.44	0/1332	0.63	1/1802 (0.1%)
30	DH	0.34	0/1332	0.70	1/1802 (0.1%)
31	BK	0.41	0/1151	0.63	0/1558
31	DK	0.40	0/1151	0.63	1/1558 (0.1%)
32	BM	0.47	0/1131	0.62	0/1525
32	DM	0.39	0/1131	0.58	0/1525
33	BN	0.47	0/943	0.61	0/1269
33	DN	0.46	0/943	0.61	0/1269
34	BO	0.54	0/1162	0.82	2/1544 (0.1%)
34	DO	0.42	0/1162	0.71	0/1544
35	BP	0.50	0/1143	0.66	0/1527
35	DP	0.45	0/1143	0.63	0/1527
36	B0	0.51	0/982	0.74	1/1312 (0.1%)
36	D0	0.46	0/974	0.63	0/1302
37	BQ	0.51	0/892	0.69	1/1187 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
37	DQ	0.44	0/892	0.73	1/1187 (0.1%)
38	BR	0.45	0/1155	0.62	0/1542
38	DR	0.43	0/1155	0.60	0/1542
39	B1	0.52	0/982	0.67	0/1306
39	D1	0.42	0/982	0.64	0/1306
40	B2	0.50	0/790	0.68	1/1057 (0.1%)
40	D2	0.42	0/790	0.69	1/1057 (0.1%)
41	BS	0.47	0/911	0.63	0/1220
41	DS	0.47	0/911	0.59	0/1220
42	BT	0.58	0/739	0.65	0/993
42	DT	0.55	0/739	0.64	0/993
43	BU	0.54	0/798	0.74	0/1064
43	DU	0.50	0/798	0.69	1/1064 (0.1%)
44	BV	0.40	0/1427	0.63	0/1935
44	DV	0.37	0/1460	0.67	1/1982 (0.1%)
45	B3	0.65	2/615 (0.3%)	0.70	0/819
45	D3	0.46	0/621	0.61	0/827
46	BZ	0.50	0/770	0.65	0/1022
46	DZ	0.49	0/770	0.68	0/1022
47	BW	0.56	1/560 (0.2%)	0.70	0/741
47	DW	0.48	0/583	0.71	1/771 (0.1%)
48	BX	0.44	0/474	0.58	0/635
48	DX	0.40	0/474	0.56	0/635
49	B4	0.65	2/545 (0.4%)	0.77	1/733 (0.1%)
49	D4	0.44	0/527	0.69	0/709
50	B5	0.52	0/473	0.76	0/639
50	D5	0.45	0/473	0.67	0/639
51	B6	0.48	0/396	0.70	0/529
51	D6	0.52	0/396	0.68	0/529
52	B7	0.59	0/438	0.74	0/575
52	D7	0.54	0/438	0.65	0/575
53	B8	0.66	0/494	0.77	0/649
53	D8	0.61	0/494	0.93	1/649 (0.2%)
All	All	0.57	63/319716 (0.0%)	0.99	976/478502 (0.2%)

The worst 5 of 63 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	193	C	P-O5'	13.92	1.73	1.59
1	AA	193	C	C5'-C4'	13.77	1.67	1.51
1	AA	1381	U	C2-N3	-13.28	1.28	1.37
22	AD	17(A)	C	C4-N4	-11.47	1.23	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	CC	17(A)	C	C4-N4	-11.41	1.23	1.33

The worst 5 of 976 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1381	U	N3-C4-C5	34.37	135.22	114.60
1	AA	193	C	C6-N1-C2	-33.39	106.94	120.30
1	AA	193	C	C5-C6-N1	30.48	136.24	121.00
1	AA	1381	U	C4-C5-C6	-26.85	103.59	119.70
22	CD	17(A)	C	N3-C4-C5	-19.72	114.01	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	16338	913	10
1	CA	32372	0	16336	884	0
2	AE	1924	0	1975	117	0
2	CE	1924	0	1975	144	0
3	AF	1605	0	1668	70	0
3	CF	1612	0	1677	118	0
4	AG	1703	0	1763	112	0
4	CG	1703	0	1764	215	0
5	AH	1155	0	1213	58	0
5	CH	1155	0	1212	56	0
6	AI	843	0	857	42	0
6	CI	843	0	857	28	0
7	AJ	1257	0	1296	74	0
7	CJ	1257	0	1296	67	0
8	AK	1116	0	1177	58	0
8	CK	1116	0	1177	43	0
9	AL	1010	0	1037	91	0
9	CL	1010	0	1037	94	0
10	AM	801	0	849	57	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	CM	801	0	849	56	1
11	AN	885	0	904	38	0
11	CN	885	0	904	39	0
12	AO	975	0	1062	76	0
12	CO	975	0	1062	44	0
13	AP	928	0	987	62	0
13	CP	933	0	992	89	0
14	AQ	492	0	529	40	0
14	CQ	492	0	531	43	0
15	AR	734	0	771	25	0
15	CR	734	0	771	32	0
16	AS	705	0	725	37	0
16	CS	705	0	725	29	0
17	AT	834	0	904	44	0
17	CT	834	0	904	28	0
18	AU	591	0	662	23	0
18	CU	591	0	662	25	0
19	AV	665	0	686	49	0
19	CV	624	0	636	80	0
20	AW	763	0	861	57	0
20	CW	763	0	861	48	0
21	AX	217	0	234	8	0
21	CX	217	0	234	20	0
22	AC	1640	0	836	20	0
22	AD	1640	0	836	97	0
22	CC	1640	0	836	23	0
22	CD	1640	0	836	90	0
23	A1	129	0	65	0	0
23	C1	129	0	65	0	0
24	BA	62707	0	31612	1372	0
24	DA	62587	0	31554	1346	0
25	BB	2617	0	1328	59	0
25	DB	2617	0	1328	85	0
26	BD	2115	0	2195	113	0
26	DD	2115	0	2195	141	0
27	BE	1568	0	1634	101	0
27	DE	1568	0	1634	207	0
28	BF	1585	0	1632	76	0
28	DF	1627	0	1680	130	0
29	BG	1474	0	1535	88	0
29	DG	1474	0	1535	105	0
30	BH	1307	0	1382	135	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	DH	1307	0	1382	122	9
31	BK	1136	0	1223	49	0
31	DK	1136	0	1223	47	0
32	BM	1104	0	1180	70	0
32	DM	1104	0	1180	50	0
33	BN	933	0	996	29	0
33	DN	933	0	996	43	0
34	BO	1145	0	1227	112	0
34	DO	1145	0	1228	155	0
35	BP	1122	0	1179	86	0
35	DP	1122	0	1179	59	0
36	B0	968	0	1033	59	0
36	D0	960	0	1021	37	0
37	BQ	882	0	943	54	0
37	DQ	882	0	943	72	0
38	BR	1141	0	1202	68	0
38	DR	1141	0	1202	65	0
39	B1	964	0	1022	64	0
39	D1	964	0	1022	69	0
40	B2	779	0	852	43	1
40	D2	779	0	852	89	0
41	BS	900	0	964	27	0
41	DS	900	0	964	27	0
42	BT	725	0	778	25	0
42	DT	725	0	778	20	0
43	BU	785	0	878	79	0
43	DU	785	0	878	57	0
44	BV	1397	0	1430	79	0
44	DV	1428	0	1454	87	0
45	B3	607	0	628	40	0
45	D3	613	0	633	35	0
46	BZ	763	0	848	30	0
46	DZ	763	0	848	34	0
47	BW	558	0	610	25	0
47	DW	581	0	629	30	0
48	BX	469	0	518	17	0
48	DX	469	0	518	19	0
49	B4	533	0	522	57	0
49	D4	515	0	510	74	0
50	B5	459	0	480	35	1
50	D5	459	0	480	25	0
51	B6	389	0	404	42	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
51	D6	389	0	404	76	0
52	B7	430	0	480	16	0
52	D7	430	0	480	13	0
53	B8	488	0	559	51	0
53	D8	488	0	560	71	0
54	A1	1	0	0	0	0
54	AA	236	0	0	0	0
54	AC	8	0	0	0	0
54	AD	1	0	0	0	0
54	AG	1	0	0	0	0
54	AH	1	0	0	0	0
54	AN	2	0	0	0	0
54	AQ	1	0	0	0	0
54	AT	1	0	0	0	0
54	B0	1	0	0	0	0
54	B1	1	0	0	0	0
54	B2	1	0	0	0	0
54	B3	2	0	0	0	0
54	B5	1	0	0	0	0
54	B7	3	0	0	0	0
54	B8	2	0	0	0	0
54	BA	632	0	0	0	0
54	BB	16	0	0	0	0
54	BD	1	0	0	0	0
54	BE	4	0	0	0	0
54	BF	2	0	0	0	0
54	BO	2	0	0	0	0
54	BU	2	0	0	0	0
54	CA	199	0	0	0	0
54	CC	9	0	0	0	0
54	CG	2	0	0	0	0
54	CL	1	0	0	0	0
54	CN	1	0	0	0	0
54	CS	1	0	0	0	0
54	CX	1	0	0	0	0
54	D1	1	0	0	0	0
54	D3	1	0	0	0	0
54	D5	1	0	0	0	0
54	D8	1	0	0	0	0
54	DA	523	0	0	0	0
54	DB	15	0	0	0	0
54	DE	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	DP	1	0	0	0	0
54	DR	1	0	0	0	0
54	DU	2	0	0	0	0
55	AA	42	0	39	2	0
55	CA	42	0	38	5	0
56	AG	1	0	0	0	0
56	AQ	1	0	0	0	0
56	CG	1	0	0	0	0
56	CQ	1	0	0	0	0
All	All	295766	0	199075	9375	11

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 21.

The worst 5 of 9375 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:BA:2751:G:C2	30:BH:3:ARG:HD3	1.42	1.55
30:DH:127:GLU:CG	30:DH:128:PRO:HD3	1.36	1.54
27:DE:11:MET:SD	27:DE:24:THR:HG22	1.47	1.52
40:D2:49:THR:HB	40:D2:50:PRO:CD	1.45	1.47
26:DD:34:VAL:HG22	26:DD:35:LYS:CE	1.44	1.46

The worst 5 of 11 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:85:U:O5'	30:DH:126:PRO:CA[3_555]	1.25	0.95
1:AA:85:U:C4'	30:DH:126:PRO:CB[3_555]	1.47	0.73
1:AA:84:U:O3'	30:DH:127:GLU:N[3_555]	1.76	0.44
1:AA:84:U:OP2	30:DH:127:GLU:CG[3_555]	1.98	0.22
1:AA:85:U:C5'	30:DH:126:PRO:CB[3_555]	2.00	0.20

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AE	235/256 (92%)	170 (72%)	41 (17%)	24 (10%)	0	3
2	CE	235/256 (92%)	165 (70%)	38 (16%)	32 (14%)	0	1
3	AF	203/239 (85%)	138 (68%)	44 (22%)	21 (10%)	0	3
3	CF	204/239 (85%)	135 (66%)	48 (24%)	21 (10%)	0	3
4	AG	206/208 (99%)	154 (75%)	35 (17%)	17 (8%)	1	5
4	CG	206/208 (99%)	150 (73%)	36 (18%)	20 (10%)	0	3
5	AH	149/162 (92%)	118 (79%)	26 (17%)	5 (3%)	3	21
5	CH	149/162 (92%)	130 (87%)	13 (9%)	6 (4%)	3	17
6	AI	99/101 (98%)	86 (87%)	9 (9%)	4 (4%)	3	17
6	CI	99/101 (98%)	87 (88%)	10 (10%)	2 (2%)	7	31
7	AJ	153/156 (98%)	127 (83%)	21 (14%)	5 (3%)	4	21
7	CJ	153/156 (98%)	120 (78%)	25 (16%)	8 (5%)	2	12
8	AK	136/138 (99%)	103 (76%)	23 (17%)	10 (7%)	1	6
8	CK	136/138 (99%)	120 (88%)	10 (7%)	6 (4%)	2	15
9	AL	125/128 (98%)	87 (70%)	26 (21%)	12 (10%)	0	3
9	CL	125/128 (98%)	90 (72%)	31 (25%)	4 (3%)	4	22
10	AM	97/105 (92%)	70 (72%)	18 (19%)	9 (9%)	0	3
10	CM	97/105 (92%)	65 (67%)	24 (25%)	8 (8%)	1	5
11	AN	117/129 (91%)	90 (77%)	19 (16%)	8 (7%)	1	7
11	CN	117/129 (91%)	96 (82%)	16 (14%)	5 (4%)	2	16
12	AO	123/128 (96%)	87 (71%)	24 (20%)	12 (10%)	0	3
12	CO	123/128 (96%)	103 (84%)	10 (8%)	10 (8%)	1	5
13	AP	114/126 (90%)	81 (71%)	20 (18%)	13 (11%)	0	2
13	CP	115/126 (91%)	75 (65%)	22 (19%)	18 (16%)	0	0
14	AQ	58/61 (95%)	40 (69%)	7 (12%)	11 (19%)	0	0
14	CQ	58/61 (95%)	40 (69%)	12 (21%)	6 (10%)	0	3
15	AR	86/89 (97%)	60 (70%)	20 (23%)	6 (7%)	1	7
15	CR	86/89 (97%)	73 (85%)	6 (7%)	7 (8%)	1	5
16	AS	82/88 (93%)	65 (79%)	16 (20%)	1 (1%)	13	44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	CS	82/88 (93%)	66 (80%)	15 (18%)	1 (1%)	13	44
17	AT	98/105 (93%)	78 (80%)	14 (14%)	6 (6%)	1	9
17	CT	98/105 (93%)	85 (87%)	11 (11%)	2 (2%)	7	31
18	AU	70/88 (80%)	59 (84%)	7 (10%)	4 (6%)	1	10
18	CU	70/88 (80%)	56 (80%)	7 (10%)	7 (10%)	0	3
19	AV	81/93 (87%)	54 (67%)	19 (24%)	8 (10%)	0	3
19	CV	76/93 (82%)	44 (58%)	17 (22%)	15 (20%)	0	0
20	AW	97/106 (92%)	72 (74%)	12 (12%)	13 (13%)	0	1
20	CW	97/106 (92%)	70 (72%)	18 (19%)	9 (9%)	0	3
21	AX	23/27 (85%)	14 (61%)	7 (30%)	2 (9%)	1	4
21	CX	23/27 (85%)	17 (74%)	3 (13%)	3 (13%)	0	1
26	BD	270/276 (98%)	231 (86%)	26 (10%)	13 (5%)	2	14
26	DD	270/276 (98%)	217 (80%)	40 (15%)	13 (5%)	2	14
27	BE	203/206 (98%)	161 (79%)	28 (14%)	14 (7%)	1	7
27	DE	203/206 (98%)	133 (66%)	33 (16%)	37 (18%)	0	0
28	BF	200/210 (95%)	175 (88%)	20 (10%)	5 (2%)	5	27
28	DF	206/210 (98%)	151 (73%)	29 (14%)	26 (13%)	0	1
29	BG	179/182 (98%)	120 (67%)	42 (24%)	17 (10%)	0	3
29	DG	179/182 (98%)	121 (68%)	38 (21%)	20 (11%)	0	2
30	BH	168/180 (93%)	124 (74%)	24 (14%)	20 (12%)	0	1
30	DH	168/180 (93%)	92 (55%)	45 (27%)	31 (18%)	0	0
31	BK	144/148 (97%)	102 (71%)	25 (17%)	17 (12%)	0	1
31	DK	144/148 (97%)	104 (72%)	28 (19%)	12 (8%)	1	5
32	BM	136/140 (97%)	101 (74%)	25 (18%)	10 (7%)	1	6
32	DM	136/140 (97%)	110 (81%)	22 (16%)	4 (3%)	4	24
33	BN	120/122 (98%)	113 (94%)	5 (4%)	2 (2%)	9	36
33	DN	120/122 (98%)	103 (86%)	14 (12%)	3 (2%)	5	27
34	BO	148/150 (99%)	99 (67%)	21 (14%)	28 (19%)	0	0
34	DO	148/150 (99%)	83 (56%)	44 (30%)	21 (14%)	0	1
35	BP	139/141 (99%)	96 (69%)	26 (19%)	17 (12%)	0	1
35	DP	139/141 (99%)	105 (76%)	19 (14%)	15 (11%)	0	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	B0	116/118 (98%)	88 (76%)	19 (16%)	9 (8%)	1	5
36	D0	115/118 (98%)	99 (86%)	13 (11%)	3 (3%)	5	26
37	BQ	109/112 (97%)	78 (72%)	19 (17%)	12 (11%)	0	2
37	DQ	109/112 (97%)	78 (72%)	20 (18%)	11 (10%)	0	3
38	BR	135/146 (92%)	101 (75%)	25 (18%)	9 (7%)	1	7
38	DR	135/146 (92%)	110 (82%)	19 (14%)	6 (4%)	2	15
39	B1	115/118 (98%)	101 (88%)	10 (9%)	4 (4%)	3	20
39	D1	115/118 (98%)	88 (76%)	18 (16%)	9 (8%)	1	5
40	B2	99/101 (98%)	78 (79%)	11 (11%)	10 (10%)	0	3
40	D2	99/101 (98%)	73 (74%)	12 (12%)	14 (14%)	0	1
41	BS	111/113 (98%)	102 (92%)	6 (5%)	3 (3%)	5	25
41	DS	111/113 (98%)	98 (88%)	8 (7%)	5 (4%)	2	15
42	BT	90/96 (94%)	78 (87%)	10 (11%)	2 (2%)	6	29
42	DT	90/96 (94%)	69 (77%)	13 (14%)	8 (9%)	1	4
43	BU	100/110 (91%)	69 (69%)	14 (14%)	17 (17%)	0	0
43	DU	100/110 (91%)	53 (53%)	22 (22%)	25 (25%)	0	0
44	BV	173/206 (84%)	117 (68%)	31 (18%)	25 (14%)	0	1
44	DV	177/206 (86%)	111 (63%)	35 (20%)	31 (18%)	0	0
45	B3	74/85 (87%)	65 (88%)	7 (10%)	2 (3%)	5	25
45	D3	75/85 (88%)	66 (88%)	7 (9%)	2 (3%)	5	25
46	BZ	95/98 (97%)	78 (82%)	10 (10%)	7 (7%)	1	6
46	DZ	95/98 (97%)	71 (75%)	14 (15%)	10 (10%)	0	3
47	BW	64/72 (89%)	52 (81%)	9 (14%)	3 (5%)	2	14
47	DW	67/72 (93%)	53 (79%)	6 (9%)	8 (12%)	0	1
48	BX	57/60 (95%)	51 (90%)	4 (7%)	2 (4%)	3	20
48	DX	57/60 (95%)	49 (86%)	5 (9%)	3 (5%)	2	12
49	B4	64/71 (90%)	34 (53%)	15 (23%)	15 (23%)	0	0
49	D4	61/71 (86%)	25 (41%)	18 (30%)	18 (30%)	0	0
50	B5	57/60 (95%)	41 (72%)	9 (16%)	7 (12%)	0	1
50	D5	57/60 (95%)	46 (81%)	7 (12%)	4 (7%)	1	7
51	B6	43/54 (80%)	24 (56%)	14 (33%)	5 (12%)	0	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
51	D6	43/54 (80%)	19 (44%)	13 (30%)	11 (26%)	0	0
52	B7	47/49 (96%)	43 (92%)	4 (8%)	0	100	100
52	D7	47/49 (96%)	45 (96%)	2 (4%)	0	100	100
53	B8	59/65 (91%)	45 (76%)	8 (14%)	6 (10%)	0	3
53	D8	59/65 (91%)	42 (71%)	8 (14%)	9 (15%)	0	0
All	All	11341/12044 (94%)	8521 (75%)	1799 (16%)	1021 (9%)	1	4

5 of 1021 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AE	29	ALA
2	AE	30	ARG
2	AE	95	GLN
2	AE	101	MET
2	AE	208	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%)	166 (81%)	39 (19%)	1	6
2	CE	205/220 (93%)	166 (81%)	39 (19%)	1	6
3	AF	159/188 (85%)	141 (89%)	18 (11%)	6	23
3	CF	160/188 (85%)	138 (86%)	22 (14%)	3	16
4	AG	180/180 (100%)	157 (87%)	23 (13%)	4	18
4	CG	180/180 (100%)	160 (89%)	20 (11%)	6	24
5	AH	116/123 (94%)	103 (89%)	13 (11%)	6	24
5	CH	116/123 (94%)	102 (88%)	14 (12%)	5	20
6	AI	90/90 (100%)	82 (91%)	8 (9%)	9	34
6	CI	90/90 (100%)	77 (86%)	13 (14%)	3	14
7	AJ	126/127 (99%)	105 (83%)	21 (17%)	2	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	CJ	126/127 (99%)	107 (85%)	19 (15%)	3	12
8	AK	119/119 (100%)	105 (88%)	14 (12%)	5	21
8	CK	119/119 (100%)	102 (86%)	17 (14%)	3	14
9	AL	98/99 (99%)	74 (76%)	24 (24%)	0	2
9	CL	98/99 (99%)	80 (82%)	18 (18%)	1	7
10	AM	89/92 (97%)	78 (88%)	11 (12%)	4	19
10	CM	89/92 (97%)	72 (81%)	17 (19%)	1	6
11	AN	90/99 (91%)	80 (89%)	10 (11%)	6	24
11	CN	90/99 (91%)	73 (81%)	17 (19%)	1	6
12	AO	104/107 (97%)	89 (86%)	15 (14%)	3	14
12	CO	104/107 (97%)	93 (89%)	11 (11%)	6	26
13	AP	94/101 (93%)	85 (90%)	9 (10%)	8	31
13	CP	94/101 (93%)	75 (80%)	19 (20%)	1	5
14	AQ	49/50 (98%)	39 (80%)	10 (20%)	1	5
14	CQ	49/50 (98%)	40 (82%)	9 (18%)	1	7
15	AR	79/80 (99%)	70 (89%)	9 (11%)	5	23
15	CR	79/80 (99%)	72 (91%)	7 (9%)	9	34
16	AS	72/74 (97%)	55 (76%)	17 (24%)	1	2
16	CS	72/74 (97%)	61 (85%)	11 (15%)	2	12
17	AT	95/97 (98%)	85 (90%)	10 (10%)	7	26
17	CT	95/97 (98%)	87 (92%)	8 (8%)	11	38
18	AU	63/77 (82%)	54 (86%)	9 (14%)	3	14
18	CU	63/77 (82%)	55 (87%)	8 (13%)	4	18
19	AV	72/80 (90%)	56 (78%)	16 (22%)	1	4
19	CV	67/80 (84%)	54 (81%)	13 (19%)	1	6
20	AW	76/82 (93%)	66 (87%)	10 (13%)	4	17
20	CW	76/82 (93%)	68 (90%)	8 (10%)	7	26
21	AX	20/22 (91%)	20 (100%)	0	100	100
21	CX	20/22 (91%)	19 (95%)	1 (5%)	24	57
26	BD	214/218 (98%)	178 (83%)	36 (17%)	2	9
26	DD	214/218 (98%)	183 (86%)	31 (14%)	3	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
27	BE	165/166 (99%)	144 (87%)	21 (13%)	4	18
27	DE	165/166 (99%)	143 (87%)	22 (13%)	4	16
28	BF	161/166 (97%)	142 (88%)	19 (12%)	5	21
28	DF	165/166 (99%)	138 (84%)	27 (16%)	2	10
29	BG	155/156 (99%)	138 (89%)	17 (11%)	6	25
29	DG	155/156 (99%)	132 (85%)	23 (15%)	3	13
30	BH	142/148 (96%)	123 (87%)	19 (13%)	4	16
30	DH	142/148 (96%)	109 (77%)	33 (23%)	1	3
31	BK	122/124 (98%)	103 (84%)	19 (16%)	2	11
31	DK	122/124 (98%)	92 (75%)	30 (25%)	0	2
32	BM	117/119 (98%)	95 (81%)	22 (19%)	1	6
32	DM	117/119 (98%)	96 (82%)	21 (18%)	2	8
33	BN	100/100 (100%)	90 (90%)	10 (10%)	7	28
33	DN	100/100 (100%)	87 (87%)	13 (13%)	4	18
34	BO	116/116 (100%)	91 (78%)	25 (22%)	1	4
34	DO	116/116 (100%)	84 (72%)	32 (28%)	0	1
35	BP	111/111 (100%)	100 (90%)	11 (10%)	8	29
35	DP	111/111 (100%)	94 (85%)	17 (15%)	2	12
36	B0	101/101 (100%)	87 (86%)	14 (14%)	3	15
36	D0	100/101 (99%)	89 (89%)	11 (11%)	6	25
37	BQ	87/88 (99%)	74 (85%)	13 (15%)	3	13
37	DQ	87/88 (99%)	69 (79%)	18 (21%)	1	5
38	BR	120/127 (94%)	105 (88%)	15 (12%)	4	18
38	DR	120/127 (94%)	98 (82%)	22 (18%)	1	7
39	B1	93/94 (99%)	79 (85%)	14 (15%)	3	12
39	D1	93/94 (99%)	79 (85%)	14 (15%)	3	12
40	B2	82/82 (100%)	69 (84%)	13 (16%)	2	11
40	D2	82/82 (100%)	62 (76%)	20 (24%)	0	2
41	BS	92/92 (100%)	80 (87%)	12 (13%)	4	18
41	DS	92/92 (100%)	75 (82%)	17 (18%)	1	7
42	BT	74/78 (95%)	63 (85%)	11 (15%)	3	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
42	DT	74/78 (95%)	66 (89%)	8 (11%)	6	25
43	BU	85/91 (93%)	62 (73%)	23 (27%)	0	1
43	DU	85/91 (93%)	59 (69%)	26 (31%)	0	0
44	BV	154/179 (86%)	126 (82%)	28 (18%)	1	7
44	DV	158/179 (88%)	136 (86%)	22 (14%)	3	15
45	B3	61/67 (91%)	54 (88%)	7 (12%)	5	22
45	D3	62/67 (92%)	58 (94%)	4 (6%)	17	47
46	BZ	82/83 (99%)	67 (82%)	15 (18%)	1	7
46	DZ	82/83 (99%)	76 (93%)	6 (7%)	14	43
47	BW	62/67 (92%)	54 (87%)	8 (13%)	4	18
47	DW	64/67 (96%)	61 (95%)	3 (5%)	26	59
48	BX	51/52 (98%)	44 (86%)	7 (14%)	3	16
48	DX	51/52 (98%)	43 (84%)	8 (16%)	2	11
49	B4	59/63 (94%)	41 (70%)	18 (30%)	0	0
49	D4	57/63 (90%)	36 (63%)	21 (37%)	0	0
50	B5	51/52 (98%)	40 (78%)	11 (22%)	1	4
50	D5	51/52 (98%)	43 (84%)	8 (16%)	2	11
51	B6	44/52 (85%)	33 (75%)	11 (25%)	0	2
51	D6	44/52 (85%)	31 (70%)	13 (30%)	0	1
52	B7	42/42 (100%)	36 (86%)	6 (14%)	3	14
52	D7	42/42 (100%)	33 (79%)	9 (21%)	1	4
53	B8	51/55 (93%)	39 (76%)	12 (24%)	1	3
53	D8	51/55 (93%)	41 (80%)	10 (20%)	1	6
All	All	9584/9992 (96%)	8081 (84%)	1503 (16%)	2	11

5 of 1503 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
49	B4	57	GLU
7	CJ	75	VAL
43	DU	62	GLU
51	B6	37	ARG
3	CF	29	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 57 such sidechains are listed below:

Mol	Chain	Res	Type
4	CG	43	HIS
12	CO	49	ASN
41	DS	40	ASN
4	CG	45	GLN
7	CJ	28	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1506/1506 (100%)	316 (20%)	26 (1%)
1	CA	1505/1506 (99%)	312 (20%)	30 (1%)
22	AC	76/77 (98%)	8 (10%)	1 (1%)
22	AD	76/77 (98%)	24 (31%)	1 (1%)
22	CC	77/77 (100%)	12 (15%)	1 (1%)
22	CD	76/77 (98%)	45 (59%)	5 (6%)
23	A1	5/6 (83%)	1 (20%)	0
23	C1	5/6 (83%)	1 (20%)	0
24	BA	2911/2912 (99%)	593 (20%)	44 (1%)
24	DA	2904/2912 (99%)	645 (22%)	39 (1%)
25	BB	121/122 (99%)	27 (22%)	0
25	DB	121/122 (99%)	32 (26%)	0
All	All	9383/9400 (99%)	2016 (21%)	147 (1%)

5 of 2016 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	6	G
1	AA	8	A
1	AA	9	G
1	AA	31	G
1	AA	32	A

5 of 147 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
24	BA	2481	G
1	CA	412	A
24	DA	2211	G
24	BA	2610	C
1	CA	197	A

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 1692 ligands modelled in this entry, 1690 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	T1C	CA	1800	54	44,45,45	0.97	5 (11%)	53,72,72	1.77	13 (24%)
55	T1C	AA	1837	54	44,45,45	0.96	5 (11%)	53,72,72	1.98	12 (22%)

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	T1C	CA	1800	54	-	9/22/80/80	0/4/4/4
55	T1C	AA	1837	54	-	7/22/80/80	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	CA	1800	T1C	C9-N9	-2.70	1.36	1.41
55	AA	1837	T1C	C9-N9	-2.61	1.36	1.41
55	AA	1837	T1C	C1C-C12	2.55	1.54	1.52
55	AA	1837	T1C	C1C-C1	-2.43	1.51	1.55
55	AA	1837	T1C	C2-C3	-2.26	1.34	1.40

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	AA	1837	T1C	C41-C1C-C1	-6.62	103.46	111.05
55	AA	1837	T1C	O12-C12-C1C	4.82	120.35	113.37
55	CA	1800	T1C	O12-C12-C1B	-4.51	117.73	123.90
55	AA	1837	T1C	O12-C12-C1B	-4.34	117.95	123.90
55	AA	1837	T1C	C11-C1B-C12	4.29	122.19	118.80

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

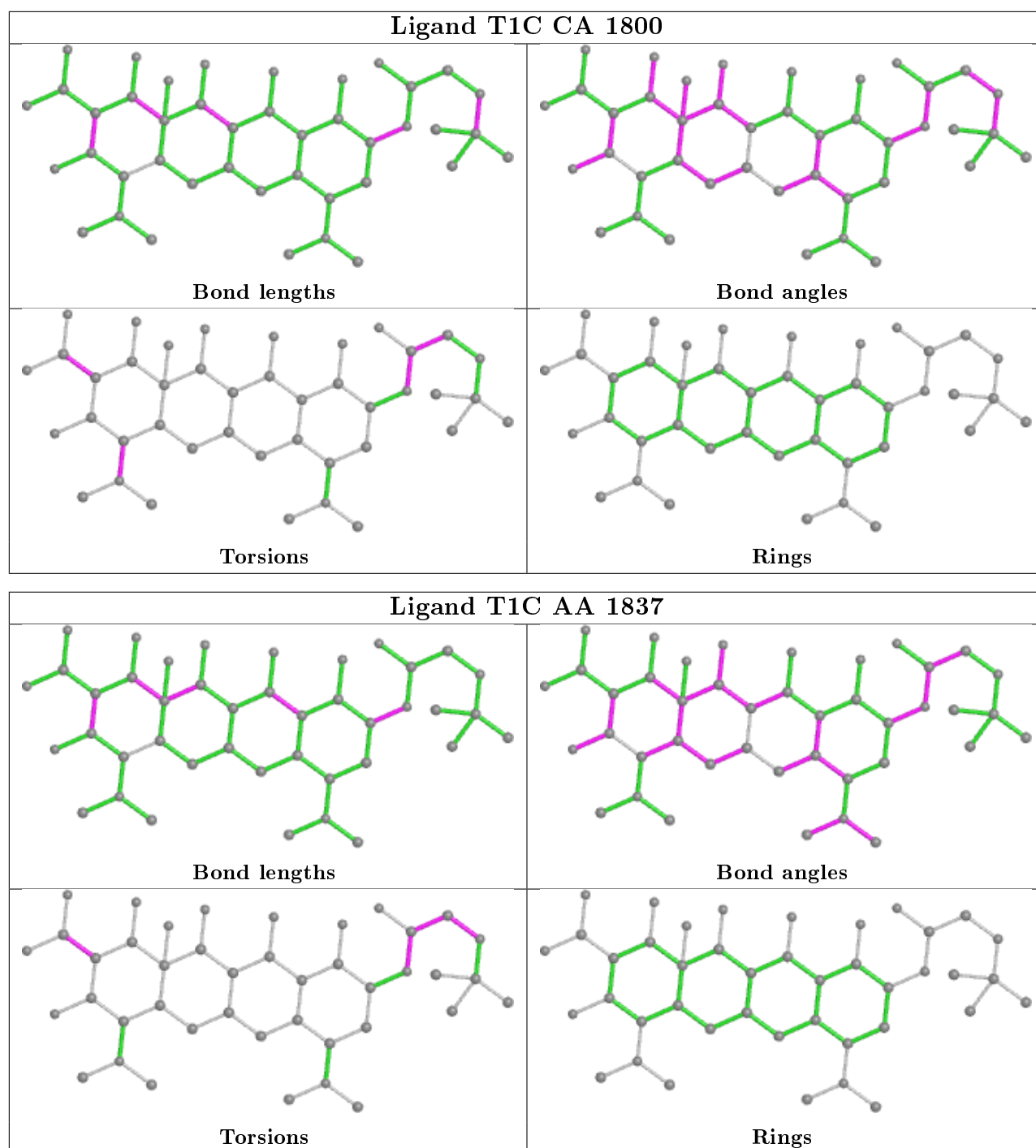
Mol	Chain	Res	Type	Atoms
55	CA	1800	T1C	C92-C91-N9-C9
55	CA	1800	T1C	O91-C91-N9-C9
55	CA	1800	T1C	C41-C4-N4-C42
55	CA	1800	T1C	C3-C2-C21-O21
55	CA	1800	T1C	C3-C2-C21-N21

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
55	CA	1800	T1C	5	0
55	AA	1837	T1C	2	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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	AA	1506/1506 (100%)	-0.71	2 (0%)	95	92	66, 112, 190, 248	0
1	CA	1506/1506 (100%)	-0.73	5 (0%)	94	88	76, 117, 189, 249	0
2	AE	237/256 (92%)	0.30	17 (7%)	15	6	116, 147, 183, 193	0
2	CE	237/256 (92%)	0.91	41 (17%)	1	0	126, 162, 192, 208	0
3	AF	205/239 (85%)	0.59	20 (9%)	7	2	99, 124, 157, 164	0
3	CF	206/239 (86%)	1.33	50 (24%)	0	0	121, 145, 174, 184	0
4	AG	208/208 (100%)	-0.43	0	100	100	95, 118, 140, 145	0
4	CG	208/208 (100%)	0.58	21 (10%)	7	2	93, 113, 133, 142	0
5	AH	151/162 (93%)	-0.03	1 (0%)	87	75	90, 110, 132, 163	0
5	CH	151/162 (93%)	0.47	9 (5%)	21	10	97, 117, 139, 165	0
6	AI	101/101 (100%)	0.97	15 (14%)	2	1	91, 112, 125, 144	0
6	CI	101/101 (100%)	-0.05	1 (0%)	82	67	90, 107, 128, 148	0
7	AJ	155/156 (99%)	0.56	20 (12%)	3	1	111, 129, 157, 167	0
7	CJ	155/156 (99%)	0.06	0	100	100	116, 133, 162, 173	0
8	AK	138/138 (100%)	-0.35	0	100	100	97, 117, 127, 137	0
8	CK	138/138 (100%)	0.19	5 (3%)	42	22	105, 122, 135, 143	0
9	AL	127/128 (99%)	0.12	2 (1%)	72	51	100, 144, 163, 167	0
9	CL	127/128 (99%)	0.11	3 (2%)	59	37	114, 155, 170, 176	0
10	AM	99/105 (94%)	0.59	10 (10%)	7	2	100, 146, 171, 175	0
10	CM	99/105 (94%)	0.81	15 (15%)	2	1	117, 159, 174, 180	0
11	AN	119/129 (92%)	1.10	20 (16%)	1	0	83, 108, 138, 168	0
11	CN	119/129 (92%)	0.21	2 (1%)	70	49	91, 112, 138, 163	0
12	AO	125/128 (97%)	-0.20	1 (0%)	86	72	78, 92, 116, 168	0
12	CO	125/128 (97%)	0.73	14 (11%)	5	2	84, 104, 129, 170	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
13	AP	116/126 (92%)	0.08	4 (3%)	45	24	100, 133, 147, 157	0
13	CP	117/126 (92%)	-0.12	6 (5%)	28	13	121, 155, 170, 177	0
14	AQ	60/61 (98%)	-0.25	0	100	100	103, 114, 127, 135	0
14	CQ	60/61 (98%)	0.82	9 (15%)	2	1	130, 139, 155, 162	0
15	AR	88/89 (98%)	-0.21	0	100	100	89, 108, 124, 127	0
15	CR	88/89 (98%)	-0.19	0	100	100	89, 113, 131, 136	0
16	AS	84/88 (95%)	-0.58	0	100	100	107, 122, 145, 171	0
16	CS	84/88 (95%)	0.29	3 (3%)	42	22	91, 107, 126, 167	0
17	AT	100/105 (95%)	-0.40	1 (1%)	82	67	96, 114, 126, 133	0
17	CT	100/105 (95%)	0.30	2 (2%)	65	44	91, 111, 128, 149	0
18	AU	72/88 (81%)	0.79	7 (9%)	7	2	95, 112, 141, 169	0
18	CU	72/88 (81%)	-0.05	2 (2%)	53	30	96, 117, 152, 173	0
19	AV	83/93 (89%)	-0.24	2 (2%)	59	37	115, 136, 151, 157	0
19	CV	78/93 (83%)	0.34	8 (10%)	6	2	135, 166, 181, 188	0
20	AW	99/106 (93%)	-0.50	0	100	100	111, 127, 157, 162	0
20	CW	99/106 (93%)	0.04	2 (2%)	65	44	91, 116, 148, 165	0
21	AX	25/27 (92%)	-0.36	0	100	100	111, 120, 140, 160	0
21	CX	25/27 (92%)	-0.45	0	100	100	117, 138, 154, 170	0
22	AC	77/77 (100%)	-0.66	0	100	100	77, 100, 135, 151	0
22	AD	77/77 (100%)	0.16	2 (2%)	56	33	93, 214, 228, 234	0
22	CC	77/77 (100%)	-0.83	0	100	100	80, 118, 151, 171	0
22	CD	77/77 (100%)	-0.62	0	100	100	93, 220, 238, 248	0
23	A1	6/6 (100%)	-0.60	0	100	100	85, 89, 129, 143	0
23	C1	6/6 (100%)	-0.52	0	100	100	103, 111, 138, 153	0
24	BA	2912/2912 (100%)	-0.38	36 (1%)	79	61	53, 82, 212, 247	0
24	DA	2906/2912 (99%)	-0.57	31 (1%)	80	64	60, 90, 232, 251	0
25	BB	122/122 (100%)	-0.60	1 (0%)	86	72	78, 106, 126, 184	0
25	DB	122/122 (100%)	-0.79	0	100	100	91, 127, 154, 200	0
26	BD	272/276 (98%)	0.13	5 (1%)	68	47	55, 75, 94, 102	0
26	DD	272/276 (98%)	-0.28	4 (1%)	73	54	58, 81, 99, 122	0
27	BE	205/206 (99%)	0.14	8 (3%)	39	20	60, 92, 135, 153	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
27	DE	205/206 (99%)	-0.18	5 (2%) 59 37	60, 97, 142, 165	0
28	BF	202/210 (96%)	0.15	4 (1%) 65 44	54, 84, 118, 133	0
28	DF	208/210 (99%)	0.68	23 (11%) 5 2	66, 102, 156, 182	0
29	BG	181/182 (99%)	1.21	43 (23%) 0 0	95, 116, 145, 154	0
29	DG	181/182 (99%)	0.43	15 (8%) 11 4	117, 141, 165, 177	0
30	BH	170/180 (94%)	0.30	6 (3%) 44 23	88, 113, 132, 151	0
30	DH	170/180 (94%)	1.23	42 (24%) 0 0	146, 200, 223, 235	0
31	BK	146/148 (98%)	0.65	16 (10%) 5 2	87, 129, 146, 151	0
31	DK	146/148 (98%)	-0.39	0 100 100	88, 132, 151, 159	0
32	BM	138/140 (98%)	0.41	8 (5%) 23 10	78, 93, 128, 145	0
32	DM	138/140 (98%)	0.07	1 (0%) 87 75	80, 107, 137, 157	0
33	BN	122/122 (100%)	0.14	1 (0%) 86 72	69, 87, 102, 112	0
33	DN	122/122 (100%)	0.25	2 (1%) 72 51	70, 91, 109, 116	0
34	BO	150/150 (100%)	0.22	5 (3%) 46 24	60, 91, 114, 167	0
34	DO	150/150 (100%)	0.93	27 (18%) 1 0	66, 105, 140, 179	0
35	BP	141/141 (100%)	0.36	5 (3%) 44 23	68, 91, 113, 135	0
35	DP	141/141 (100%)	0.27	6 (4%) 35 17	80, 106, 130, 152	0
36	B0	118/118 (100%)	0.20	1 (0%) 86 72	72, 89, 104, 118	0
36	D0	117/118 (99%)	-0.06	0 100 100	71, 89, 108, 119	0
37	BQ	111/112 (99%)	0.71	13 (11%) 4 2	85, 104, 127, 137	0
37	DQ	111/112 (99%)	0.14	5 (4%) 33 16	98, 121, 142, 151	0
38	BR	137/146 (93%)	-0.00	5 (3%) 42 22	80, 102, 150, 169	0
38	DR	137/146 (93%)	-0.04	1 (0%) 87 75	80, 99, 159, 185	0
39	B1	117/118 (99%)	-0.03	3 (2%) 56 33	63, 83, 112, 138	0
39	D1	117/118 (99%)	-0.03	0 100 100	72, 101, 136, 155	0
40	B2	101/101 (100%)	0.43	5 (4%) 28 13	64, 102, 126, 145	0
40	D2	101/101 (100%)	0.99	16 (15%) 2 1	71, 123, 139, 148	0
41	BS	113/113 (100%)	0.19	3 (2%) 54 31	63, 80, 110, 161	0
41	DS	113/113 (100%)	0.26	2 (1%) 68 47	68, 83, 113, 161	0
42	BT	92/96 (95%)	0.50	4 (4%) 35 17	64, 78, 101, 111	0
42	DT	92/96 (95%)	0.23	5 (5%) 25 12	77, 94, 118, 128	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
43	BU	102/110 (92%)	0.62	9 (8%) 10 4	75, 99, 149, 163	0
43	DU	102/110 (92%)	1.53	30 (29%) 0 0	93, 118, 160, 182	0
44	BV	175/206 (84%)	1.89	62 (35%) 0 0	97, 131, 195, 201	0
44	DV	179/206 (86%)	1.72	57 (31%) 0 0	118, 157, 213, 219	0
45	B3	76/85 (89%)	0.30	1 (1%) 77 59	69, 85, 101, 140	0
45	D3	77/85 (90%)	0.24	2 (2%) 56 33	74, 95, 111, 151	0
46	BZ	97/98 (98%)	1.04	11 (11%) 5 2	65, 85, 132, 164	0
46	DZ	97/98 (98%)	-0.20	0 100 100	67, 91, 135, 157	0
47	BW	66/72 (91%)	0.23	1 (1%) 73 54	70, 87, 108, 132	0
47	DW	69/72 (95%)	0.51	4 (5%) 23 10	90, 112, 133, 164	0
48	BX	59/60 (98%)	0.25	4 (6%) 17 7	73, 86, 121, 137	0
48	DX	59/60 (98%)	0.74	6 (10%) 6 2	79, 102, 145, 162	0
49	B4	66/71 (92%)	2.76	42 (63%) 0 0	122, 158, 180, 186	0
49	D4	63/71 (88%)	2.48	38 (60%) 0 0	154, 187, 197, 205	0
50	B5	59/60 (98%)	0.59	9 (15%) 2 1	57, 90, 166, 172	0
50	D5	59/60 (98%)	0.62	7 (11%) 4 2	68, 91, 178, 192	0
51	B6	45/54 (83%)	9.22	45 (100%) 0 0	128, 153, 163, 164	0
51	D6	45/54 (83%)	4.96	42 (93%) 0 0	138, 164, 181, 183	0
52	B7	49/49 (100%)	0.05	2 (4%) 37 18	55, 61, 92, 120	0
52	D7	49/49 (100%)	0.12	1 (2%) 65 44	63, 70, 107, 130	0
53	B8	61/65 (93%)	0.38	3 (4%) 29 14	66, 81, 98, 124	0
53	D8	61/65 (93%)	0.42	0 100 100	73, 87, 106, 121	0
All	All	20927/21444 (97%)	-0.01	1055 (5%) 28 13	53, 106, 186, 251	0

The worst 5 of 1055 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
51	B6	16	CYS	21.4
44	DV	143	GLY	18.4
51	B6	15	GLU	17.4
34	DO	150	ALA	16.1
51	B6	43	CYS	15.5

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(\AA^2)	Q<0.9
54	MG	AA	1722	1/1	0.24	0.34	96,96,96,96	0
54	MG	DA	3250	1/1	0.26	0.33	105,105,105,105	0
54	MG	CA	1798	1/1	0.31	0.21	115,115,115,115	0
54	MG	DA	3296	1/1	0.31	0.20	104,104,104,104	0
54	MG	CA	1787	1/1	0.31	0.35	136,136,136,136	0
54	MG	AC	105	1/1	0.32	0.23	100,100,100,100	0
54	MG	DA	3500	1/1	0.36	0.18	98,98,98,98	0
54	MG	BA	3091	1/1	0.39	0.33	128,128,128,128	0
54	MG	DA	3446	1/1	0.39	0.19	99,99,99,99	0
54	MG	DA	3086	1/1	0.41	0.24	109,109,109,109	0
54	MG	DA	3117	1/1	0.41	0.26	102,102,102,102	0
54	MG	B8	101	1/1	0.43	0.28	91,91,91,91	0
54	MG	AA	1675	1/1	0.46	0.37	112,112,112,112	0
54	MG	DA	3025	1/1	0.46	0.17	91,91,91,91	0
54	MG	CA	1732	1/1	0.48	0.31	108,108,108,108	0
54	MG	AA	1614	1/1	0.48	0.17	132,132,132,132	0
54	MG	BA	3510	1/1	0.49	0.51	97,97,97,97	0
54	MG	BA	3288	1/1	0.50	0.41	115,115,115,115	0
54	MG	BA	3468	1/1	0.50	0.28	99,99,99,99	0
54	MG	CA	1755	1/1	0.52	0.23	104,104,104,104	0
54	MG	DA	3432	1/1	0.52	0.23	102,102,102,102	0
54	MG	BA	3509	1/1	0.52	0.76	102,102,102,102	0
54	MG	AA	1743	1/1	0.54	0.24	100,100,100,100	0
54	MG	CA	1709	1/1	0.54	0.24	97,97,97,97	0
54	MG	CA	1684	1/1	0.54	0.21	91,91,91,91	0
54	MG	DA	3353	1/1	0.55	0.28	83,83,83,83	0
54	MG	AA	1717	1/1	0.55	0.28	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	BA	3464	1/1	0.55	0.36	101,101,101,101	0
54	MG	CA	1658	1/1	0.55	0.24	104,104,104,104	0
54	MG	CA	1781	1/1	0.55	0.25	148,148,148,148	0
54	MG	DA	3439	1/1	0.56	0.13	95,95,95,95	0
54	MG	BA	3447	1/1	0.57	0.29	83,83,83,83	0
54	MG	BA	3280	1/1	0.58	0.32	106,106,106,106	0
54	MG	BA	3438	1/1	0.58	0.22	90,90,90,90	0
54	MG	DA	3357	1/1	0.59	0.12	123,123,123,123	0
54	MG	DA	3406	1/1	0.59	0.29	113,113,113,113	0
54	MG	DA	3002	1/1	0.59	0.16	87,87,87,87	0
54	MG	DB	212	1/1	0.59	0.21	101,101,101,101	0
54	MG	CA	1618	1/1	0.60	0.19	108,108,108,108	0
54	MG	DA	3042	1/1	0.60	0.19	78,78,78,78	0
54	MG	BA	3418	1/1	0.60	0.39	104,104,104,104	0
54	MG	DA	3391	1/1	0.60	0.22	107,107,107,107	0
54	MG	CA	1785	1/1	0.60	0.48	101,101,101,101	0
54	MG	CA	1676	1/1	0.61	0.20	90,90,90,90	0
54	MG	AA	1709	1/1	0.61	0.20	106,106,106,106	0
54	MG	AA	1836	1/1	0.61	0.16	91,91,91,91	0
54	MG	BA	3231	1/1	0.61	0.21	89,89,89,89	0
54	MG	DA	3370	1/1	0.61	0.40	87,87,87,87	0
54	MG	CA	1739	1/1	0.61	0.26	120,120,120,120	0
54	MG	AA	1818	1/1	0.62	0.53	121,121,121,121	0
54	MG	BA	3456	1/1	0.62	0.13	225,225,225,225	0
54	MG	DA	3040	1/1	0.62	0.16	103,103,103,103	0
54	MG	CA	1697	1/1	0.63	0.30	95,95,95,95	0
54	MG	DA	3017	1/1	0.63	0.34	105,105,105,105	0
54	MG	CA	1660	1/1	0.64	0.15	101,101,101,101	0
54	MG	AA	1816	1/1	0.64	0.36	93,93,93,93	0
54	MG	DA	3149	1/1	0.64	0.24	79,79,79,79	0
54	MG	BA	3341	1/1	0.64	0.21	67,67,67,67	0
54	MG	BA	3531	1/1	0.64	0.31	83,83,83,83	0
54	MG	BA	3289	1/1	0.64	0.32	94,94,94,94	0
54	MG	AA	1612	1/1	0.64	0.19	131,131,131,131	0
54	MG	CA	1715	1/1	0.64	0.21	102,102,102,102	0
54	MG	BA	3519	1/1	0.65	0.38	115,115,115,115	0
54	MG	DA	3517	1/1	0.65	0.39	80,80,80,80	0
54	MG	BA	3522	1/1	0.66	0.46	100,100,100,100	0
54	MG	DB	214	1/1	0.66	0.12	101,101,101,101	0
54	MG	CA	1602	1/1	0.66	0.18	91,91,91,91	0
54	MG	BA	3149	1/1	0.66	0.27	91,91,91,91	0
54	MG	DA	3281	1/1	0.66	0.19	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	BA	3453	1/1	0.66	0.17	78,78,78,78	0
54	MG	BA	3481	1/1	0.66	0.20	79,79,79,79	0
54	MG	AA	1637	1/1	0.66	0.33	122,122,122,122	0
54	MG	AA	1700	1/1	0.66	0.20	84,84,84,84	0
54	MG	BA	3163	1/1	0.66	0.29	94,94,94,94	0
54	MG	BA	3196	1/1	0.67	0.26	85,85,85,85	0
54	MG	AA	1785	1/1	0.67	0.32	146,146,146,146	0
54	MG	DA	3358	1/1	0.67	0.18	113,113,113,113	0
54	MG	AA	1610	1/1	0.67	0.16	102,102,102,102	0
54	MG	CA	1639	1/1	0.67	0.18	95,95,95,95	0
54	MG	AA	1788	1/1	0.67	0.25	91,91,91,91	0
54	MG	BA	3114	1/1	0.67	0.16	98,98,98,98	0
54	MG	CA	1778	1/1	0.67	0.23	107,107,107,107	0
54	MG	AA	1773	1/1	0.67	0.42	125,125,125,125	0
54	MG	BA	3408	1/1	0.68	0.30	79,79,79,79	0
54	MG	DA	3390	1/1	0.68	0.23	76,76,76,76	0
54	MG	BA	3151	1/1	0.68	0.37	91,91,91,91	0
54	MG	BA	3489	1/1	0.68	0.18	84,84,84,84	0
54	MG	CA	1615	1/1	0.68	0.25	113,113,113,113	0
54	MG	CA	1724	1/1	0.68	0.30	94,94,94,94	0
54	MG	BA	3621	1/1	0.68	0.20	93,93,93,93	0
54	MG	DB	206	1/1	0.68	0.32	104,104,104,104	0
54	MG	AA	1714	1/1	0.68	0.21	88,88,88,88	0
54	MG	DA	3460	1/1	0.69	1.04	100,100,100,100	0
54	MG	AA	1677	1/1	0.69	0.37	109,109,109,109	0
54	MG	BA	3039	1/1	0.69	0.29	76,76,76,76	0
54	MG	BA	3440	1/1	0.69	0.32	73,73,73,73	0
54	MG	AA	1735	1/1	0.69	0.29	104,104,104,104	0
54	MG	BA	3362	1/1	0.69	0.30	83,83,83,83	0
54	MG	DA	3253	1/1	0.69	0.20	88,88,88,88	0
54	MG	AA	1740	1/1	0.70	0.42	83,83,83,83	0
54	MG	DA	3113	1/1	0.70	0.36	83,83,83,83	0
54	MG	DA	3327	1/1	0.70	0.22	75,75,75,75	0
54	MG	DA	3459	1/1	0.70	0.33	87,87,87,87	0
54	MG	AA	1782	1/1	0.70	0.42	124,124,124,124	0
54	MG	BA	3427	1/1	0.70	0.10	160,160,160,160	0
54	MG	BA	3090	1/1	0.70	0.26	85,85,85,85	0
54	MG	BA	3599	1/1	0.70	0.35	85,85,85,85	0
54	MG	BA	3099	1/1	0.70	0.14	68,68,68,68	0
54	MG	AA	1786	1/1	0.70	0.11	145,145,145,145	0
54	MG	BA	3367	1/1	0.70	0.23	91,91,91,91	0
54	MG	BA	3623	1/1	0.70	0.25	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	3457	1/1	0.70	0.22	84,84,84,84	0
54	MG	AD	101	1/1	0.70	0.27	114,114,114,114	0
54	MG	AA	1808	1/1	0.70	0.35	125,125,125,125	0
54	MG	BA	3419	1/1	0.70	0.28	81,81,81,81	0
54	MG	BA	3334	1/1	0.70	0.19	84,84,84,84	0
54	MG	BA	3450	1/1	0.71	0.11	166,166,166,166	0
54	MG	DB	211	1/1	0.71	0.39	90,90,90,90	0
54	MG	AA	1706	1/1	0.71	0.21	94,94,94,94	0
54	MG	CA	1751	1/1	0.71	0.20	95,95,95,95	0
54	MG	BA	3490	1/1	0.71	0.32	102,102,102,102	0
54	MG	DA	3278	1/1	0.71	0.22	91,91,91,91	0
54	MG	CA	1608	1/1	0.71	0.17	94,94,94,94	0
54	MG	CA	1613	1/1	0.71	0.31	86,86,86,86	0
54	MG	DA	3392	1/1	0.71	0.12	82,82,82,82	0
54	MG	BA	3277	1/1	0.71	0.30	89,89,89,89	0
54	MG	CA	1716	1/1	0.71	0.73	103,103,103,103	0
54	MG	BA	3432	1/1	0.72	0.27	81,81,81,81	0
54	MG	CG	301	1/1	0.72	0.21	113,113,113,113	0
54	MG	BA	3580	1/1	0.72	0.42	68,68,68,68	0
54	MG	BA	3089	1/1	0.72	0.36	87,87,87,87	0
54	MG	DA	3151	1/1	0.72	0.16	106,106,106,106	0
54	MG	BA	3392	1/1	0.72	0.23	91,91,91,91	0
54	MG	DA	3410	1/1	0.72	0.15	67,67,67,67	0
54	MG	DB	208	1/1	0.72	0.24	94,94,94,94	0
54	MG	DA	3282	1/1	0.72	0.30	88,88,88,88	0
54	MG	DA	3301	1/1	0.72	0.20	140,140,140,140	0
54	MG	BA	3222	1/1	0.72	0.25	62,62,62,62	0
54	MG	BA	3316	1/1	0.72	0.30	91,91,91,91	0
54	MG	AA	1765	1/1	0.72	0.39	122,122,122,122	0
54	MG	DA	3058	1/1	0.72	0.19	84,84,84,84	0
54	MG	BA	3332	1/1	0.72	0.36	92,92,92,92	0
54	MG	CC	107	1/1	0.72	0.22	105,105,105,105	0
54	MG	BA	3543	1/1	0.72	0.30	98,98,98,98	0
54	MG	AG	301	1/1	0.72	0.08	122,122,122,122	0
54	MG	BA	3130	1/1	0.73	0.29	105,105,105,105	0
54	MG	BB	214	1/1	0.73	0.15	99,99,99,99	0
54	MG	DA	3037	1/1	0.73	0.35	101,101,101,101	0
54	MG	DA	3348	1/1	0.73	0.27	90,90,90,90	0
54	MG	AA	1759	1/1	0.73	0.18	101,101,101,101	0
54	MG	AA	1751	1/1	0.73	0.25	90,90,90,90	0
54	MG	BA	3072	1/1	0.73	0.33	81,81,81,81	0
54	MG	BA	3364	1/1	0.73	0.32	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	AA	1606	1/1	0.73	0.15	101,101,101,101	0
54	MG	BA	3376	1/1	0.73	0.22	84,84,84,84	0
54	MG	DA	3443	1/1	0.73	0.12	85,85,85,85	0
54	MG	AA	1718	1/1	0.73	0.23	87,87,87,87	0
54	MG	DA	3064	1/1	0.73	0.39	88,88,88,88	0
54	MG	BA	3157	1/1	0.73	0.21	72,72,72,72	0
54	MG	BA	3391	1/1	0.73	0.35	85,85,85,85	0
54	MG	CA	1768	1/1	0.73	0.21	97,97,97,97	0
54	MG	DA	3274	1/1	0.73	0.37	100,100,100,100	0
54	MG	AA	1647	1/1	0.74	0.37	92,92,92,92	0
54	MG	DA	3434	1/1	0.74	0.22	92,92,92,92	0
54	MG	CA	1719	1/1	0.74	0.12	104,104,104,104	0
54	MG	BA	3301	1/1	0.74	0.32	91,91,91,91	0
54	MG	DA	3442	1/1	0.74	0.18	105,105,105,105	0
54	MG	DA	3444	1/1	0.74	0.11	133,133,133,133	0
54	MG	DA	3111	1/1	0.74	0.35	105,105,105,105	0
54	MG	DA	3379	1/1	0.74	0.30	88,88,88,88	0
54	MG	BA	3353	1/1	0.74	0.46	95,95,95,95	0
54	MG	DA	3519	1/1	0.74	0.12	81,81,81,81	0
54	MG	DA	3289	1/1	0.74	0.34	110,110,110,110	0
54	MG	BA	3342	1/1	0.74	0.23	85,85,85,85	0
54	MG	BA	3230	1/1	0.75	0.19	71,71,71,71	0
54	MG	BA	3180	1/1	0.75	0.50	92,92,92,92	0
54	MG	BA	3380	1/1	0.75	0.24	74,74,74,74	0
54	MG	CA	1767	1/1	0.75	0.31	80,80,80,80	0
54	MG	CA	1708	1/1	0.75	0.19	98,98,98,98	0
54	MG	DA	3324	1/1	0.75	0.45	90,90,90,90	0
54	MG	BA	3442	1/1	0.75	0.23	89,89,89,89	0
54	MG	BA	3533	1/1	0.75	0.25	89,89,89,89	0
54	MG	DA	3501	1/1	0.75	0.17	82,82,82,82	0
54	MG	CA	1725	1/1	0.75	0.19	115,115,115,115	0
54	MG	DA	3382	1/1	0.75	0.34	94,94,94,94	0
54	MG	BA	3597	1/1	0.75	0.29	103,103,103,103	0
54	MG	BA	3499	1/1	0.75	0.21	82,82,82,82	0
54	MG	BA	3503	1/1	0.75	0.42	117,117,117,117	0
54	MG	CA	1707	1/1	0.75	0.27	88,88,88,88	0
54	MG	AA	1694	1/1	0.75	0.29	87,87,87,87	0
54	MG	CA	1695	1/1	0.75	0.12	119,119,119,119	0
54	MG	CA	1603	1/1	0.76	0.33	115,115,115,115	0
54	MG	BA	3360	1/1	0.76	0.24	85,85,85,85	0
54	MG	CC	109	1/1	0.76	0.22	111,111,111,111	0
54	MG	DA	3461	1/1	0.76	0.21	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	BA	3397	1/1	0.76	0.36	84,84,84,84	0
54	MG	BA	3469	1/1	0.76	0.44	94,94,94,94	0
54	MG	BA	3206	1/1	0.76	0.30	89,89,89,89	0
54	MG	AA	1817	1/1	0.76	0.13	137,137,137,137	0
54	MG	BA	3365	1/1	0.76	0.17	86,86,86,86	0
54	MG	BA	3465	1/1	0.76	0.20	79,79,79,79	0
54	MG	DA	3304	1/1	0.76	0.21	88,88,88,88	0
54	MG	DA	3005	1/1	0.76	0.36	99,99,99,99	0
54	MG	AA	1688	1/1	0.76	0.35	118,118,118,118	0
54	MG	AA	1777	1/1	0.76	0.12	117,117,117,117	0
54	MG	DA	3309	1/1	0.76	0.14	64,64,64,64	0
54	MG	AA	1797	1/1	0.76	0.39	102,102,102,102	0
54	MG	AA	1693	1/1	0.76	0.20	106,106,106,106	0
54	MG	BA	3566	1/1	0.76	0.44	70,70,70,70	0
54	MG	BA	3349	1/1	0.76	0.14	64,64,64,64	0
54	MG	CA	1795	1/1	0.76	0.11	87,87,87,87	0
54	MG	DA	3496	1/1	0.76	0.17	86,86,86,86	0
54	MG	BA	3394	1/1	0.77	0.22	102,102,102,102	0
54	MG	BA	3109	1/1	0.77	0.32	89,89,89,89	0
54	MG	BA	3404	1/1	0.77	0.29	90,90,90,90	0
54	MG	AA	1730	1/1	0.77	0.23	90,90,90,90	0
54	MG	BA	3327	1/1	0.77	0.35	85,85,85,85	0
54	MG	BA	3345	1/1	0.77	0.32	91,91,91,91	0
54	MG	AA	1754	1/1	0.77	0.18	91,91,91,91	0
54	MG	BA	3273	1/1	0.77	0.20	80,80,80,80	0
54	MG	DA	3492	1/1	0.77	0.22	96,96,96,96	0
54	MG	AA	1734	1/1	0.77	0.33	135,135,135,135	0
54	MG	AA	1755	1/1	0.77	0.21	88,88,88,88	0
54	MG	DA	3072	1/1	0.77	0.11	109,109,109,109	0
54	MG	DA	3023	1/1	0.77	0.15	76,76,76,76	0
54	MG	AA	1679	1/1	0.77	0.33	86,86,86,86	0
54	MG	BA	3249	1/1	0.78	0.23	74,74,74,74	0
54	MG	DE	303	1/1	0.78	0.12	85,85,85,85	0
54	MG	BA	3594	1/1	0.78	0.66	81,81,81,81	0
54	MG	CA	1620	1/1	0.78	0.25	75,75,75,75	0
54	MG	BA	3183	1/1	0.78	0.37	75,75,75,75	0
54	MG	DA	3316	1/1	0.78	0.30	76,76,76,76	0
54	MG	BA	3245	1/1	0.78	0.32	67,67,67,67	0
54	MG	DA	3144	1/1	0.78	0.23	79,79,79,79	0
54	MG	DA	3329	1/1	0.78	0.46	88,88,88,88	0
54	MG	AA	1829	1/1	0.78	0.19	81,81,81,81	0
54	MG	AA	1684	1/1	0.78	0.37	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	DA	3277	1/1	0.78	0.36	76,76,76,76	0
54	MG	DA	3455	1/1	0.78	0.36	80,80,80,80	0
54	MG	DA	3493	1/1	0.78	0.11	90,90,90,90	0
54	MG	CA	1752	1/1	0.78	0.11	94,94,94,94	0
54	MG	CA	1713	1/1	0.78	0.18	109,109,109,109	0
54	MG	AA	1621	1/1	0.78	0.32	101,101,101,101	0
54	MG	DA	3187	1/1	0.78	0.27	83,83,83,83	0
54	MG	BA	3588	1/1	0.78	0.44	77,77,77,77	0
54	MG	DA	3325	1/1	0.78	0.25	92,92,92,92	0
54	MG	DA	3134	1/1	0.78	0.13	96,96,96,96	0
54	MG	BA	3493	1/1	0.78	0.27	74,74,74,74	0
54	MG	BA	3393	1/1	0.78	0.51	89,89,89,89	0
56	ZN	CG	303	1/1	0.78	0.27	139,139,139,139	0
54	MG	AA	1692	1/1	0.78	0.20	94,94,94,94	0
54	MG	BA	3237	1/1	0.78	0.49	64,64,64,64	0
54	MG	DA	3416	1/1	0.79	0.30	86,86,86,86	0
54	MG	BA	3518	1/1	0.79	0.54	87,87,87,87	0
54	MG	BA	3381	1/1	0.79	0.27	89,89,89,89	0
54	MG	DA	3137	1/1	0.79	0.36	86,86,86,86	0
54	MG	BA	3423	1/1	0.79	0.40	100,100,100,100	0
54	MG	DA	3270	1/1	0.79	0.41	90,90,90,90	0
54	MG	BA	3223	1/1	0.79	0.19	84,84,84,84	0
54	MG	AA	1736	1/1	0.79	0.23	92,92,92,92	0
54	MG	DA	3161	1/1	0.79	0.17	84,84,84,84	0
54	MG	DA	3214	1/1	0.79	0.25	69,69,69,69	0
54	MG	DA	3084	1/1	0.79	0.15	67,67,67,67	0
54	MG	DA	3056	1/1	0.79	0.24	97,97,97,97	0
54	MG	DA	3411	1/1	0.79	0.34	88,88,88,88	0
54	MG	AA	1758	1/1	0.79	0.22	71,71,71,71	0
54	MG	DA	3029	1/1	0.79	0.18	96,96,96,96	0
54	MG	CA	1698	1/1	0.79	0.19	96,96,96,96	0
54	MG	DA	3254	1/1	0.79	0.26	79,79,79,79	0
54	MG	AA	1649	1/1	0.79	0.31	81,81,81,81	0
54	MG	DA	3520	1/1	0.79	0.33	99,99,99,99	0
54	MG	CA	1629	1/1	0.79	0.12	107,107,107,107	0
54	MG	DA	3428	1/1	0.79	0.16	86,86,86,86	0
54	MG	BA	3300	1/1	0.79	0.42	95,95,95,95	0
54	MG	BA	3517	1/1	0.79	0.37	90,90,90,90	0
54	MG	DA	3024	1/1	0.79	0.15	110,110,110,110	0
54	MG	BA	3361	1/1	0.79	0.26	76,76,76,76	0
54	MG	AA	1725	1/1	0.79	0.17	105,105,105,105	0
54	MG	AA	1731	1/1	0.79	0.14	97,97,97,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	CA	1769	1/1	0.79	0.29	101,101,101,101	0
54	MG	AC	104	1/1	0.80	0.26	100,100,100,100	0
54	MG	DA	3374	1/1	0.80	0.25	87,87,87,87	0
54	MG	BA	3429	1/1	0.80	0.55	103,103,103,103	0
54	MG	CA	1765	1/1	0.80	0.19	122,122,122,122	0
54	MG	AA	1814	1/1	0.80	0.16	91,91,91,91	0
54	MG	BB	206	1/1	0.80	0.21	84,84,84,84	0
54	MG	BA	3290	1/1	0.80	0.19	82,82,82,82	0
54	MG	BU	202	1/1	0.80	0.20	71,71,71,71	0
54	MG	BE	303	1/1	0.80	0.30	89,89,89,89	0
54	MG	BA	3248	1/1	0.80	0.21	76,76,76,76	0
54	MG	BA	3619	1/1	0.80	0.32	87,87,87,87	0
54	MG	AA	1800	1/1	0.80	0.21	89,89,89,89	0
54	MG	CA	1681	1/1	0.80	0.33	88,88,88,88	0
54	MG	DA	3071	1/1	0.80	0.13	107,107,107,107	0
54	MG	BA	3550	1/1	0.80	0.23	98,98,98,98	0
54	MG	CC	105	1/1	0.80	0.38	86,86,86,86	0
54	MG	DA	3258	1/1	0.80	0.37	86,86,86,86	0
54	MG	BA	3336	1/1	0.80	0.21	72,72,72,72	0
54	MG	BA	3240	1/1	0.80	0.23	84,84,84,84	0
54	MG	BA	3604	1/1	0.80	0.28	92,92,92,92	0
54	MG	AA	1732	1/1	0.80	0.11	104,104,104,104	0
54	MG	AA	1723	1/1	0.80	0.21	82,82,82,82	0
54	MG	CA	1796	1/1	0.80	0.11	81,81,81,81	0
54	MG	CA	1642	1/1	0.80	0.12	116,116,116,116	0
54	MG	AA	1727	1/1	0.80	0.21	88,88,88,88	0
54	MG	BA	3555	1/1	0.80	0.15	105,105,105,105	0
54	MG	BA	3523	1/1	0.80	0.35	82,82,82,82	0
54	MG	DA	3360	1/1	0.80	0.36	86,86,86,86	0
54	MG	CA	1689	1/1	0.80	0.15	98,98,98,98	0
54	MG	DA	3420	1/1	0.80	0.21	84,84,84,84	0
54	MG	BA	3618	1/1	0.80	0.20	87,87,87,87	0
54	MG	BA	3400	1/1	0.80	0.17	72,72,72,72	0
54	MG	BA	3111	1/1	0.80	0.46	85,85,85,85	0
54	MG	AA	1793	1/1	0.81	0.27	71,71,71,71	0
54	MG	DA	3007	1/1	0.81	0.34	76,76,76,76	0
54	MG	CA	1621	1/1	0.81	0.21	82,82,82,82	0
54	MG	CA	1791	1/1	0.81	0.14	95,95,95,95	0
54	MG	DA	3240	1/1	0.81	0.16	86,86,86,86	0
54	MG	AA	1828	1/1	0.81	0.24	107,107,107,107	0
54	MG	AA	1674	1/1	0.81	0.24	93,93,93,93	0
54	MG	CA	1782	1/1	0.81	0.32	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	3458	1/1	0.81	0.12	91,91,91,91	0
54	MG	DA	3013	1/1	0.81	0.12	95,95,95,95	0
54	MG	DE	302	1/1	0.81	0.22	96,96,96,96	0
54	MG	DA	3290	1/1	0.81	0.22	75,75,75,75	0
54	MG	AA	1673	1/1	0.81	0.13	131,131,131,131	0
54	MG	DA	3409	1/1	0.81	0.30	95,95,95,95	0
54	MG	DB	213	1/1	0.81	0.50	111,111,111,111	0
54	MG	BA	3603	1/1	0.81	0.23	93,93,93,93	0
54	MG	CC	104	1/1	0.81	0.20	103,103,103,103	0
54	MG	BA	3221	1/1	0.81	0.34	93,93,93,93	0
54	MG	BA	3630	1/1	0.81	0.21	93,93,93,93	0
54	MG	BA	3228	1/1	0.81	0.17	62,62,62,62	0
54	MG	DA	3279	1/1	0.81	0.17	70,70,70,70	0
54	MG	AA	1616	1/1	0.81	0.33	81,81,81,81	0
54	MG	BA	3462	1/1	0.81	0.27	94,94,94,94	0
54	MG	BB	212	1/1	0.81	0.34	82,82,82,82	0
54	MG	AA	1687	1/1	0.81	0.14	137,137,137,137	0
54	MG	BA	3374	1/1	0.81	0.36	74,74,74,74	0
54	MG	BA	3150	1/1	0.81	0.47	76,76,76,76	0
54	MG	BA	3436	1/1	0.81	0.25	75,75,75,75	0
54	MG	CA	1760	1/1	0.81	0.31	109,109,109,109	0
54	MG	BA	3313	1/1	0.81	0.48	94,94,94,94	0
54	MG	BA	3585	1/1	0.81	0.44	77,77,77,77	0
54	MG	AA	1683	1/1	0.81	0.25	97,97,97,97	0
54	MG	BA	3629	1/1	0.81	0.26	100,100,100,100	0
54	MG	DA	3424	1/1	0.81	0.47	114,114,114,114	0
54	MG	BA	3118	1/1	0.81	0.48	83,83,83,83	0
54	MG	BA	3355	1/1	0.81	0.40	86,86,86,86	0
54	MG	AA	1833	1/1	0.81	0.11	98,98,98,98	0
54	MG	CA	1749	1/1	0.81	0.24	91,91,91,91	0
54	MG	AA	1671	1/1	0.82	0.38	81,81,81,81	0
54	MG	BA	3516	1/1	0.82	0.49	90,90,90,90	0
54	MG	DA	3036	1/1	0.82	0.40	114,114,114,114	0
54	MG	DA	3085	1/1	0.82	0.41	89,89,89,89	0
54	MG	DA	3389	1/1	0.82	0.13	82,82,82,82	0
54	MG	BA	3279	1/1	0.82	0.39	68,68,68,68	0
54	MG	AA	1768	1/1	0.82	0.15	89,89,89,89	0
54	MG	BA	3414	1/1	0.82	0.79	102,102,102,102	0
54	MG	BA	3530	1/1	0.82	0.26	85,85,85,85	0
54	MG	DA	3184	1/1	0.82	0.26	87,87,87,87	0
54	MG	BA	3094	1/1	0.82	0.29	103,103,103,103	0
54	MG	BA	3375	1/1	0.82	0.46	99,99,99,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	DA	3049	1/1	0.82	0.28	92,92,92,92	0
54	MG	DA	3387	1/1	0.82	0.18	89,89,89,89	0
54	MG	BA	3614	1/1	0.82	0.21	92,92,92,92	0
54	MG	DA	3077	1/1	0.82	0.35	110,110,110,110	0
54	MG	DA	3089	1/1	0.82	0.32	81,81,81,81	0
54	MG	DA	3150	1/1	0.82	0.29	91,91,91,91	0
54	MG	BB	213	1/1	0.82	0.28	103,103,103,103	0
54	MG	CA	1604	1/1	0.82	0.11	91,91,91,91	0
54	MG	DA	3096	1/1	0.82	0.43	88,88,88,88	0
54	MG	BB	211	1/1	0.82	0.27	99,99,99,99	0
54	MG	DA	3006	1/1	0.82	0.39	95,95,95,95	0
54	MG	DA	3377	1/1	0.82	0.18	85,85,85,85	0
54	MG	DA	3488	1/1	0.82	0.14	77,77,77,77	0
54	MG	CA	1678	1/1	0.82	0.31	75,75,75,75	0
54	MG	DA	3067	1/1	0.82	0.43	93,93,93,93	0
54	MG	DA	3311	1/1	0.82	0.42	74,74,74,74	0
54	MG	AA	1812	1/1	0.82	0.51	99,99,99,99	0
54	MG	BA	3100	1/1	0.82	0.21	105,105,105,105	0
54	MG	BA	3573	1/1	0.82	0.19	87,87,87,87	0
54	MG	DA	3026	1/1	0.82	0.23	76,76,76,76	0
54	MG	AA	1772	1/1	0.82	0.32	110,110,110,110	0
54	MG	CA	1766	1/1	0.82	0.23	74,74,74,74	0
54	MG	BA	3068	1/1	0.83	0.36	94,94,94,94	0
54	MG	CA	1679	1/1	0.83	0.24	97,97,97,97	0
54	MG	DA	3168	1/1	0.83	0.11	69,69,69,69	0
54	MG	CA	1747	1/1	0.83	0.34	96,96,96,96	0
54	MG	BA	3583	1/1	0.83	0.21	88,88,88,88	0
54	MG	BA	3622	1/1	0.83	0.24	97,97,97,97	0
54	MG	BA	3596	1/1	0.83	0.24	85,85,85,85	0
54	MG	BA	3141	1/1	0.83	0.31	76,76,76,76	0
54	MG	AA	1748	1/1	0.83	0.15	152,152,152,152	0
54	MG	DA	3082	1/1	0.83	0.15	97,97,97,97	0
54	MG	AA	1636	1/1	0.83	0.21	76,76,76,76	0
54	MG	AA	1641	1/1	0.83	0.22	74,74,74,74	0
54	MG	BA	3270	1/1	0.83	0.41	91,91,91,91	0
54	MG	DA	3429	1/1	0.83	0.27	103,103,103,103	0
54	MG	AA	1787	1/1	0.83	0.09	89,89,89,89	0
54	MG	DA	3153	1/1	0.83	0.31	88,88,88,88	0
54	MG	CA	1626	1/1	0.83	0.24	115,115,115,115	0
54	MG	DB	207	1/1	0.83	0.27	133,133,133,133	0
54	MG	AA	1660	1/1	0.83	0.16	68,68,68,68	0
54	MG	DA	3462	1/1	0.83	0.28	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	1835	1/1	0.83	0.30	100,100,100,100	0
54	MG	BA	3426	1/1	0.83	0.36	100,100,100,100	0
54	MG	A1	101	1/1	0.83	0.19	94,94,94,94	0
54	MG	BA	3534	1/1	0.83	0.44	85,85,85,85	0
54	MG	BA	3257	1/1	0.83	0.36	73,73,73,73	0
54	MG	BA	3537	1/1	0.83	0.13	65,65,65,65	0
54	MG	BA	3308	1/1	0.83	0.18	108,108,108,108	0
54	MG	BA	3121	1/1	0.83	0.24	98,98,98,98	0
54	MG	AA	1811	1/1	0.83	0.63	102,102,102,102	0
54	MG	DA	3407	1/1	0.83	0.16	94,94,94,94	0
54	MG	DA	3155	1/1	0.83	0.22	74,74,74,74	0
54	MG	DA	3154	1/1	0.83	0.17	102,102,102,102	0
54	MG	AA	1681	1/1	0.83	0.20	101,101,101,101	0
54	MG	AA	1638	1/1	0.83	0.19	109,109,109,109	0
54	MG	BA	3424	1/1	0.83	0.26	86,86,86,86	0
54	MG	BA	3390	1/1	0.83	0.37	95,95,95,95	0
54	MG	CA	1640	1/1	0.83	0.24	99,99,99,99	0
54	MG	AA	1617	1/1	0.83	0.25	97,97,97,97	0
54	MG	DA	3167	1/1	0.83	0.31	105,105,105,105	0
54	MG	DA	3018	1/1	0.83	0.12	90,90,90,90	0
54	MG	BA	3547	1/1	0.83	0.45	84,84,84,84	0
54	MG	DA	3192	1/1	0.84	0.27	92,92,92,92	0
54	MG	BA	3428	1/1	0.84	0.12	90,90,90,90	0
54	MG	AN	202	1/1	0.84	0.08	88,88,88,88	0
54	MG	BA	3191	1/1	0.84	0.26	78,78,78,78	0
54	MG	BA	3417	1/1	0.84	0.41	82,82,82,82	0
54	MG	DA	3051	1/1	0.84	0.36	78,78,78,78	0
54	MG	CA	1622	1/1	0.84	0.40	113,113,113,113	0
54	MG	CA	1641	1/1	0.84	0.30	78,78,78,78	0
54	MG	DA	3020	1/1	0.84	0.28	81,81,81,81	0
54	MG	CA	1799	1/1	0.84	0.10	115,115,115,115	0
54	MG	BA	3225	1/1	0.84	0.22	75,75,75,75	0
54	MG	CA	1624	1/1	0.84	0.11	92,92,92,92	0
54	MG	DA	3326	1/1	0.84	0.27	82,82,82,82	0
54	MG	CC	108	1/1	0.84	0.12	120,120,120,120	0
54	MG	BA	3347	1/1	0.84	0.40	86,86,86,86	0
54	MG	CA	1616	1/1	0.84	0.11	102,102,102,102	0
54	MG	BA	3227	1/1	0.84	0.10	101,101,101,101	0
54	MG	CA	1771	1/1	0.84	0.34	96,96,96,96	0
54	MG	AA	1767	1/1	0.84	0.21	82,82,82,82	0
54	MG	BA	3525	1/1	0.84	0.30	47,47,47,47	0
54	MG	CA	1735	1/1	0.84	0.30	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	BA	3410	1/1	0.84	0.44	83,83,83,83	0
54	MG	CA	1779	1/1	0.84	0.23	97,97,97,97	0
54	MG	BA	3296	1/1	0.84	0.39	81,81,81,81	0
54	MG	BA	3131	1/1	0.84	0.40	80,80,80,80	0
54	MG	BA	3287	1/1	0.84	0.46	70,70,70,70	0
54	MG	AA	1825	1/1	0.84	0.15	92,92,92,92	0
54	MG	CA	1701	1/1	0.84	0.24	90,90,90,90	0
54	MG	BA	3322	1/1	0.84	0.27	76,76,76,76	0
54	MG	BA	3416	1/1	0.84	0.15	92,92,92,92	0
54	MG	D1	201	1/1	0.84	0.27	72,72,72,72	0
54	MG	BA	3165	1/1	0.85	0.37	48,48,48,48	0
54	MG	AA	1790	1/1	0.85	0.26	97,97,97,97	0
54	MG	CA	1704	1/1	0.85	0.32	99,99,99,99	0
54	MG	AA	1634	1/1	0.85	0.22	97,97,97,97	0
54	MG	BA	3318	1/1	0.85	0.38	71,71,71,71	0
54	MG	CA	1614	1/1	0.85	0.15	100,100,100,100	0
54	MG	DA	3445	1/1	0.85	0.10	96,96,96,96	0
54	MG	DB	202	1/1	0.85	0.18	116,116,116,116	0
54	MG	DA	3142	1/1	0.85	0.28	83,83,83,83	0
54	MG	BA	3385	1/1	0.85	0.36	79,79,79,79	0
54	MG	DA	3287	1/1	0.85	0.18	102,102,102,102	0
54	MG	DA	3399	1/1	0.85	0.13	103,103,103,103	0
54	MG	BA	3540	1/1	0.85	0.20	78,78,78,78	0
54	MG	BA	3087	1/1	0.85	0.21	72,72,72,72	0
54	MG	BA	3167	1/1	0.85	0.23	68,68,68,68	0
54	MG	DA	3384	1/1	0.85	0.32	81,81,81,81	0
54	MG	DA	3196	1/1	0.85	0.20	72,72,72,72	0
54	MG	DA	3129	1/1	0.85	0.24	79,79,79,79	0
54	MG	DA	3418	1/1	0.85	0.16	97,97,97,97	0
54	MG	DA	3386	1/1	0.85	0.26	71,71,71,71	0
54	MG	DA	3333	1/1	0.85	0.38	90,90,90,90	0
54	MG	DA	3019	1/1	0.85	0.15	79,79,79,79	0
54	MG	AA	1715	1/1	0.85	0.35	112,112,112,112	0
54	MG	DA	3223	1/1	0.85	0.35	73,73,73,73	0
54	MG	AA	1801	1/1	0.85	0.28	113,113,113,113	0
54	MG	BB	215	1/1	0.85	0.15	110,110,110,110	0
54	MG	AA	1654	1/1	0.85	0.28	99,99,99,99	0
54	MG	DA	3275	1/1	0.85	0.20	76,76,76,76	0
54	MG	BA	3626	1/1	0.85	0.20	87,87,87,87	0
54	MG	BA	3528	1/1	0.85	0.20	74,74,74,74	0
54	MG	BA	3529	1/1	0.85	0.24	87,87,87,87	0
54	MG	AA	1711	1/1	0.85	0.10	132,132,132,132	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	AA	1733	1/1	0.85	0.15	88,88,88,88	0
54	MG	BA	3263	1/1	0.85	0.19	73,73,73,73	0
54	MG	DA	3383	1/1	0.85	0.32	87,87,87,87	0
54	MG	AA	1810	1/1	0.85	0.26	89,89,89,89	0
54	MG	DA	3299	1/1	0.85	0.29	99,99,99,99	0
54	MG	DA	3515	1/1	0.85	0.29	101,101,101,101	0
54	MG	AA	1678	1/1	0.85	0.27	87,87,87,87	0
54	MG	DB	215	1/1	0.85	0.11	120,120,120,120	0
54	MG	DA	3314	1/1	0.85	0.25	91,91,91,91	0
54	MG	BA	3135	1/1	0.85	0.39	85,85,85,85	0
54	MG	DA	3356	1/1	0.85	0.12	84,84,84,84	0
54	MG	BA	3092	1/1	0.85	0.37	72,72,72,72	0
54	MG	B8	102	1/1	0.85	0.57	107,107,107,107	0
54	MG	DA	3186	1/1	0.85	0.19	84,84,84,84	0
54	MG	AA	1631	1/1	0.85	0.28	92,92,92,92	0
54	MG	DA	3238	1/1	0.85	0.19	65,65,65,65	0
54	MG	DA	3330	1/1	0.85	0.38	95,95,95,95	0
54	MG	DB	209	1/1	0.85	0.14	97,97,97,97	0
54	MG	BA	3372	1/1	0.85	0.36	81,81,81,81	0
54	MG	BA	3344	1/1	0.85	0.13	91,91,91,91	0
54	MG	DA	3038	1/1	0.85	0.13	119,119,119,119	0
54	MG	BA	3326	1/1	0.85	0.31	89,89,89,89	0
54	MG	DA	3449	1/1	0.85	0.22	88,88,88,88	0
54	MG	BA	3217	1/1	0.85	0.29	98,98,98,98	0
54	MG	DA	3162	1/1	0.85	0.13	81,81,81,81	0
54	MG	DA	3139	1/1	0.85	0.20	63,63,63,63	0
54	MG	BA	3388	1/1	0.85	0.49	82,82,82,82	0
54	MG	BA	3160	1/1	0.85	0.46	92,92,92,92	0
54	MG	BA	3181	1/1	0.85	0.32	64,64,64,64	0
54	MG	CA	1750	1/1	0.85	0.33	97,97,97,97	0
54	MG	BA	3304	1/1	0.85	0.41	81,81,81,81	0
54	MG	CA	1653	1/1	0.85	0.21	124,124,124,124	0
54	MG	BA	3425	1/1	0.85	0.14	87,87,87,87	0
54	MG	DA	3095	1/1	0.85	0.15	88,88,88,88	0
54	MG	AA	1774	1/1	0.86	0.27	79,79,79,79	0
54	MG	DA	3283	1/1	0.86	0.16	69,69,69,69	0
54	MG	CA	1748	1/1	0.86	0.13	110,110,110,110	0
54	MG	DA	3039	1/1	0.86	0.35	80,80,80,80	0
54	MG	AA	1698	1/1	0.86	0.21	85,85,85,85	0
54	MG	DA	3045	1/1	0.86	0.30	93,93,93,93	0
54	MG	BA	3076	1/1	0.86	0.41	86,86,86,86	0
54	MG	BA	3488	1/1	0.86	0.37	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	CL	201	1/1	0.86	0.32	104,104,104,104	0
54	MG	BA	3377	1/1	0.86	0.17	81,81,81,81	0
54	MG	BA	3284	1/1	0.86	0.23	76,76,76,76	0
54	MG	AA	1713	1/1	0.86	0.42	82,82,82,82	0
54	MG	BA	3496	1/1	0.86	0.31	97,97,97,97	0
54	MG	AA	1799	1/1	0.86	0.45	111,111,111,111	0
54	MG	AA	1643	1/1	0.86	0.17	91,91,91,91	0
54	MG	BA	3359	1/1	0.86	0.24	83,83,83,83	0
54	MG	AA	1710	1/1	0.86	0.12	118,118,118,118	0
54	MG	CA	1635	1/1	0.86	0.11	93,93,93,93	0
54	MG	BA	3513	1/1	0.86	0.30	78,78,78,78	0
54	MG	BA	3500	1/1	0.86	0.17	92,92,92,92	0
54	MG	AA	1824	1/1	0.86	0.29	93,93,93,93	0
54	MG	BA	3161	1/1	0.86	0.35	70,70,70,70	0
54	MG	DA	3078	1/1	0.86	0.20	65,65,65,65	0
54	MG	DA	3222	1/1	0.86	0.52	82,82,82,82	0
54	MG	CA	1770	1/1	0.86	0.14	65,65,65,65	0
54	MG	DA	3300	1/1	0.86	0.26	83,83,83,83	0
54	MG	BA	3315	1/1	0.86	0.30	83,83,83,83	0
54	MG	DA	3366	1/1	0.86	0.30	78,78,78,78	0
54	MG	BA	3062	1/1	0.86	0.25	106,106,106,106	0
54	MG	DA	3244	1/1	0.86	0.51	89,89,89,89	0
54	MG	CA	1636	1/1	0.86	0.27	100,100,100,100	0
54	MG	DA	3319	1/1	0.86	0.09	97,97,97,97	0
54	MG	CA	1728	1/1	0.86	0.29	76,76,76,76	0
54	MG	CA	1664	1/1	0.86	0.22	169,169,169,169	0
54	MG	AA	1757	1/1	0.86	0.14	102,102,102,102	0
54	MG	BA	3545	1/1	0.86	0.19	76,76,76,76	0
54	MG	BA	3286	1/1	0.86	0.41	73,73,73,73	0
54	MG	AA	1724	1/1	0.86	0.58	126,126,126,126	0
54	MG	AA	1642	1/1	0.86	0.27	88,88,88,88	0
54	MG	AA	1605	1/1	0.86	0.07	103,103,103,103	0
54	MG	DA	3053	1/1	0.86	0.30	70,70,70,70	0
54	MG	DA	3373	1/1	0.86	0.30	107,107,107,107	0
54	MG	BB	205	1/1	0.86	0.36	91,91,91,91	0
54	MG	AA	1686	1/1	0.86	0.27	88,88,88,88	0
54	MG	BA	3498	1/1	0.86	0.27	94,94,94,94	0
54	MG	B3	101	1/1	0.86	0.46	84,84,84,84	0
54	MG	DB	201	1/1	0.86	0.35	90,90,90,90	0
54	MG	BA	3460	1/1	0.86	0.08	189,189,189,189	0
54	MG	BA	3589	1/1	0.86	0.28	66,66,66,66	0
54	MG	CA	1754	1/1	0.86	0.38	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	AA	1761	1/1	0.86	0.16	94,94,94,94	0
54	MG	BA	3088	1/1	0.86	0.30	84,84,84,84	0
54	MG	CA	1630	1/1	0.86	0.11	91,91,91,91	0
54	MG	BA	3441	1/1	0.86	0.23	95,95,95,95	0
54	MG	BF	302	1/1	0.86	0.19	71,71,71,71	0
54	MG	DA	3423	1/1	0.86	0.14	83,83,83,83	0
54	MG	BA	3506	1/1	0.86	0.33	74,74,74,74	0
54	MG	DA	3511	1/1	0.86	0.31	77,77,77,77	0
54	MG	DA	3490	1/1	0.86	0.06	77,77,77,77	0
54	MG	BA	3494	1/1	0.87	0.24	72,72,72,72	0
54	MG	B3	102	1/1	0.87	0.17	80,80,80,80	0
54	MG	DA	3451	1/1	0.87	0.32	81,81,81,81	0
54	MG	AA	1753	1/1	0.87	0.17	97,97,97,97	0
54	MG	CA	1761	1/1	0.87	0.18	103,103,103,103	0
54	MG	DA	3485	1/1	0.87	0.29	77,77,77,77	0
54	MG	DA	3272	1/1	0.87	0.17	65,65,65,65	0
54	MG	DA	3044	1/1	0.87	0.14	78,78,78,78	0
54	MG	BA	3030	1/1	0.87	0.35	70,70,70,70	0
54	MG	DA	3522	1/1	0.87	0.23	81,81,81,81	0
54	MG	DA	3221	1/1	0.87	0.32	74,74,74,74	0
54	MG	DA	3292	1/1	0.87	0.31	78,78,78,78	0
54	MG	DA	3364	1/1	0.87	0.11	102,102,102,102	0
54	MG	BA	3474	1/1	0.87	0.14	86,86,86,86	0
54	MG	CA	1762	1/1	0.87	0.14	83,83,83,83	0
54	MG	BA	3412	1/1	0.87	0.43	78,78,78,78	0
54	MG	DA	3345	1/1	0.87	0.16	91,91,91,91	0
54	MG	AA	1721	1/1	0.87	0.35	95,95,95,95	0
54	MG	BA	3051	1/1	0.87	0.35	74,74,74,74	0
54	MG	DA	3004	1/1	0.87	0.43	105,105,105,105	0
54	MG	DA	3306	1/1	0.87	0.14	88,88,88,88	0
54	MG	DA	3337	1/1	0.87	0.45	80,80,80,80	0
54	MG	BA	3570	1/1	0.87	0.13	65,65,65,65	0
54	MG	AA	1627	1/1	0.87	0.46	76,76,76,76	0
54	MG	DA	3127	1/1	0.87	0.08	91,91,91,91	0
54	MG	DA	3331	1/1	0.87	0.28	79,79,79,79	0
54	MG	DA	3422	1/1	0.87	0.12	83,83,83,83	0
54	MG	BA	3439	1/1	0.87	0.40	70,70,70,70	0
54	MG	CG	302	1/1	0.87	0.09	114,114,114,114	0
54	MG	BA	3324	1/1	0.87	0.28	70,70,70,70	0
54	MG	CA	1623	1/1	0.87	0.07	142,142,142,142	0
54	MG	DA	3516	1/1	0.87	0.28	76,76,76,76	0
54	MG	BA	3444	1/1	0.87	0.30	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	CA	1705	1/1	0.87	0.11	135,135,135,135	0
54	MG	DA	3401	1/1	0.87	0.30	93,93,93,93	0
54	MG	BA	3413	1/1	0.87	0.32	87,87,87,87	0
54	MG	BA	3124	1/1	0.87	0.34	85,85,85,85	0
54	MG	AA	1685	1/1	0.87	0.27	73,73,73,73	0
54	MG	AA	1822	1/1	0.87	0.17	101,101,101,101	0
54	MG	CA	1737	1/1	0.87	0.16	93,93,93,93	0
54	MG	BA	3320	1/1	0.87	0.45	82,82,82,82	0
54	MG	AA	1738	1/1	0.87	0.41	120,120,120,120	0
54	MG	DA	3426	1/1	0.87	0.18	95,95,95,95	0
54	MG	DA	3341	1/1	0.87	0.30	68,68,68,68	0
54	MG	DA	3495	1/1	0.87	0.16	125,125,125,125	0
54	MG	BA	3250	1/1	0.87	0.26	61,61,61,61	0
54	MG	DA	3293	1/1	0.87	0.36	72,72,72,72	0
54	MG	BA	3386	1/1	0.87	0.20	76,76,76,76	0
54	MG	BA	3170	1/1	0.88	0.19	57,57,57,57	0
54	MG	BA	3601	1/1	0.88	0.16	83,83,83,83	0
54	MG	BA	3319	1/1	0.88	0.25	82,82,82,82	0
54	MG	DA	3178	1/1	0.88	0.38	70,70,70,70	0
54	MG	B7	101	1/1	0.88	0.38	69,69,69,69	0
54	MG	DA	3521	1/1	0.88	0.40	104,104,104,104	0
54	MG	BA	3548	1/1	0.88	0.36	76,76,76,76	0
54	MG	DA	3332	1/1	0.88	0.20	94,94,94,94	0
54	MG	DA	3417	1/1	0.88	0.25	81,81,81,81	0
54	MG	BA	3232	1/1	0.88	0.21	95,95,95,95	0
54	MG	CA	1764	1/1	0.88	0.21	89,89,89,89	0
54	MG	BA	3093	1/1	0.88	0.14	72,72,72,72	0
54	MG	AA	1802	1/1	0.88	0.08	100,100,100,100	0
54	MG	CA	1694	1/1	0.88	0.14	91,91,91,91	0
54	MG	AA	1745	1/1	0.88	0.40	78,78,78,78	0
54	MG	BA	3058	1/1	0.88	0.25	68,68,68,68	0
54	MG	DA	3435	1/1	0.88	0.09	134,134,134,134	0
54	MG	CA	1722	1/1	0.88	0.33	104,104,104,104	0
54	MG	DA	3414	1/1	0.88	0.23	92,92,92,92	0
54	MG	CS	101	1/1	0.88	0.19	95,95,95,95	0
54	MG	AA	1719	1/1	0.88	0.20	98,98,98,98	0
54	MG	BA	3229	1/1	0.88	0.39	64,64,64,64	0
54	MG	DA	3436	1/1	0.88	0.32	92,92,92,92	0
54	MG	BA	3065	1/1	0.88	0.46	68,68,68,68	0
54	MG	BA	3329	1/1	0.88	0.44	62,62,62,62	0
54	MG	AA	1796	1/1	0.88	0.41	76,76,76,76	0
54	MG	AA	1695	1/1	0.88	0.13	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	3358	1/1	0.88	0.33	82,82,82,82	0
54	MG	CA	1757	1/1	0.88	0.10	100,100,100,100	0
54	MG	BA	3079	1/1	0.88	0.26	103,103,103,103	0
54	MG	DA	3350	1/1	0.88	0.37	85,85,85,85	0
54	MG	CA	1702	1/1	0.88	0.23	84,84,84,84	0
54	MG	DA	3075	1/1	0.88	0.28	93,93,93,93	0
54	MG	BA	3466	1/1	0.88	0.16	81,81,81,81	0
54	MG	CA	1631	1/1	0.88	0.11	102,102,102,102	0
54	MG	CA	1745	1/1	0.88	0.30	102,102,102,102	0
54	MG	DA	3466	1/1	0.88	0.15	123,123,123,123	0
54	MG	DA	3425	1/1	0.88	0.15	82,82,82,82	0
54	MG	BA	3166	1/1	0.88	0.26	72,72,72,72	0
54	MG	AA	1624	1/1	0.88	0.14	92,92,92,92	0
54	MG	BA	3197	1/1	0.88	0.28	89,89,89,89	0
54	MG	BA	3368	1/1	0.88	0.18	98,98,98,98	0
54	MG	BA	3452	1/1	0.88	0.28	108,108,108,108	0
54	MG	BA	3507	1/1	0.88	0.28	79,79,79,79	0
54	MG	DA	3380	1/1	0.88	0.17	90,90,90,90	0
54	MG	BA	3205	1/1	0.88	0.28	51,51,51,51	0
54	MG	AA	1807	1/1	0.88	0.46	79,79,79,79	0
54	MG	BA	3352	1/1	0.88	0.27	112,112,112,112	0
54	MG	DA	3400	1/1	0.88	0.20	95,95,95,95	0
54	MG	DA	3308	1/1	0.88	0.24	78,78,78,78	0
54	MG	AA	1620	1/1	0.88	0.07	140,140,140,140	0
54	MG	BA	3054	1/1	0.88	0.29	100,100,100,100	0
54	MG	BA	3343	1/1	0.88	0.42	73,73,73,73	0
54	MG	BA	3458	1/1	0.88	0.47	78,78,78,78	0
54	MG	DA	3016	1/1	0.89	0.17	74,74,74,74	0
54	MG	DA	3066	1/1	0.89	0.17	80,80,80,80	0
54	MG	BA	3406	1/1	0.89	0.19	88,88,88,88	0
54	MG	BA	3578	1/1	0.89	0.26	73,73,73,73	0
54	MG	BA	3171	1/1	0.89	0.52	92,92,92,92	0
54	MG	DA	3081	1/1	0.89	0.21	91,91,91,91	0
54	MG	CA	1699	1/1	0.89	0.36	80,80,80,80	0
54	MG	BA	3049	1/1	0.89	0.20	59,59,59,59	0
54	MG	DA	3158	1/1	0.89	0.34	71,71,71,71	0
54	MG	BA	3330	1/1	0.89	0.49	91,91,91,91	0
54	MG	BA	3169	1/1	0.89	0.14	65,65,65,65	0
54	MG	B7	102	1/1	0.89	0.29	78,78,78,78	0
54	MG	DA	3318	1/1	0.89	0.33	88,88,88,88	0
54	MG	BA	3389	1/1	0.89	0.26	74,74,74,74	0
54	MG	DA	3101	1/1	0.89	0.32	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	AA	1696	1/1	0.89	0.16	80,80,80,80	0
54	MG	DA	3498	1/1	0.89	0.11	71,71,71,71	0
54	MG	CA	1775	1/1	0.89	0.14	84,84,84,84	0
54	MG	DA	3093	1/1	0.89	0.28	88,88,88,88	0
54	MG	DA	3166	1/1	0.89	0.17	91,91,91,91	0
54	MG	BA	3024	1/1	0.89	0.35	56,56,56,56	0
54	MG	AA	1672	1/1	0.89	0.46	86,86,86,86	0
54	MG	AA	1794	1/1	0.89	0.48	93,93,93,93	0
54	MG	AA	1804	1/1	0.89	0.41	81,81,81,81	0
54	MG	DA	3266	1/1	0.89	0.15	87,87,87,87	0
54	MG	BA	3616	1/1	0.89	0.22	73,73,73,73	0
54	MG	AA	1739	1/1	0.89	0.12	191,191,191,191	0
54	MG	DA	3171	1/1	0.89	0.38	64,64,64,64	0
54	MG	BA	3463	1/1	0.89	0.31	84,84,84,84	0
54	MG	D5	101	1/1	0.89	0.13	63,63,63,63	0
54	MG	BA	3052	1/1	0.89	0.55	81,81,81,81	0
54	MG	AA	1697	1/1	0.89	0.18	90,90,90,90	0
54	MG	DA	3323	1/1	0.89	0.16	84,84,84,84	0
54	MG	BA	3437	1/1	0.89	0.20	81,81,81,81	0
54	MG	CA	1692	1/1	0.89	0.29	93,93,93,93	0
54	MG	DA	3497	1/1	0.89	0.30	86,86,86,86	0
54	MG	BE	304	1/1	0.89	0.10	90,90,90,90	0
54	MG	DA	3502	1/1	0.89	0.16	67,67,67,67	0
54	MG	DA	3349	1/1	0.89	0.23	78,78,78,78	0
54	MG	BA	3307	1/1	0.89	0.30	75,75,75,75	0
54	MG	AC	102	1/1	0.89	0.38	102,102,102,102	0
54	MG	DA	3032	1/1	0.89	0.20	79,79,79,79	0
54	MG	DA	3453	1/1	0.89	0.45	92,92,92,92	0
54	MG	BA	3539	1/1	0.89	0.32	59,59,59,59	0
54	MG	CA	1648	1/1	0.89	0.24	88,88,88,88	0
54	MG	BA	3085	1/1	0.89	0.27	75,75,75,75	0
54	MG	BA	3219	1/1	0.89	0.21	82,82,82,82	0
54	MG	DA	3003	1/1	0.89	0.08	77,77,77,77	0
54	MG	BA	3204	1/1	0.89	0.38	106,106,106,106	0
54	MG	CA	1726	1/1	0.89	0.30	82,82,82,82	0
54	MG	CA	1774	1/1	0.89	0.15	105,105,105,105	0
54	MG	DA	3437	1/1	0.89	0.32	101,101,101,101	0
54	MG	DA	3047	1/1	0.89	0.14	91,91,91,91	0
54	MG	CA	1700	1/1	0.89	0.10	133,133,133,133	0
54	MG	DA	3477	1/1	0.89	0.14	67,67,67,67	0
54	MG	BA	3350	1/1	0.89	0.47	72,72,72,72	0
54	MG	AA	1645	1/1	0.89	0.29	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	BA	3095	1/1	0.89	0.46	57,57,57,57	0
54	MG	DA	3286	1/1	0.89	0.20	63,63,63,63	0
54	MG	DA	3268	1/1	0.89	0.36	76,76,76,76	0
54	MG	BA	3213	1/1	0.89	0.15	61,61,61,61	0
54	MG	CA	1703	1/1	0.89	0.44	85,85,85,85	0
54	MG	AA	1669	1/1	0.89	0.38	76,76,76,76	0
54	MG	BA	3325	1/1	0.89	0.14	79,79,79,79	0
54	MG	CA	1777	1/1	0.89	0.15	78,78,78,78	0
54	MG	DA	3430	1/1	0.89	0.20	110,110,110,110	0
54	MG	BA	3598	1/1	0.89	0.20	75,75,75,75	0
54	MG	BA	3536	1/1	0.89	0.29	74,74,74,74	0
54	MG	BA	3405	1/1	0.89	0.48	72,72,72,72	0
54	MG	DA	3463	1/1	0.89	0.31	75,75,75,75	0
54	MG	BA	3138	1/1	0.89	0.32	65,65,65,65	0
54	MG	DA	3242	1/1	0.89	0.44	66,66,66,66	0
54	MG	BA	3045	1/1	0.89	0.16	64,64,64,64	0
54	MG	BA	3328	1/1	0.89	0.33	68,68,68,68	0
54	MG	BA	3306	1/1	0.89	0.51	94,94,94,94	0
54	MG	BA	3297	1/1	0.89	0.33	86,86,86,86	0
54	MG	AA	1819	1/1	0.89	0.17	92,92,92,92	0
54	MG	CA	1643	1/1	0.89	0.24	86,86,86,86	0
54	MG	BA	3331	1/1	0.89	0.19	88,88,88,88	0
54	MG	AA	1798	1/1	0.89	0.40	93,93,93,93	0
54	MG	BA	3378	1/1	0.89	0.42	80,80,80,80	0
54	MG	DA	3243	1/1	0.89	0.30	71,71,71,71	0
54	MG	AN	201	1/1	0.89	0.09	91,91,91,91	0
54	MG	DA	3190	1/1	0.90	0.31	67,67,67,67	0
54	MG	AA	1613	1/1	0.90	0.34	97,97,97,97	0
54	MG	BA	3470	1/1	0.90	0.26	90,90,90,90	0
54	MG	BA	3346	1/1	0.90	0.17	74,74,74,74	0
54	MG	DA	3335	1/1	0.90	0.26	91,91,91,91	0
54	MG	BA	3275	1/1	0.90	0.33	90,90,90,90	0
54	MG	CA	1780	1/1	0.90	0.26	74,74,74,74	0
54	MG	DR	201	1/1	0.90	0.35	82,82,82,82	0
54	MG	CA	1741	1/1	0.90	0.14	114,114,114,114	0
54	MG	BO	201	1/1	0.90	0.19	79,79,79,79	0
54	MG	CA	1649	1/1	0.90	0.29	88,88,88,88	0
54	MG	BA	3600	1/1	0.90	0.25	65,65,65,65	0
54	MG	BA	3117	1/1	0.90	0.38	57,57,57,57	0
54	MG	BA	3264	1/1	0.90	0.31	78,78,78,78	0
54	MG	DA	3427	1/1	0.90	0.24	74,74,74,74	0
54	MG	BA	3508	1/1	0.90	0.19	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	CC	106	1/1	0.90	0.13	98,98,98,98	0
54	MG	CC	101	1/1	0.90	0.10	110,110,110,110	0
54	MG	BB	209	1/1	0.90	0.24	112,112,112,112	0
54	MG	DA	3367	1/1	0.90	0.34	89,89,89,89	0
54	MG	BA	3147	1/1	0.90	0.34	73,73,73,73	0
54	MG	AA	1795	1/1	0.90	0.33	86,86,86,86	0
54	MG	DA	3074	1/1	0.90	0.44	102,102,102,102	0
54	MG	BA	3174	1/1	0.90	0.27	63,63,63,63	0
54	MG	BA	3224	1/1	0.90	0.46	76,76,76,76	0
54	MG	DA	3369	1/1	0.90	0.28	91,91,91,91	0
54	MG	DA	3261	1/1	0.90	0.38	97,97,97,97	0
55	T1C	AA	1837	42/42	0.90	0.15	81,103,111,117	0
54	MG	DA	3041	1/1	0.90	0.11	82,82,82,82	0
54	MG	AA	1741	1/1	0.90	0.13	99,99,99,99	0
54	MG	BA	3134	1/1	0.90	0.30	66,66,66,66	0
54	MG	BA	3504	1/1	0.90	0.10	90,90,90,90	0
54	MG	BA	3527	1/1	0.90	0.21	78,78,78,78	0
54	MG	DA	3216	1/1	0.90	0.14	78,78,78,78	0
54	MG	AA	1803	1/1	0.90	0.36	75,75,75,75	0
54	MG	BA	3590	1/1	0.90	0.16	83,83,83,83	0
54	MG	DA	3217	1/1	0.90	0.35	89,89,89,89	0
54	MG	DA	3523	1/1	0.90	0.18	90,90,90,90	0
54	MG	CA	1625	1/1	0.90	0.12	115,115,115,115	0
54	MG	DA	3088	1/1	0.90	0.29	110,110,110,110	0
54	MG	BA	3403	1/1	0.90	0.33	103,103,103,103	0
54	MG	DA	3310	1/1	0.90	0.35	85,85,85,85	0
54	MG	DA	3394	1/1	0.90	0.20	75,75,75,75	0
54	MG	AA	1655	1/1	0.90	0.43	97,97,97,97	0
54	MG	BA	3195	1/1	0.90	0.20	43,43,43,43	0
54	MG	BA	3338	1/1	0.90	0.22	77,77,77,77	0
54	MG	DA	3265	1/1	0.90	0.18	91,91,91,91	0
54	MG	BA	3274	1/1	0.90	0.24	81,81,81,81	0
54	MG	BA	3625	1/1	0.90	0.19	113,113,113,113	0
54	MG	DA	3104	1/1	0.90	0.14	71,71,71,71	0
54	MG	DA	3456	1/1	0.90	0.10	105,105,105,105	0
54	MG	DA	3494	1/1	0.90	0.30	72,72,72,72	0
54	MG	DA	3398	1/1	0.90	0.19	84,84,84,84	0
54	MG	BA	3552	1/1	0.90	0.07	79,79,79,79	0
54	MG	CA	1786	1/1	0.90	0.25	83,83,83,83	0
54	MG	AA	1630	1/1	0.90	0.23	88,88,88,88	0
54	MG	DA	3182	1/1	0.90	0.33	74,74,74,74	0
54	MG	BA	3581	1/1	0.90	0.16	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	AC	108	1/1	0.90	0.17	95,95,95,95	0
54	MG	BB	208	1/1	0.90	0.17	89,89,89,89	0
54	MG	CA	1772	1/1	0.90	0.13	128,128,128,128	0
54	MG	AA	1667	1/1	0.90	0.52	82,82,82,82	0
54	MG	DA	3125	1/1	0.90	0.30	71,71,71,71	0
54	MG	AA	1827	1/1	0.90	0.12	112,112,112,112	0
54	MG	DU	201	1/1	0.90	0.24	89,89,89,89	0
54	MG	B1	201	1/1	0.90	0.30	68,68,68,68	0
54	MG	AA	1726	1/1	0.90	0.17	95,95,95,95	0
54	MG	AH	201	1/1	0.90	0.20	91,91,91,91	0
54	MG	BA	3271	1/1	0.90	0.14	98,98,98,98	0
54	MG	BA	3309	1/1	0.90	0.38	69,69,69,69	0
54	MG	CA	1652	1/1	0.90	0.31	106,106,106,106	0
54	MG	BA	3253	1/1	0.90	0.31	82,82,82,82	0
54	MG	BA	3356	1/1	0.90	0.56	81,81,81,81	0
54	MG	DA	3513	1/1	0.90	0.34	81,81,81,81	0
54	MG	BA	3479	1/1	0.90	0.34	80,80,80,80	0
54	MG	BA	3218	1/1	0.90	0.25	90,90,90,90	0
54	MG	DA	3347	1/1	0.90	0.11	79,79,79,79	0
54	MG	DA	3227	1/1	0.90	0.16	67,67,67,67	0
54	MG	AA	1608	1/1	0.90	0.35	91,91,91,91	0
54	MG	DB	203	1/1	0.90	0.27	81,81,81,81	0
54	MG	BA	3546	1/1	0.90	0.15	98,98,98,98	0
54	MG	BA	3487	1/1	0.90	0.17	72,72,72,72	0
55	T1C	CA	1800	42/42	0.90	0.15	101,116,124,127	0
54	MG	DA	3483	1/1	0.90	0.32	79,79,79,79	0
54	MG	BA	3434	1/1	0.90	0.15	86,86,86,86	0
54	MG	AA	1805	1/1	0.90	0.41	91,91,91,91	0
54	MG	BA	3333	1/1	0.91	0.17	83,83,83,83	0
54	MG	BA	3340	1/1	0.91	0.27	84,84,84,84	0
54	MG	DA	3448	1/1	0.91	0.41	89,89,89,89	0
54	MG	BA	3495	1/1	0.91	0.12	80,80,80,80	0
54	MG	BA	3177	1/1	0.91	0.20	87,87,87,87	0
54	MG	AA	1813	1/1	0.91	0.25	88,88,88,88	0
54	MG	CA	1758	1/1	0.91	0.21	94,94,94,94	0
54	MG	CA	1655	1/1	0.91	0.34	93,93,93,93	0
54	MG	BA	3384	1/1	0.91	0.26	73,73,73,73	0
54	MG	BA	3544	1/1	0.91	0.17	83,83,83,83	0
54	MG	DA	3194	1/1	0.91	0.43	54,54,54,54	0
54	MG	BA	3136	1/1	0.91	0.21	60,60,60,60	0
54	MG	CA	1644	1/1	0.91	0.27	85,85,85,85	0
54	MG	DA	3145	1/1	0.91	0.19	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	AA	1702	1/1	0.91	0.24	80,80,80,80	0
54	MG	DA	3246	1/1	0.91	0.28	89,89,89,89	0
54	MG	DA	3046	1/1	0.91	0.22	78,78,78,78	0
54	MG	BA	3371	1/1	0.91	0.26	77,77,77,77	0
54	MG	BA	3207	1/1	0.91	0.33	78,78,78,78	0
54	MG	DA	3487	1/1	0.91	0.15	95,95,95,95	0
54	MG	DA	3177	1/1	0.91	0.34	65,65,65,65	0
54	MG	CA	1714	1/1	0.91	0.12	161,161,161,161	0
54	MG	DA	3148	1/1	0.91	0.17	86,86,86,86	0
54	MG	DA	3068	1/1	0.91	0.34	86,86,86,86	0
54	MG	DA	3193	1/1	0.91	0.17	76,76,76,76	0
54	MG	BA	3473	1/1	0.91	0.48	84,84,84,84	0
54	MG	DA	3122	1/1	0.91	0.31	84,84,84,84	0
54	MG	BA	3382	1/1	0.91	0.47	89,89,89,89	0
54	MG	BA	3485	1/1	0.91	0.20	79,79,79,79	0
54	MG	BA	3433	1/1	0.91	0.12	94,94,94,94	0
54	MG	DA	3121	1/1	0.91	0.33	109,109,109,109	0
54	MG	DA	3213	1/1	0.91	0.21	64,64,64,64	0
54	MG	BA	3168	1/1	0.91	0.35	85,85,85,85	0
54	MG	BB	203	1/1	0.91	0.36	70,70,70,70	0
54	MG	BA	3258	1/1	0.91	0.40	74,74,74,74	0
54	MG	AA	1831	1/1	0.91	0.31	91,91,91,91	0
54	MG	BA	3592	1/1	0.91	0.24	73,73,73,73	0
54	MG	CA	1686	1/1	0.91	0.17	96,96,96,96	0
54	MG	BA	3431	1/1	0.91	0.11	88,88,88,88	0
54	MG	BA	3312	1/1	0.91	0.49	84,84,84,84	0
54	MG	AA	1763	1/1	0.91	0.41	89,89,89,89	0
54	MG	DA	3454	1/1	0.91	0.29	90,90,90,90	0
54	MG	BA	3283	1/1	0.91	0.34	78,78,78,78	0
54	MG	BA	3535	1/1	0.91	0.19	79,79,79,79	0
54	MG	DU	202	1/1	0.91	0.10	96,96,96,96	0
54	MG	BA	3446	1/1	0.91	0.47	94,94,94,94	0
54	MG	CA	1788	1/1	0.91	0.22	91,91,91,91	0
54	MG	BA	3609	1/1	0.91	0.27	80,80,80,80	0
54	MG	AA	1780	1/1	0.91	0.28	90,90,90,90	0
54	MG	BA	3006	1/1	0.91	0.35	56,56,56,56	0
54	MG	DA	3136	1/1	0.91	0.24	63,63,63,63	0
54	MG	BA	3074	1/1	0.91	0.16	76,76,76,76	0
54	MG	D3	101	1/1	0.91	0.34	78,78,78,78	0
54	MG	BA	3182	1/1	0.91	0.41	81,81,81,81	0
54	MG	BA	3034	1/1	0.91	0.38	78,78,78,78	0
54	MG	BA	3335	1/1	0.91	0.27	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	DA	3365	1/1	0.91	0.25	73,73,73,73	0
54	MG	DA	3368	1/1	0.91	0.24	82,82,82,82	0
54	MG	DA	3034	1/1	0.91	0.12	82,82,82,82	0
54	MG	DP	201	1/1	0.91	0.10	76,76,76,76	0
54	MG	DA	3486	1/1	0.91	0.15	78,78,78,78	0
54	MG	DA	3203	1/1	0.91	0.31	73,73,73,73	0
54	MG	DA	3352	1/1	0.91	0.14	71,71,71,71	0
54	MG	BA	3492	1/1	0.91	0.17	87,87,87,87	0
54	MG	AA	1712	1/1	0.91	0.36	94,94,94,94	0
54	MG	BB	216	1/1	0.91	0.07	111,111,111,111	0
54	MG	DE	301	1/1	0.91	0.20	67,67,67,67	0
54	MG	DA	3393	1/1	0.91	0.31	92,92,92,92	0
54	MG	BA	3071	1/1	0.91	0.24	90,90,90,90	0
54	MG	BA	3617	1/1	0.91	0.20	83,83,83,83	0
54	MG	BA	3451	1/1	0.91	0.45	93,93,93,93	0
54	MG	AA	1622	1/1	0.91	0.40	70,70,70,70	0
54	MG	DA	3152	1/1	0.91	0.14	86,86,86,86	0
54	MG	CA	1706	1/1	0.91	0.21	90,90,90,90	0
54	MG	AA	1665	1/1	0.91	0.41	82,82,82,82	0
54	MG	DA	3489	1/1	0.91	0.15	79,79,79,79	0
54	MG	AA	1652	1/1	0.91	0.40	93,93,93,93	0
54	MG	CA	1711	1/1	0.91	0.21	100,100,100,100	0
54	MG	BA	3203	1/1	0.91	0.45	75,75,75,75	0
54	MG	CA	1647	1/1	0.91	0.18	84,84,84,84	0
54	MG	DA	3070	1/1	0.91	0.29	68,68,68,68	0
54	MG	CA	1687	1/1	0.91	0.19	84,84,84,84	0
54	MG	BA	3060	1/1	0.91	0.22	92,92,92,92	0
54	MG	BA	3122	1/1	0.91	0.38	98,98,98,98	0
54	MG	AQ	101	1/1	0.91	0.29	94,94,94,94	0
54	MG	DA	3008	1/1	0.91	0.20	77,77,77,77	0
54	MG	AA	1701	1/1	0.91	0.13	96,96,96,96	0
54	MG	CA	1721	1/1	0.91	0.27	74,74,74,74	0
54	MG	AC	103	1/1	0.91	0.34	83,83,83,83	0
54	MG	AA	1682	1/1	0.91	0.29	103,103,103,103	0
54	MG	CA	1736	1/1	0.91	0.10	90,90,90,90	0
54	MG	DA	3057	1/1	0.91	0.31	70,70,70,70	0
54	MG	DA	3507	1/1	0.91	0.15	117,117,117,117	0
54	MG	BA	3192	1/1	0.91	0.26	100,100,100,100	0
54	MG	BA	3615	1/1	0.91	0.12	83,83,83,83	0
54	MG	BA	3421	1/1	0.92	0.34	73,73,73,73	0
54	MG	BA	3461	1/1	0.92	0.26	73,73,73,73	0
54	MG	AA	1644	1/1	0.92	0.35	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	DA	3320	1/1	0.92	0.05	105,105,105,105	0
54	MG	BA	3243	1/1	0.92	0.38	63,63,63,63	0
54	MG	BA	3582	1/1	0.92	0.39	78,78,78,78	0
54	MG	CA	1723	1/1	0.92	0.41	82,82,82,82	0
54	MG	BA	3471	1/1	0.92	0.40	78,78,78,78	0
54	MG	BA	3398	1/1	0.92	0.30	78,78,78,78	0
54	MG	BA	3119	1/1	0.92	0.30	84,84,84,84	0
54	MG	CA	1797	1/1	0.92	0.35	101,101,101,101	0
54	MG	DA	3073	1/1	0.92	0.17	66,66,66,66	0
54	MG	DA	3419	1/1	0.92	0.15	97,97,97,97	0
54	MG	CA	1763	1/1	0.92	0.28	80,80,80,80	0
54	MG	BA	3187	1/1	0.92	0.45	71,71,71,71	0
54	MG	CA	1674	1/1	0.92	0.22	87,87,87,87	0
54	MG	BA	3059	1/1	0.92	0.25	78,78,78,78	0
54	MG	DA	3226	1/1	0.92	0.29	75,75,75,75	0
54	MG	AA	1670	1/1	0.92	0.22	86,86,86,86	0
54	MG	BA	3514	1/1	0.92	0.27	76,76,76,76	0
54	MG	BA	3554	1/1	0.92	0.18	94,94,94,94	0
54	MG	DA	3262	1/1	0.92	0.19	95,95,95,95	0
54	MG	AA	1815	1/1	0.92	0.41	98,98,98,98	0
54	MG	BA	3046	1/1	0.92	0.28	60,60,60,60	0
54	MG	BA	3055	1/1	0.92	0.37	84,84,84,84	0
54	MG	DA	3231	1/1	0.92	0.17	74,74,74,74	0
54	MG	DA	3431	1/1	0.92	0.09	81,81,81,81	0
54	MG	DA	3375	1/1	0.92	0.10	96,96,96,96	0
54	MG	BA	3586	1/1	0.92	0.39	71,71,71,71	0
54	MG	CA	1659	1/1	0.92	0.17	92,92,92,92	0
54	MG	DA	3164	1/1	0.92	0.25	84,84,84,84	0
54	MG	BA	3482	1/1	0.92	0.40	84,84,84,84	0
54	MG	DA	3172	1/1	0.92	0.36	66,66,66,66	0
54	MG	DA	3484	1/1	0.92	0.19	69,69,69,69	0
54	MG	DB	205	1/1	0.92	0.25	84,84,84,84	0
54	MG	DA	3065	1/1	0.92	0.38	82,82,82,82	0
54	MG	DA	3012	1/1	0.92	0.35	87,87,87,87	0
54	MG	BA	3542	1/1	0.92	0.22	77,77,77,77	0
54	MG	BA	3565	1/1	0.92	0.36	45,45,45,45	0
54	MG	CA	1753	1/1	0.92	0.17	105,105,105,105	0
54	MG	BA	3602	1/1	0.92	0.26	71,71,71,71	0
54	MG	BA	3568	1/1	0.92	0.23	55,55,55,55	0
54	MG	BA	3448	1/1	0.92	0.24	79,79,79,79	0
54	MG	DA	3191	1/1	0.92	0.34	62,62,62,62	0
54	MG	BA	3337	1/1	0.92	0.43	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	CA	1601	1/1	0.92	0.29	95,95,95,95	0
54	MG	DB	210	1/1	0.92	0.26	95,95,95,95	0
54	MG	CA	1789	1/1	0.92	0.14	82,82,82,82	0
54	MG	BA	3043	1/1	0.92	0.34	57,57,57,57	0
54	MG	AA	1716	1/1	0.92	0.28	106,106,106,106	0
54	MG	BA	3198	1/1	0.92	0.41	71,71,71,71	0
54	MG	BA	3608	1/1	0.92	0.15	89,89,89,89	0
54	MG	CA	1619	1/1	0.92	0.10	75,75,75,75	0
54	MG	CA	1672	1/1	0.92	0.28	79,79,79,79	0
54	MG	DA	3175	1/1	0.92	0.21	71,71,71,71	0
54	MG	AA	1664	1/1	0.92	0.52	81,81,81,81	0
54	MG	BA	3120	1/1	0.92	0.17	76,76,76,76	0
54	MG	DA	3055	1/1	0.92	0.21	51,51,51,51	0
54	MG	DA	3465	1/1	0.92	0.30	50,50,50,50	0
54	MG	BA	3407	1/1	0.92	0.47	85,85,85,85	0
54	MG	DA	3452	1/1	0.92	0.35	95,95,95,95	0
54	MG	AA	1744	1/1	0.92	0.26	81,81,81,81	0
54	MG	BA	3411	1/1	0.92	0.26	80,80,80,80	0
54	MG	DA	3504	1/1	0.92	0.29	79,79,79,79	0
54	MG	CA	1784	1/1	0.92	0.31	95,95,95,95	0
54	MG	BA	3317	1/1	0.92	0.26	87,87,87,87	0
54	MG	AA	1720	1/1	0.92	0.11	113,113,113,113	0
54	MG	DA	3342	1/1	0.92	0.28	90,90,90,90	0
54	MG	BB	210	1/1	0.92	0.38	76,76,76,76	0
54	MG	DA	3043	1/1	0.92	0.31	88,88,88,88	0
54	MG	BA	3574	1/1	0.92	0.19	60,60,60,60	0
54	MG	CA	1675	1/1	0.92	0.14	96,96,96,96	0
54	MG	DA	3255	1/1	0.92	0.32	62,62,62,62	0
54	MG	DA	3336	1/1	0.92	0.47	90,90,90,90	0
54	MG	BA	3475	1/1	0.92	0.13	79,79,79,79	0
54	MG	BA	3115	1/1	0.92	0.41	74,74,74,74	0
54	MG	BA	3233	1/1	0.92	0.08	82,82,82,82	0
54	MG	BA	3311	1/1	0.92	0.21	73,73,73,73	0
54	MG	DA	3048	1/1	0.92	0.33	61,61,61,61	0
54	MG	DA	3312	1/1	0.92	0.28	81,81,81,81	0
54	MG	DB	204	1/1	0.92	0.15	87,87,87,87	0
54	MG	BA	3399	1/1	0.92	0.22	77,77,77,77	0
54	MG	AA	1646	1/1	0.92	0.37	105,105,105,105	0
54	MG	DA	3031	1/1	0.92	0.20	72,72,72,72	0
54	MG	BA	3106	1/1	0.92	0.51	73,73,73,73	0
54	MG	DA	3131	1/1	0.92	0.21	77,77,77,77	0
54	MG	BA	3112	1/1	0.92	0.46	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	DA	3322	1/1	0.92	0.23	104,104,104,104	0
54	MG	BA	3524	1/1	0.92	0.26	77,77,77,77	0
54	MG	DA	3143	1/1	0.92	0.10	84,84,84,84	0
54	MG	BF	301	1/1	0.92	0.08	76,76,76,76	0
54	MG	AA	1648	1/1	0.92	0.10	115,115,115,115	0
54	MG	DA	3233	1/1	0.92	0.15	75,75,75,75	0
54	MG	BA	3605	1/1	0.92	0.29	72,72,72,72	0
54	MG	BA	3272	1/1	0.92	0.19	53,53,53,53	0
54	MG	BA	3241	1/1	0.92	0.13	70,70,70,70	0
54	MG	AA	1791	1/1	0.92	0.23	96,96,96,96	0
54	MG	DA	3362	1/1	0.92	0.39	79,79,79,79	0
54	MG	CA	1661	1/1	0.92	0.23	88,88,88,88	0
54	MG	CA	1717	1/1	0.93	0.21	86,86,86,86	0
54	MG	AA	1659	1/1	0.93	0.24	56,56,56,56	0
54	MG	BA	3194	1/1	0.93	0.26	64,64,64,64	0
54	MG	CA	1673	1/1	0.93	0.31	74,74,74,74	0
54	MG	AA	1707	1/1	0.93	0.10	127,127,127,127	0
54	MG	DA	3083	1/1	0.93	0.34	90,90,90,90	0
54	MG	BA	3409	1/1	0.93	0.23	73,73,73,73	0
54	MG	CA	1632	1/1	0.93	0.20	88,88,88,88	0
54	MG	CA	1627	1/1	0.93	0.07	111,111,111,111	0
54	MG	AA	1729	1/1	0.93	0.22	102,102,102,102	0
54	MG	DA	3315	1/1	0.93	0.33	95,95,95,95	0
54	MG	DA	3421	1/1	0.93	0.45	86,86,86,86	0
54	MG	DA	3185	1/1	0.93	0.29	77,77,77,77	0
54	MG	BA	3152	1/1	0.93	0.15	80,80,80,80	0
54	MG	BA	3383	1/1	0.93	0.25	86,86,86,86	0
54	MG	DA	3165	1/1	0.93	0.32	64,64,64,64	0
54	MG	DA	3147	1/1	0.93	0.26	79,79,79,79	0
54	MG	DA	3135	1/1	0.93	0.14	79,79,79,79	0
54	MG	DA	3415	1/1	0.93	0.25	92,92,92,92	0
54	MG	DA	3474	1/1	0.93	0.22	65,65,65,65	0
54	MG	BA	3303	1/1	0.93	0.31	69,69,69,69	0
54	MG	BA	3549	1/1	0.93	0.11	74,74,74,74	0
56	ZN	CQ	101	1/1	0.93	0.12	123,123,123,123	0
54	MG	CN	201	1/1	0.93	0.07	95,95,95,95	0
54	MG	DA	3408	1/1	0.93	0.17	76,76,76,76	0
54	MG	DA	3376	1/1	0.93	0.24	62,62,62,62	0
54	MG	BA	3125	1/1	0.93	0.28	75,75,75,75	0
54	MG	CA	1688	1/1	0.93	0.26	88,88,88,88	0
54	MG	DA	3508	1/1	0.93	0.38	65,65,65,65	0
54	MG	CA	1720	1/1	0.93	0.24	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	DA	3090	1/1	0.93	0.18	119,119,119,119	0
54	MG	AA	1771	1/1	0.93	0.17	94,94,94,94	0
54	MG	BA	3294	1/1	0.93	0.37	75,75,75,75	0
54	MG	CA	1633	1/1	0.93	0.23	85,85,85,85	0
54	MG	BA	3532	1/1	0.93	0.25	82,82,82,82	0
54	MG	BA	3261	1/1	0.93	0.20	65,65,65,65	0
54	MG	DA	3035	1/1	0.93	0.12	92,92,92,92	0
54	MG	BA	3044	1/1	0.93	0.28	60,60,60,60	0
54	MG	CA	1693	1/1	0.93	0.50	89,89,89,89	0
54	MG	DA	3288	1/1	0.93	0.28	77,77,77,77	0
54	MG	BA	3624	1/1	0.93	0.16	98,98,98,98	0
54	MG	CA	1773	1/1	0.93	0.24	113,113,113,113	0
54	MG	BA	3063	1/1	0.93	0.20	67,67,67,67	0
54	MG	BA	3050	1/1	0.93	0.22	79,79,79,79	0
54	MG	DA	3344	1/1	0.93	0.30	82,82,82,82	0
54	MG	CA	1682	1/1	0.93	0.27	94,94,94,94	0
54	MG	DA	3180	1/1	0.93	0.32	68,68,68,68	0
54	MG	DA	3195	1/1	0.93	0.23	82,82,82,82	0
54	MG	DA	3146	1/1	0.93	0.13	86,86,86,86	0
54	MG	BA	3036	1/1	0.93	0.40	73,73,73,73	0
54	MG	DA	3412	1/1	0.93	0.20	89,89,89,89	0
54	MG	BA	3292	1/1	0.93	0.13	78,78,78,78	0
54	MG	BA	3017	1/1	0.93	0.31	53,53,53,53	0
54	MG	BA	3247	1/1	0.93	0.36	59,59,59,59	0
56	ZN	AG	302	1/1	0.93	0.29	115,115,115,115	0
54	MG	DA	3294	1/1	0.93	0.25	77,77,77,77	0
54	MG	AA	1705	1/1	0.93	0.10	104,104,104,104	0
54	MG	BA	3255	1/1	0.93	0.19	69,69,69,69	0
54	MG	BA	3354	1/1	0.93	0.19	83,83,83,83	0
54	MG	AA	1769	1/1	0.93	0.27	122,122,122,122	0
54	MG	DA	3241	1/1	0.93	0.32	74,74,74,74	0
54	MG	BA	3102	1/1	0.93	0.29	80,80,80,80	0
54	MG	BA	3512	1/1	0.93	0.15	87,87,87,87	0
54	MG	DA	3063	1/1	0.93	0.19	95,95,95,95	0
54	MG	BO	202	1/1	0.93	0.15	68,68,68,68	0
54	MG	DA	3303	1/1	0.93	0.07	94,94,94,94	0
54	MG	BA	3576	1/1	0.93	0.18	93,93,93,93	0
54	MG	CA	1669	1/1	0.93	0.28	81,81,81,81	0
54	MG	BA	3236	1/1	0.93	0.34	74,74,74,74	0
54	MG	DA	3305	1/1	0.93	0.34	78,78,78,78	0
54	MG	DA	3291	1/1	0.93	0.37	84,84,84,84	0
54	MG	AA	1762	1/1	0.93	0.39	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	BA	3628	1/1	0.93	0.33	78,78,78,78	0
54	MG	DA	3518	1/1	0.93	0.35	83,83,83,83	0
54	MG	BA	3373	1/1	0.93	0.24	85,85,85,85	0
54	MG	BA	3351	1/1	0.93	0.20	62,62,62,62	0
54	MG	DA	3112	1/1	0.93	0.30	58,58,58,58	0
54	MG	BA	3402	1/1	0.93	0.20	83,83,83,83	0
54	MG	DA	3438	1/1	0.93	0.25	82,82,82,82	0
54	MG	DA	3239	1/1	0.93	0.28	64,64,64,64	0
54	MG	DA	3050	1/1	0.93	0.19	67,67,67,67	0
54	MG	CA	1743	1/1	0.93	0.10	85,85,85,85	0
54	MG	CA	1710	1/1	0.93	0.18	102,102,102,102	0
54	MG	DA	3235	1/1	0.93	0.33	74,74,74,74	0
54	MG	AA	1690	1/1	0.93	0.19	131,131,131,131	0
54	MG	DA	3080	1/1	0.93	0.21	74,74,74,74	0
54	MG	DA	3413	1/1	0.93	0.17	84,84,84,84	0
54	MG	BA	3366	1/1	0.93	0.37	65,65,65,65	0
54	MG	AA	1703	1/1	0.93	0.27	61,61,61,61	0
54	MG	BA	3056	1/1	0.93	0.34	109,109,109,109	0
54	MG	BA	3259	1/1	0.93	0.38	56,56,56,56	0
54	MG	DA	3321	1/1	0.93	0.31	78,78,78,78	0
54	MG	BA	3357	1/1	0.93	0.48	77,77,77,77	0
54	MG	AA	1628	1/1	0.93	0.32	96,96,96,96	0
54	MG	AA	1776	1/1	0.93	0.29	102,102,102,102	0
54	MG	BA	3415	1/1	0.93	0.36	80,80,80,80	0
54	MG	DA	3467	1/1	0.93	0.27	72,72,72,72	0
54	MG	BA	3129	1/1	0.93	0.27	84,84,84,84	0
54	MG	DA	3198	1/1	0.93	0.30	57,57,57,57	0
54	MG	AA	1611	1/1	0.93	0.10	118,118,118,118	0
54	MG	CA	1744	1/1	0.93	0.10	70,70,70,70	0
54	MG	BA	3310	1/1	0.93	0.20	70,70,70,70	0
54	MG	CA	1734	1/1	0.93	0.25	78,78,78,78	0
54	MG	AA	1662	1/1	0.93	0.16	71,71,71,71	0
54	MG	CA	1609	1/1	0.94	0.14	121,121,121,121	0
54	MG	BA	3266	1/1	0.94	0.30	72,72,72,72	0
54	MG	BA	3520	1/1	0.94	0.15	86,86,86,86	0
54	MG	CA	1638	1/1	0.94	0.28	100,100,100,100	0
54	MG	BE	302	1/1	0.94	0.11	76,76,76,76	0
54	MG	BA	3370	1/1	0.94	0.18	100,100,100,100	0
54	MG	DA	3388	1/1	0.94	0.25	78,78,78,78	0
54	MG	CA	1646	1/1	0.94	0.13	92,92,92,92	0
54	MG	DA	3197	1/1	0.94	0.11	82,82,82,82	0
54	MG	AA	1832	1/1	0.94	0.27	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	DA	3313	1/1	0.94	0.34	54,54,54,54	0
54	MG	DA	3339	1/1	0.94	0.10	76,76,76,76	0
54	MG	CA	1665	1/1	0.94	0.16	82,82,82,82	0
54	MG	BA	3577	1/1	0.94	0.17	72,72,72,72	0
54	MG	DA	3405	1/1	0.94	0.10	153,153,153,153	0
54	MG	BA	3235	1/1	0.94	0.35	79,79,79,79	0
54	MG	DA	3264	1/1	0.94	0.16	68,68,68,68	0
54	MG	CA	1605	1/1	0.94	0.23	87,87,87,87	0
54	MG	AA	1625	1/1	0.94	0.27	83,83,83,83	0
54	MG	AA	1821	1/1	0.94	0.21	96,96,96,96	0
54	MG	DA	3247	1/1	0.94	0.34	76,76,76,76	0
54	MG	AA	1651	1/1	0.94	0.25	86,86,86,86	0
54	MG	BA	3132	1/1	0.94	0.12	65,65,65,65	0
54	MG	BA	3538	1/1	0.94	0.12	76,76,76,76	0
54	MG	BA	3146	1/1	0.94	0.29	75,75,75,75	0
54	MG	AA	1756	1/1	0.94	0.33	121,121,121,121	0
54	MG	CA	1637	1/1	0.94	0.10	97,97,97,97	0
54	MG	AA	1789	1/1	0.94	0.33	109,109,109,109	0
54	MG	BA	3234	1/1	0.94	0.11	79,79,79,79	0
54	MG	DA	3464	1/1	0.94	0.14	89,89,89,89	0
54	MG	BU	201	1/1	0.94	0.11	95,95,95,95	0
54	MG	CA	1645	1/1	0.94	0.35	78,78,78,78	0
54	MG	BB	201	1/1	0.94	0.27	77,77,77,77	0
54	MG	DA	3021	1/1	0.94	0.30	63,63,63,63	0
54	MG	DA	3210	1/1	0.94	0.32	57,57,57,57	0
54	MG	BA	3186	1/1	0.94	0.38	69,69,69,69	0
54	MG	BA	3363	1/1	0.94	0.21	79,79,79,79	0
54	MG	BA	3082	1/1	0.94	0.35	80,80,80,80	0
54	MG	BA	3005	1/1	0.94	0.38	59,59,59,59	0
54	MG	BA	3153	1/1	0.94	0.16	76,76,76,76	0
54	MG	BA	3295	1/1	0.94	0.37	78,78,78,78	0
54	MG	CA	1759	1/1	0.94	0.32	100,100,100,100	0
54	MG	BA	3220	1/1	0.94	0.11	76,76,76,76	0
54	MG	CA	1690	1/1	0.94	0.26	86,86,86,86	0
54	MG	CA	1776	1/1	0.94	0.27	98,98,98,98	0
54	MG	CA	1718	1/1	0.94	0.12	100,100,100,100	0
54	MG	BA	3265	1/1	0.94	0.39	82,82,82,82	0
54	MG	DA	3028	1/1	0.94	0.28	74,74,74,74	0
54	MG	BA	3097	1/1	0.94	0.49	69,69,69,69	0
54	MG	AA	1708	1/1	0.94	0.13	96,96,96,96	0
54	MG	BA	3501	1/1	0.94	0.23	90,90,90,90	0
54	MG	BA	3379	1/1	0.94	0.21	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	3246	1/1	0.94	0.38	62,62,62,62	0
54	MG	DA	3248	1/1	0.94	0.28	93,93,93,93	0
54	MG	CA	1607	1/1	0.94	0.27	81,81,81,81	0
54	MG	AA	1626	1/1	0.94	0.30	84,84,84,84	0
54	MG	BA	3239	1/1	0.94	0.30	71,71,71,71	0
54	MG	B7	103	1/1	0.94	0.27	79,79,79,79	0
54	MG	DA	3378	1/1	0.94	0.28	70,70,70,70	0
54	MG	AA	1668	1/1	0.94	0.40	81,81,81,81	0
54	MG	BA	3435	1/1	0.94	0.15	94,94,94,94	0
54	MG	AA	1749	1/1	0.94	0.12	130,130,130,130	0
54	MG	AC	106	1/1	0.94	0.24	104,104,104,104	0
54	MG	BA	3162	1/1	0.94	0.21	85,85,85,85	0
54	MG	AA	1602	1/1	0.94	0.22	82,82,82,82	0
54	MG	AA	1666	1/1	0.94	0.40	88,88,88,88	0
54	MG	DA	3138	1/1	0.94	0.11	121,121,121,121	0
54	MG	DA	3245	1/1	0.94	0.31	76,76,76,76	0
54	MG	DA	3503	1/1	0.94	0.29	76,76,76,76	0
54	MG	CA	1742	1/1	0.94	0.27	90,90,90,90	0
54	MG	BA	3077	1/1	0.94	0.31	82,82,82,82	0
54	MG	BA	3190	1/1	0.94	0.32	75,75,75,75	0
54	MG	BA	3401	1/1	0.94	0.12	73,73,73,73	0
54	MG	BA	3348	1/1	0.94	0.07	140,140,140,140	0
54	MG	DA	3510	1/1	0.94	0.15	77,77,77,77	0
54	MG	BA	3560	1/1	0.94	0.29	54,54,54,54	0
54	MG	AA	1639	1/1	0.94	0.33	88,88,88,88	0
54	MG	BA	3083	1/1	0.94	0.22	68,68,68,68	0
54	MG	DA	3105	1/1	0.94	0.24	65,65,65,65	0
54	MG	BA	3057	1/1	0.94	0.36	70,70,70,70	0
54	MG	BA	3455	1/1	0.94	0.17	74,74,74,74	0
54	MG	AA	1728	1/1	0.94	0.41	70,70,70,70	0
54	MG	CA	1671	1/1	0.94	0.14	77,77,77,77	0
54	MG	BA	3480	1/1	0.94	0.32	75,75,75,75	0
54	MG	DA	3069	1/1	0.94	0.27	85,85,85,85	0
54	MG	CA	1651	1/1	0.94	0.13	114,114,114,114	0
54	MG	BA	3159	1/1	0.94	0.33	69,69,69,69	0
54	MG	DA	3132	1/1	0.94	0.27	80,80,80,80	0
54	MG	BA	3595	1/1	0.94	0.12	91,91,91,91	0
54	MG	BA	3075	1/1	0.94	0.25	82,82,82,82	0
54	MG	DA	3079	1/1	0.94	0.07	95,95,95,95	0
54	MG	DA	3109	1/1	0.94	0.30	61,61,61,61	0
54	MG	CA	1685	1/1	0.94	0.18	82,82,82,82	0
54	MG	DA	3033	1/1	0.94	0.21	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	BA	3477	1/1	0.94	0.21	92,92,92,92	0
54	MG	AA	1775	1/1	0.94	0.15	113,113,113,113	0
54	MG	BA	3066	1/1	0.94	0.20	60,60,60,60	0
54	MG	DA	3505	1/1	0.94	0.25	73,73,73,73	0
54	MG	DA	3473	1/1	0.94	0.22	70,70,70,70	0
54	MG	CA	1628	1/1	0.94	0.06	110,110,110,110	0
54	MG	BA	3627	1/1	0.94	0.34	69,69,69,69	0
54	MG	AA	1650	1/1	0.94	0.36	87,87,87,87	0
54	MG	DA	3107	1/1	0.94	0.18	56,56,56,56	0
54	MG	CA	1656	1/1	0.94	0.16	127,127,127,127	0
54	MG	AA	1783	1/1	0.94	0.47	88,88,88,88	0
54	MG	DA	3355	1/1	0.94	0.39	84,84,84,84	0
54	MG	DA	3499	1/1	0.94	0.12	92,92,92,92	0
54	MG	AA	1779	1/1	0.94	0.43	78,78,78,78	0
54	MG	DA	3359	1/1	0.94	0.43	91,91,91,91	0
54	MG	BA	3612	1/1	0.94	0.21	67,67,67,67	0
54	MG	BA	3631	1/1	0.94	0.24	96,96,96,96	0
54	MG	CC	102	1/1	0.94	0.31	77,77,77,77	0
54	MG	CA	1654	1/1	0.94	0.23	107,107,107,107	0
54	MG	D8	101	1/1	0.95	0.26	80,80,80,80	0
54	MG	BA	3561	1/1	0.95	0.34	57,57,57,57	0
54	MG	BA	3484	1/1	0.95	0.27	76,76,76,76	0
54	MG	AA	1766	1/1	0.95	0.14	98,98,98,98	0
54	MG	DA	3260	1/1	0.95	0.39	72,72,72,72	0
54	MG	DA	3346	1/1	0.95	0.20	93,93,93,93	0
54	MG	DA	3285	1/1	0.95	0.24	57,57,57,57	0
54	MG	CA	1667	1/1	0.95	0.30	70,70,70,70	0
54	MG	BA	3004	1/1	0.95	0.28	72,72,72,72	0
54	MG	AA	1633	1/1	0.95	0.29	90,90,90,90	0
54	MG	BA	3061	1/1	0.95	0.23	84,84,84,84	0
54	MG	CA	1794	1/1	0.95	0.15	112,112,112,112	0
54	MG	AT	201	1/1	0.95	0.11	87,87,87,87	0
54	MG	BA	3387	1/1	0.95	0.26	90,90,90,90	0
54	MG	BA	3137	1/1	0.95	0.22	54,54,54,54	0
54	MG	DA	3480	1/1	0.95	0.33	64,64,64,64	0
54	MG	BD	301	1/1	0.95	0.09	91,91,91,91	0
54	MG	DA	3094	1/1	0.95	0.16	107,107,107,107	0
54	MG	BA	3305	1/1	0.95	0.45	79,79,79,79	0
54	MG	BA	3459	1/1	0.95	0.32	78,78,78,78	0
54	MG	DA	3009	1/1	0.95	0.22	71,71,71,71	0
54	MG	DA	3506	1/1	0.95	0.38	91,91,91,91	0
54	MG	BB	207	1/1	0.95	0.22	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	CC	103	1/1	0.95	0.27	73,73,73,73	0
54	MG	AA	1691	1/1	0.95	0.12	107,107,107,107	0
54	MG	DA	3228	1/1	0.95	0.23	70,70,70,70	0
54	MG	DA	3179	1/1	0.95	0.24	73,73,73,73	0
54	MG	AA	1629	1/1	0.95	0.08	134,134,134,134	0
54	MG	DA	3372	1/1	0.95	0.11	84,84,84,84	0
54	MG	BA	3035	1/1	0.95	0.32	52,52,52,52	0
54	MG	CA	1666	1/1	0.95	0.06	76,76,76,76	0
54	MG	DA	3267	1/1	0.95	0.29	78,78,78,78	0
54	MG	AA	1689	1/1	0.95	0.36	73,73,73,73	0
54	MG	BA	3551	1/1	0.95	0.17	93,93,93,93	0
54	MG	DA	3284	1/1	0.95	0.27	76,76,76,76	0
54	MG	DA	3338	1/1	0.95	0.45	105,105,105,105	0
54	MG	BA	3526	1/1	0.95	0.10	97,97,97,97	0
54	MG	AA	1742	1/1	0.95	0.23	82,82,82,82	0
54	MG	DA	3133	1/1	0.95	0.09	76,76,76,76	0
54	MG	CA	1783	1/1	0.95	0.32	80,80,80,80	0
54	MG	BA	3019	1/1	0.95	0.34	48,48,48,48	0
54	MG	DA	3099	1/1	0.95	0.32	60,60,60,60	0
54	MG	DA	3450	1/1	0.95	0.07	94,94,94,94	0
54	MG	DA	3100	1/1	0.95	0.39	64,64,64,64	0
54	MG	DA	3385	1/1	0.95	0.30	63,63,63,63	0
54	MG	BA	3476	1/1	0.95	0.20	71,71,71,71	0
54	MG	AA	1619	1/1	0.95	0.23	96,96,96,96	0
54	MG	DA	3174	1/1	0.95	0.21	52,52,52,52	0
54	MG	AA	1806	1/1	0.95	0.43	87,87,87,87	0
54	MG	DA	3361	1/1	0.95	0.31	77,77,77,77	0
54	MG	BA	3021	1/1	0.95	0.32	63,63,63,63	0
54	MG	BB	204	1/1	0.95	0.40	87,87,87,87	0
54	MG	DA	3060	1/1	0.95	0.36	78,78,78,78	0
54	MG	CA	1731	1/1	0.95	0.19	70,70,70,70	0
54	MG	DA	3302	1/1	0.95	0.21	64,64,64,64	0
54	MG	CA	1663	1/1	0.95	0.13	90,90,90,90	0
54	MG	DA	3334	1/1	0.95	0.24	84,84,84,84	0
54	MG	BA	3148	1/1	0.95	0.32	85,85,85,85	0
54	MG	DA	3340	1/1	0.95	0.27	83,83,83,83	0
54	MG	CA	1733	1/1	0.95	0.40	79,79,79,79	0
54	MG	BA	3078	1/1	0.95	0.41	63,63,63,63	0
54	MG	DA	3140	1/1	0.95	0.29	80,80,80,80	0
54	MG	AA	1653	1/1	0.95	0.35	89,89,89,89	0
54	MG	DA	3010	1/1	0.95	0.33	74,74,74,74	0
54	MG	AA	1601	1/1	0.95	0.29	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	DA	3509	1/1	0.95	0.26	64,64,64,64	0
54	MG	BA	3032	1/1	0.95	0.33	56,56,56,56	0
54	MG	DA	3479	1/1	0.95	0.17	68,68,68,68	0
54	MG	DA	3249	1/1	0.95	0.19	74,74,74,74	0
54	MG	DA	3297	1/1	0.95	0.40	84,84,84,84	0
54	MG	BA	3587	1/1	0.95	0.12	88,88,88,88	0
54	MG	AA	1826	1/1	0.95	0.12	117,117,117,117	0
54	MG	BA	3268	1/1	0.95	0.36	86,86,86,86	0
54	MG	DA	3163	1/1	0.95	0.32	66,66,66,66	0
54	MG	CA	1662	1/1	0.95	0.10	110,110,110,110	0
54	MG	DA	3273	1/1	0.95	0.25	54,54,54,54	0
54	MG	CA	1650	1/1	0.95	0.14	93,93,93,93	0
54	MG	DA	3169	1/1	0.95	0.29	74,74,74,74	0
54	MG	BA	3067	1/1	0.95	0.21	60,60,60,60	0
54	MG	BA	3511	1/1	0.95	0.12	80,80,80,80	0
54	MG	DA	3027	1/1	0.95	0.17	93,93,93,93	0
54	MG	AA	1656	1/1	0.95	0.34	73,73,73,73	0
54	MG	AA	1834	1/1	0.95	0.26	86,86,86,86	0
54	MG	DA	3022	1/1	0.95	0.21	61,61,61,61	0
54	MG	CA	1677	1/1	0.95	0.31	73,73,73,73	0
54	MG	DA	3472	1/1	0.95	0.13	88,88,88,88	0
54	MG	DA	3491	1/1	0.95	0.19	71,71,71,71	0
54	MG	BA	3486	1/1	0.95	0.40	73,73,73,73	0
54	MG	BA	3420	1/1	0.95	0.14	65,65,65,65	0
54	MG	BA	3096	1/1	0.95	0.39	56,56,56,56	0
54	MG	BA	3299	1/1	0.95	0.36	79,79,79,79	0
54	MG	BA	3164	1/1	0.95	0.43	83,83,83,83	0
54	MG	AA	1746	1/1	0.95	0.19	110,110,110,110	0
54	MG	BA	3238	1/1	0.95	0.44	63,63,63,63	0
54	MG	BA	3215	1/1	0.95	0.46	74,74,74,74	0
54	MG	DA	3087	1/1	0.95	0.38	79,79,79,79	0
54	MG	DA	3059	1/1	0.95	0.29	87,87,87,87	0
54	MG	AA	1764	1/1	0.95	0.37	111,111,111,111	0
54	MG	AA	1752	1/1	0.95	0.13	134,134,134,134	0
54	MG	BA	3126	1/1	0.95	0.41	73,73,73,73	0
54	MG	BA	3606	1/1	0.95	0.10	81,81,81,81	0
54	MG	AC	107	1/1	0.95	0.22	94,94,94,94	0
56	ZN	AQ	102	1/1	0.95	0.08	138,138,138,138	0
54	MG	BA	3505	1/1	0.95	0.20	51,51,51,51	0
54	MG	DA	3188	1/1	0.95	0.22	82,82,82,82	0
54	MG	DA	3441	1/1	0.96	0.15	111,111,111,111	0
54	MG	DA	3130	1/1	0.96	0.31	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	DA	3476	1/1	0.96	0.22	66,66,66,66	0
54	MG	BA	3033	1/1	0.96	0.35	62,62,62,62	0
54	MG	BA	3430	1/1	0.96	0.19	93,93,93,93	0
54	MG	CA	1634	1/1	0.96	0.24	87,87,87,87	0
54	MG	BA	3178	1/1	0.96	0.36	51,51,51,51	0
54	MG	AA	1770	1/1	0.96	0.11	110,110,110,110	0
54	MG	BA	3216	1/1	0.96	0.30	62,62,62,62	0
54	MG	DA	3259	1/1	0.96	0.39	78,78,78,78	0
54	MG	BA	3593	1/1	0.96	0.28	78,78,78,78	0
54	MG	CX	101	1/1	0.96	0.24	101,101,101,101	0
54	MG	BE	301	1/1	0.96	0.33	59,59,59,59	0
54	MG	DA	3475	1/1	0.96	0.35	66,66,66,66	0
54	MG	AA	1699	1/1	0.96	0.10	96,96,96,96	0
54	MG	BA	3285	1/1	0.96	0.39	67,67,67,67	0
54	MG	AA	1618	1/1	0.96	0.26	82,82,82,82	0
54	MG	AA	1658	1/1	0.96	0.25	68,68,68,68	0
54	MG	DA	3251	1/1	0.96	0.25	87,87,87,87	0
54	MG	DA	3014	1/1	0.96	0.32	67,67,67,67	0
54	MG	AA	1781	1/1	0.96	0.12	103,103,103,103	0
54	MG	AA	1737	1/1	0.96	0.32	95,95,95,95	0
54	MG	DA	3123	1/1	0.96	0.36	92,92,92,92	0
54	MG	DA	3257	1/1	0.96	0.37	56,56,56,56	0
54	MG	DA	3215	1/1	0.96	0.29	68,68,68,68	0
54	MG	AA	1676	1/1	0.96	0.27	109,109,109,109	0
54	MG	BA	3015	1/1	0.96	0.13	88,88,88,88	0
54	MG	BA	3267	1/1	0.96	0.34	75,75,75,75	0
54	MG	DA	3097	1/1	0.96	0.15	89,89,89,89	0
54	MG	DA	3124	1/1	0.96	0.26	71,71,71,71	0
54	MG	BA	3291	1/1	0.96	0.22	85,85,85,85	0
54	MG	BA	3632	1/1	0.96	0.13	114,114,114,114	0
54	MG	DA	3276	1/1	0.96	0.21	91,91,91,91	0
54	MG	AA	1661	1/1	0.96	0.26	81,81,81,81	0
54	MG	DA	3207	1/1	0.96	0.31	72,72,72,72	0
54	MG	DA	3295	1/1	0.96	0.19	128,128,128,128	0
54	MG	DA	3447	1/1	0.96	0.12	80,80,80,80	0
54	MG	CA	1617	1/1	0.96	0.21	109,109,109,109	0
54	MG	BA	3080	1/1	0.96	0.21	82,82,82,82	0
54	MG	BA	3154	1/1	0.96	0.36	59,59,59,59	0
54	MG	BA	3084	1/1	0.96	0.15	109,109,109,109	0
54	MG	AA	1830	1/1	0.96	0.12	89,89,89,89	0
54	MG	BA	3564	1/1	0.96	0.14	71,71,71,71	0
54	MG	BA	3491	1/1	0.96	0.12	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	DA	3234	1/1	0.96	0.12	94,94,94,94	0
54	MG	DE	304	1/1	0.96	0.21	66,66,66,66	0
54	MG	BA	3584	1/1	0.96	0.13	66,66,66,66	0
54	MG	DA	3512	1/1	0.96	0.22	63,63,63,63	0
54	MG	AA	1760	1/1	0.96	0.19	87,87,87,87	0
54	MG	BA	3145	1/1	0.96	0.43	61,61,61,61	0
54	MG	DA	3440	1/1	0.96	0.12	86,86,86,86	0
54	MG	DA	3159	1/1	0.96	0.24	67,67,67,67	0
54	MG	DA	3106	1/1	0.96	0.24	66,66,66,66	0
54	MG	BA	3185	1/1	0.96	0.53	62,62,62,62	0
54	MG	B2	201	1/1	0.96	0.16	104,104,104,104	0
54	MG	AA	1784	1/1	0.96	0.13	82,82,82,82	0
54	MG	AA	1704	1/1	0.96	0.33	88,88,88,88	0
54	MG	DA	3204	1/1	0.96	0.35	71,71,71,71	0
54	MG	BA	3143	1/1	0.96	0.41	63,63,63,63	0
54	MG	DA	3230	1/1	0.96	0.28	64,64,64,64	0
54	MG	CA	1727	1/1	0.96	0.06	128,128,128,128	0
54	MG	DA	3470	1/1	0.96	0.22	54,54,54,54	0
54	MG	BA	3497	1/1	0.96	0.41	72,72,72,72	0
54	MG	AA	1809	1/1	0.96	0.30	105,105,105,105	0
54	MG	BA	3127	1/1	0.96	0.28	90,90,90,90	0
54	MG	BA	3105	1/1	0.96	0.36	60,60,60,60	0
54	MG	DA	3402	1/1	0.96	0.15	91,91,91,91	0
54	MG	CA	1612	1/1	0.96	0.06	94,94,94,94	0
54	MG	DA	3001	1/1	0.96	0.34	77,77,77,77	0
54	MG	DA	3224	1/1	0.96	0.46	49,49,49,49	0
54	MG	BA	3199	1/1	0.96	0.32	80,80,80,80	0
54	MG	DA	3212	1/1	0.96	0.32	48,48,48,48	0
54	MG	BA	3103	1/1	0.96	0.29	76,76,76,76	0
54	MG	BA	3069	1/1	0.96	0.25	68,68,68,68	0
54	MG	BA	3369	1/1	0.96	0.49	68,68,68,68	0
54	MG	BA	3086	1/1	0.96	0.50	73,73,73,73	0
54	MG	BA	3256	1/1	0.96	0.53	80,80,80,80	0
54	MG	DA	3354	1/1	0.96	0.19	126,126,126,126	0
54	MG	AA	1603	1/1	0.96	0.23	89,89,89,89	0
54	MG	DA	3381	1/1	0.96	0.22	93,93,93,93	0
54	MG	DA	3103	1/1	0.96	0.21	66,66,66,66	0
54	MG	CA	1611	1/1	0.96	0.40	106,106,106,106	0
54	MG	DA	3115	1/1	0.96	0.33	66,66,66,66	0
54	MG	DA	3199	1/1	0.96	0.26	63,63,63,63	0
54	MG	AA	1778	1/1	0.96	0.47	70,70,70,70	0
54	MG	DA	3514	1/1	0.96	0.22	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	BA	3133	1/1	0.96	0.34	72,72,72,72	0
54	MG	DA	3091	1/1	0.96	0.29	73,73,73,73	0
54	MG	DA	3202	1/1	0.96	0.28	60,60,60,60	0
54	MG	CA	1790	1/1	0.96	0.31	105,105,105,105	0
54	MG	BA	3339	1/1	0.96	0.43	85,85,85,85	0
54	MG	CA	1683	1/1	0.96	0.38	86,86,86,86	0
54	MG	DA	3110	1/1	0.96	0.33	60,60,60,60	0
54	MG	BA	3278	1/1	0.96	0.43	64,64,64,64	0
54	MG	DA	3351	1/1	0.96	0.15	85,85,85,85	0
54	MG	BA	3293	1/1	0.96	0.22	89,89,89,89	0
54	MG	BA	3454	1/1	0.96	0.38	92,92,92,92	0
54	MG	BA	3478	1/1	0.96	0.41	64,64,64,64	0
54	MG	BA	3139	1/1	0.96	0.45	48,48,48,48	0
54	MG	DA	3189	1/1	0.96	0.39	56,56,56,56	0
54	MG	BA	3142	1/1	0.96	0.30	66,66,66,66	0
54	MG	DA	3061	1/1	0.96	0.15	67,67,67,67	0
54	MG	BA	3449	1/1	0.96	0.35	70,70,70,70	0
54	MG	BA	3226	1/1	0.96	0.13	64,64,64,64	0
54	MG	DA	3269	1/1	0.96	0.32	97,97,97,97	0
54	MG	DA	3141	1/1	0.96	0.32	88,88,88,88	0
54	MG	BA	3269	1/1	0.96	0.20	49,49,49,49	0
54	MG	BA	3251	1/1	0.96	0.36	48,48,48,48	0
54	MG	BA	3026	1/1	0.96	0.30	59,59,59,59	0
54	MG	AA	1747	1/1	0.96	0.29	88,88,88,88	0
54	MG	BA	3002	1/1	0.96	0.35	58,58,58,58	0
54	MG	DA	3363	1/1	0.96	0.32	92,92,92,92	0
54	MG	BA	3445	1/1	0.96	0.48	64,64,64,64	0
54	MG	DA	3108	1/1	0.96	0.29	65,65,65,65	0
54	MG	BA	3023	1/1	0.96	0.30	45,45,45,45	0
54	MG	DA	3015	1/1	0.96	0.37	64,64,64,64	0
54	MG	BA	3314	1/1	0.96	0.38	81,81,81,81	0
54	MG	DA	3307	1/1	0.96	0.15	75,75,75,75	0
54	MG	BA	3064	1/1	0.97	0.30	63,63,63,63	0
54	MG	AA	1607	1/1	0.97	0.17	89,89,89,89	0
54	MG	BA	3208	1/1	0.97	0.48	67,67,67,67	0
54	MG	AA	1615	1/1	0.97	0.16	114,114,114,114	0
54	MG	DA	3156	1/1	0.97	0.32	49,49,49,49	0
54	MG	DA	3280	1/1	0.97	0.27	44,44,44,44	0
54	MG	BA	3396	1/1	0.97	0.18	117,117,117,117	0
54	MG	DA	3482	1/1	0.97	0.31	54,54,54,54	0
54	MG	DA	3114	1/1	0.97	0.28	70,70,70,70	0
54	MG	BA	3041	1/1	0.97	0.48	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	BA	3298	1/1	0.97	0.32	43,43,43,43	0
54	MG	BA	3579	1/1	0.97	0.50	51,51,51,51	0
54	MG	AA	1632	1/1	0.97	0.17	94,94,94,94	0
54	MG	DA	3128	1/1	0.97	0.29	56,56,56,56	0
54	MG	DA	3120	1/1	0.97	0.25	60,60,60,60	0
54	MG	DA	3076	1/1	0.97	0.27	93,93,93,93	0
54	MG	DA	3201	1/1	0.97	0.37	66,66,66,66	0
54	MG	BA	3620	1/1	0.97	0.15	63,63,63,63	0
54	MG	BA	3567	1/1	0.97	0.30	62,62,62,62	0
54	MG	BA	3201	1/1	0.97	0.28	66,66,66,66	0
54	MG	AA	1820	1/1	0.97	0.06	112,112,112,112	0
54	MG	BA	3053	1/1	0.97	0.29	90,90,90,90	0
54	MG	DA	3396	1/1	0.97	0.26	73,73,73,73	0
54	MG	BA	3031	1/1	0.97	0.32	58,58,58,58	0
54	MG	BA	3212	1/1	0.97	0.43	52,52,52,52	0
54	MG	AA	1657	1/1	0.97	0.38	58,58,58,58	0
54	MG	AA	1823	1/1	0.97	0.09	151,151,151,151	0
54	MG	AA	1609	1/1	0.97	0.30	61,61,61,61	0
54	MG	BA	3193	1/1	0.97	0.39	56,56,56,56	0
54	MG	BA	3010	1/1	0.97	0.34	45,45,45,45	0
54	MG	CA	1606	1/1	0.97	0.21	83,83,83,83	0
54	MG	DA	3011	1/1	0.97	0.15	103,103,103,103	0
54	MG	DA	3371	1/1	0.97	0.34	98,98,98,98	0
54	MG	BA	3188	1/1	0.97	0.28	47,47,47,47	0
54	MG	BA	3070	1/1	0.97	0.15	64,64,64,64	0
54	MG	DA	3225	1/1	0.97	0.33	57,57,57,57	0
54	MG	BA	3515	1/1	0.97	0.33	93,93,93,93	0
54	MG	BA	3028	1/1	0.97	0.38	59,59,59,59	0
54	MG	BA	3395	1/1	0.97	0.36	84,84,84,84	0
54	MG	BA	3003	1/1	0.97	0.33	61,61,61,61	0
54	MG	DA	3317	1/1	0.97	0.26	67,67,67,67	0
54	MG	BA	3009	1/1	0.97	0.17	66,66,66,66	0
54	MG	DA	3209	1/1	0.97	0.31	61,61,61,61	0
54	MG	BA	3276	1/1	0.97	0.45	91,91,91,91	0
54	MG	CA	1730	1/1	0.97	0.19	117,117,117,117	0
54	MG	DA	3298	1/1	0.97	0.27	73,73,73,73	0
54	MG	BA	3210	1/1	0.97	0.29	59,59,59,59	0
54	MG	BA	3557	1/1	0.97	0.36	44,44,44,44	0
54	MG	BA	3443	1/1	0.97	0.12	116,116,116,116	0
54	MG	BA	3262	1/1	0.97	0.23	61,61,61,61	0
54	MG	DA	3328	1/1	0.97	0.14	98,98,98,98	0
54	MG	BA	3184	1/1	0.97	0.28	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	BA	3040	1/1	0.97	0.34	58,58,58,58	0
54	MG	DA	3092	1/1	0.97	0.41	85,85,85,85	0
54	MG	DA	3232	1/1	0.97	0.31	54,54,54,54	0
54	MG	DA	3183	1/1	0.97	0.32	70,70,70,70	0
54	MG	DA	3263	1/1	0.97	0.38	62,62,62,62	0
54	MG	DA	3433	1/1	0.97	0.30	91,91,91,91	0
54	MG	B5	1701	1/1	0.97	0.28	60,60,60,60	0
54	MG	DA	3219	1/1	0.97	0.33	70,70,70,70	0
54	MG	BA	3022	1/1	0.97	0.37	66,66,66,66	0
54	MG	BA	3025	1/1	0.97	0.33	61,61,61,61	0
54	MG	BA	3591	1/1	0.97	0.33	69,69,69,69	0
54	MG	CA	1740	1/1	0.97	0.17	103,103,103,103	0
54	MG	BA	3607	1/1	0.97	0.40	62,62,62,62	0
54	MG	BA	3081	1/1	0.97	0.20	72,72,72,72	0
54	MG	BA	3123	1/1	0.97	0.41	74,74,74,74	0
54	MG	BA	3110	1/1	0.97	0.28	58,58,58,58	0
54	MG	BA	3572	1/1	0.97	0.44	45,45,45,45	0
54	MG	DA	3343	1/1	0.97	0.42	72,72,72,72	0
54	MG	DA	3200	1/1	0.97	0.36	58,58,58,58	0
54	MG	BA	3013	1/1	0.97	0.28	65,65,65,65	0
54	MG	BA	3179	1/1	0.97	0.52	60,60,60,60	0
54	MG	CA	1610	1/1	0.97	0.17	97,97,97,97	0
54	MG	DA	3229	1/1	0.97	0.36	57,57,57,57	0
54	MG	CA	1738	1/1	0.97	0.42	74,74,74,74	0
54	MG	DA	3211	1/1	0.97	0.27	52,52,52,52	0
54	MG	AA	1680	1/1	0.97	0.13	105,105,105,105	0
54	MG	BA	3472	1/1	0.97	0.28	114,114,114,114	0
54	MG	BA	3483	1/1	0.97	0.28	105,105,105,105	0
54	MG	AA	1663	1/1	0.97	0.16	72,72,72,72	0
54	MG	AA	1750	1/1	0.97	0.09	92,92,92,92	0
54	MG	DA	3054	1/1	0.97	0.36	65,65,65,65	0
54	MG	CA	1792	1/1	0.97	0.18	105,105,105,105	0
54	MG	BA	3571	1/1	0.97	0.35	45,45,45,45	0
54	MG	DA	3471	1/1	0.97	0.31	51,51,51,51	0
54	MG	AA	1792	1/1	0.97	0.22	108,108,108,108	0
54	MG	BA	3553	1/1	0.97	0.33	50,50,50,50	0
54	MG	BA	3173	1/1	0.97	0.23	60,60,60,60	0
54	MG	BA	3323	1/1	0.97	0.33	87,87,87,87	0
54	MG	BA	3521	1/1	0.97	0.40	81,81,81,81	0
54	MG	BA	3281	1/1	0.97	0.37	72,72,72,72	0
54	MG	AC	101	1/1	0.97	0.24	68,68,68,68	0
54	MG	BA	3144	1/1	0.97	0.34	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	AA	1635	1/1	0.97	0.15	111,111,111,111	0
54	MG	BA	3467	1/1	0.97	0.27	62,62,62,62	0
54	MG	CA	1696	1/1	0.97	0.10	121,121,121,121	0
54	MG	DA	3098	1/1	0.97	0.09	112,112,112,112	0
54	MG	CA	1756	1/1	0.97	0.39	76,76,76,76	0
54	MG	BA	3321	1/1	0.97	0.43	100,100,100,100	0
54	MG	DA	3126	1/1	0.97	0.25	67,67,67,67	0
54	MG	CA	1746	1/1	0.97	0.36	97,97,97,97	0
54	MG	BA	3569	1/1	0.97	0.40	51,51,51,51	0
54	MG	DA	3102	1/1	0.97	0.24	68,68,68,68	0
54	MG	BB	202	1/1	0.97	0.20	101,101,101,101	0
54	MG	BA	3252	1/1	0.97	0.49	63,63,63,63	0
54	MG	BA	3107	1/1	0.98	0.39	76,76,76,76	0
54	MG	DA	3160	1/1	0.98	0.32	69,69,69,69	0
54	MG	BA	3128	1/1	0.98	0.11	85,85,85,85	0
54	MG	BA	3575	1/1	0.98	0.33	52,52,52,52	0
54	MG	BA	3200	1/1	0.98	0.39	76,76,76,76	0
54	MG	BA	3422	1/1	0.98	0.33	52,52,52,52	0
54	MG	BA	3556	1/1	0.98	0.38	49,49,49,49	0
54	MG	CA	1712	1/1	0.98	0.14	99,99,99,99	0
54	MG	AA	1604	1/1	0.98	0.14	88,88,88,88	0
54	MG	DA	3205	1/1	0.98	0.32	80,80,80,80	0
54	MG	BA	3001	1/1	0.98	0.40	57,57,57,57	0
54	MG	BA	3242	1/1	0.98	0.32	59,59,59,59	0
54	MG	AA	1640	1/1	0.98	0.33	77,77,77,77	0
54	MG	DA	3119	1/1	0.98	0.30	58,58,58,58	0
54	MG	BA	3176	1/1	0.98	0.15	73,73,73,73	0
54	MG	CA	1691	1/1	0.98	0.30	89,89,89,89	0
54	MG	DA	3173	1/1	0.98	0.29	53,53,53,53	0
54	MG	DA	3236	1/1	0.98	0.30	56,56,56,56	0
54	MG	DA	3469	1/1	0.98	0.38	50,50,50,50	0
54	MG	BA	3302	1/1	0.98	0.42	59,59,59,59	0
54	MG	BA	3254	1/1	0.98	0.31	72,72,72,72	0
54	MG	DA	3271	1/1	0.98	0.16	67,67,67,67	0
54	MG	CA	1680	1/1	0.98	0.05	104,104,104,104	0
54	MG	BA	3563	1/1	0.98	0.40	59,59,59,59	0
54	MG	BA	3562	1/1	0.98	0.40	53,53,53,53	0
54	MG	DA	3030	1/1	0.98	0.05	64,64,64,64	0
54	MG	BA	3048	1/1	0.98	0.29	67,67,67,67	0
54	MG	BA	3282	1/1	0.98	0.43	60,60,60,60	0
54	MG	CA	1657	1/1	0.98	0.24	114,114,114,114	0
54	MG	BA	3558	1/1	0.98	0.34	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	DA	3256	1/1	0.98	0.30	60,60,60,60	0
54	MG	BA	3042	1/1	0.98	0.19	62,62,62,62	0
54	MG	DA	3403	1/1	0.98	0.12	62,62,62,62	0
54	MG	BA	3012	1/1	0.98	0.28	66,66,66,66	0
54	MG	CA	1670	1/1	0.98	0.35	73,73,73,73	0
54	MG	BA	3073	1/1	0.98	0.10	73,73,73,73	0
54	MG	BA	3037	1/1	0.98	0.17	68,68,68,68	0
54	MG	BA	3175	1/1	0.98	0.27	61,61,61,61	0
54	MG	BA	3156	1/1	0.98	0.35	57,57,57,57	0
54	MG	DA	3116	1/1	0.98	0.26	60,60,60,60	0
54	MG	BA	3541	1/1	0.98	0.33	74,74,74,74	0
54	MG	DA	3052	1/1	0.98	0.35	60,60,60,60	0
54	MG	BA	3613	1/1	0.98	0.18	64,64,64,64	0
54	MG	DA	3206	1/1	0.98	0.36	73,73,73,73	0
54	MG	DA	3397	1/1	0.98	0.41	52,52,52,52	0
54	MG	BA	3113	1/1	0.98	0.28	54,54,54,54	0
54	MG	DA	3468	1/1	0.98	0.43	47,47,47,47	0
54	MG	DA	3481	1/1	0.98	0.27	55,55,55,55	0
54	MG	BA	3202	1/1	0.98	0.28	71,71,71,71	0
54	MG	BA	3029	1/1	0.98	0.33	62,62,62,62	0
54	MG	DA	3218	1/1	0.98	0.39	56,56,56,56	0
54	MG	BA	3559	1/1	0.98	0.43	65,65,65,65	0
54	MG	BA	3018	1/1	0.98	0.36	55,55,55,55	0
54	MG	AA	1623	1/1	0.98	0.17	82,82,82,82	0
54	MG	CA	1729	1/1	0.98	0.08	108,108,108,108	0
54	MG	DA	3170	1/1	0.98	0.23	58,58,58,58	0
54	MG	BA	3214	1/1	0.98	0.29	56,56,56,56	0
54	MG	BA	3116	1/1	0.98	0.25	84,84,84,84	0
54	MG	BA	3155	1/1	0.98	0.40	55,55,55,55	0
54	MG	CA	1793	1/1	0.98	0.33	82,82,82,82	0
54	MG	BA	3027	1/1	0.98	0.28	53,53,53,53	0
54	MG	BA	3104	1/1	0.98	0.34	45,45,45,45	0
54	MG	CA	1668	1/1	0.98	0.39	61,61,61,61	0
54	MG	BA	3140	1/1	0.98	0.41	47,47,47,47	0
54	MG	BA	3502	1/1	0.98	0.21	113,113,113,113	0
54	MG	BA	3108	1/1	0.98	0.28	56,56,56,56	0
54	MG	DA	3118	1/1	0.99	0.15	57,57,57,57	0
54	MG	DA	3478	1/1	0.99	0.40	63,63,63,63	0
54	MG	BA	3172	1/1	0.99	0.47	62,62,62,62	0
54	MG	BA	3011	1/1	0.99	0.35	49,49,49,49	0
54	MG	BA	3047	1/1	0.99	0.31	77,77,77,77	0
54	MG	DA	3176	1/1	0.99	0.38	58,58,58,58	0

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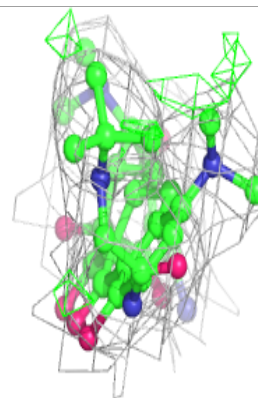
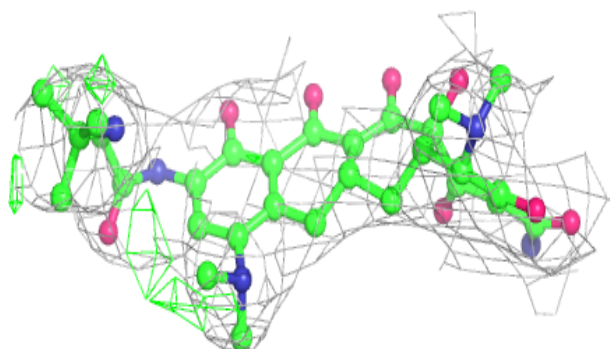
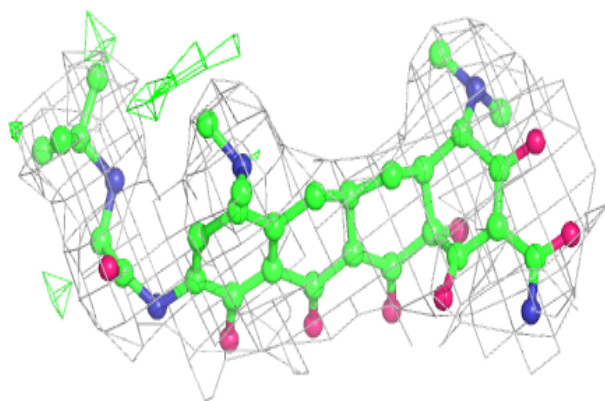
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	DA	3208	1/1	0.99	0.29	57,57,57,57	0
54	MG	BA	3211	1/1	0.99	0.24	48,48,48,48	0
54	MG	DA	3062	1/1	0.99	0.31	60,60,60,60	0
54	MG	DA	3237	1/1	0.99	0.35	52,52,52,52	0
54	MG	BA	3158	1/1	0.99	0.18	79,79,79,79	0
54	MG	BA	3007	1/1	0.99	0.39	59,59,59,59	0
54	MG	BA	3260	1/1	0.99	0.38	62,62,62,62	0
54	MG	DA	3157	1/1	0.99	0.30	58,58,58,58	0
54	MG	BA	3008	1/1	0.99	0.44	59,59,59,59	0
54	MG	BA	3014	1/1	0.99	0.36	49,49,49,49	0
54	MG	BA	3610	1/1	0.99	0.28	55,55,55,55	0
54	MG	DA	3181	1/1	0.99	0.27	78,78,78,78	0
54	MG	BA	3457	1/1	0.99	0.50	49,49,49,49	0
54	MG	BA	3038	1/1	0.99	0.30	53,53,53,53	0
54	MG	BA	3209	1/1	0.99	0.37	64,64,64,64	0
54	MG	DA	3395	1/1	0.99	0.07	103,103,103,103	0
54	MG	BA	3244	1/1	0.99	0.33	53,53,53,53	0
54	MG	BA	3101	1/1	0.99	0.42	42,42,42,42	0
54	MG	BA	3020	1/1	0.99	0.40	49,49,49,49	0
54	MG	DA	3220	1/1	0.99	0.26	60,60,60,60	0
54	MG	BA	3098	1/1	0.99	0.37	45,45,45,45	0
54	MG	BA	3016	1/1	0.99	0.40	57,57,57,57	0
54	MG	BA	3611	1/1	0.99	0.23	55,55,55,55	0
54	MG	BA	3189	1/1	0.99	0.41	52,52,52,52	0
54	MG	DA	3404	1/1	0.99	0.22	86,86,86,86	0
54	MG	B0	201	1/1	0.99	0.26	67,67,67,67	0
54	MG	DA	3252	1/1	0.99	0.23	67,67,67,67	0

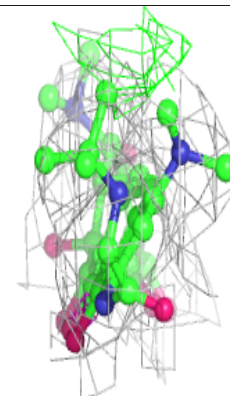
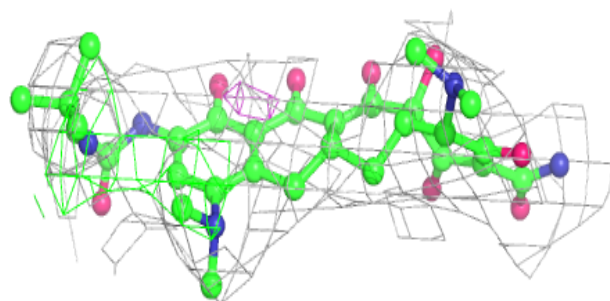
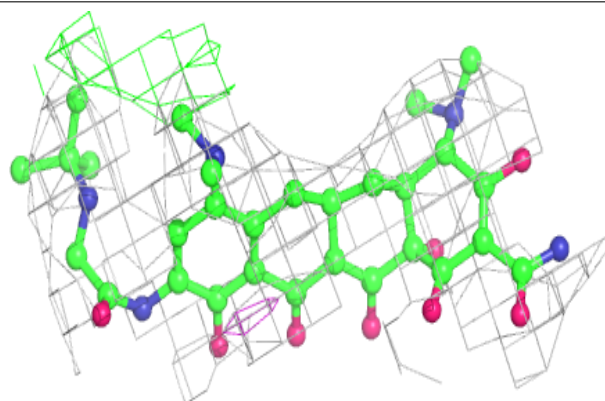
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around T1C AA 1837:

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

**Electron density around T1C CA 1800:**

$2mF_o-DF_c$ (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.