



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 04:50 PM UTC

PDB ID : 4V9N / pdb_00004v9n
Title : Crystal structure of the 70S ribosome bound with the Q253P mutant of release factor RF2.
Authors : Santos, N.; Zhu, J.; Donohue, J.P.; Korostelev, A.A.; Noller, H.F.
Deposited on : 2013-04-26
Resolution : 3.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

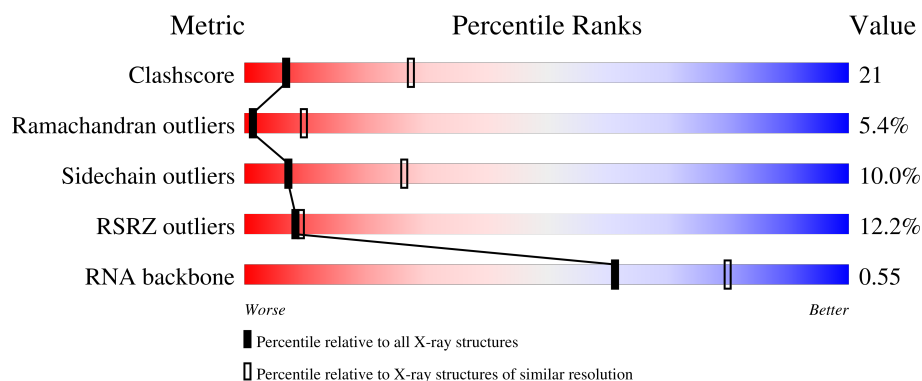
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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))
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)
RNA backbone	3983	1157 (3.80-3.00)

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

Mol	Chain	Length	Quality of chain
1	AA	1504	3% 44% 46% 10%
1	CA	1504	9% 44% 46% 10%
2	AV	10	30% 50% 50%
2	CV	10	40% 40% 60%
3	AW	77	% 60% 35% 5%

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Mol	Chain	Length	Quality of chain
3	CW	77	
4	AY	362	
4	CY	362	
5	AB	234	
5	CB	234	
6	AC	206	
6	CC	206	
7	AD	208	
7	CD	208	
8	AE	151	
8	CE	151	
9	AF	101	
9	CF	101	
10	AG	155	
10	CG	155	
11	AH	138	
11	CH	138	
12	AI	127	
12	CI	127	
13	AJ	98	
13	CJ	98	
14	AK	114	
14	CK	114	
15	AL	122	
15	CL	122	

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Mol	Chain	Length	Quality of chain
16	AM	117	
16	CM	117	
17	AN	60	
17	CN	60	
18	AO	88	
18	CO	88	
19	AP	83	
19	CP	83	
20	AQ	99	
20	CQ	99	
21	AR	70	
21	CR	70	
22	AS	78	
22	CS	78	
23	AT	99	
23	CT	99	
24	AU	24	
24	CU	24	
25	BA	2879	
25	DA	2879	
26	BB	119	
26	DB	119	
27	BD	271	
27	DD	271	
28	BE	204	

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Mol	Chain	Length	Quality of chain
28	DE	204	
29	BF	202	
29	DF	202	
30	BG	181	
30	DG	181	
31	BH	159	
31	DH	159	
32	BI	145	
32	DI	145	
33	BK	147	
33	DK	147	
34	BN	137	
34	DN	137	
35	BO	122	
35	DO	122	
36	BP	146	
36	DP	146	
37	BQ	134	
37	DQ	134	
38	BR	117	
38	DR	117	
39	BS	98	
39	DS	98	
40	BT	137	
40	DT	137	

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Mol	Chain	Length	Quality of chain
41	BU	117	
41	DU	117	
42	BV	101	
42	DV	101	
43	BW	112	
43	DW	112	
44	BX	92	
44	DX	92	
45	BY	100	
45	DY	100	
46	BZ	187	
46	DZ	187	
47	B0	76	
47	D0	76	
48	B1	88	
48	D1	88	
49	B2	62	
49	D2	62	
50	B3	59	
50	D3	59	
51	B4	30	
51	D4	30	
52	B5	52	
52	D5	52	
53	B6	44	

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Mol	Chain	Length	Quality of chain
53	D6	44	
54	B7	48	
54	D7	48	
55	B8	63	
55	D8	63	

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
56	MG	AA	1770	-	-	-	X
56	MG	AA	1778	-	-	-	X
56	MG	AT	201	-	-	-	X
56	MG	BA	2924	-	-	-	X
56	MG	BA	2931	-	-	-	X
56	MG	BA	3080	-	-	-	X
56	MG	BA	3591	-	-	-	X
56	MG	BA	3685	-	-	-	X
56	MG	CA	1603	-	-	-	X
56	MG	CA	1728	-	-	-	X
56	MG	DA	3409	-	-	-	X
56	MG	DA	3428	-	-	-	X

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 294074 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 rRNA (1504-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1504	Total	C	N	O	P	0	0	0
			32332	14391	5994	10444	1503			
1	CA	1504	Total	C	N	O	P	0	0	0
			32332	14391	5994	10444	1503			

- Molecule 2 is a RNA chain called messenger RNA (5'-R(*AP*AP*UP*GP*UP*AP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AV	10	Total	C	N	O	P	0	0	0
			214	98	44	63	9			
2	CV	10	Total	C	N	O	P	0	0	0
			214	98	44	63	9			

- Molecule 3 is a RNA chain called P-site tRNA-fMet.

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

- Molecule 4 is a protein called Bacterial peptide chain release factor 2 (RF-2).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AY	362	Total	C	N	O	S	0	0	0
			2874	1794	517	555	8			
4	CY	362	Total	C	N	O	S	0	0	0
			2874	1794	517	555	8			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AY	253	PRO	GLN	engineered mutation	UNP Q72GJ6
CY	253	PRO	GLN	engineered mutation	UNP Q72GJ6

- Molecule 5 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AB	234	Total	C	N	O	S	0	0	0
			1901	1213	341	342	5			
5	CB	234	Total	C	N	O	S	0	0	0
			1901	1213	341	342	5			

- Molecule 6 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AC	206	Total	C	N	O	S	0	0	0
			1613	1016	314	282	1			
6	CC	206	Total	C	N	O	S	0	0	0
			1613	1016	314	282	1			

- Molecule 7 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AD	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			
7	CD	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			

- Molecule 8 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AE	151	Total	C	N	O	S	0	0	0
			1156	729	218	205	4			
8	CE	151	Total	C	N	O	S	0	0	0
			1156	729	218	205	4			

- Molecule 9 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	AF	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			
9	CF	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			

- Molecule 10 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AG	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			
10	CG	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			

- Molecule 11 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	AH	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			
11	CH	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			

- Molecule 12 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
12	AI	127	Total	C	N	O	0	0	0
			1011	639	198	174			
12	CI	127	Total	C	N	O	0	0	0
			1011	639	198	174			

- Molecule 13 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AJ	98	Total	C	N	O	S	0	0	0
			795	499	156	139	1			
13	CJ	98	Total	C	N	O	S	0	0	0
			795	499	156	139	1			

- Molecule 14 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AK	114	Total	C	N	O	S	0	0	0
			843	522	159	159	3			
14	CK	114	Total	C	N	O	S	0	0	0
			843	522	159	159	3			

- Molecule 15 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AL	122	Total	C	N	O	S	0	0	0
			957	603	193	160	1			
15	CL	122	Total	C	N	O	S	0	0	0
			957	603	193	160	1			

- Molecule 16 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AM	117	Total	C	N	O	S	0	0	0
			934	577	192	163	2			
16	CM	117	Total	C	N	O	S	0	0	0
			934	577	192	163	2			

- Molecule 17 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AN	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			
17	CN	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			

- Molecule 18 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	AO	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			
18	CO	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			

- Molecule 19 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AP	83	Total	C	N	O	S	0	0	0
			701	443	139	118	1			
19	CP	83	Total	C	N	O	S	0	0	0
			701	443	139	118	1			

- Molecule 20 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AQ	99	Total	C	N	O	S	0	0	0
			824	528	152	142	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	CQ	99	Total	C	N	O	S	0	0	0
			824	528	152	142	2			

- Molecule 21 is a protein called 30S ribosomal protein S18.

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

- Molecule 22 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AS	78	Total	C	N	O	S	0	0	0
			630	403	114	111	2			
22	CS	78	Total	C	N	O	S	0	0	0
			630	403	114	111	2			

- Molecule 23 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AT	99	Total	C	N	O	S	0	0	0
			762	469	162	129	2			
23	CT	99	Total	C	N	O	S	0	0	0
			762	469	162	129	2			

- Molecule 24 is a protein called 30S ribosomal protein Thx.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
24	AU	24	Total	C	N	O	0	0	0
			209	128	50	31			
24	CU	24	Total	C	N	O	0	0	0
			209	128	50	31			

- Molecule 25 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	BA	2789	Total	C	N	O	P	0	0	0
			60059	26734	11225	19312	2788			
25	DA	2789	Total	C	N	O	P	0	0	0
			60059	26734	11225	19312	2788			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BA	276	C	A	conflict	GB AE017221.1
BA	277	A	C	conflict	GB AE017221.1
BA	1141A	U	C	conflict	GB AE017221.1
BA	2825	U	G	conflict	GB AE017221.1
DA	276	C	A	conflict	GB AE017221.1
DA	277	A	C	conflict	GB AE017221.1
DA	1141A	U	C	conflict	GB AE017221.1
DA	2825	U	G	conflict	GB AE017221.1

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	BD	271	Total	C	N	O	S	0	0	0
			2105	1329	416	357	3			
27	DD	271	Total	C	N	O	S	0	0	0
			2105	1329	416	357	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	BE	204	Total	C	N	O	S	0	0	0
			1564	988	299	271	6			
28	DE	204	Total	C	N	O	S	0	0	0
			1564	988	299	271	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	BF	202	Total	C	N	O	S	0	0	0
			1587	1011	297	276	3			
29	DF	202	Total	C	N	O	S	0	0	0
			1587	1011	297	276	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	BG	181	Total	C	N	O	S	0	0	0
			1475	943	268	260	4			
30	DG	181	Total	C	N	O	S	0	0	0
			1475	943	268	260	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	BH	159	Total	C	N	O	S	0	0	0
			1223	773	228	221	1			
31	DH	159	Total	C	N	O	S	0	0	0
			1223	773	228	221	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	BI	145	Total	C	N	O	S	0	0	0
			1133	724	200	208	1			
32	DI	145	Total	C	N	O	S	0	0	0
			1133	724	200	208	1			

- Molecule 33 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	BK	147	Total	C	N	O	S	0	0	0
			1088	692	191	199	6			
33	DK	147	Total	C	N	O	S	0	0	0
			1088	692	191	199	6			

- Molecule 34 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	BN	137	Total	C	N	O	S	0	0	0
			1097	707	205	182	3			
34	DN	137	Total	C	N	O	S	0	0	0
			1097	707	205	182	3			

- Molecule 35 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BO	122	Total	C	N	O	S	0	0	0
			932	587	171	170	4			
35	DO	122	Total	C	N	O	S	0	0	0
			932	587	171	170	4			

- Molecule 36 is a protein called 50S ribosomal protein L15.

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

- Molecule 37 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	BQ	134	Total	C	N	O	S	0	0	0
			1065	680	201	179	5			
37	DQ	134	Total	C	N	O	S	0	0	0
			1065	680	201	179	5			

- Molecule 38 is a protein called 50S ribosomal protein L17.

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

- Molecule 39 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BS	98	Total	C	N	O		0	0	0
			771	486	154	131				
39	DS	98	Total	C	N	O		0	0	0
			771	486	154	131				

- Molecule 40 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	BT	137	Total	C	N	O	S	0	0	0
			1144	713	234	196	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	DT	137	Total	C	N	O	S	0	0	0
			1144	713	234	196	1			

- Molecule 41 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BU	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			
41	DU	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			

- Molecule 42 is a protein called 50S ribosomal protein L21.

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

- Molecule 43 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BW	112	Total	C	N	O	S	0	0	0
			891	560	175	154	2			
43	DW	112	Total	C	N	O	S	0	0	0
			891	560	175	154	2			

- Molecule 44 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
44	BX	92	Total	C	N	O	0	0	0
			726	471	131	124			
44	DX	92	Total	C	N	O	0	0	0
			726	471	131	124			

- Molecule 45 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	BY	100	Total	C	N	O	S	0	0	0
			776	500	148	124	4			
45	DY	100	Total	C	N	O	S	0	0	0
			776	500	148	124	4			

- Molecule 46 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	BZ	187	Total	C	N	O	S	0	0	0
			1483	945	264	272	2			
46	DZ	187	Total	C	N	O	S	0	0	0
			1483	945	264	272	2			

- Molecule 47 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	B0	76	Total	C	N	O	S	0	0	0
			605	376	126	102	1			
47	D0	76	Total	C	N	O	S	0	0	0
			605	376	126	102	1			

- Molecule 48 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
48	B1	88	Total	C	N	O	0	0	0
			695	435	141	119			
48	D1	88	Total	C	N	O	0	0	0
			695	435	141	119			

- Molecule 49 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	B2	62	Total	C	N	O	S	0	0	0
			521	325	102	92	2			
49	D2	62	Total	C	N	O	S	0	0	0
			521	325	102	92	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	B3	59	Total	C	N	O	S	0	0	0
			468	298	90	79	1			
50	D3	59	Total	C	N	O	S	0	0	0
			468	298	90	79	1			

- Molecule 51 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	B4	30	Total	C	N	O	S	0	0	0
			226	142	36	44	4			
51	D4	30	Total	C	N	O	S	0	0	0
			226	142	36	44	4			

- Molecule 52 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	B5	52	Total	C	N	O	S	0	0	0
			405	255	79	66	5			
52	D5	52	Total	C	N	O	S	0	0	0
			405	255	79	66	5			

- Molecule 53 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	B6	44	Total	C	N	O	S	0	0	0
			381	235	77	65	4			
53	D6	44	Total	C	N	O	S	0	0	0
			381	235	77	65	4			

- Molecule 54 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	B7	48	Total	C	N	O	S	0	0	0
			419	257	104	56	2			
54	D7	48	Total	C	N	O	S	0	0	0
			419	257	104	56	2			

- Molecule 55 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	B8	63	Total	C	N	O	S	0	0	0
			508	326	101	79	2			
55	D8	63	Total	C	N	O	S	0	0	0
			508	326	101	79	2			

- Molecule 56 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	AA	393	Total	Mg	0	0
			393	393		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	AV	1	Total 1	Mg 1	0	0
56	AW	18	Total 18	Mg 18	0	0
56	AY	3	Total 3	Mg 3	0	0
56	AC	1	Total 1	Mg 1	0	0
56	AG	1	Total 1	Mg 1	0	0
56	AO	1	Total 1	Mg 1	0	0
56	AQ	1	Total 1	Mg 1	0	0
56	AT	3	Total 3	Mg 3	0	0
56	BA	824	Total 824	Mg 824	0	0
56	BB	23	Total 23	Mg 23	0	0
56	BD	1	Total 1	Mg 1	0	0
56	BE	1	Total 1	Mg 1	0	0
56	BF	1	Total 1	Mg 1	0	0
56	BP	1	Total 1	Mg 1	0	0
56	BT	1	Total 1	Mg 1	0	0
56	BX	2	Total 2	Mg 2	0	0
56	BY	1	Total 1	Mg 1	0	0
56	B0	2	Total 2	Mg 2	0	0
56	B1	1	Total 1	Mg 1	0	0
56	B3	1	Total 1	Mg 1	0	0
56	B5	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	B8	2	Total 2	Mg 2	0	0
56	CA	326	Total 326	Mg 326	0	0
56	CV	2	Total 2	Mg 2	0	0
56	CW	16	Total 16	Mg 16	0	0
56	CY	2	Total 2	Mg 2	0	0
56	CD	1	Total 1	Mg 1	0	0
56	CM	1	Total 1	Mg 1	0	0
56	CR	1	Total 1	Mg 1	0	0
56	DA	732	Total 732	Mg 732	0	0
56	DB	20	Total 20	Mg 20	0	0
56	DD	1	Total 1	Mg 1	0	0
56	DE	1	Total 1	Mg 1	0	0
56	DF	2	Total 2	Mg 2	0	0
56	DH	1	Total 1	Mg 1	0	0
56	DI	2	Total 2	Mg 2	0	0
56	DN	1	Total 1	Mg 1	0	0
56	DP	2	Total 2	Mg 2	0	0
56	DQ	4	Total 4	Mg 4	0	0
56	DV	1	Total 1	Mg 1	0	0
56	DW	2	Total 2	Mg 2	0	0
56	DX	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	D0	1	Total 1	Mg 1	0	0
56	D1	1	Total 1	Mg 1	0	0
56	D5	3	Total 3	Mg 3	0	0
56	D7	2	Total 2	Mg 2	0	0

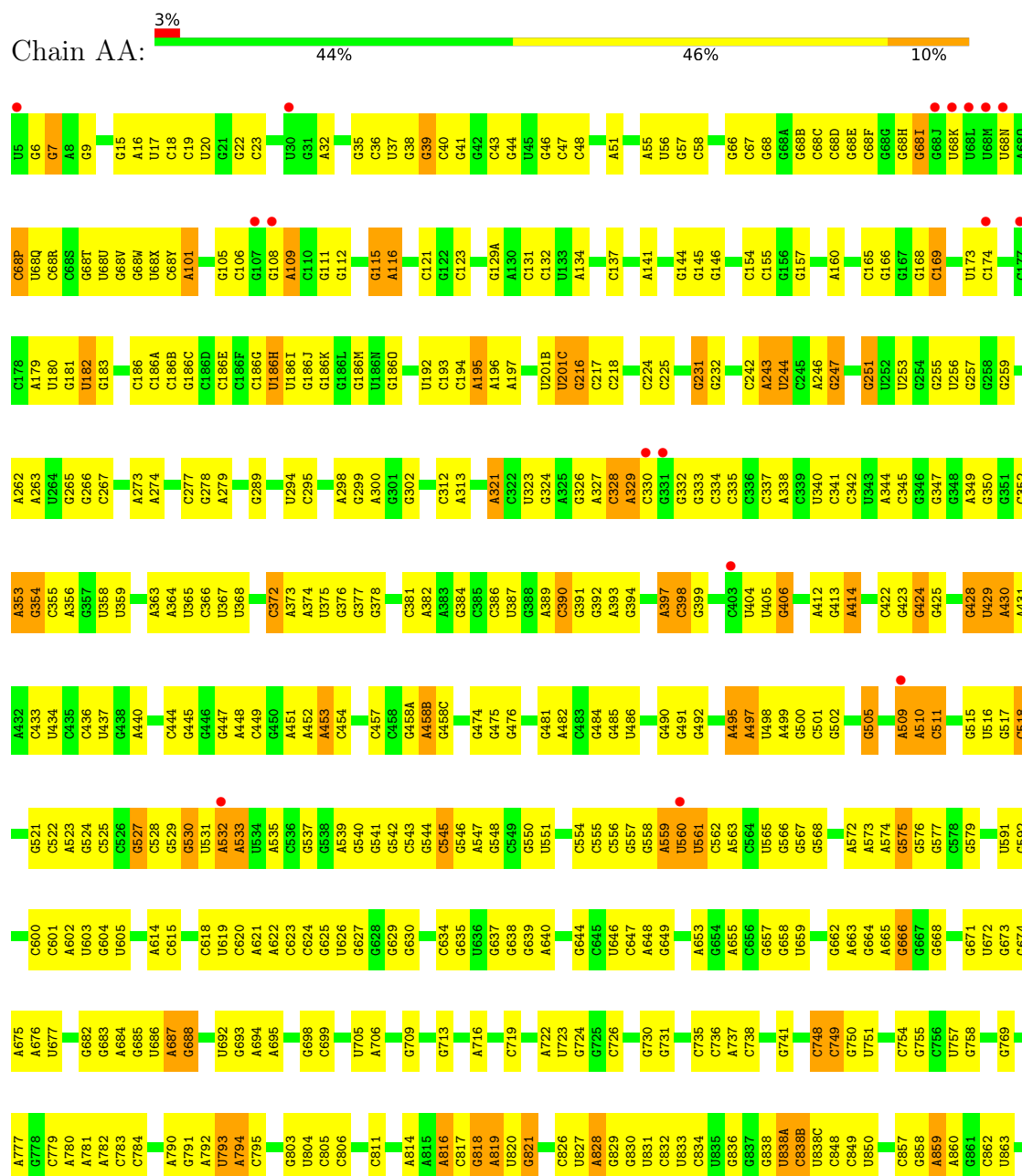
- Molecule 57 is ZINC ION (CCD ID: ZN) (formula: Zn).

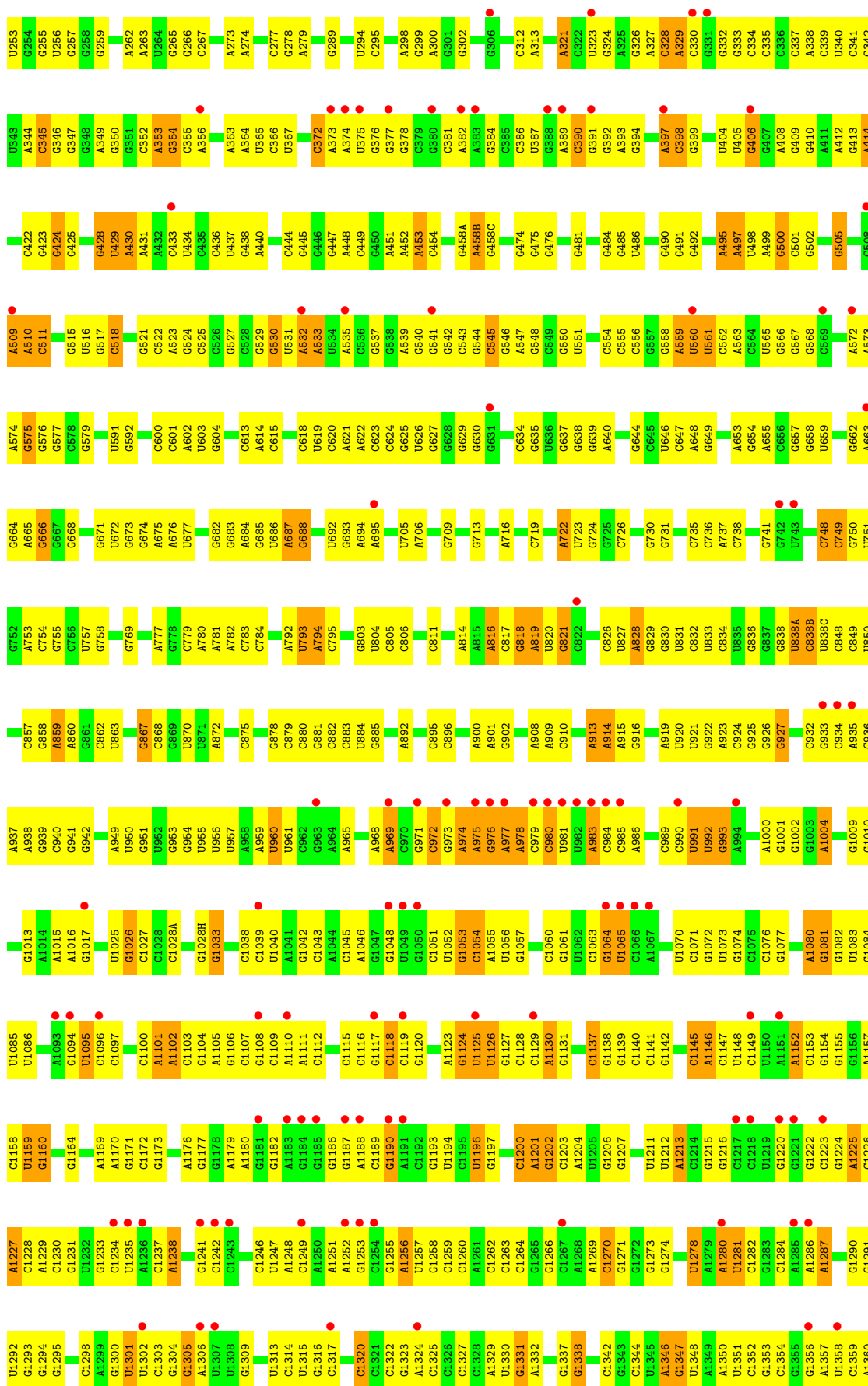
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	AD	1	Total 1	Zn 1	0	0
57	AN	1	Total 1	Zn 1	0	0
57	CD	1	Total 1	Zn 1	0	0
57	CN	1	Total 1	Zn 1	0	0

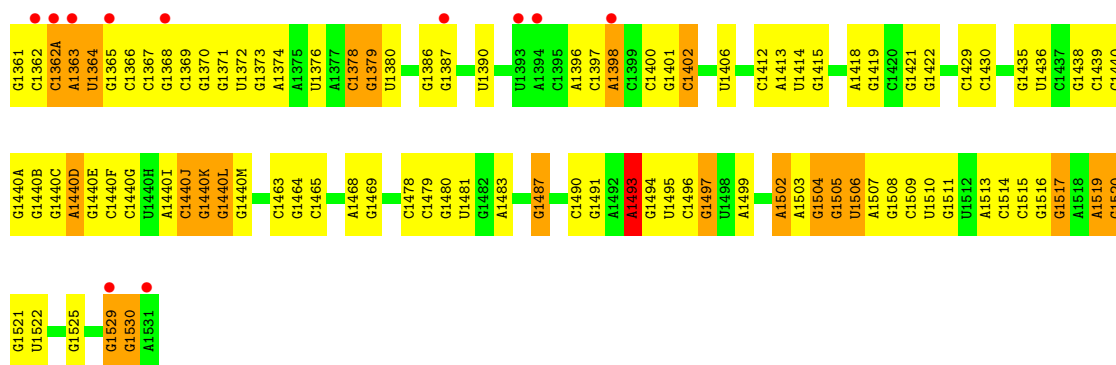
3 Residue-property plots

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

• Molecule 1: 16S rRNA (1504-MER)







- Molecule 2: messenger RNA (5'-R(*AP*AP*UP*GP*UP*AP*G)-3')



- Molecule 2: messenger RNA (5'-R(*AP*AP*UP*GP*UP*AP*G)-3')



- Molecule 3: P-site tRNA-fMet

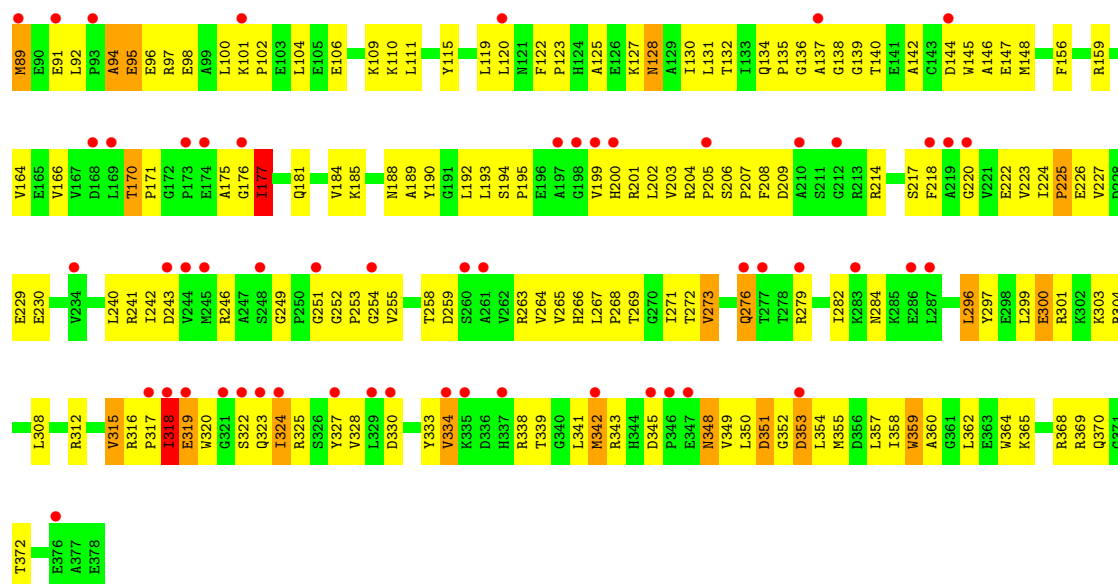


- Molecule 3: P-site tRNA-fMet

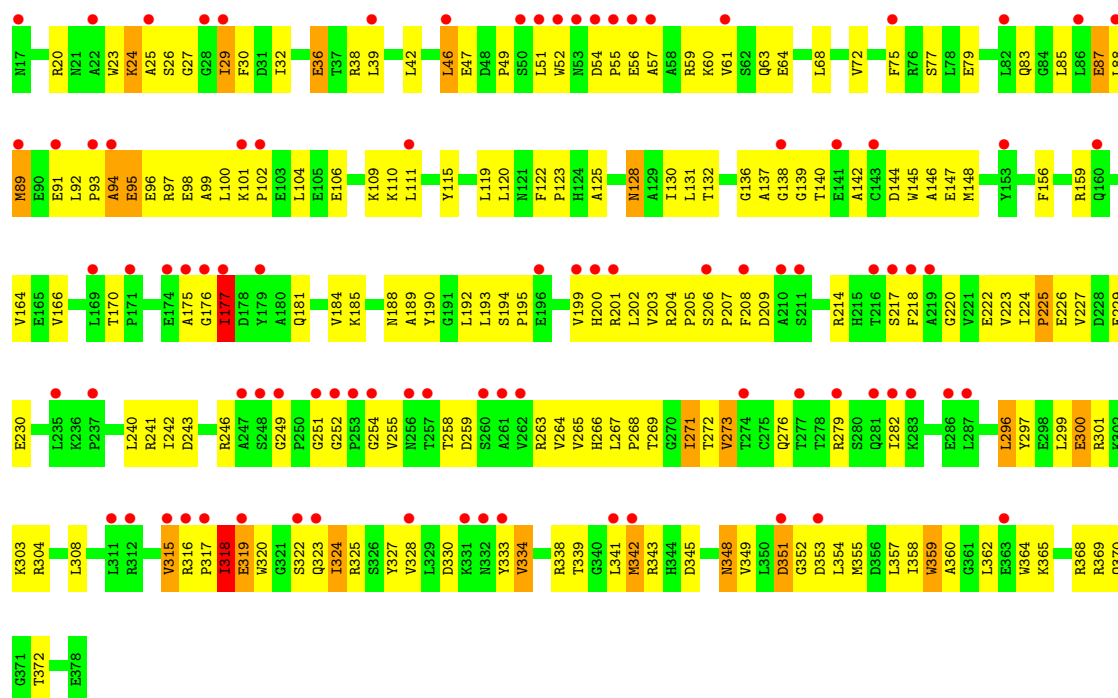


- Molecule 4: Bacterial peptide chain release factor 2 (RF-2)

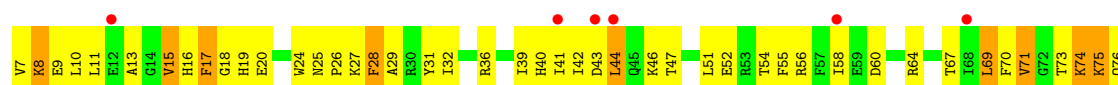


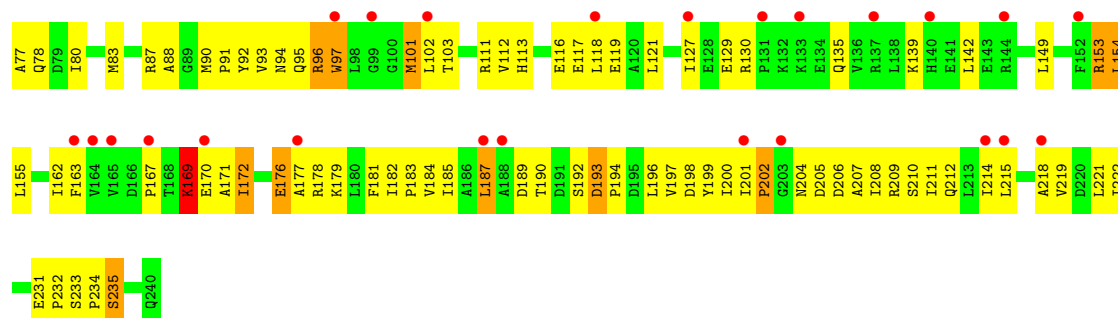


• Molecule 4: Bacterial peptide chain release factor 2 (RF-2)

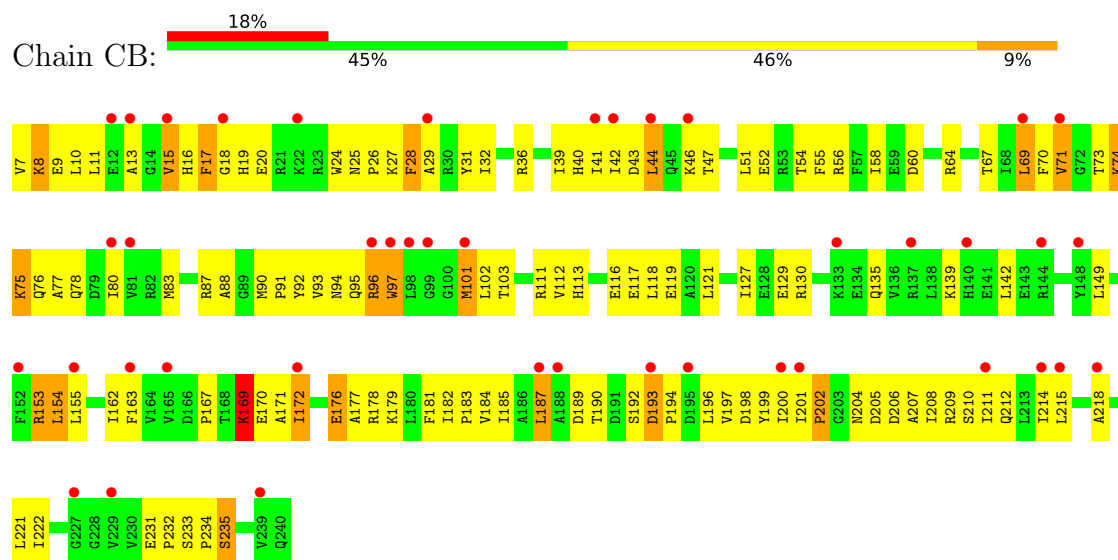


• Molecule 5: 30S ribosomal protein S2

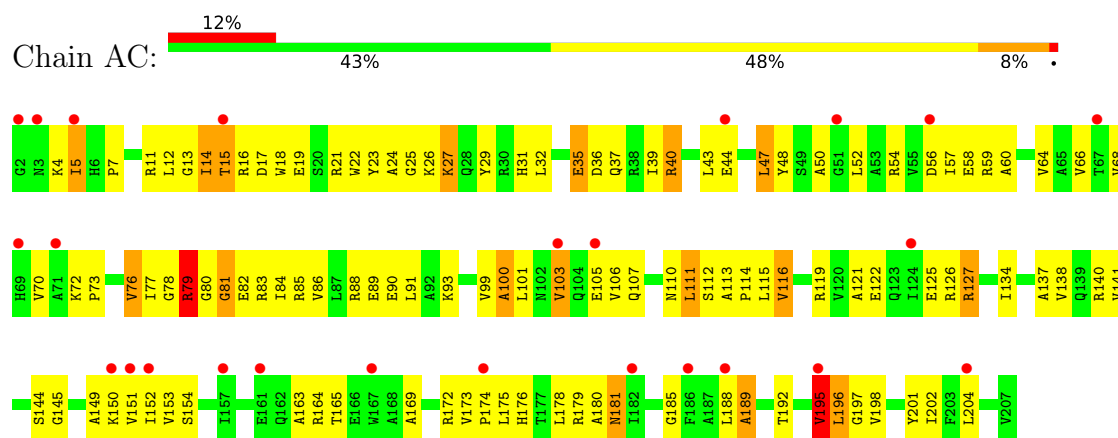




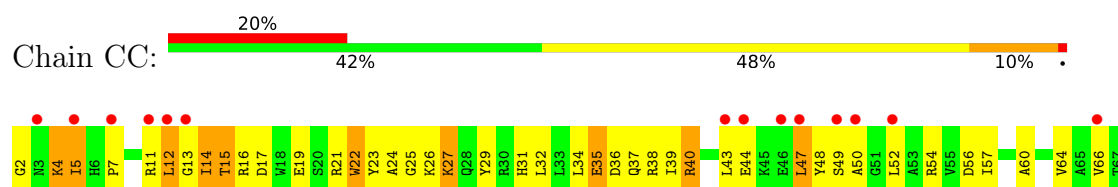
• Molecule 5: 30S ribosomal protein S2

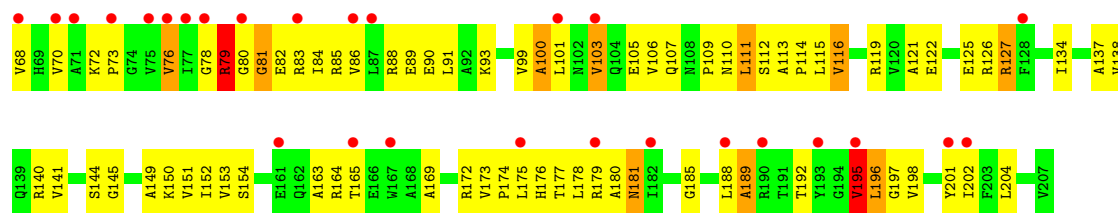


• Molecule 6: 30S ribosomal protein S3

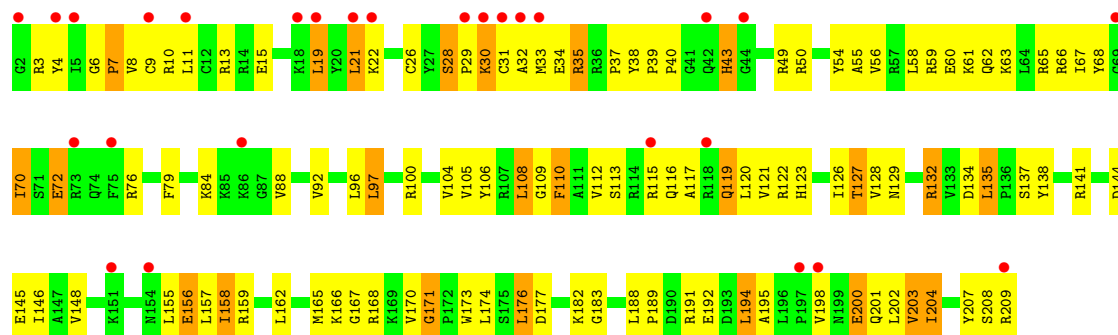


• Molecule 6: 30S ribosomal protein S3

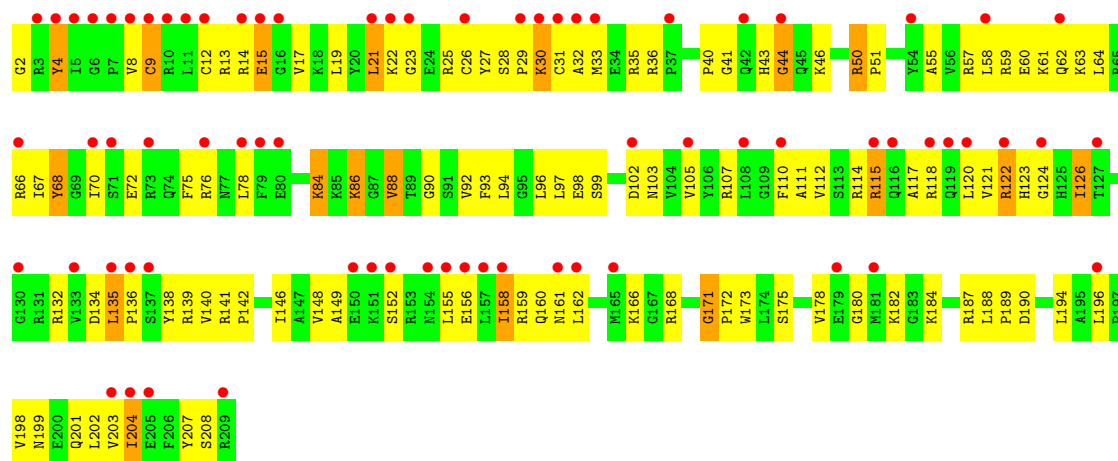
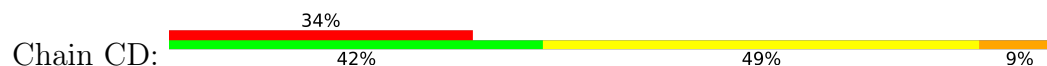




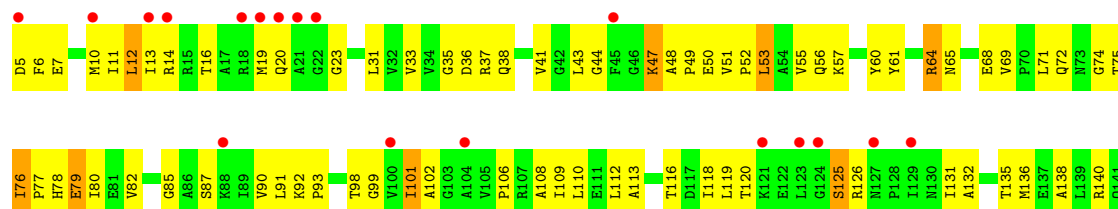
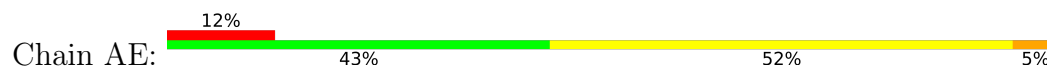
• Molecule 7: 30S ribosomal protein S4



• Molecule 7: 30S ribosomal protein S4



• Molecule 8: 30S ribosomal protein S5



L142
R143
T144
K145
A146
D147
V148
E149
R150
L151
K152
K153
G154
E155

• Molecule 8: 30S ribosomal protein S5

Chain CE: 25%
46% 48% 6%

D5
F6
E7
M10
I11
I12
I13
R14
R18
M19
Q20
K21
G22
G23
R24
F28
L31
V32
V33
V34
G35
D36
R37
Q38
V41
G42
L43
G44
F45
G46
A47
A48
P49
E50
V51
P52
L53
A54
V55
Q56
K57
Y60
Y61
R64
N65
E68
V69
P70
L71
Q72
N73
G74

L142
R143
T144
D147
V148
E149
R150
L151
K152
K153
G154
E155

• Molecule 9: 30S ribosomal protein S6

Chain AF: 18%
54% 41% 5%

R1
R2
R3
V6
N7
I8
I9
L10
M11
P12
M13
L14
D15
L19
K23
Q27
Y33
V37
E38
F39
V40
G44
L45
R46
Y50
D55
P56
Q57
G58
Y59
F60
L61
W62
Y63
Q64
V65
E66
P67
P68
E69
D70
R71
V72
L75
A76
L79
R80
I81
R82

• Molecule 9: 30S ribosomal protein S6

Chain CF: 5%
55% 41%

R1
R2
R3
N7
I8
V9
L10
M11
P12
M13
L14
D15
Q16
Q18
L19
K23
Q27
Y33
V37
E38
F39
V40
G44
L45
R46
D55
P56
Q57
G58
Y59
F60
L61
W62
Y63
Q64
V65
E66
P67
P68
E69
D70
R71
V72
L75
A76
L79
R80
I81
R82

• Molecule 10: 30S ribosomal protein S7

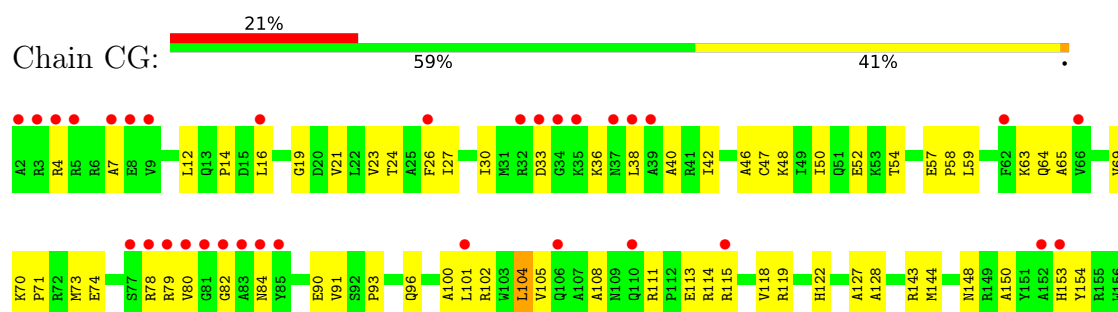
Chain AG: 11%
55% 45%

A2
R3
R4
R5
R6
A7
L12
Q13
P14
D15
L16
G19
D20
V21
L22
V23
T24
A25
F26
I27
I30
M31
R32
D33
G34
K35
K36
N37
L38
A39
A40
R41
I42
A46
C47
K48
I49
I50
Q51
E52
K53
T54
E57
P58
L59
K63
Q64
A65
V69
K70
P71
R72
M73

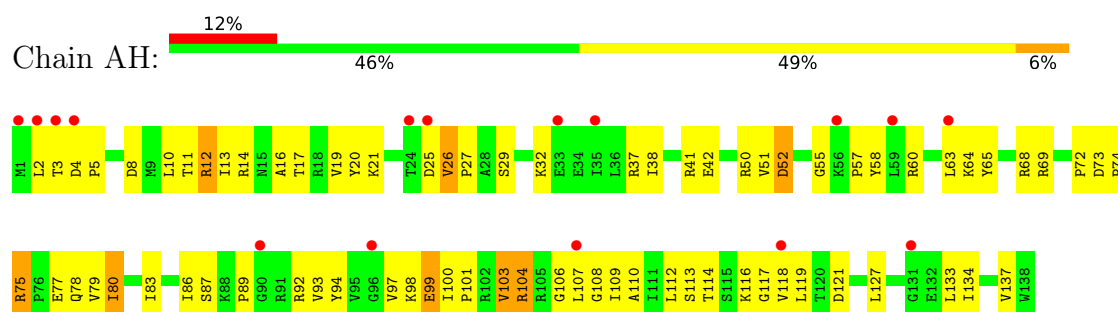
E74
R78
R79
V80
G81
G82
R83
N84
Y85
P88
M89
E90
V91
S92
P93
Q96
A100
L101
R102
W103
L104
V105
Q106
A107
A108
R111
P112
E113
R114
R115
V118
R119
H122
D126
A127
A128
G132
G133
A134
K138
E142
R143
M144
A150
H153
Y154
R155



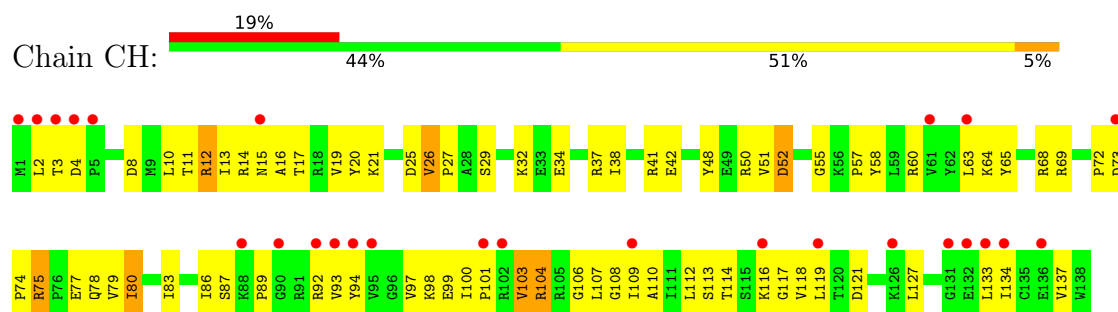
• Molecule 10: 30S ribosomal protein S7



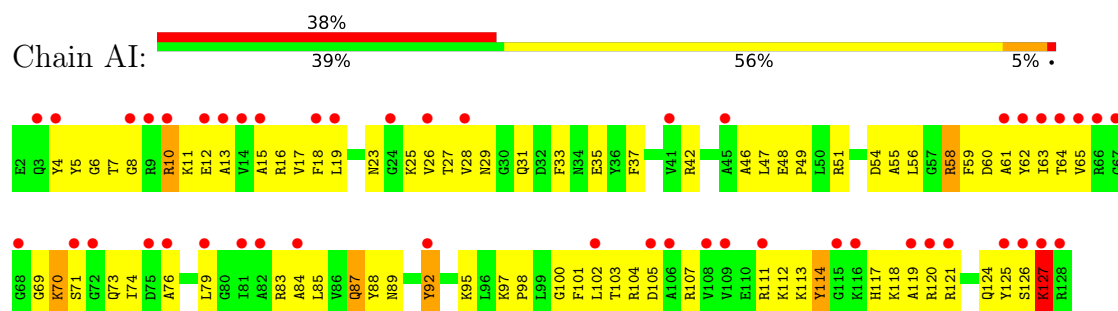
• Molecule 11: 30S ribosomal protein S8



• Molecule 11: 30S ribosomal protein S8

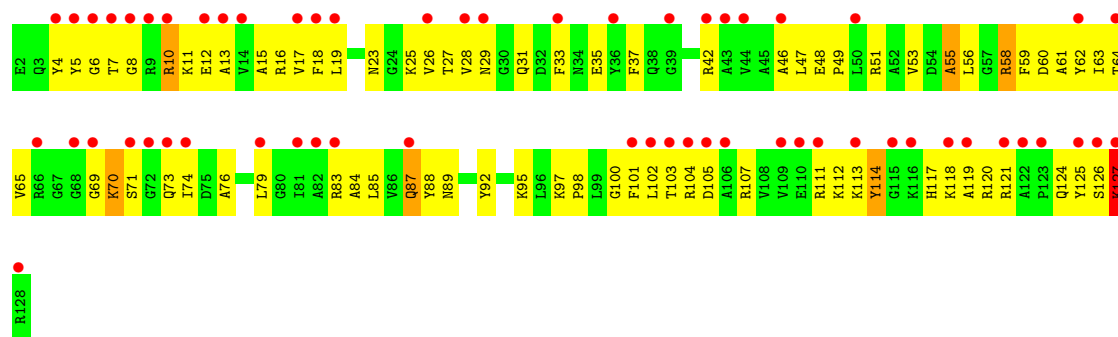


• Molecule 12: 30S ribosomal protein S9

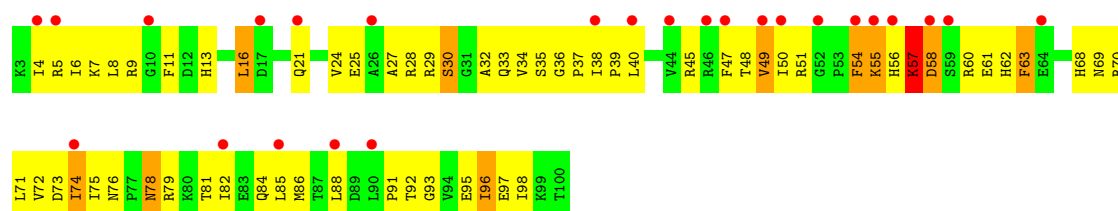


• Molecule 12: 30S ribosomal protein S9

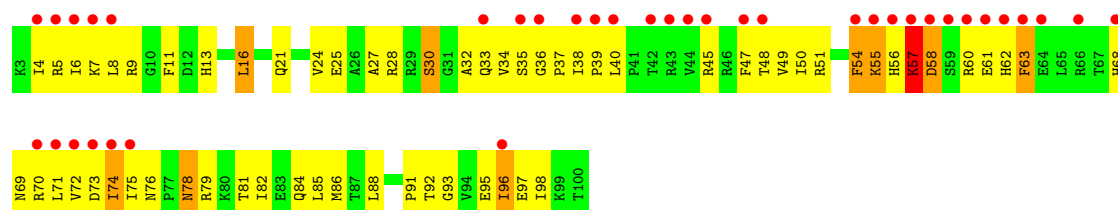




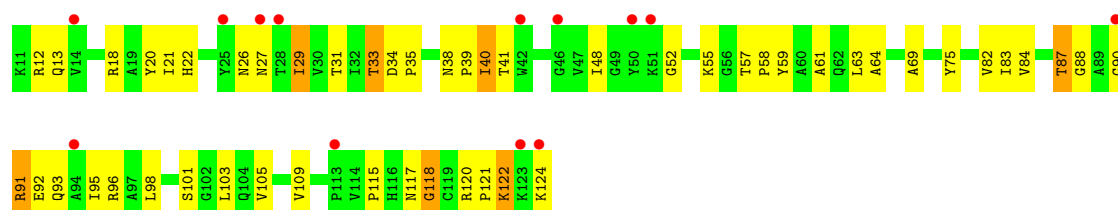
• Molecule 13: 30S ribosomal protein S10



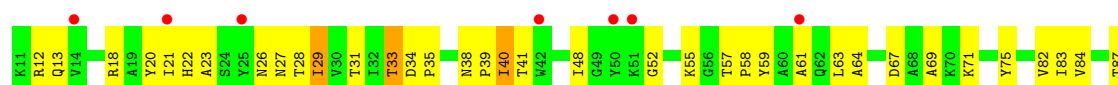
• Molecule 13: 30S ribosomal protein S10



• Molecule 14: 30S ribosomal protein S11



• Molecule 14: 30S ribosomal protein S11





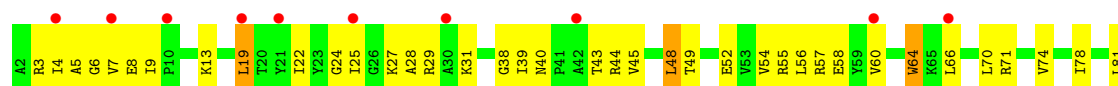
- Molecule 15: 30S ribosomal protein S12



- Molecule 15: 30S ribosomal protein S12



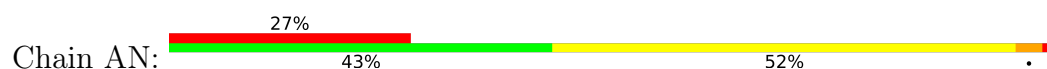
- Molecule 16: 30S ribosomal protein S13

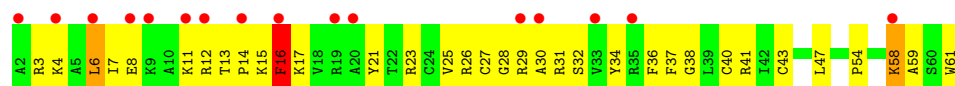


- Molecule 16: 30S ribosomal protein S13

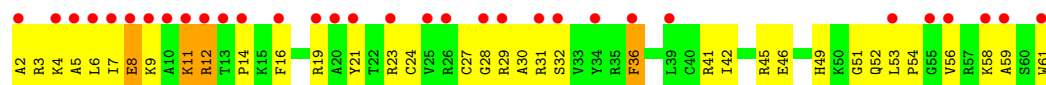


- Molecule 17: 30S ribosomal protein S14

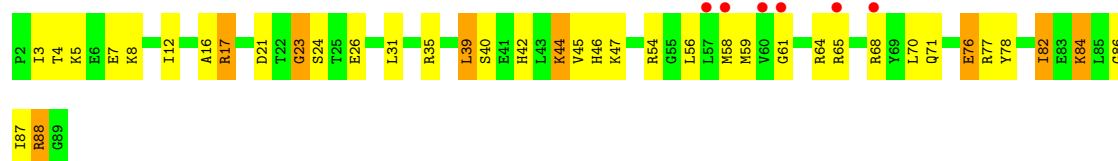




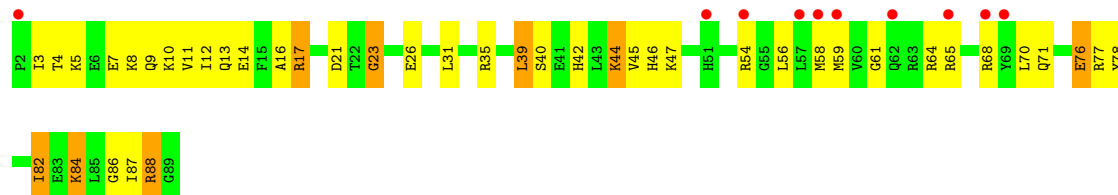
- Molecule 17: 30S ribosomal protein S14



- Molecule 18: 30S ribosomal protein S15



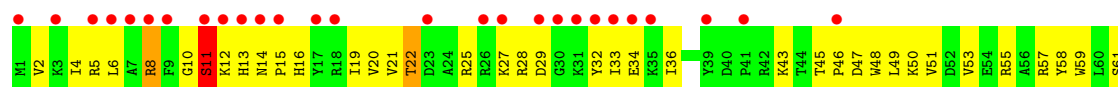
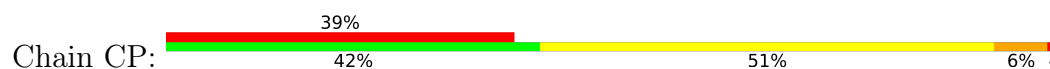
- Molecule 18: 30S ribosomal protein S15

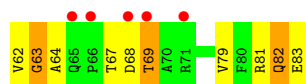


- Molecule 19: 30S ribosomal protein S16

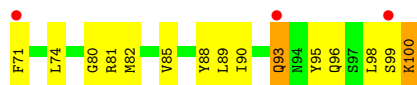
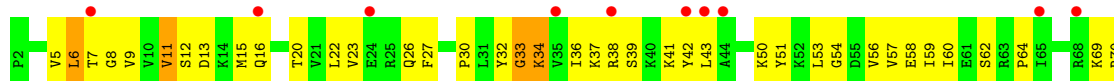


- Molecule 19: 30S ribosomal protein S16

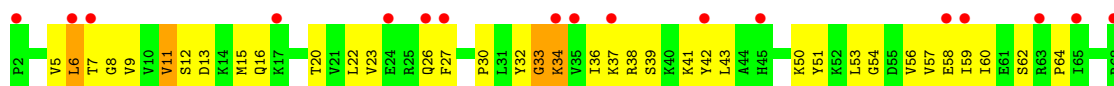




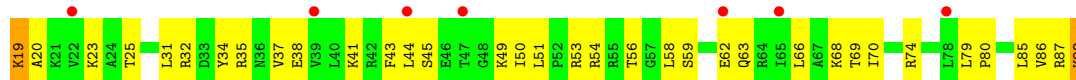
- Molecule 20: 30S ribosomal protein S17



- Molecule 20: 30S ribosomal protein S17



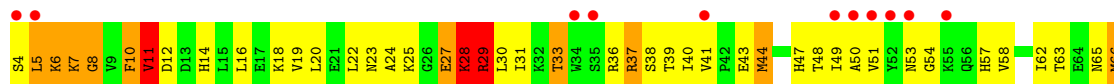
- Molecule 21: 30S ribosomal protein S18



- Molecule 21: 30S ribosomal protein S18

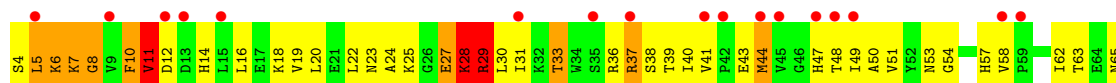


- Molecule 22: 30S ribosomal protein S19





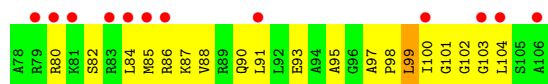
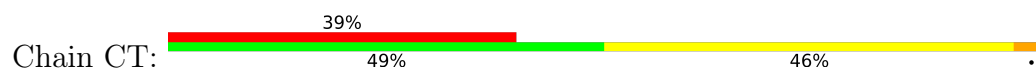
- Molecule 22: 30S ribosomal protein S19



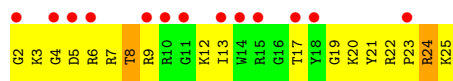
- Molecule 23: 30S ribosomal protein S20



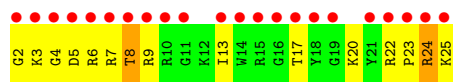
- Molecule 23: 30S ribosomal protein S20



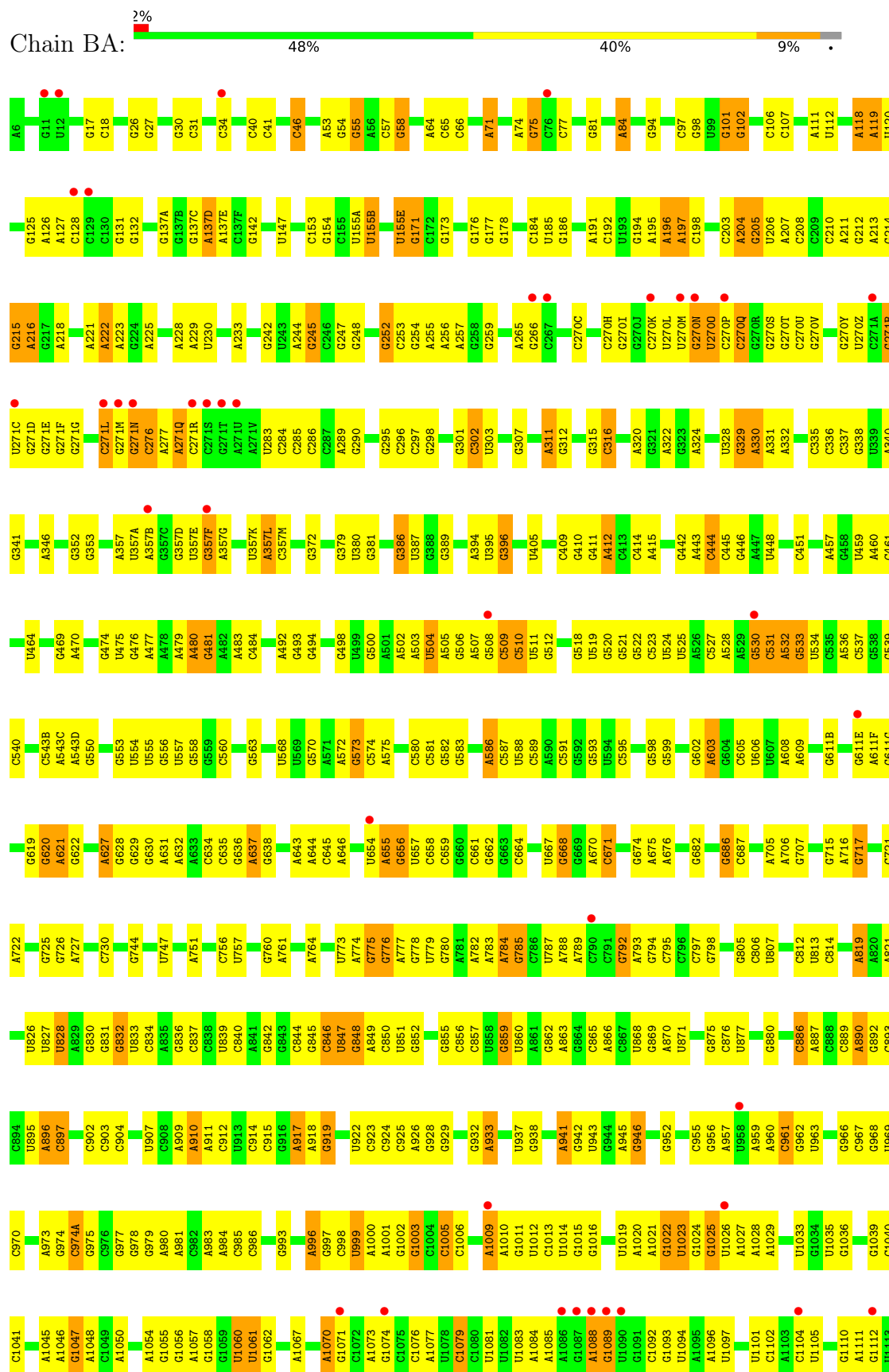
- Molecule 24: 30S ribosomal protein Thx



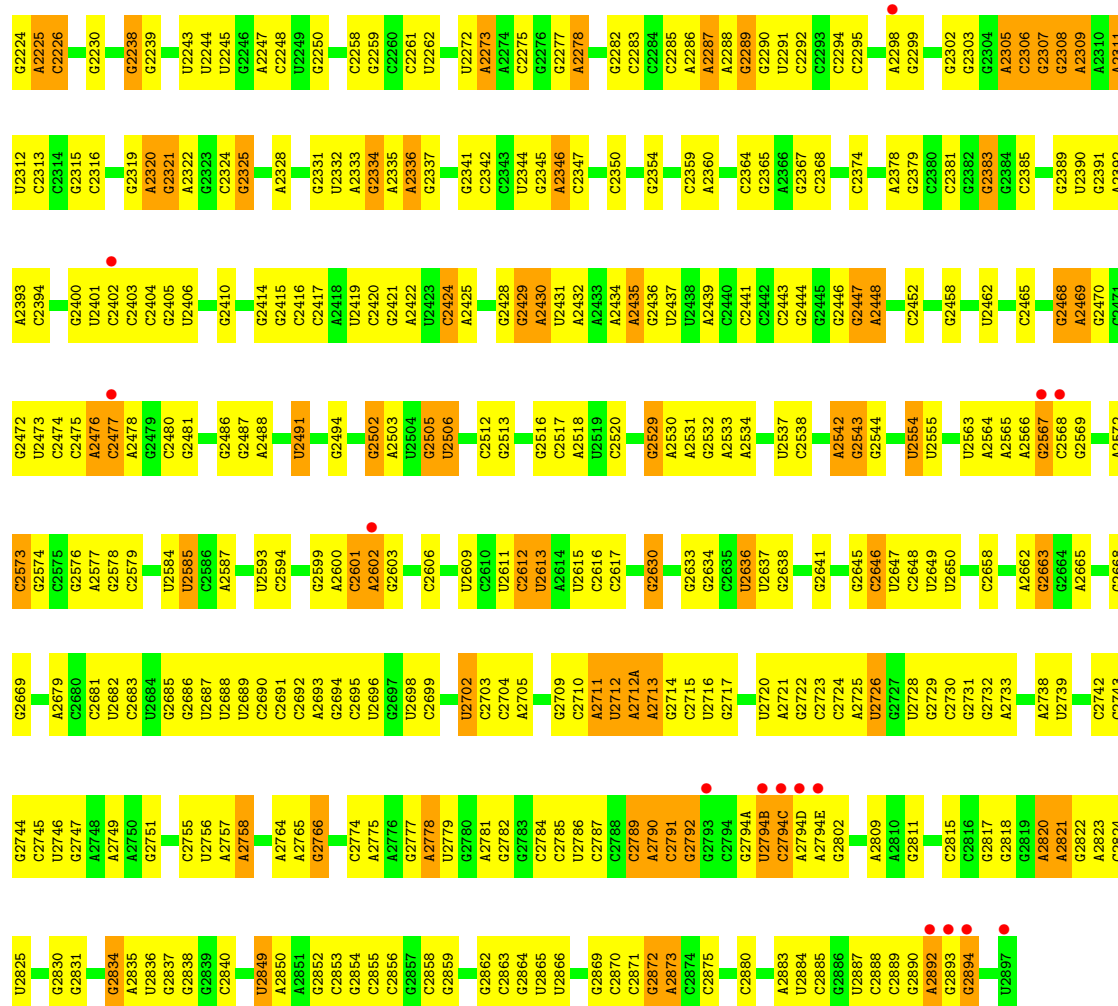
- Molecule 24: 30S ribosomal protein Thx



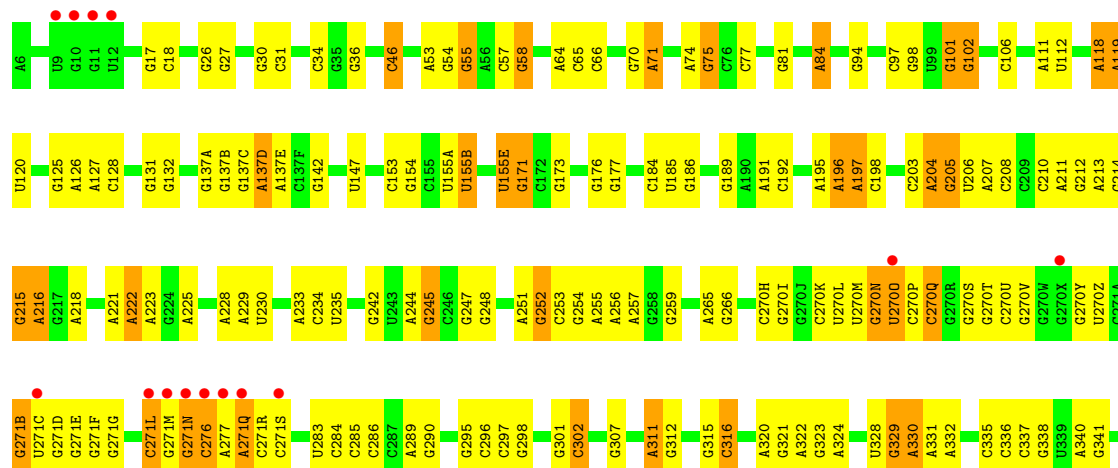
• Molecule 25: 23S ribosomal RNA



[illegible]

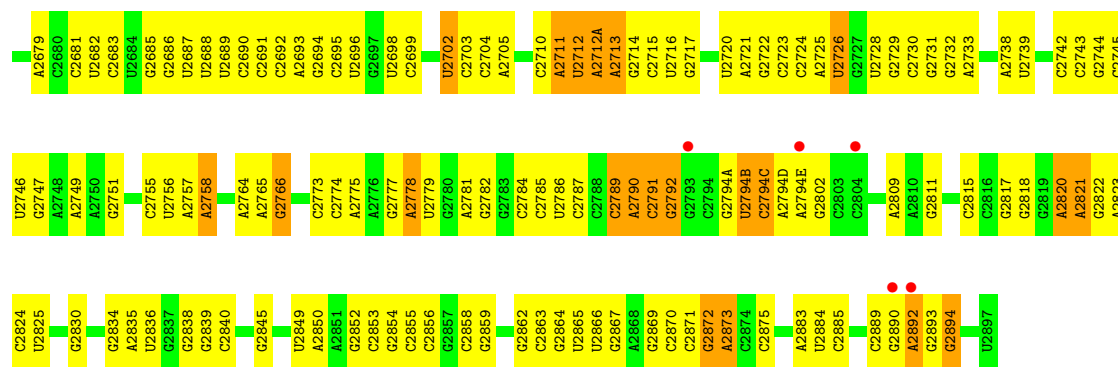


• Molecule 25: 23S ribosomal RNA

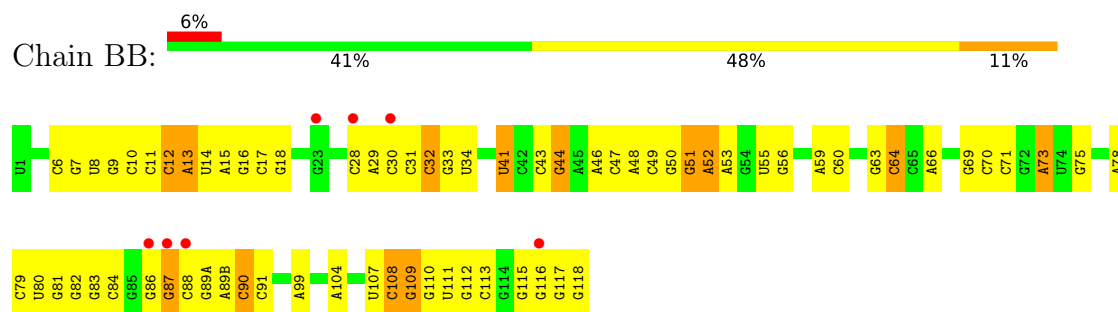


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A1460	A1286	G1285	G1186	A1111	C1041	G968	C894	U912	A716	A620	A543C	G469	G353
C1461	A1287	A1288	U1188	G1112	A1045	U969	A896	A819	G717	C624	A543D	A470	
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G1463	G1386	C1290	G1190	G1117	G1047	A973	A899	U827	A722	G628	U554	G475	U357A
C1464	C1387	C1291	G1191	C1118	A1048	G974	A900	U828	G725	G629	U555	G476	G357C
G1465	G1388	C1292	G1192	G1119	C1049	C974A	A901	A829	G726	G630	U556	A477	G357D
C1466	G1389	C1293	A1194	C1120	A1050	G975	C902	G830	A727	A631	U557	A478	U357E
G1467	G1390	G1201	G1195	G1121	A1051	C976	C903	G831		A632	U558	A479	G357F
C1468	U1394	G1202	G1196	G1122	A1052	G977	C904	G832	G730	A633	G559	A480	A357G
A1468A	G1203	G1203	A1126	A1126	G1055	A880	U907	U833		C634	C560	A481	G357J
C1468B	U1204	U1204	A1127	A1127	G1056	A983	C908	U834	G744	C635	A482	A482	U357K
A1468J	U1205	U1205	A1128	A1128	A1057	A984	A909	A835		G636	C484	A357L	A357M
G1468K	A1210	A1210	U1130	U1130	G1059	C985	A910	G836	U747	A637		A492	G372
G1483	U1211	U1211	C1135	C1135	U1060	C991	A911	C837	A751	G638	U568	A493	
G1484	G1212	G1212	G1136	G1136	U1061	C992	C912	C838		U639	U569	G494	
G1485	G1215	G1215	G1137	G1137	G1062	G993	C914	U839	C756	A643	A571	G498	G379
A1486	G1138	G1138	G1138	G1138	G1063		C915	C840	U757	A644	A572	U499	U380
G1487	G1139	G1139	G1139	G1139	A1067	A996	G916	G842		C645	C574	G500	G381
C1488	C1217	C1217	C1140	C1140	A1067	G997	A917	G843	G760	A646	A575	A501	
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A1490	G1219	G1219	U1141	U1141	G1071	U999	G919	C845	A764	A655	C580	A503	G387
A1491	A1219A	A1219A	U1141A	U1141A	G1072	A1000	U922	C846		G656	C581	A504	G388
G1492	C1220	C1220	A1142	A1142	A1073	A1001	C923	U847	U773	U657	G582	A505	G389
C1493	C1221	C1221	A1143	A1143	G1074	G1002	C924	G848	U774	C658	G583	G506	A394
G1494	C1222	C1222	G1144	G1144	G1075	G1003	C925	A849	G775	C659		A507	U395
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A1495	G1228	G1228	C1146	C1146	G1077	C1005	A926	U851		A777	C587	C509	
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U1497	G1230	G1230	G1150	G1150	G1079	C1007	G929	C857	U779	G663	C589	U511	
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C1504	G1333	G1333	C1152	C1152	A1083	A1010	G931	G859	A782	U667	G592	G518	G410
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A1506A	G1343	G1343	A1155	A1155	A1086	U1014	U937	C865	G785	A670	C595	G521	C413
A1506B	G1344	G1344	C1161	C1161	G1087	G1015	G938	C866	G786	C671			C414
G1506C	G1345	G1345	G1162	G1162	A1088	G1016	U937	C867	U787	C672	G599	U524	A415
A1506D	G1346	G1346	G1163	G1163	G1089		A841	C868	A788	C673	U525	U524	G442
G1506E	A1349	A1349	G1164	G1164	U1090	U1019	G942	U868	A789	G674	A526	U525	G443
C1506F	U1352	U1352	U1165	U1165	C1091	A1020	U943	G869		A675	C527	A526	A443
U1506G	G1356	G1356	C1166	C1166	G1092	A1021	G946	U871	G792	A676	A528	A528	C444
C1506H	U1265	U1265	U1167	U1167	U1093	G1022	G946		A793	G681	G604	A529	C445
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G1506J	U1263	U1263	G1172	G1172	U1096	G1025	C955	C876	C795	G683	U607	G531	U447
G1506K	A1268	A1268	A1173	A1173	U1097	U1026	G956	C877	C796	G684	A608	A532	U448
C1506L	G1270	G1270	U1174	U1174	C1102	A1027	A957	U877	C797	G686	A609	G533	A449
G1506M	A1272	A1272	G1175	G1175	U1101	U1028	G957	G880	G798	C687	U534	U534	G450
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A1529	A1453	A1453	A1182	A1182	G1108	G1036	C961	C888	G707	G707	G611E	G538	A459
G1530	U1454	U1454	A1183	A1183	U1108		U963	C889	G808	C708	A611F	G539	A460
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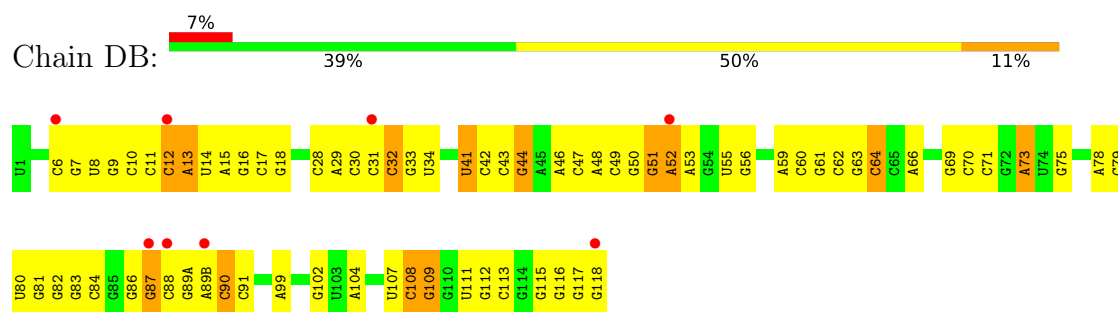




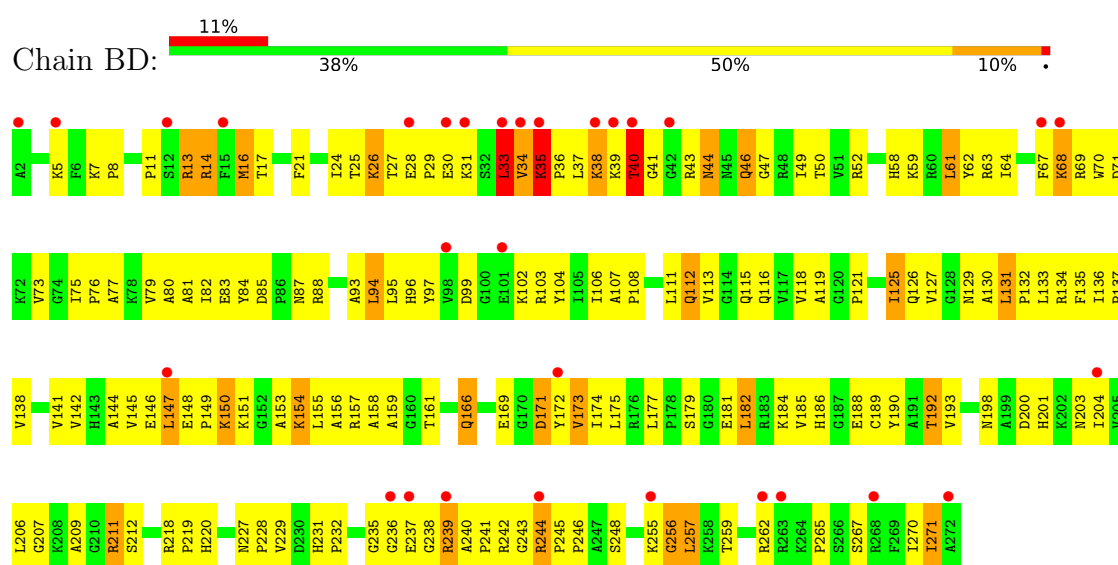
• Molecule 26: 5S ribosomal RNA



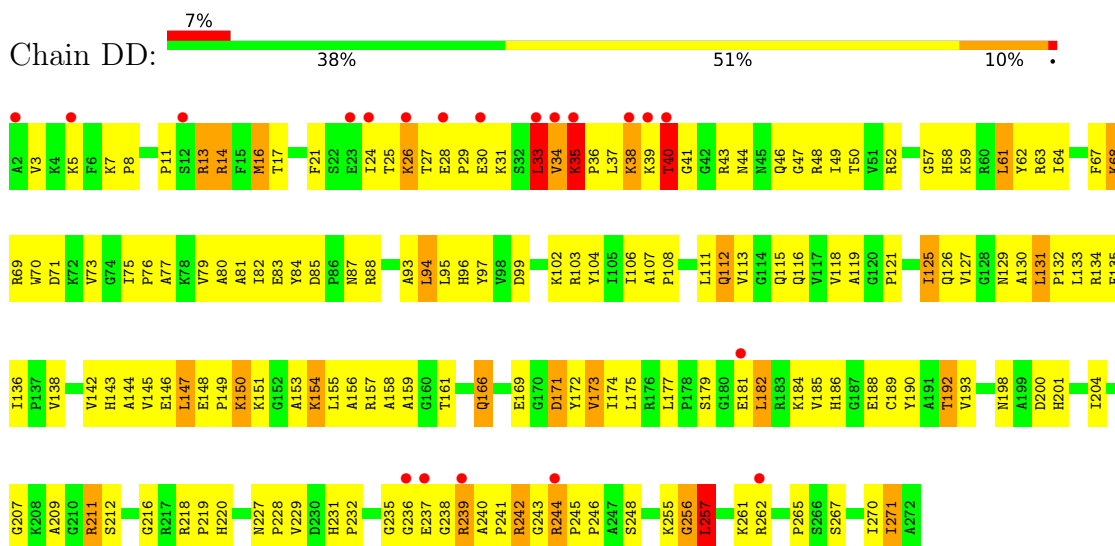
• Molecule 26: 5S ribosomal RNA



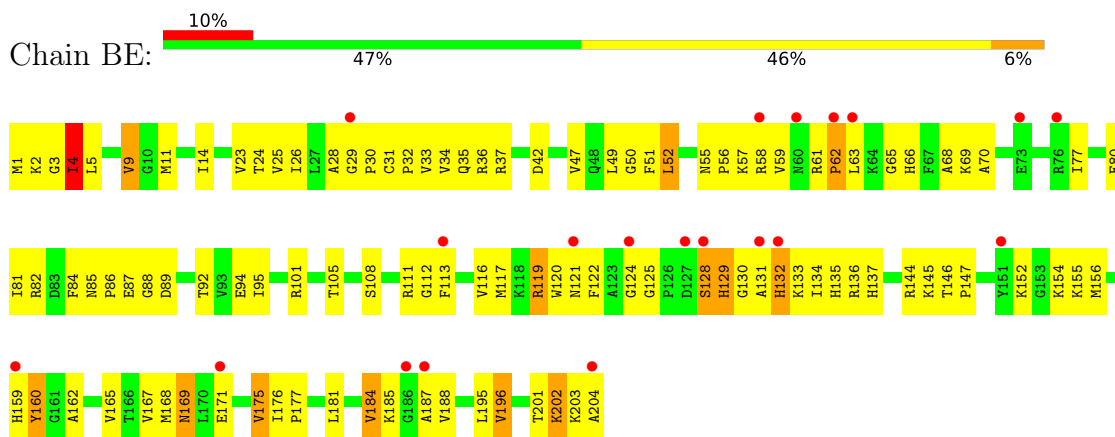
• Molecule 27: 50S ribosomal protein L2



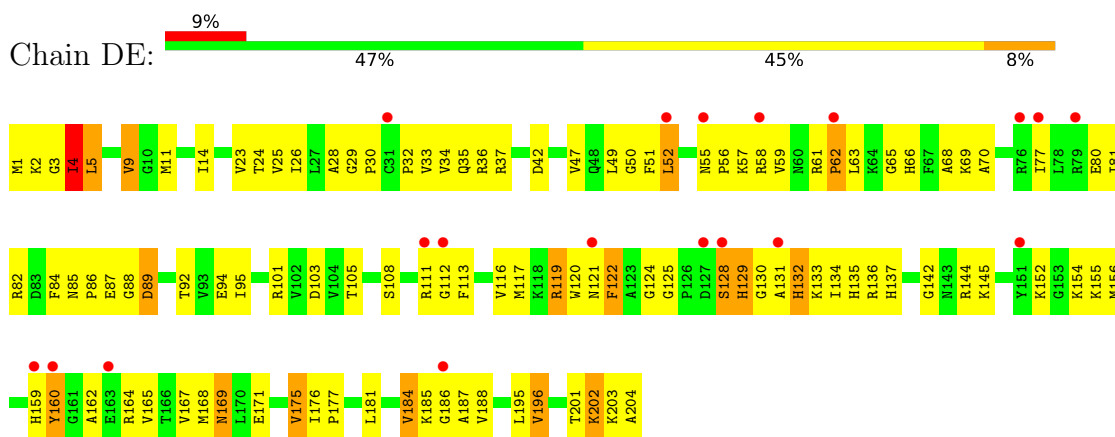
- Molecule 27: 50S ribosomal protein L2



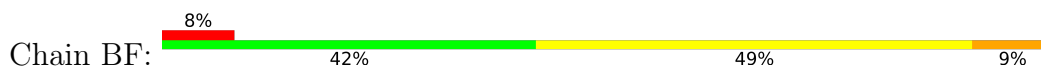
- Molecule 28: 50S ribosomal protein L3

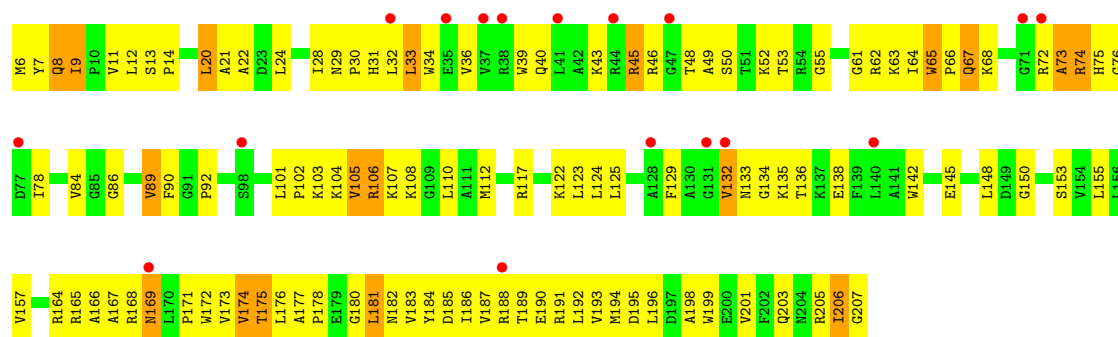


- Molecule 28: 50S ribosomal protein L3

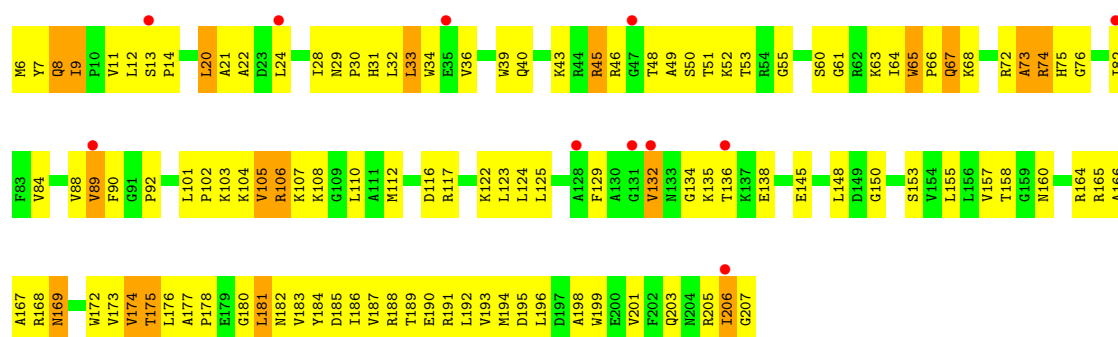
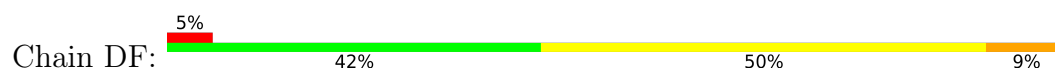


- Molecule 29: 50S ribosomal protein L4

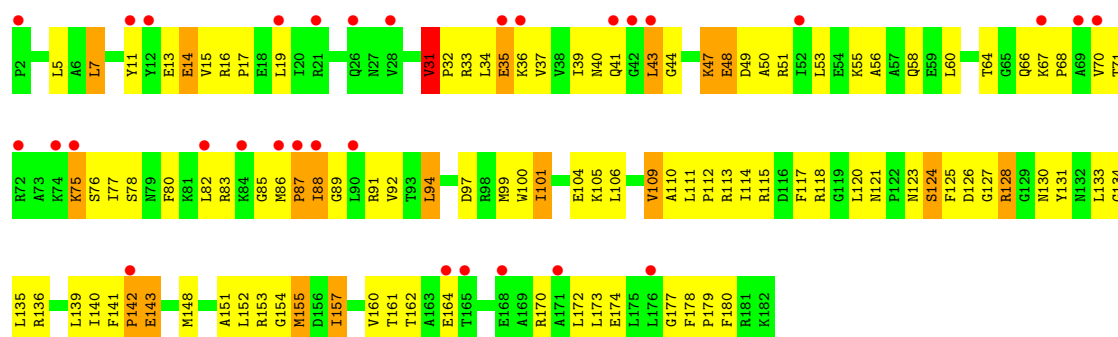
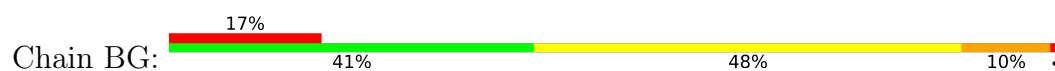




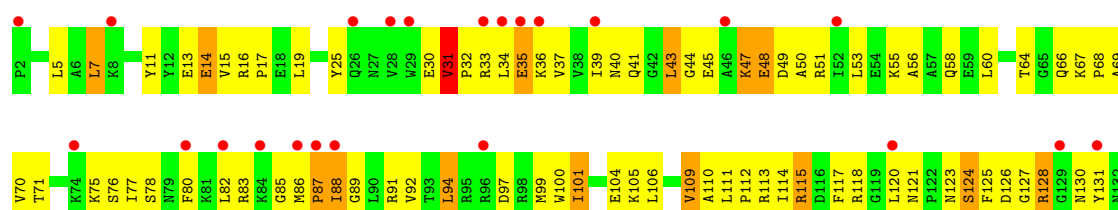
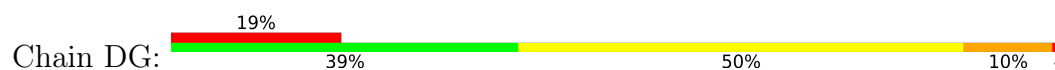
• Molecule 29: 50S ribosomal protein L4

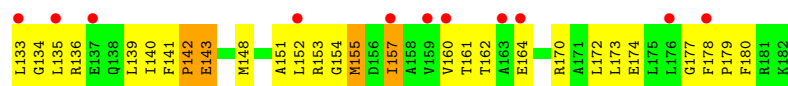


• Molecule 30: 50S ribosomal protein L5

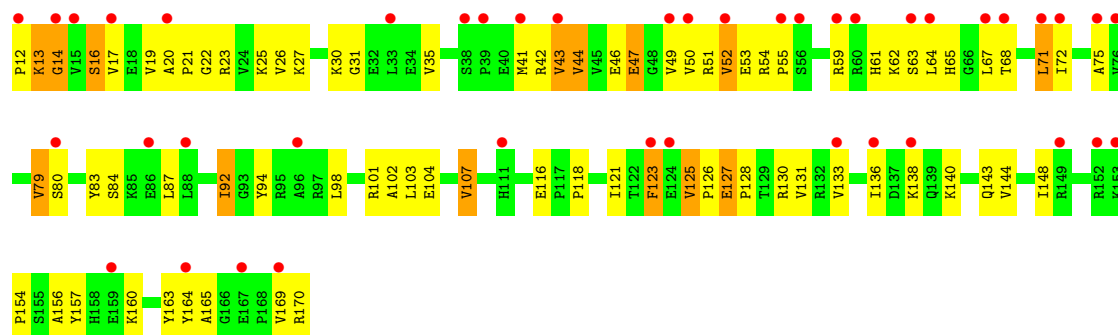


• Molecule 30: 50S ribosomal protein L5

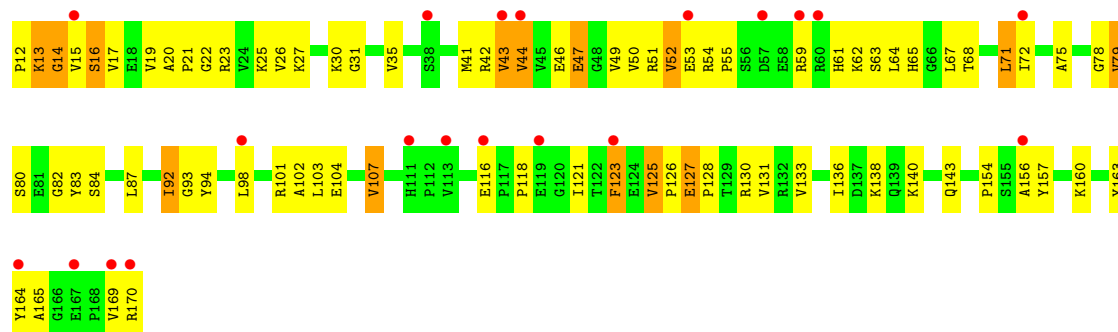




• Molecule 31: 50S ribosomal protein L6



• Molecule 31: 50S ribosomal protein L6

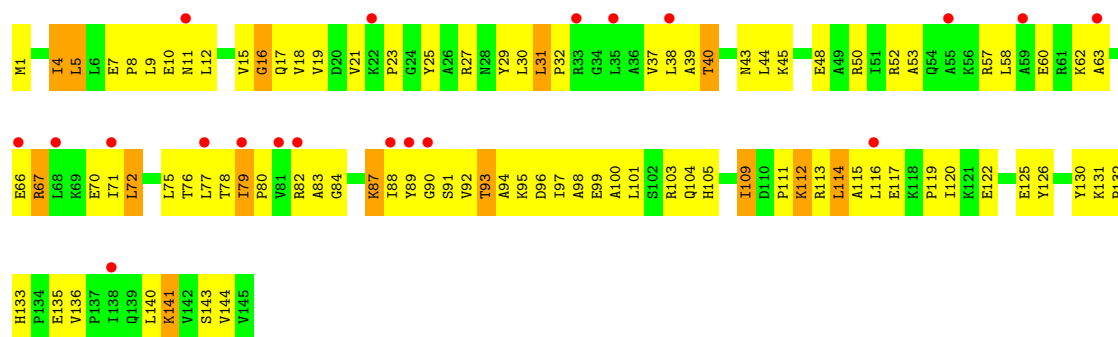


• Molecule 32: 50S ribosomal protein L9

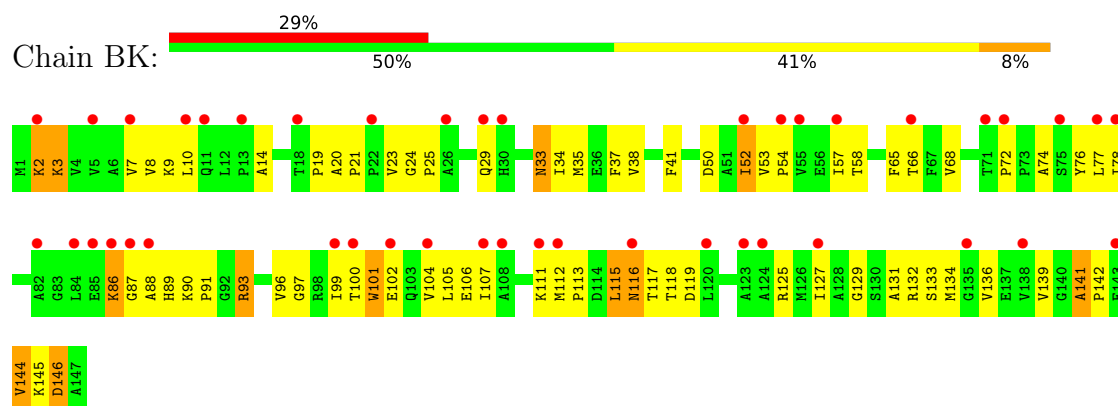


• Molecule 32: 50S ribosomal protein L9

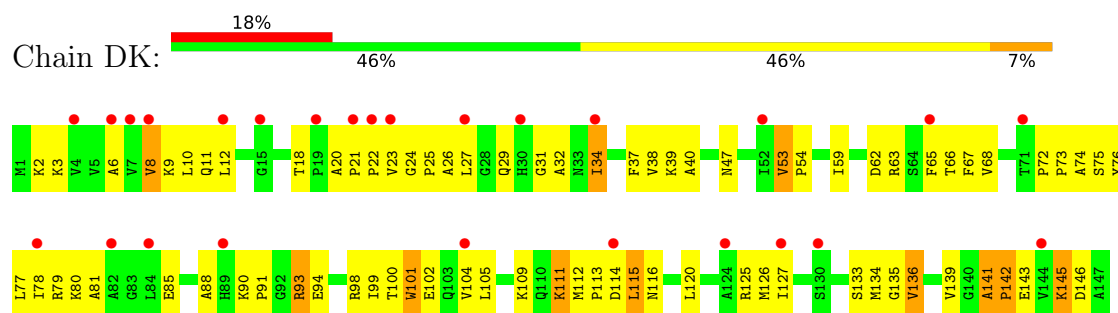




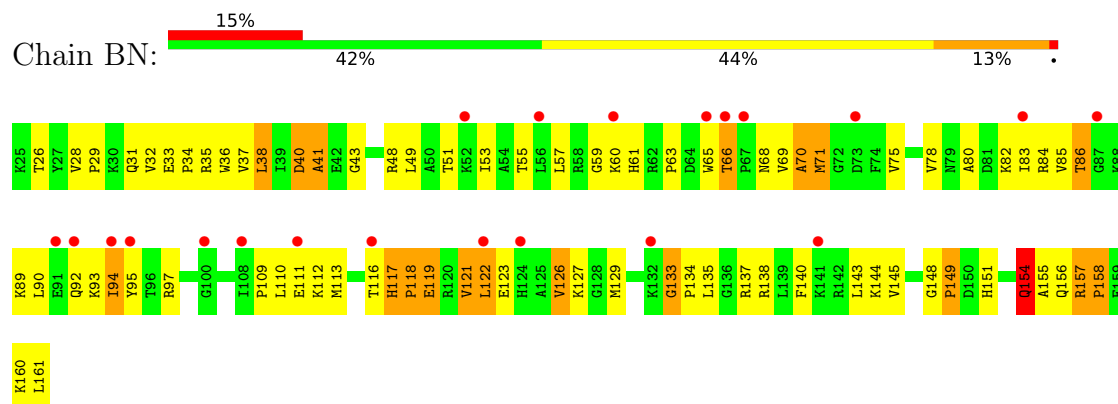
- Molecule 33: 50S ribosomal protein L11



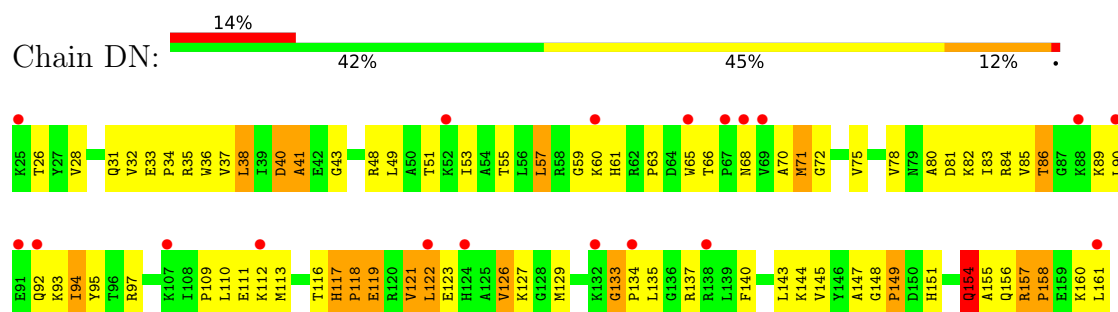
- Molecule 33: 50S ribosomal protein L11



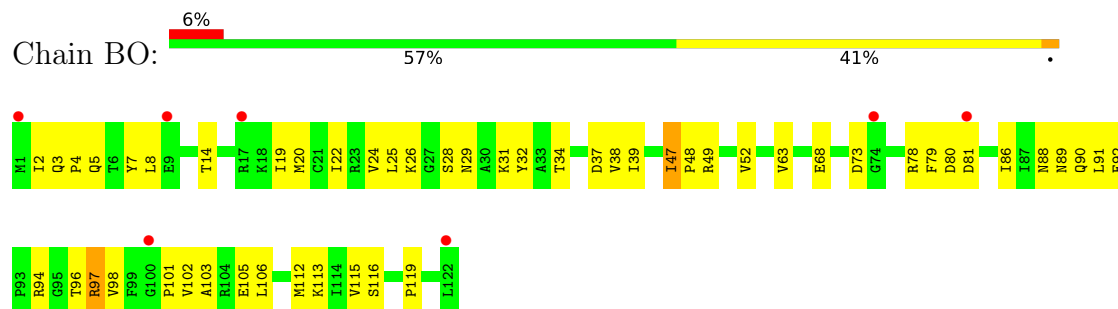
- Molecule 34: 50S ribosomal protein L13



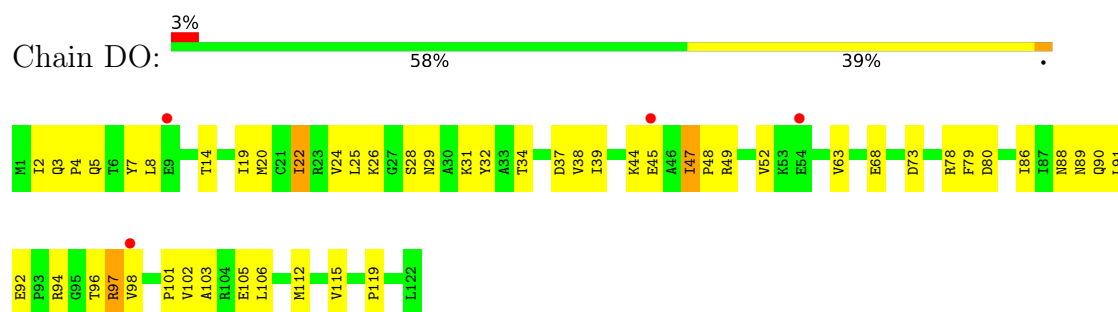
- Molecule 34: 50S ribosomal protein L13



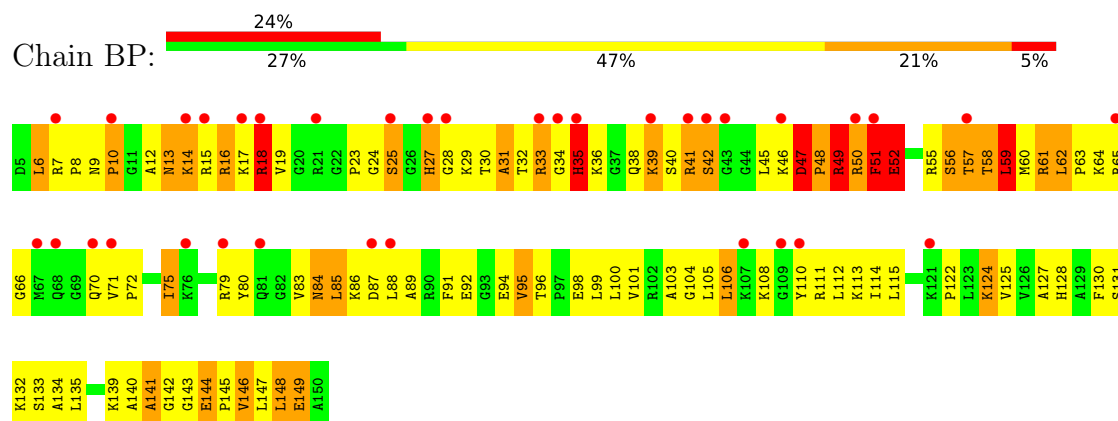
• Molecule 35: 50S ribosomal protein L14



• Molecule 35: 50S ribosomal protein L14

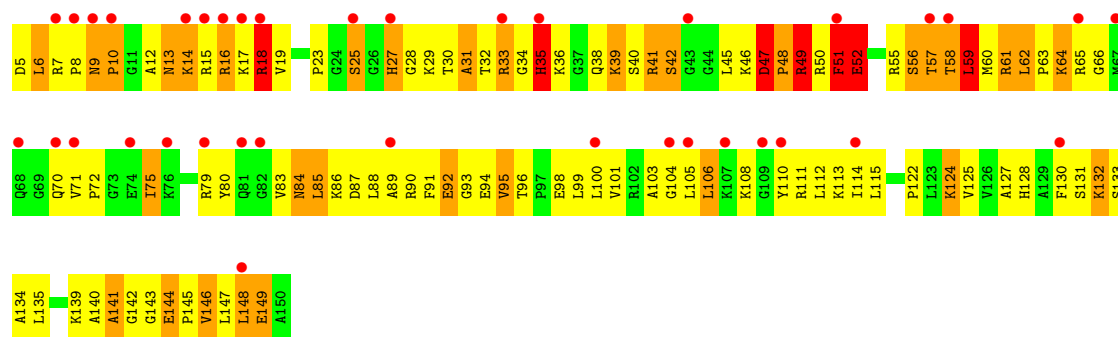


• Molecule 36: 50S ribosomal protein L15

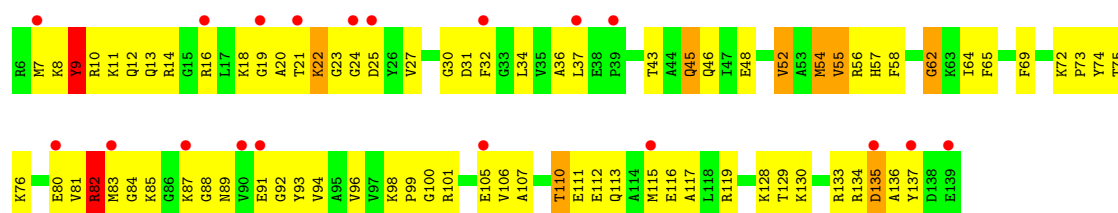
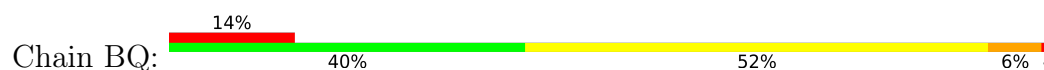


• Molecule 36: 50S ribosomal protein L15

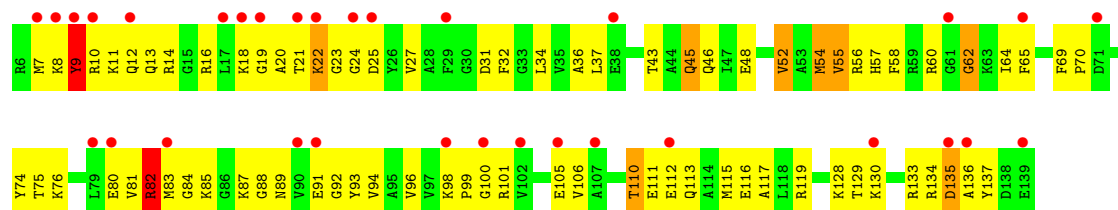
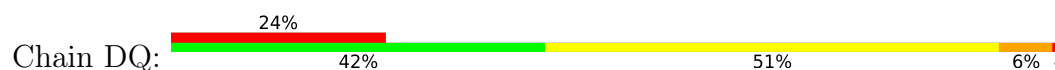




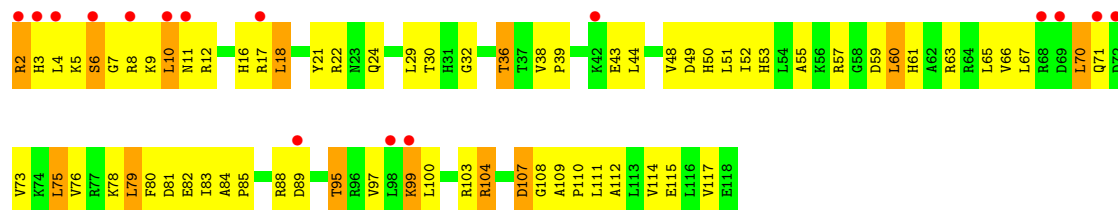
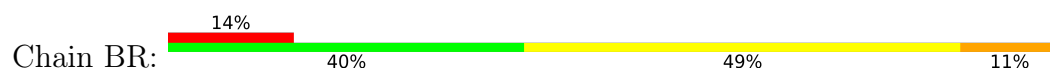
• Molecule 37: 50S ribosomal protein L16



• Molecule 37: 50S ribosomal protein L16

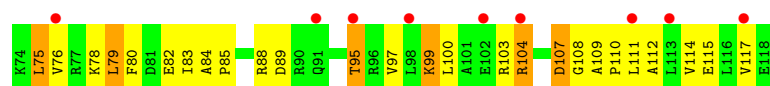


• Molecule 38: 50S ribosomal protein L17

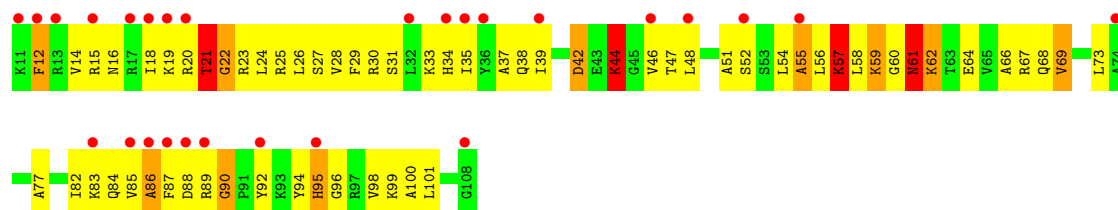


• Molecule 38: 50S ribosomal protein L17

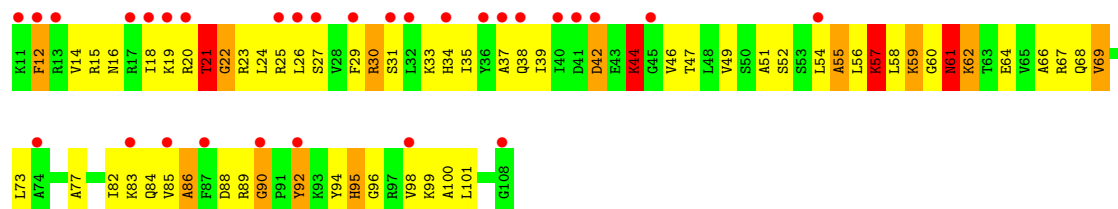




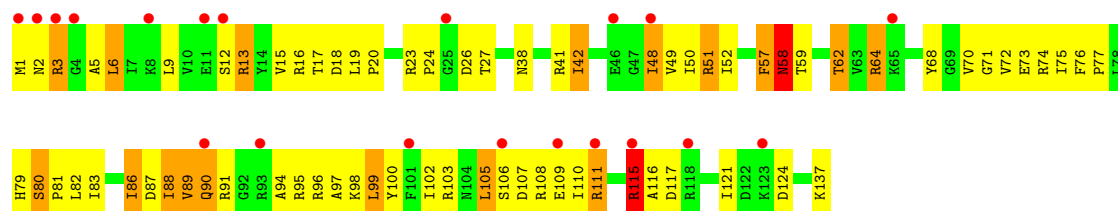
• Molecule 39: 50S ribosomal protein L18



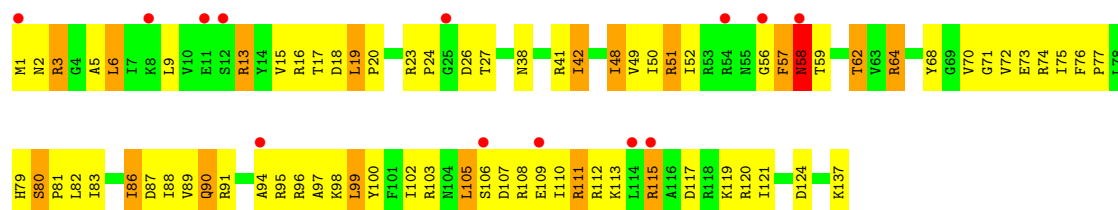
• Molecule 39: 50S ribosomal protein L18



• Molecule 40: 50S ribosomal protein L19

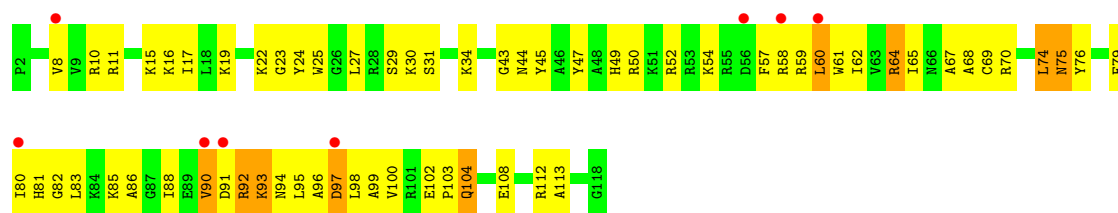


• Molecule 40: 50S ribosomal protein L19

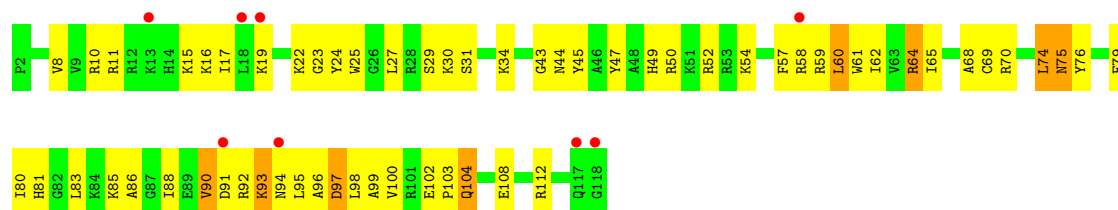


• Molecule 41: 50S ribosomal protein L20

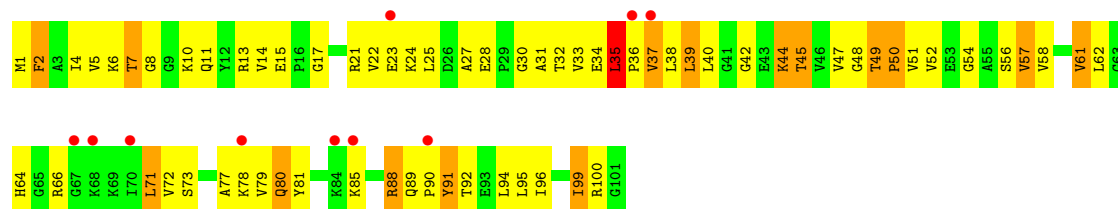




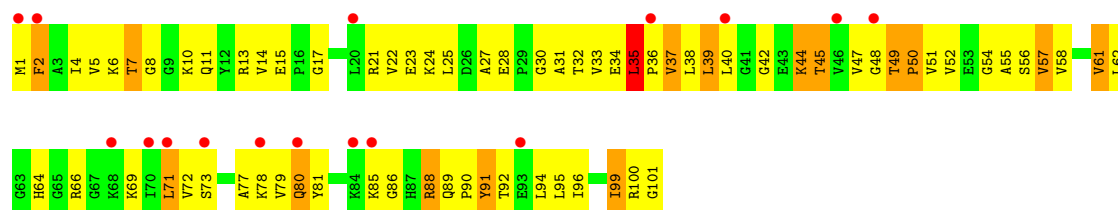
• Molecule 41: 50S ribosomal protein L20



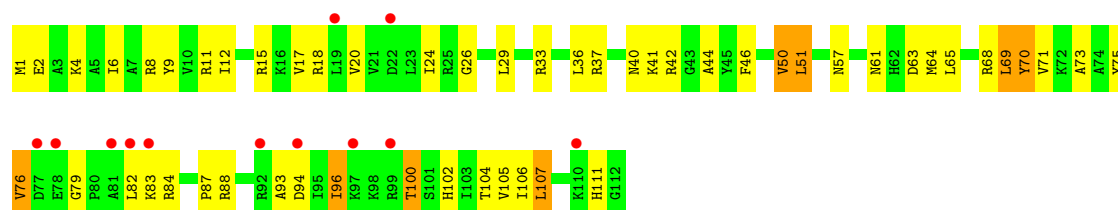
• Molecule 42: 50S ribosomal protein L21



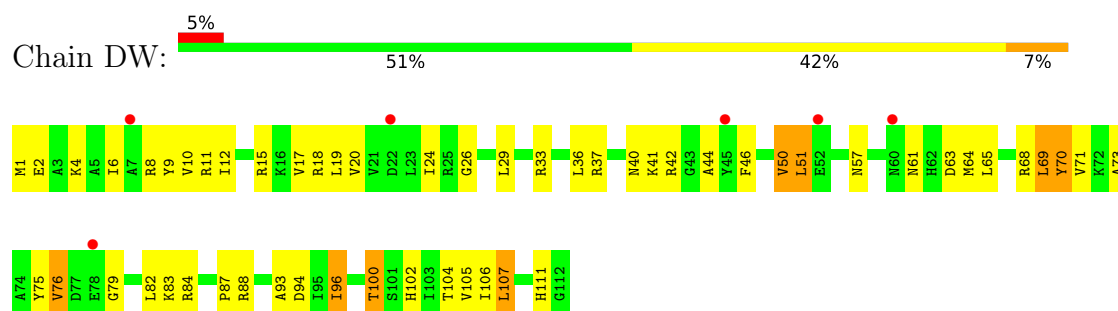
• Molecule 42: 50S ribosomal protein L21



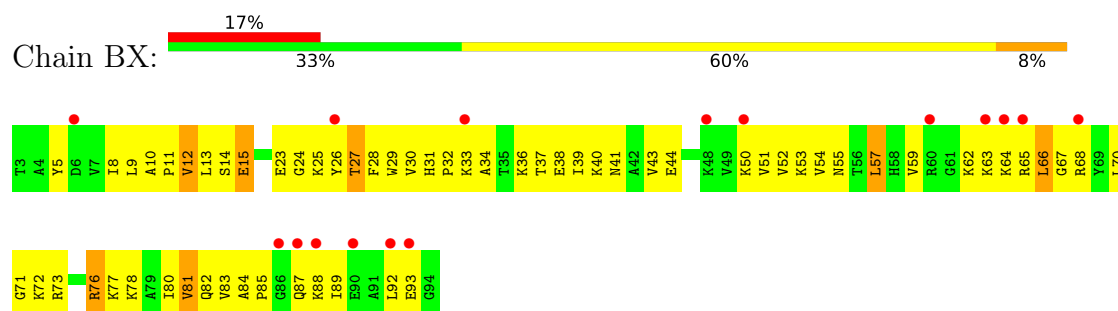
• Molecule 43: 50S ribosomal protein L22



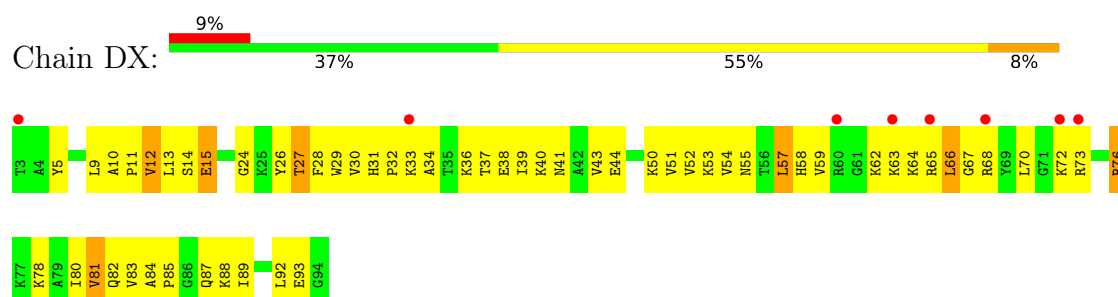
- Molecule 43: 50S ribosomal protein L22



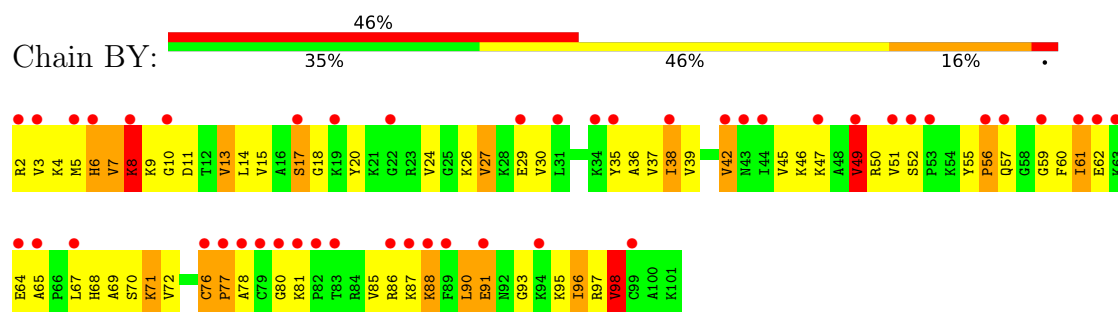
- Molecule 44: 50S ribosomal protein L23



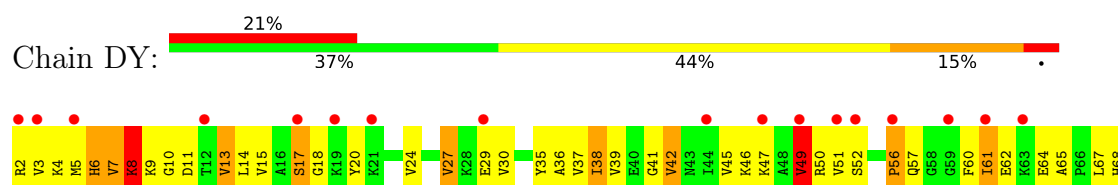
- Molecule 44: 50S ribosomal protein L23

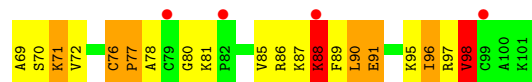


- Molecule 45: 50S ribosomal protein L24

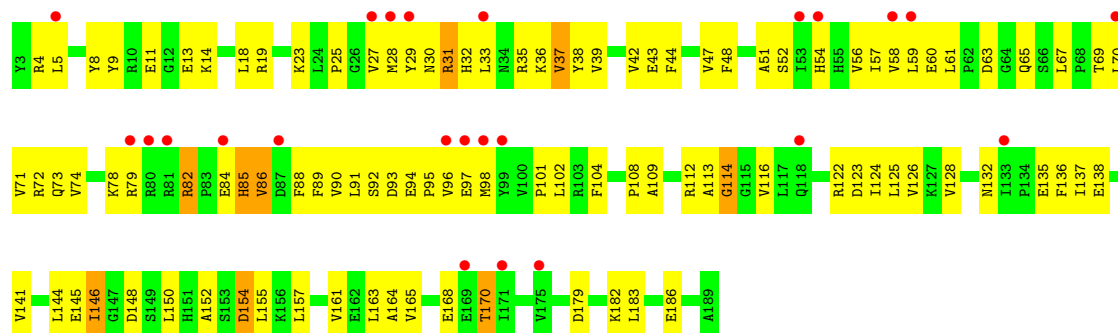


- Molecule 45: 50S ribosomal protein L24

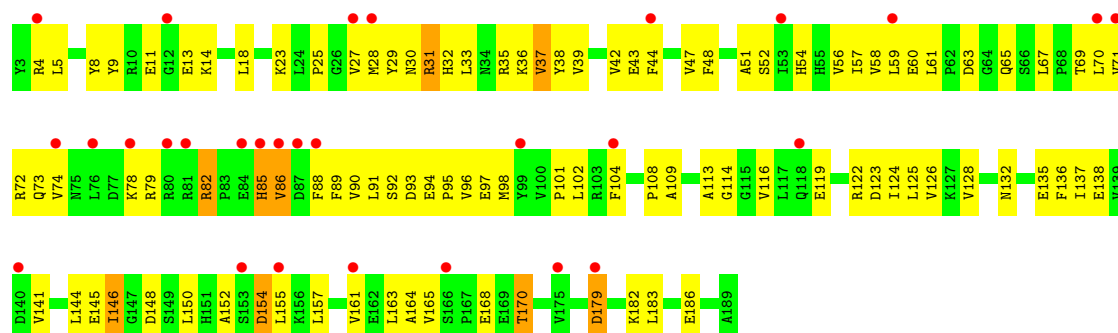




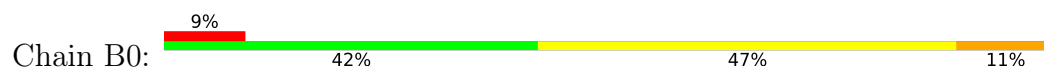
• Molecule 46: 50S ribosomal protein L25



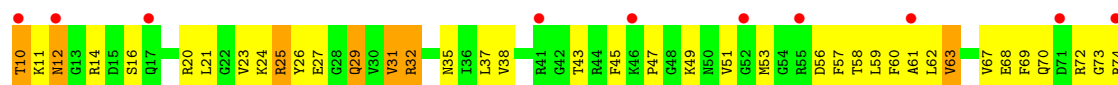
• Molecule 46: 50S ribosomal protein L25

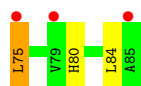


• Molecule 47: 50S ribosomal protein L27

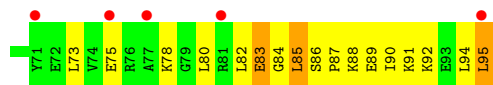
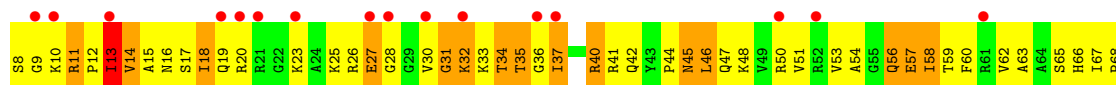


• Molecule 47: 50S ribosomal protein L27

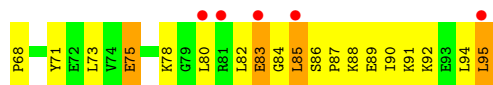
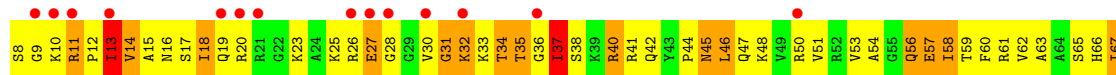




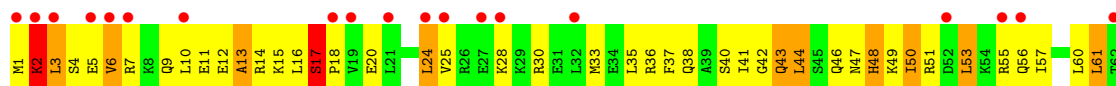
• Molecule 48: 50S ribosomal protein L28



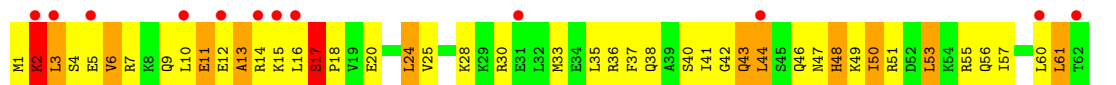
• Molecule 48: 50S ribosomal protein L28



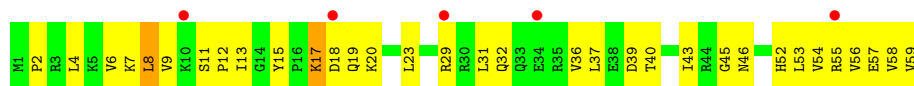
• Molecule 49: 50S ribosomal protein L29



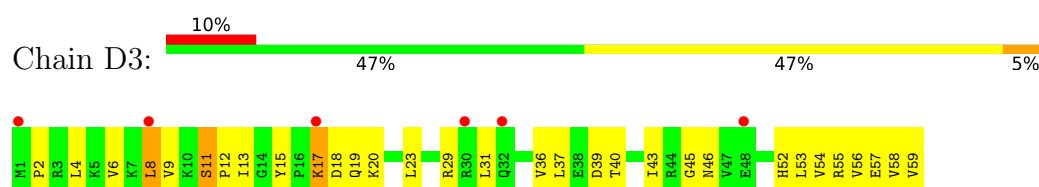
• Molecule 49: 50S ribosomal protein L29



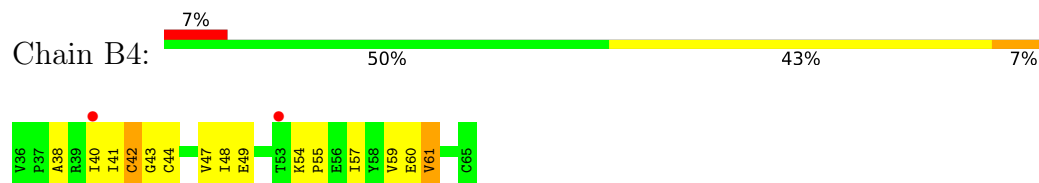
• Molecule 50: 50S ribosomal protein L30



• Molecule 50: 50S ribosomal protein L30



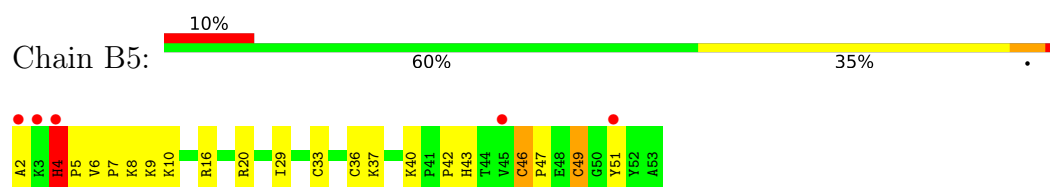
- Molecule 51: 50S ribosomal protein L31



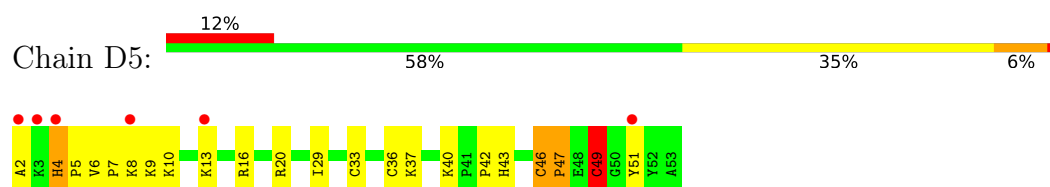
- Molecule 51: 50S ribosomal protein L31



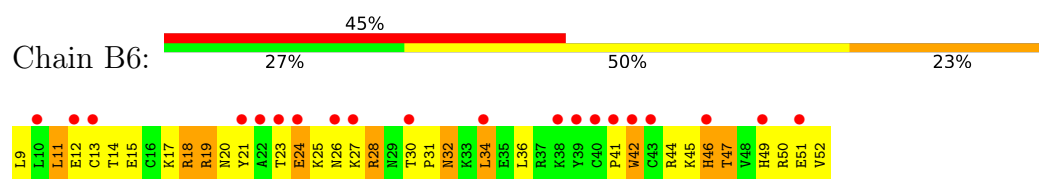
- Molecule 52: 50S ribosomal protein L32



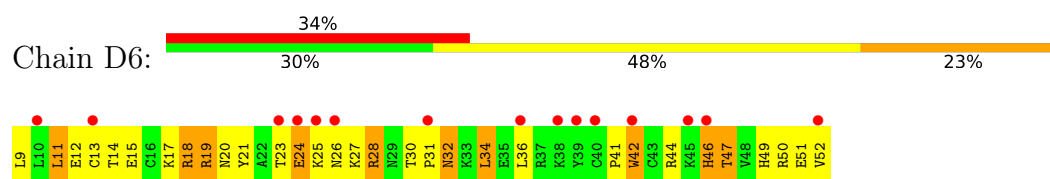
- Molecule 52: 50S ribosomal protein L32



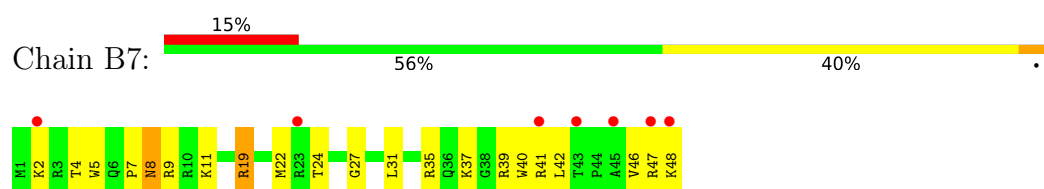
- Molecule 53: 50S ribosomal protein L33



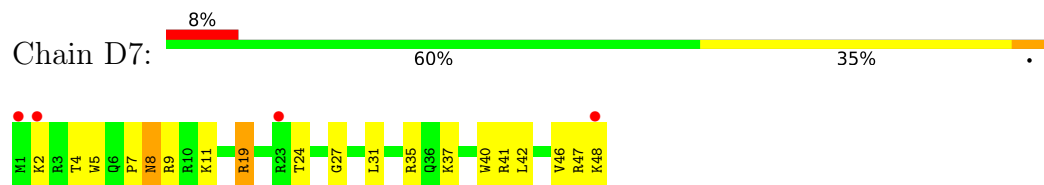
- Molecule 53: 50S ribosomal protein L33



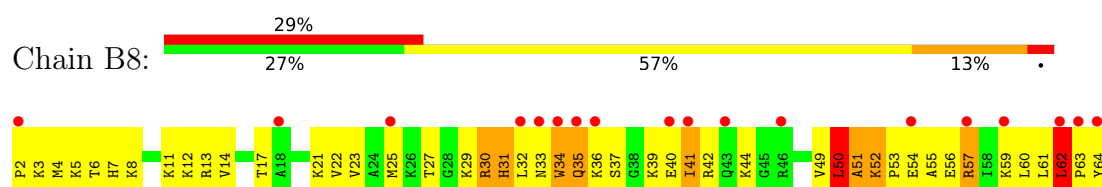
- Molecule 54: 50S ribosomal protein L34



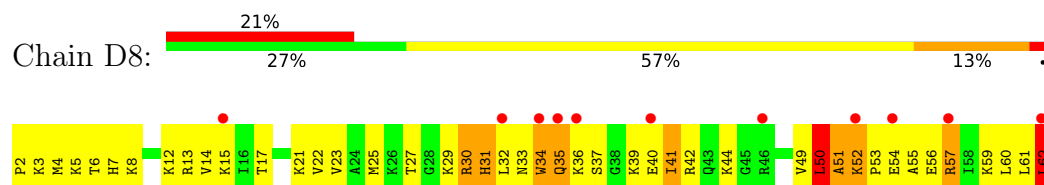
- Molecule 54: 50S ribosomal protein L34



- Molecule 55: 50S ribosomal protein L35



- Molecule 55: 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	212.07Å 454.40Å 618.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.67 – 3.40 49.67 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.67-3.40) 99.6 (49.67-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 3.33Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486), CNS	Depositor
R, R_{free}	0.234 , 0.268 0.241 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	83.6	Xtriage
Anisotropy	0.218	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 100.6	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	0.91	EDS
Total number of atoms	294074	wwPDB-VP
Average B, all atoms (Å ²)	109.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.50% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	AA	0.16	2/36194 (0.0%)	0.29	0/56493
1	CA	0.16	2/36194 (0.0%)	0.29	0/56493
2	AV	0.15	0/241	0.34	0/374
2	CV	0.13	0/241	0.33	0/374
3	AW	0.14	0/1832	0.28	0/2855
3	CW	0.15	0/1832	0.28	0/2855
4	AY	0.29	0/2925	0.72	2/3953 (0.1%)
4	CY	0.29	0/2925	0.72	2/3953 (0.1%)
5	AB	0.28	0/1936	0.72	2/2609 (0.1%)
5	CB	0.27	0/1936	0.72	2/2609 (0.1%)
6	AC	0.28	0/1637	0.65	0/2205
6	CC	0.28	0/1637	0.65	0/2205
7	AD	0.33	0/1733	0.80	4/2318 (0.2%)
7	CD	0.29	0/1733	0.74	2/2318 (0.1%)
8	AE	0.32	0/1172	0.81	2/1576 (0.1%)
8	CE	0.32	0/1172	0.81	2/1576 (0.1%)
9	AF	0.28	0/856	0.71	2/1154 (0.2%)
9	CF	0.30	0/856	0.72	2/1154 (0.2%)
10	AG	0.29	0/1276	0.69	0/1709
10	CG	0.29	0/1276	0.69	0/1709
11	AH	0.29	0/1136	0.76	1/1527 (0.1%)
11	CH	0.28	0/1136	0.75	1/1527 (0.1%)
12	AI	0.27	0/1029	0.71	0/1378
12	CI	0.27	0/1029	0.71	0/1378
13	AJ	0.27	0/808	0.76	1/1085 (0.1%)
13	CJ	0.27	0/808	0.76	1/1085 (0.1%)
14	AK	0.31	0/857	0.81	0/1157
14	CK	0.31	0/857	0.81	2/1157 (0.2%)
15	AL	0.33	0/973	0.78	2/1301 (0.2%)
15	CL	0.33	0/973	0.78	2/1301 (0.2%)
16	AM	0.28	0/944	0.74	1/1265 (0.1%)
16	CM	0.29	0/944	0.75	1/1265 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AN	0.29	0/501	0.74	0/664
17	CN	0.34	0/501	0.69	0/664
18	AO	0.32	0/745	0.69	0/992
18	CO	0.31	0/745	0.70	0/992
19	AP	0.31	0/717	0.71	0/963
19	CP	0.29	0/717	0.70	0/963
20	AQ	0.28	0/837	0.71	0/1117
20	CQ	0.27	0/837	0.71	0/1117
21	AR	0.29	0/579	0.74	0/768
21	CR	0.29	0/579	0.76	0/768
22	AS	0.28	0/643	0.64	0/865
22	CS	0.28	0/643	0.64	0/865
23	AT	0.31	0/764	0.70	0/1006
23	CT	0.29	0/764	0.70	0/1006
24	AU	0.26	0/213	0.71	0/277
24	CU	0.26	0/213	0.71	0/277
25	BA	0.22	6/67268 (0.0%)	0.33	0/105011
25	DA	0.25	6/67268 (0.0%)	0.34	0/105011
26	BB	0.14	0/2853	0.29	0/4451
26	DB	0.15	0/2853	0.29	0/4451
27	BD	0.42	0/2155	0.86	5/2905 (0.2%)
27	DD	0.44	0/2155	0.86	5/2905 (0.2%)
28	BE	0.37	0/1597	0.85	3/2153 (0.1%)
28	DE	0.38	0/1597	0.86	3/2153 (0.1%)
29	BF	0.37	0/1622	0.83	2/2194 (0.1%)
29	DF	0.38	0/1622	0.83	2/2194 (0.1%)
30	BG	0.28	0/1500	0.71	2/2017 (0.1%)
30	DG	0.29	0/1500	0.71	2/2017 (0.1%)
31	BH	0.29	0/1246	0.77	2/1682 (0.1%)
31	DH	0.33	0/1246	0.79	2/1682 (0.1%)
32	BI	0.30	0/1148	0.76	3/1552 (0.2%)
32	DI	0.32	0/1148	0.77	1/1552 (0.1%)
33	BK	0.31	0/1108	0.72	1/1500 (0.1%)
33	DK	0.30	0/1108	0.70	1/1500 (0.1%)
34	BN	0.34	0/1124	0.80	4/1515 (0.3%)
34	DN	0.36	0/1124	0.79	4/1515 (0.3%)
35	BO	0.35	0/942	0.79	0/1268
35	DO	0.38	0/942	0.83	0/1268
36	BP	0.43	0/1131	0.91	3/1504 (0.2%)
36	DP	0.44	0/1131	0.92	4/1504 (0.3%)
37	BQ	0.40	0/1085	0.84	2/1449 (0.1%)
37	DQ	0.40	0/1085	0.85	2/1449 (0.1%)
38	BR	0.37	0/974	0.77	1/1302 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DR	0.37	0/974	0.77	1/1302 (0.1%)
39	BS	0.31	0/779	0.70	0/1036
39	DS	0.31	0/779	0.70	0/1036
40	BT	0.33	0/1158	0.79	2/1544 (0.1%)
40	DT	0.34	0/1158	0.79	2/1544 (0.1%)
41	BU	0.40	0/982	0.78	2/1306 (0.2%)
41	DU	0.41	0/982	0.77	1/1306 (0.1%)
42	BV	0.35	0/790	0.74	0/1057
42	DV	0.35	0/790	0.73	0/1057
43	BW	0.40	0/902	0.76	0/1209
43	DW	0.40	0/902	0.76	0/1209
44	BX	0.34	0/740	0.74	0/993
44	DX	0.40	0/740	0.76	0/993
45	BY	0.37	0/789	0.87	3/1051 (0.3%)
45	DY	0.40	0/789	0.86	3/1051 (0.3%)
46	BZ	0.29	0/1515	0.75	0/2056
46	DZ	0.30	0/1515	0.75	0/2056
47	B0	0.32	0/613	0.78	0/816
47	D0	0.33	0/613	0.77	0/816
48	B1	0.45	0/702	0.92	3/932 (0.3%)
48	D1	0.49	0/702	0.94	4/932 (0.4%)
49	B2	0.35	0/523	0.74	0/690
49	D2	0.43	0/523	0.76	0/690
50	B3	0.32	0/473	0.79	0/634
50	D3	0.34	0/473	0.79	2/634 (0.3%)
51	B4	0.29	0/229	0.69	0/309
51	D4	0.30	0/229	0.70	0/309
52	B5	0.38	0/419	0.83	2/567 (0.4%)
52	D5	0.39	0/419	0.82	2/567 (0.4%)
53	B6	0.29	0/388	0.72	1/518 (0.2%)
53	D6	0.29	0/388	0.72	1/518 (0.2%)
54	B7	0.44	0/427	0.89	0/561
54	D7	0.49	0/427	0.90	0/561
55	B8	0.38	0/516	0.82	2/679 (0.3%)
55	D8	0.42	0/516	0.82	2/679 (0.3%)
All	All	0.26	16/316492 (0.0%)	0.49	121/472144 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
36	BP	0	1
36	DP	0	1
38	BR	0	1
38	DR	0	1
48	B1	0	1
48	D1	0	1
52	B5	0	1
All	All	0	7

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	BA	1913	A	P-OP1	-7.81	1.33	1.49
1	AA	1493	A	P-OP2	-7.65	1.33	1.49
25	BA	1912	A	P-OP2	-7.65	1.33	1.49
25	DA	1912	A	P-OP1	-7.60	1.33	1.49
1	CA	1493	A	P-OP1	-7.48	1.33	1.49

The worst 5 of 121 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	DE	125	GLY	CA-C-N	9.50	129.26	119.76
28	DE	125	GLY	C-N-CA	9.50	129.26	119.76
28	BE	125	GLY	CA-C-N	9.31	129.07	119.76
28	BE	125	GLY	C-N-CA	9.31	129.07	119.76
41	DU	97	ASP	N-CA-C	-8.03	103.49	113.28

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
48	B1	26	ARG	Peptide
52	B5	4	HIS	Peptide
36	BP	51	PHE	Peptide
38	BR	10	LEU	Peptide
36	DP	51	PHE	Peptide

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	32332	0	16318	785	0
1	CA	32332	0	16318	798	0
2	AV	214	0	110	7	0
2	CV	214	0	110	8	0
3	AW	1640	0	837	26	0
3	CW	1640	0	837	24	0
4	AY	2874	0	2866	176	0
4	CY	2874	0	2866	172	0
5	AB	1901	0	1951	123	0
5	CB	1901	0	1951	122	0
6	AC	1613	0	1677	105	0
6	CC	1613	0	1677	107	0
7	AD	1703	0	1764	109	0
7	CD	1703	0	1765	123	0
8	AE	1156	0	1213	83	0
8	CE	1156	0	1213	81	0
9	AF	843	0	857	39	0
9	CF	843	0	857	38	0
10	AG	1257	0	1296	47	0
10	CG	1257	0	1296	44	0
11	AH	1116	0	1177	74	0
11	CH	1116	0	1177	78	0
12	AI	1011	0	1043	74	0
12	CI	1011	0	1043	73	0
13	AJ	795	0	840	76	0
13	CJ	795	0	840	75	0
14	AK	843	0	859	39	0
14	CK	843	0	859	40	0
15	AL	957	0	1046	75	0
15	CL	957	0	1046	73	0
16	AM	934	0	992	51	0
16	CM	934	0	992	57	0
17	AN	492	0	530	51	0
17	CN	492	0	530	39	0
18	AO	734	0	771	34	0
18	CO	734	0	771	35	0
19	AP	701	0	720	52	0
19	CP	701	0	720	50	0
20	AQ	824	0	893	43	0
20	CQ	824	0	893	45	0
21	AR	574	0	644	37	0
21	CR	574	0	644	38	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	AS	630	0	652	59	0
22	CS	630	0	652	60	0
23	AT	762	0	859	39	0
23	CT	762	0	859	41	0
24	AU	209	0	221	16	0
24	CU	209	0	221	17	0
25	BA	60059	0	30274	1279	0
25	DA	60059	0	30274	1286	0
26	BB	2551	0	1295	82	0
26	DB	2551	0	1295	83	0
27	BD	2105	0	2182	186	0
27	DD	2105	0	2182	191	0
28	BE	1564	0	1629	129	0
28	DE	1564	0	1629	130	0
29	BF	1587	0	1632	105	0
29	DF	1587	0	1632	112	0
30	BG	1475	0	1537	112	0
30	DG	1475	0	1537	119	0
31	BH	1223	0	1282	82	0
31	DH	1223	0	1282	82	0
32	BI	1133	0	1220	101	0
32	DI	1133	0	1220	112	0
33	BK	1088	0	1138	59	0
33	DK	1088	0	1138	64	0
34	BN	1097	0	1168	82	0
34	DN	1097	0	1168	76	0
35	BO	932	0	994	47	0
35	DO	932	0	994	47	0
36	BP	1114	0	1187	190	0
36	DP	1114	0	1187	202	0
37	BQ	1065	0	1114	86	0
37	DQ	1065	0	1114	88	0
38	BR	960	0	1021	87	0
38	DR	960	0	1021	80	0
39	BS	771	0	832	63	0
39	DS	771	0	832	64	0
40	BT	1144	0	1211	80	0
40	DT	1144	0	1211	78	0
41	BU	964	0	1022	86	0
41	DU	964	0	1022	83	0
42	BV	779	0	852	89	0
42	DV	779	0	852	84	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	BW	891	0	951	59	0
43	DW	891	0	951	62	0
44	BX	726	0	778	69	0
44	DX	726	0	778	68	0
45	BY	776	0	870	83	0
45	DY	776	0	870	84	0
46	BZ	1483	0	1507	92	0
46	DZ	1483	0	1507	91	0
47	B0	605	0	628	37	0
47	D0	605	0	628	33	0
48	B1	695	0	764	67	0
48	D1	695	0	764	78	0
49	B2	521	0	575	55	0
49	D2	521	0	575	58	0
50	B3	468	0	523	29	0
50	D3	468	0	523	27	0
51	B4	226	0	227	14	0
51	D4	226	0	225	15	0
52	B5	405	0	420	27	0
52	D5	405	0	420	31	0
53	B6	381	0	391	30	0
53	D6	381	0	391	28	0
54	B7	419	0	467	23	0
54	D7	419	0	467	22	0
55	B8	508	0	576	61	0
55	D8	508	0	576	64	0
56	AA	393	0	0	0	0
56	AC	1	0	0	0	0
56	AG	1	0	0	0	0
56	AO	1	0	0	0	0
56	AQ	1	0	0	0	0
56	AT	3	0	0	0	0
56	AV	1	0	0	0	0
56	AW	18	0	0	0	0
56	AY	3	0	0	0	0
56	B0	2	0	0	0	0
56	B1	1	0	0	0	0
56	B3	1	0	0	0	0
56	B5	1	0	0	0	0
56	B8	2	0	0	0	0
56	BA	824	0	0	0	0
56	BB	23	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	BD	1	0	0	0	0
56	BE	1	0	0	0	0
56	BF	1	0	0	0	0
56	BP	1	0	0	0	0
56	BT	1	0	0	0	0
56	BX	2	0	0	0	0
56	BY	1	0	0	0	0
56	CA	326	0	0	0	0
56	CD	1	0	0	0	0
56	CM	1	0	0	0	0
56	CR	1	0	0	0	0
56	CV	2	0	0	0	0
56	CW	16	0	0	0	0
56	CY	2	0	0	0	0
56	D0	1	0	0	0	0
56	D1	1	0	0	0	0
56	D5	3	0	0	0	0
56	D7	2	0	0	0	0
56	DA	732	0	0	0	0
56	DB	20	0	0	0	0
56	DD	1	0	0	0	0
56	DE	1	0	0	0	0
56	DF	2	0	0	0	0
56	DH	1	0	0	0	0
56	DI	2	0	0	0	0
56	DN	1	0	0	0	0
56	DP	2	0	0	0	0
56	DQ	4	0	0	0	0
56	DV	1	0	0	0	0
56	DW	2	0	0	0	0
56	DX	1	0	0	0	0
57	AD	1	0	0	0	0
57	AN	1	0	0	0	0
57	CD	1	0	0	0	0
57	CN	1	0	0	0	0
All	All	294074	0	200805	10482	0

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 10482 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:559:A:H4'	1:CA:560:U:H3'	1.26	1.16
25:BA:1899:G:N2	25:BA:1902:C:H41	1.43	1.15
45:DY:76:CYS:SG	45:DY:77:PRO:HD2	1.91	1.11
25:DA:1899:G:N2	25:DA:1902:C:H41	1.48	1.10
1:AA:559:A:H4'	1:AA:560:U:H3'	1.26	1.09

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	AY	360/362 (99%)	301 (84%)	41 (11%)	18 (5%)	1	10
4	CY	360/362 (99%)	301 (84%)	42 (12%)	17 (5%)	2	12
5	AB	232/234 (99%)	185 (80%)	37 (16%)	10 (4%)	2	13
5	CB	232/234 (99%)	184 (79%)	38 (16%)	10 (4%)	2	13
6	AC	204/206 (99%)	144 (71%)	40 (20%)	20 (10%)	0	3
6	CC	204/206 (99%)	145 (71%)	38 (19%)	21 (10%)	0	2
7	AD	206/208 (99%)	165 (80%)	32 (16%)	9 (4%)	2	13
7	CD	206/208 (99%)	166 (81%)	29 (14%)	11 (5%)	1	10
8	AE	149/151 (99%)	113 (76%)	32 (22%)	4 (3%)	4	20
8	CE	149/151 (99%)	116 (78%)	29 (20%)	4 (3%)	4	20
9	AF	99/101 (98%)	82 (83%)	16 (16%)	1 (1%)	12	40
9	CF	99/101 (98%)	82 (83%)	16 (16%)	1 (1%)	12	40
10	AG	153/155 (99%)	136 (89%)	13 (8%)	4 (3%)	4	21
10	CG	153/155 (99%)	136 (89%)	13 (8%)	4 (3%)	4	21
11	AH	136/138 (99%)	111 (82%)	23 (17%)	2 (2%)	8	30
11	CH	136/138 (99%)	113 (83%)	21 (15%)	2 (2%)	8	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	AI	125/127 (98%)	90 (72%)	27 (22%)	8 (6%)	1	7
12	CI	125/127 (98%)	90 (72%)	27 (22%)	8 (6%)	1	7
13	AJ	96/98 (98%)	72 (75%)	18 (19%)	6 (6%)	1	7
13	CJ	96/98 (98%)	72 (75%)	18 (19%)	6 (6%)	1	7
14	AK	112/114 (98%)	93 (83%)	14 (12%)	5 (4%)	2	12
14	CK	112/114 (98%)	93 (83%)	15 (13%)	4 (4%)	2	16
15	AL	120/122 (98%)	94 (78%)	21 (18%)	5 (4%)	2	14
15	CL	120/122 (98%)	93 (78%)	22 (18%)	5 (4%)	2	14
16	AM	115/117 (98%)	97 (84%)	15 (13%)	3 (3%)	4	21
16	CM	115/117 (98%)	97 (84%)	15 (13%)	3 (3%)	4	21
17	AN	58/60 (97%)	47 (81%)	9 (16%)	2 (3%)	3	17
17	CN	58/60 (97%)	43 (74%)	11 (19%)	4 (7%)	1	6
18	AO	86/88 (98%)	75 (87%)	8 (9%)	3 (4%)	3	16
18	CO	86/88 (98%)	75 (87%)	8 (9%)	3 (4%)	3	16
19	AP	81/83 (98%)	62 (76%)	16 (20%)	3 (4%)	2	16
19	CP	81/83 (98%)	61 (75%)	17 (21%)	3 (4%)	2	16
20	AQ	97/99 (98%)	82 (84%)	11 (11%)	4 (4%)	2	15
20	CQ	97/99 (98%)	83 (86%)	10 (10%)	4 (4%)	2	15
21	AR	68/70 (97%)	49 (72%)	17 (25%)	2 (3%)	3	19
21	CR	68/70 (97%)	50 (74%)	16 (24%)	2 (3%)	3	19
22	AS	76/78 (97%)	53 (70%)	15 (20%)	8 (10%)	0	2
22	CS	76/78 (97%)	53 (70%)	15 (20%)	8 (10%)	0	2
23	AT	97/99 (98%)	75 (77%)	14 (14%)	8 (8%)	0	4
23	CT	97/99 (98%)	75 (77%)	14 (14%)	8 (8%)	0	4
24	AU	22/24 (92%)	13 (59%)	7 (32%)	2 (9%)	0	3
24	CU	22/24 (92%)	13 (59%)	7 (32%)	2 (9%)	0	3
27	BD	269/271 (99%)	227 (84%)	29 (11%)	13 (5%)	2	11
27	DD	269/271 (99%)	227 (84%)	29 (11%)	13 (5%)	2	11
28	BE	202/204 (99%)	167 (83%)	26 (13%)	9 (4%)	2	12
28	DE	202/204 (99%)	165 (82%)	27 (13%)	10 (5%)	1	10
29	BF	200/202 (99%)	172 (86%)	21 (10%)	7 (4%)	3	16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	DF	200/202 (99%)	171 (86%)	24 (12%)	5 (2%)	4	21
30	BG	179/181 (99%)	141 (79%)	28 (16%)	10 (6%)	1	9
30	DG	179/181 (99%)	141 (79%)	28 (16%)	10 (6%)	1	9
31	BH	157/159 (99%)	130 (83%)	19 (12%)	8 (5%)	1	10
31	DH	157/159 (99%)	131 (83%)	18 (12%)	8 (5%)	1	10
32	BI	143/145 (99%)	113 (79%)	25 (18%)	5 (4%)	3	16
32	DI	143/145 (99%)	115 (80%)	23 (16%)	5 (4%)	3	16
33	BK	145/147 (99%)	99 (68%)	41 (28%)	5 (3%)	3	17
33	DK	145/147 (99%)	103 (71%)	31 (21%)	11 (8%)	1	5
34	BN	135/137 (98%)	96 (71%)	29 (22%)	10 (7%)	1	5
34	DN	135/137 (98%)	96 (71%)	29 (22%)	10 (7%)	1	5
35	BO	120/122 (98%)	103 (86%)	14 (12%)	3 (2%)	4	21
35	DO	120/122 (98%)	103 (86%)	14 (12%)	3 (2%)	4	21
36	BP	144/146 (99%)	91 (63%)	32 (22%)	21 (15%)	0	0
36	DP	144/146 (99%)	93 (65%)	31 (22%)	20 (14%)	0	1
37	BQ	132/134 (98%)	104 (79%)	22 (17%)	6 (4%)	2	12
37	DQ	132/134 (98%)	105 (80%)	22 (17%)	5 (4%)	2	15
38	BR	115/117 (98%)	96 (84%)	17 (15%)	2 (2%)	7	28
38	DR	115/117 (98%)	97 (84%)	16 (14%)	2 (2%)	7	28
39	BS	96/98 (98%)	62 (65%)	20 (21%)	14 (15%)	0	0
39	DS	96/98 (98%)	60 (62%)	22 (23%)	14 (15%)	0	0
40	BT	135/137 (98%)	100 (74%)	24 (18%)	11 (8%)	1	4
40	DT	135/137 (98%)	101 (75%)	23 (17%)	11 (8%)	1	4
41	BU	115/117 (98%)	99 (86%)	13 (11%)	3 (3%)	4	21
41	DU	115/117 (98%)	101 (88%)	11 (10%)	3 (3%)	4	21
42	BV	99/101 (98%)	75 (76%)	18 (18%)	6 (6%)	1	7
42	DV	99/101 (98%)	74 (75%)	19 (19%)	6 (6%)	1	7
43	BW	110/112 (98%)	98 (89%)	12 (11%)	0	100	100
43	DW	110/112 (98%)	95 (86%)	15 (14%)	0	100	100
44	BX	90/92 (98%)	82 (91%)	7 (8%)	1 (1%)	11	38
44	DX	90/92 (98%)	81 (90%)	8 (9%)	1 (1%)	11	38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
45	BY	98/100 (98%)	68 (69%)	14 (14%)	16 (16%)	0	0
45	DY	98/100 (98%)	68 (69%)	13 (13%)	17 (17%)	0	0
46	BZ	185/187 (99%)	158 (85%)	21 (11%)	6 (3%)	3	17
46	DZ	185/187 (99%)	158 (85%)	21 (11%)	6 (3%)	3	17
47	B0	74/76 (97%)	63 (85%)	7 (10%)	4 (5%)	1	10
47	D0	74/76 (97%)	63 (85%)	7 (10%)	4 (5%)	1	10
48	B1	86/88 (98%)	59 (69%)	14 (16%)	13 (15%)	0	0
48	D1	86/88 (98%)	59 (69%)	14 (16%)	13 (15%)	0	0
49	B2	60/62 (97%)	45 (75%)	7 (12%)	8 (13%)	0	1
49	D2	60/62 (97%)	45 (75%)	7 (12%)	8 (13%)	0	1
50	B3	57/59 (97%)	51 (90%)	5 (9%)	1 (2%)	6	26
50	D3	57/59 (97%)	51 (90%)	5 (9%)	1 (2%)	6	26
51	B4	28/30 (93%)	16 (57%)	10 (36%)	2 (7%)	1	6
51	D4	28/30 (93%)	16 (57%)	10 (36%)	2 (7%)	1	6
52	B5	50/52 (96%)	42 (84%)	5 (10%)	3 (6%)	1	7
52	D5	50/52 (96%)	42 (84%)	5 (10%)	3 (6%)	1	7
53	B6	42/44 (96%)	29 (69%)	8 (19%)	5 (12%)	0	2
53	D6	42/44 (96%)	29 (69%)	8 (19%)	5 (12%)	0	2
54	B7	46/48 (96%)	42 (91%)	4 (9%)	0	100	100
54	D7	46/48 (96%)	43 (94%)	3 (6%)	0	100	100
55	B8	61/63 (97%)	47 (77%)	7 (12%)	7 (12%)	0	2
55	D8	61/63 (97%)	47 (77%)	7 (12%)	7 (12%)	0	2
All	All	12130/12330 (98%)	9635 (79%)	1836 (15%)	659 (5%)	1	10

5 of 659 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	AY	55	PRO
4	AY	95	GLU
4	AY	175	ALA
4	AY	225	PRO
4	AY	315	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	AY	305/305 (100%)	281 (92%)	24 (8%)	11	36
4	CY	305/305 (100%)	281 (92%)	24 (8%)	11	36
5	AB	202/202 (100%)	185 (92%)	17 (8%)	10	34
5	CB	202/202 (100%)	185 (92%)	17 (8%)	10	34
6	AC	160/160 (100%)	149 (93%)	11 (7%)	14	40
6	CC	160/160 (100%)	149 (93%)	11 (7%)	14	40
7	AD	180/180 (100%)	156 (87%)	24 (13%)	4	15
7	CD	180/180 (100%)	166 (92%)	14 (8%)	11	37
8	AE	116/116 (100%)	109 (94%)	7 (6%)	17	43
8	CE	116/116 (100%)	109 (94%)	7 (6%)	17	43
9	AF	90/90 (100%)	85 (94%)	5 (6%)	19	46
9	CF	90/90 (100%)	85 (94%)	5 (6%)	19	46
10	AG	126/126 (100%)	123 (98%)	3 (2%)	43	62
10	CG	126/126 (100%)	123 (98%)	3 (2%)	43	62
11	AH	119/119 (100%)	111 (93%)	8 (7%)	15	41
11	CH	119/119 (100%)	111 (93%)	8 (7%)	15	41
12	AI	98/98 (100%)	90 (92%)	8 (8%)	10	35
12	CI	98/98 (100%)	90 (92%)	8 (8%)	10	35
13	AJ	88/88 (100%)	80 (91%)	8 (9%)	9	30
13	CJ	88/88 (100%)	80 (91%)	8 (9%)	9	30
14	AK	86/86 (100%)	81 (94%)	5 (6%)	18	45
14	CK	86/86 (100%)	81 (94%)	5 (6%)	18	45
15	AL	103/103 (100%)	96 (93%)	7 (7%)	14	40
15	CL	103/103 (100%)	96 (93%)	7 (7%)	14	40
16	AM	94/94 (100%)	85 (90%)	9 (10%)	8	28
16	CM	94/94 (100%)	85 (90%)	9 (10%)	8	28

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	AN	49/49 (100%)	46 (94%)	3 (6%)	17	43
17	CN	49/49 (100%)	47 (96%)	2 (4%)	27	52
18	AO	79/79 (100%)	72 (91%)	7 (9%)	9	31
18	CO	79/79 (100%)	72 (91%)	7 (9%)	9	31
19	AP	72/72 (100%)	65 (90%)	7 (10%)	8	28
19	CP	72/72 (100%)	65 (90%)	7 (10%)	8	28
20	AQ	94/94 (100%)	88 (94%)	6 (6%)	16	42
20	CQ	94/94 (100%)	88 (94%)	6 (6%)	16	42
21	AR	61/61 (100%)	59 (97%)	2 (3%)	33	57
21	CR	61/61 (100%)	59 (97%)	2 (3%)	33	57
22	AS	69/69 (100%)	55 (80%)	14 (20%)	1	4
22	CS	69/69 (100%)	55 (80%)	14 (20%)	1	4
23	AT	76/76 (100%)	72 (95%)	4 (5%)	20	47
23	CT	76/76 (100%)	72 (95%)	4 (5%)	20	47
24	AU	19/19 (100%)	18 (95%)	1 (5%)	20	47
24	CU	19/19 (100%)	18 (95%)	1 (5%)	20	47
27	BD	213/213 (100%)	184 (86%)	29 (14%)	3	15
27	DD	213/213 (100%)	185 (87%)	28 (13%)	4	16
28	BE	165/165 (100%)	151 (92%)	14 (8%)	10	33
28	DE	165/165 (100%)	150 (91%)	15 (9%)	9	30
29	BF	161/161 (100%)	143 (89%)	18 (11%)	6	21
29	DF	161/161 (100%)	143 (89%)	18 (11%)	6	21
30	BG	155/155 (100%)	140 (90%)	15 (10%)	8	28
30	DG	155/155 (100%)	140 (90%)	15 (10%)	8	28
31	BH	132/132 (100%)	122 (92%)	10 (8%)	12	38
31	DH	132/132 (100%)	122 (92%)	10 (8%)	12	38
32	BI	122/122 (100%)	109 (89%)	13 (11%)	6	23
32	DI	122/122 (100%)	109 (89%)	13 (11%)	6	23
33	BK	111/111 (100%)	100 (90%)	11 (10%)	7	26
33	DK	111/111 (100%)	103 (93%)	8 (7%)	13	39
34	BN	116/116 (100%)	99 (85%)	17 (15%)	3	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	DN	116/116 (100%)	100 (86%)	16 (14%)	3	14
35	BO	100/100 (100%)	94 (94%)	6 (6%)	17	43
35	DO	100/100 (100%)	93 (93%)	7 (7%)	14	40
36	BP	112/112 (100%)	83 (74%)	29 (26%)	0	1
36	DP	112/112 (100%)	82 (73%)	30 (27%)	0	1
37	BQ	105/105 (100%)	94 (90%)	11 (10%)	6	23
37	DQ	105/105 (100%)	94 (90%)	11 (10%)	6	23
38	BR	100/100 (100%)	86 (86%)	14 (14%)	3	13
38	DR	100/100 (100%)	87 (87%)	13 (13%)	4	16
39	BS	77/77 (100%)	66 (86%)	11 (14%)	3	13
39	DS	77/77 (100%)	66 (86%)	11 (14%)	3	13
40	BT	121/121 (100%)	101 (84%)	20 (16%)	2	10
40	DT	121/121 (100%)	100 (83%)	21 (17%)	2	8
41	BU	93/93 (100%)	87 (94%)	6 (6%)	15	42
41	DU	93/93 (100%)	87 (94%)	6 (6%)	15	42
42	BV	82/82 (100%)	67 (82%)	15 (18%)	2	7
42	DV	82/82 (100%)	67 (82%)	15 (18%)	2	7
43	BW	91/91 (100%)	80 (88%)	11 (12%)	5	19
43	DW	91/91 (100%)	79 (87%)	12 (13%)	4	16
44	BX	74/74 (100%)	65 (88%)	9 (12%)	5	19
44	DX	74/74 (100%)	65 (88%)	9 (12%)	5	19
45	BY	84/84 (100%)	75 (89%)	9 (11%)	6	23
45	DY	84/84 (100%)	75 (89%)	9 (11%)	6	23
46	BZ	162/162 (100%)	152 (94%)	10 (6%)	16	43
46	DZ	162/162 (100%)	152 (94%)	10 (6%)	16	43
47	B0	61/61 (100%)	51 (84%)	10 (16%)	2	10
47	D0	61/61 (100%)	50 (82%)	11 (18%)	2	7
48	B1	73/73 (100%)	59 (81%)	14 (19%)	1	6
48	D1	73/73 (100%)	59 (81%)	14 (19%)	1	6
49	B2	58/58 (100%)	50 (86%)	8 (14%)	3	14
49	D2	58/58 (100%)	50 (86%)	8 (14%)	3	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
50	B3	51/51 (100%)	47 (92%)	4 (8%)	11	37
50	D3	51/51 (100%)	47 (92%)	4 (8%)	11	37
51	B4	27/27 (100%)	26 (96%)	1 (4%)	30	55
51	D4	27/27 (100%)	26 (96%)	1 (4%)	30	55
52	B5	45/45 (100%)	43 (96%)	2 (4%)	25	51
52	D5	45/45 (100%)	43 (96%)	2 (4%)	25	51
53	B6	43/43 (100%)	36 (84%)	7 (16%)	2	10
53	D6	43/43 (100%)	36 (84%)	7 (16%)	2	10
54	B7	41/41 (100%)	34 (83%)	7 (17%)	2	9
54	D7	41/41 (100%)	35 (85%)	6 (15%)	3	12
55	B8	53/53 (100%)	48 (91%)	5 (9%)	8	29
55	D8	53/53 (100%)	48 (91%)	5 (9%)	8	29
All	All	10228/10228 (100%)	9208 (90%)	1020 (10%)	7	26

5 of 1020 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
47	B0	29	GLN
40	DT	51	ARG
7	CD	84	LYS
39	DS	83	LYS
45	DY	27	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 287 such sidechains are listed below:

Mol	Chain	Res	Type
34	DN	154	GLN
55	D8	43	GLN
36	DP	84	ASN
43	DW	61	ASN
38	BR	53	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1503/1504 (99%)	216 (14%)	20 (1%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	CA	1503/1504 (99%)	217 (14%)	20 (1%)
2	AV	9/10 (90%)	2 (22%)	0
2	CV	9/10 (90%)	2 (22%)	0
25	BA	2787/2879 (96%)	431 (15%)	19 (0%)
25	DA	2787/2879 (96%)	432 (15%)	19 (0%)
26	BB	118/119 (99%)	15 (12%)	0
26	DB	118/119 (99%)	15 (12%)	0
3	AW	76/77 (98%)	7 (9%)	0
3	CW	76/77 (98%)	7 (9%)	0
All	All	8986/9178 (97%)	1344 (14%)	78 (0%)

5 of 1344 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	7	G
1	AA	9	G
1	AA	32	A
1	AA	39	G
1	AA	41	G

5 of 78 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	CA	1362(A)	C
25	DA	1786	A
25	DA	352	G
25	DA	1022	G
25	DA	2447	G

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2414 ligands modelled in this entry, 2414 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	1504/1504 (100%)	0.38	46 (3%) 51 38	46, 108, 215, 381	0
1	CA	1504/1504 (100%)	0.75	139 (9%) 14 14	48, 122, 235, 451	0
2	AV	10/10 (100%)	1.26	3 (30%) 1 2	76, 120, 198, 250	0
2	CV	10/10 (100%)	2.19	4 (40%) 1 1	74, 123, 204, 230	0
3	AW	77/77 (100%)	0.17	1 (1%) 75 61	73, 106, 160, 212	0
3	CW	77/77 (100%)	0.13	1 (1%) 75 61	65, 104, 140, 219	0
4	AY	362/362 (100%)	1.17	72 (19%) 3 4	72, 164, 304, 366	0
4	CY	362/362 (100%)	1.29	90 (24%) 2 3	69, 180, 326, 473	0
5	AB	234/234 (100%)	0.87	30 (12%) 7 9	84, 152, 249, 335	0
5	CB	234/234 (100%)	1.17	42 (17%) 3 5	84, 173, 267, 348	0
6	AC	206/206 (100%)	0.91	25 (12%) 8 9	69, 141, 224, 325	0
6	CC	206/206 (100%)	1.29	41 (19%) 3 4	88, 154, 252, 385	0
7	AD	208/208 (100%)	0.80	27 (12%) 7 8	46, 104, 158, 201	0
7	CD	208/208 (100%)	1.79	71 (34%) 1 1	78, 146, 224, 346	0
8	AE	151/151 (100%)	0.75	18 (11%) 9 10	61, 102, 156, 274	0
8	CE	151/151 (100%)	1.31	38 (25%) 1 3	84, 125, 202, 274	0
9	AF	101/101 (100%)	1.17	18 (17%) 4 5	92, 150, 222, 283	0
9	CF	101/101 (100%)	0.69	5 (4%) 34 25	60, 104, 157, 216	0
10	AG	155/155 (100%)	0.79	17 (10%) 10 11	81, 147, 220, 290	0
10	CG	155/155 (100%)	1.19	33 (21%) 2 4	91, 147, 209, 352	0
11	AH	138/138 (100%)	0.85	16 (11%) 9 10	58, 110, 163, 235	0
11	CH	138/138 (100%)	1.32	26 (18%) 3 4	74, 130, 191, 271	0
12	AI	127/127 (100%)	1.74	48 (37%) 1 1	94, 172, 247, 329	0
12	CI	127/127 (100%)	1.98	59 (46%) 0 1	85, 174, 242, 307	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å²)		Q<0.9	
13	AJ	98/98 (100%)	1.48	25 (25%)	1	3	85, 172, 278, 357	0
13	CJ	98/98 (100%)	1.87	37 (37%)	1	1	86, 197, 311, 435	0
14	AK	114/114 (100%)	0.64	13 (11%)	10	10	59, 110, 172, 233	0
14	CK	114/114 (100%)	0.80	14 (12%)	8	9	55, 99, 165, 372	0
15	AL	122/122 (100%)	0.95	17 (13%)	6	8	44, 85, 148, 192	0
15	CL	122/122 (100%)	1.27	25 (20%)	2	4	48, 99, 149, 268	0
16	AM	117/117 (100%)	1.11	18 (15%)	5	7	81, 166, 258, 377	0
16	CM	117/117 (100%)	1.51	28 (23%)	2	3	109, 159, 244, 340	0
17	AN	60/60 (100%)	1.50	16 (26%)	1	2	72, 128, 174, 224	0
17	CN	60/60 (100%)	2.25	32 (53%)	0	0	80, 151, 191, 265	0
18	AO	88/88 (100%)	0.70	6 (6%)	23	19	67, 109, 157, 188	0
18	CO	88/88 (100%)	0.84	10 (11%)	10	10	58, 106, 146, 168	0
19	AP	83/83 (100%)	1.10	14 (16%)	4	5	65, 99, 135, 245	0
19	CP	83/83 (100%)	2.14	32 (38%)	1	1	78, 139, 192, 243	0
20	AQ	99/99 (100%)	0.85	13 (13%)	7	8	63, 102, 157, 211	0
20	CQ	99/99 (100%)	1.20	22 (22%)	2	4	76, 116, 167, 283	0
21	AR	70/70 (100%)	0.92	7 (10%)	12	12	76, 134, 215, 266	0
21	CR	70/70 (100%)	0.51	3 (4%)	40	29	70, 112, 182, 225	0
22	AS	78/78 (100%)	1.26	17 (21%)	2	4	113, 164, 229, 318	0
22	CS	78/78 (100%)	1.50	21 (26%)	1	2	112, 174, 250, 339	0
23	AT	99/99 (100%)	1.22	20 (20%)	3	4	68, 115, 202, 272	0
23	CT	99/99 (100%)	2.00	39 (39%)	1	1	84, 134, 222, 336	0
24	AU	24/24 (100%)	2.50	13 (54%)	0	0	102, 150, 217, 233	0
24	CU	24/24 (100%)	4.31	22 (91%)	0	0	126, 169, 229, 236	0
25	BA	2789/2879 (96%)	0.23	66 (2%)	59	45	36, 76, 211, 411	0
25	DA	2789/2879 (96%)	0.09	63 (2%)	61	46	27, 65, 189, 401	0
26	BB	119/119 (100%)	0.76	7 (5%)	28	22	63, 129, 186, 245	0
26	DB	119/119 (100%)	0.76	8 (6%)	24	19	73, 119, 167, 276	0
27	BD	271/271 (100%)	0.72	30 (11%)	10	11	31, 66, 114, 224	0
27	DD	271/271 (100%)	0.50	20 (7%)	20	17	14, 56, 107, 221	0
28	BE	204/204 (100%)	0.75	20 (9%)	13	13	35, 82, 148, 377	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	DE	204/204 (100%)	0.66	19 (9%) 14 14	29, 74, 138, 256	0
29	BF	202/202 (100%)	0.69	17 (8%) 17 15	28, 81, 163, 345	0
29	DF	202/202 (100%)	0.45	11 (5%) 31 24	13, 69, 145, 300	0
30	BG	181/181 (100%)	1.21	31 (17%) 4 5	78, 147, 221, 323	0
30	DG	181/181 (100%)	1.23	34 (18%) 3 4	73, 136, 220, 288	0
31	BH	159/159 (100%)	1.44	42 (26%) 1 3	86, 172, 263, 376	0
31	DH	159/159 (100%)	0.77	20 (12%) 8 9	48, 100, 157, 286	0
32	BI	145/145 (100%)	2.45	83 (57%) 0 0	74, 188, 473, 558	0
32	DI	145/145 (100%)	0.99	20 (13%) 6 8	47, 118, 209, 462	0
33	BK	147/147 (100%)	1.45	43 (29%) 1 2	155, 266, 359, 430	0
33	DK	147/147 (100%)	1.32	26 (17%) 4 5	115, 275, 372, 435	0
34	BN	137/137 (100%)	1.01	21 (15%) 5 7	51, 89, 139, 220	0
34	DN	137/137 (100%)	0.95	19 (13%) 6 8	37, 84, 149, 192	0
35	BO	122/122 (100%)	0.50	7 (5%) 29 22	44, 77, 121, 158	0
35	DO	122/122 (100%)	0.43	4 (3%) 49 36	31, 67, 117, 149	0
36	BP	146/146 (100%)	1.43	35 (23%) 2 3	27, 100, 201, 293	0
36	DP	146/146 (100%)	1.35	37 (25%) 1 3	23, 85, 172, 304	0
37	BQ	134/134 (100%)	1.14	19 (14%) 6 8	45, 86, 159, 419	0
37	DQ	134/134 (100%)	1.31	32 (23%) 2 3	41, 83, 175, 469	0
38	BR	117/117 (100%)	1.11	16 (13%) 6 8	37, 83, 141, 190	0
38	DR	117/117 (100%)	1.05	23 (19%) 3 4	32, 74, 137, 174	0
39	BS	98/98 (100%)	1.38	27 (27%) 1 2	61, 135, 212, 245	0
39	DS	98/98 (100%)	1.47	30 (30%) 1 2	72, 116, 180, 203	0
40	BT	137/137 (100%)	0.94	20 (14%) 6 7	54, 95, 195, 362	0
40	DT	137/137 (100%)	0.68	13 (9%) 14 13	34, 90, 194, 343	0
41	BU	117/117 (100%)	0.73	8 (6%) 23 19	36, 73, 137, 173	0
41	DU	117/117 (100%)	0.80	8 (6%) 23 19	35, 74, 125, 363	0
42	BV	101/101 (100%)	0.84	10 (9%) 13 12	49, 93, 159, 283	0
42	DV	101/101 (100%)	1.00	16 (15%) 5 6	34, 96, 153, 283	0
43	BW	112/112 (100%)	0.80	12 (10%) 11 11	28, 66, 124, 378	0
43	DW	112/112 (100%)	0.57	6 (5%) 31 24	38, 66, 125, 210	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	BX	92/92 (100%)	1.18	16 (17%) 4 5	61, 87, 139, 179	0
44	DX	92/92 (100%)	0.50	8 (8%) 16 14	34, 66, 106, 168	0
45	BY	100/100 (100%)	1.99	46 (46%) 0 1	46, 112, 248, 418	0
45	DY	100/100 (100%)	1.49	21 (21%) 2 4	50, 92, 223, 452	0
46	BZ	187/187 (100%)	0.93	24 (12%) 7 9	75, 130, 200, 267	0
46	DZ	187/187 (100%)	1.09	29 (15%) 5 7	56, 123, 182, 260	0
47	B0	76/76 (100%)	1.02	7 (9%) 14 14	54, 84, 150, 259	0
47	D0	76/76 (100%)	1.19	13 (17%) 4 5	37, 80, 115, 238	0
48	B1	88/88 (100%)	1.43	21 (23%) 2 3	46, 90, 156, 264	0
48	D1	88/88 (100%)	1.32	19 (21%) 2 4	23, 69, 147, 267	0
49	B2	62/62 (100%)	1.62	19 (30%) 1 2	67, 119, 210, 257	0
49	D2	62/62 (100%)	0.93	12 (19%) 3 4	33, 75, 176, 304	0
50	B3	59/59 (100%)	0.77	5 (8%) 16 15	52, 80, 144, 224	0
50	D3	59/59 (100%)	0.85	6 (10%) 12 12	42, 81, 143, 236	0
51	B4	30/30 (100%)	0.76	2 (6%) 24 19	107, 184, 297, 335	0
51	D4	30/30 (100%)	0.75	0 100 100	125, 215, 272, 361	0
52	B5	52/52 (100%)	0.96	5 (9%) 13 13	32, 75, 181, 213	0
52	D5	52/52 (100%)	0.84	6 (11%) 9 10	20, 77, 172, 269	0
53	B6	44/44 (100%)	1.86	20 (45%) 0 1	118, 225, 304, 330	0
53	D6	44/44 (100%)	1.75	15 (34%) 1 1	136, 208, 276, 330	0
54	B7	48/48 (100%)	0.87	7 (14%) 6 7	35, 60, 131, 156	0
54	D7	48/48 (100%)	0.38	4 (8%) 17 15	19, 36, 94, 156	0
55	B8	63/63 (100%)	1.51	18 (28%) 1 2	38, 78, 155, 190	0
55	D8	63/63 (100%)	1.42	13 (20%) 2 4	33, 62, 142, 213	0
All	All	21328/21508 (99%)	0.77	2593 (12%) 8 9	13, 103, 238, 558	0

The worst 5 of 2593 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	CD	4	TYR	12.0
24	CU	4	GLY	10.9
44	BX	86	GLY	10.3
37	DQ	24	GLY	10.3
39	DS	11	LYS	9.8

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BA	3022	1/1	-0.08	0.12	168,168,168,168	0
56	MG	AA	1697	1/1	0.02	0.21	148,148,148,148	0
56	MG	CA	1912	1/1	0.02	0.16	152,152,152,152	0
56	MG	CA	1842	1/1	0.03	0.31	137,137,137,137	0
56	MG	BA	3503	1/1	0.06	0.25	195,195,195,195	0
56	MG	BA	3718	1/1	0.23	0.26	163,163,163,163	0
56	MG	CA	1633	1/1	0.23	0.11	143,143,143,143	0
56	MG	BA	3016	1/1	0.25	0.12	168,168,168,168	0
56	MG	BA	3123	1/1	0.26	0.15	156,156,156,156	0
56	MG	BA	3713	1/1	0.26	0.15	123,123,123,123	0
56	MG	CA	1743	1/1	0.29	0.20	169,169,169,169	0
56	MG	DA	3432	1/1	0.29	0.33	104,104,104,104	0
56	MG	DA	3632	1/1	0.29	0.21	135,135,135,135	0
56	MG	CA	1865	1/1	0.30	0.15	108,108,108,108	0
56	MG	CA	1677	1/1	0.32	0.22	138,138,138,138	0
56	MG	DA	3107	1/1	0.33	0.12	139,139,139,139	0
56	MG	CA	1607	1/1	0.33	0.19	138,138,138,138	0
56	MG	CA	1631	1/1	0.33	0.13	119,119,119,119	0
56	MG	BB	223	1/1	0.34	0.11	242,242,242,242	0
56	MG	BA	3119	1/1	0.34	0.14	133,133,133,133	0
56	MG	BA	2972	1/1	0.34	0.10	122,122,122,122	0
56	MG	BA	3248	1/1	0.34	0.24	102,102,102,102	0
56	MG	CA	1860	1/1	0.36	0.14	133,133,133,133	0
56	MG	BA	3105	1/1	0.36	0.12	122,122,122,122	0
56	MG	CA	1650	1/1	0.37	0.17	170,170,170,170	0
56	MG	BA	3082	1/1	0.37	0.11	119,119,119,119	0
56	MG	CW	112	1/1	0.38	0.19	103,103,103,103	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	CA	1732	1/1	0.39	0.33	131,131,131,131	0
56	MG	AA	1796	1/1	0.40	0.25	129,129,129,129	0
56	MG	CA	1747	1/1	0.40	0.36	122,122,122,122	0
56	MG	AA	1804	1/1	0.42	0.20	108,108,108,108	0
56	MG	CA	1681	1/1	0.42	0.13	136,136,136,136	0
56	MG	CA	1686	1/1	0.42	0.10	286,286,286,286	0
56	MG	DA	3112	1/1	0.42	0.23	141,141,141,141	0
56	MG	DA	3348	1/1	0.42	0.13	165,165,165,165	0
56	MG	BA	2915	1/1	0.42	0.11	102,102,102,102	0
56	MG	CA	1734	1/1	0.42	0.16	196,196,196,196	0
56	MG	DA	2975	1/1	0.43	0.31	79,79,79,79	0
56	MG	DA	3086	1/1	0.45	0.09	120,120,120,120	0
56	MG	AA	1945	1/1	0.45	0.19	115,115,115,115	0
56	MG	BA	3592	1/1	0.45	0.15	132,132,132,132	0
56	MG	BA	2918	1/1	0.46	0.19	191,191,191,191	0
56	MG	CA	1719	1/1	0.46	0.10	106,106,106,106	0
56	MG	CA	1809	1/1	0.46	0.20	117,117,117,117	0
56	MG	CA	1823	1/1	0.46	0.10	166,166,166,166	0
56	MG	CA	1856	1/1	0.47	0.22	136,136,136,136	0
56	MG	AA	1726	1/1	0.47	0.27	141,141,141,141	0
56	MG	BB	211	1/1	0.47	0.25	132,132,132,132	0
56	MG	BA	3078	1/1	0.47	0.18	117,117,117,117	0
56	MG	DB	209	1/1	0.47	0.17	143,143,143,143	0
56	MG	DB	218	1/1	0.47	0.16	111,111,111,111	0
56	MG	BA	2973	1/1	0.48	0.34	160,160,160,160	0
56	MG	CA	1669	1/1	0.48	0.39	118,118,118,118	0
56	MG	AA	1780	1/1	0.48	0.24	105,105,105,105	0
56	MG	CA	1864	1/1	0.48	0.15	157,157,157,157	0
56	MG	CA	1614	1/1	0.49	0.25	122,122,122,122	0
56	MG	CA	1728	1/1	0.49	0.46	195,195,195,195	0
56	MG	AA	1724	1/1	0.50	0.14	133,133,133,133	0
56	MG	BA	3011	1/1	0.50	0.18	82,82,82,82	0
56	MG	DA	2921	1/1	0.50	0.11	113,113,113,113	0
56	MG	AA	1702	1/1	0.51	0.18	97,97,97,97	0
56	MG	BA	3091	1/1	0.51	0.26	125,125,125,125	0
56	MG	CA	1630	1/1	0.51	0.13	177,177,177,177	0
56	MG	CA	1843	1/1	0.51	0.15	103,103,103,103	0
56	MG	CA	1605	1/1	0.51	0.12	159,159,159,159	0
56	MG	AA	1831	1/1	0.52	0.25	203,203,203,203	0
56	MG	DA	3043	1/1	0.52	0.30	77,77,77,77	0
56	MG	BB	208	1/1	0.52	0.15	82,82,82,82	0
56	MG	BA	3137	1/1	0.52	0.20	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	AA	1764	1/1	0.52	0.28	103,103,103,103	0
56	MG	BA	3369	1/1	0.53	0.23	74,74,74,74	0
56	MG	AA	1809	1/1	0.53	0.20	106,106,106,106	0
56	MG	BA	2997	1/1	0.54	0.13	104,104,104,104	0
56	MG	CA	1699	1/1	0.54	0.21	152,152,152,152	0
56	MG	BA	3533	1/1	0.54	0.18	97,97,97,97	0
56	MG	BA	3494	1/1	0.54	0.12	73,73,73,73	0
56	MG	DA	3346	1/1	0.54	0.12	90,90,90,90	0
56	MG	DA	3447	1/1	0.55	0.12	89,89,89,89	0
56	MG	DA	3453	1/1	0.55	0.16	85,85,85,85	0
56	MG	DA	2940	1/1	0.55	0.14	94,94,94,94	0
56	MG	CA	1898	1/1	0.55	0.36	126,126,126,126	0
56	MG	AA	1725	1/1	0.55	0.13	121,121,121,121	0
56	MG	BA	3062	1/1	0.56	0.13	110,110,110,110	0
56	MG	DA	2972	1/1	0.56	0.27	187,187,187,187	0
56	MG	AA	1619	1/1	0.56	0.20	69,69,69,69	0
56	MG	AA	1723	1/1	0.56	0.19	106,106,106,106	0
56	MG	CA	1873	1/1	0.56	0.18	207,207,207,207	0
56	MG	AY	401	1/1	0.57	0.08	119,119,119,119	0
56	MG	CA	1672	1/1	0.57	0.28	78,78,78,78	0
56	MG	BA	3435	1/1	0.57	0.17	112,112,112,112	0
56	MG	AA	1900	1/1	0.57	0.20	213,213,213,213	0
56	MG	BA	3607	1/1	0.57	0.09	105,105,105,105	0
56	MG	CA	1895	1/1	0.58	0.21	126,126,126,126	0
56	MG	BA	3300	1/1	0.58	0.11	89,89,89,89	0
56	MG	AA	1897	1/1	0.58	0.40	80,80,80,80	0
56	MG	CA	1701	1/1	0.58	0.19	88,88,88,88	0
56	MG	AV	101	1/1	0.59	0.17	109,109,109,109	0
56	MG	DA	3405	1/1	0.59	0.14	91,91,91,91	0
56	MG	AA	1777	1/1	0.59	0.13	101,101,101,101	0
56	MG	BA	3159	1/1	0.59	0.17	151,151,151,151	0
56	MG	AA	1728	1/1	0.59	0.10	130,130,130,130	0
56	MG	BA	3514	1/1	0.59	0.24	80,80,80,80	0
56	MG	AA	1850	1/1	0.59	0.10	98,98,98,98	0
56	MG	BA	3542	1/1	0.59	0.10	116,116,116,116	0
56	MG	CA	1644	1/1	0.60	0.11	120,120,120,120	0
56	MG	AA	1605	1/1	0.60	0.10	142,142,142,142	0
56	MG	BA	3067	1/1	0.60	0.37	142,142,142,142	0
56	MG	BA	3021	1/1	0.60	0.14	111,111,111,111	0
56	MG	CA	1712	1/1	0.60	0.14	106,106,106,106	0
56	MG	AA	1794	1/1	0.60	0.12	151,151,151,151	0
56	MG	CA	1724	1/1	0.60	0.24	108,108,108,108	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	CA	1733	1/1	0.61	0.13	197,197,197,197	0
56	MG	BA	3711	1/1	0.61	0.15	104,104,104,104	0
56	MG	DA	3054	1/1	0.61	0.14	93,93,93,93	0
56	MG	BA	3276	1/1	0.62	0.16	107,107,107,107	0
56	MG	DA	3373	1/1	0.62	0.10	86,86,86,86	0
56	MG	DA	2999	1/1	0.62	0.10	102,102,102,102	0
56	MG	AW	109	1/1	0.62	0.27	91,91,91,91	0
56	MG	CA	1739	1/1	0.62	0.16	122,122,122,122	0
56	MG	AA	1717	1/1	0.62	0.15	99,99,99,99	0
56	MG	DA	3595	1/1	0.62	0.11	106,106,106,106	0
56	MG	BA	2935	1/1	0.62	0.22	89,89,89,89	0
56	MG	BA	3482	1/1	0.62	0.40	74,74,74,74	0
56	MG	DB	217	1/1	0.62	0.21	121,121,121,121	0
56	MG	CA	1613	1/1	0.62	0.18	71,71,71,71	0
56	MG	BA	3696	1/1	0.63	0.26	96,96,96,96	0
56	MG	BA	3433	1/1	0.63	0.08	97,97,97,97	0
56	MG	BA	3256	1/1	0.63	0.14	91,91,91,91	0
56	MG	CA	1897	1/1	0.63	0.14	227,227,227,227	0
56	MG	CA	1698	1/1	0.63	0.08	100,100,100,100	0
56	MG	AA	1721	1/1	0.63	0.18	128,128,128,128	0
56	MG	DA	3626	1/1	0.63	0.09	117,117,117,117	0
56	MG	AA	1682	1/1	0.63	0.12	124,124,124,124	0
56	MG	DA	2914	1/1	0.63	0.20	97,97,97,97	0
56	MG	AA	1986	1/1	0.63	0.23	69,69,69,69	0
56	MG	CA	1717	1/1	0.63	0.12	121,121,121,121	0
56	MG	BA	3230	1/1	0.64	0.22	103,103,103,103	0
56	MG	AA	1957	1/1	0.64	0.26	109,109,109,109	0
56	MG	BA	3609	1/1	0.64	0.14	149,149,149,149	0
56	MG	CA	1729	1/1	0.64	0.11	139,139,139,139	0
56	MG	AA	1752	1/1	0.64	0.10	183,183,183,183	0
56	MG	AA	1931	1/1	0.64	0.17	102,102,102,102	0
56	MG	AA	1848	1/1	0.64	0.08	125,125,125,125	0
56	MG	DA	3484	1/1	0.64	0.18	98,98,98,98	0
56	MG	BA	3519	1/1	0.64	0.11	93,93,93,93	0
56	MG	CA	1885	1/1	0.64	0.09	270,270,270,270	0
56	MG	CA	1892	1/1	0.64	0.17	150,150,150,150	0
56	MG	AW	113	1/1	0.64	0.12	96,96,96,96	0
56	MG	BA	3085	1/1	0.64	0.19	116,116,116,116	0
56	MG	BB	216	1/1	0.64	0.07	109,109,109,109	0
56	MG	CA	1657	1/1	0.65	0.18	95,95,95,95	0
56	MG	CA	1806	1/1	0.65	0.14	95,95,95,95	0
56	MG	BA	3610	1/1	0.65	0.16	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	AA	1638	1/1	0.65	0.19	132,132,132,132	0
56	MG	DA	3521	1/1	0.65	0.10	93,93,93,93	0
56	MG	DA	3586	1/1	0.65	0.23	133,133,133,133	0
56	MG	CA	1674	1/1	0.65	0.11	107,107,107,107	0
56	MG	DA	2941	1/1	0.65	0.08	93,93,93,93	0
56	MG	BA	3462	1/1	0.65	0.36	95,95,95,95	0
56	MG	DA	3351	1/1	0.65	0.09	116,116,116,116	0
56	MG	BA	3020	1/1	0.65	0.10	107,107,107,107	0
56	MG	BB	217	1/1	0.65	0.17	99,99,99,99	0
56	MG	DA	3386	1/1	0.66	0.11	102,102,102,102	0
56	MG	BA	2950	1/1	0.66	0.23	87,87,87,87	0
56	MG	BA	3310	1/1	0.66	0.21	117,117,117,117	0
56	MG	BA	3035	1/1	0.66	0.10	158,158,158,158	0
56	MG	BA	3092	1/1	0.66	0.15	99,99,99,99	0
56	MG	AA	1993	1/1	0.66	0.10	73,73,73,73	0
56	MG	DA	3380	1/1	0.66	0.16	85,85,85,85	0
56	MG	BA	3722	1/1	0.67	0.14	80,80,80,80	0
56	MG	CA	1606	1/1	0.67	0.18	115,115,115,115	0
56	MG	AA	1642	1/1	0.67	0.26	120,120,120,120	0
56	MG	BA	3709	1/1	0.67	0.11	97,97,97,97	0
56	MG	DA	3456	1/1	0.67	0.14	116,116,116,116	0
56	MG	BA	3003	1/1	0.67	0.11	113,113,113,113	0
56	MG	CA	1706	1/1	0.67	0.08	88,88,88,88	0
56	MG	CA	1737	1/1	0.67	0.20	98,98,98,98	0
56	MG	CY	401	1/1	0.67	0.27	103,103,103,103	0
56	MG	CA	1625	1/1	0.67	0.30	125,125,125,125	0
56	MG	BA	3179	1/1	0.67	0.38	98,98,98,98	0
56	MG	CA	1872	1/1	0.67	0.11	88,88,88,88	0
56	MG	AT	201	1/1	0.67	0.41	117,117,117,117	0
56	MG	CA	1884	1/1	0.67	0.27	79,79,79,79	0
56	MG	BA	3465	1/1	0.68	0.20	114,114,114,114	0
56	MG	BA	2958	1/1	0.68	0.24	103,103,103,103	0
56	MG	AA	1890	1/1	0.68	0.21	124,124,124,124	0
56	MG	DA	3249	1/1	0.68	0.15	120,120,120,120	0
56	MG	DA	3499	1/1	0.68	0.22	98,98,98,98	0
56	MG	DA	3502	1/1	0.68	0.36	73,73,73,73	0
56	MG	AA	1921	1/1	0.68	0.19	68,68,68,68	0
56	MG	CA	1615	1/1	0.68	0.15	110,110,110,110	0
56	MG	AA	1950	1/1	0.68	0.13	102,102,102,102	0
56	MG	BA	3205	1/1	0.68	0.10	95,95,95,95	0
56	MG	DA	2997	1/1	0.68	0.20	132,132,132,132	0
56	MG	CA	1910	1/1	0.68	0.15	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	CA	1731	1/1	0.68	0.09	139,139,139,139	0
56	MG	CA	1807	1/1	0.68	0.16	195,195,195,195	0
56	MG	BA	3059	1/1	0.69	0.25	43,43,43,43	0
56	MG	CA	1921	1/1	0.69	0.10	108,108,108,108	0
56	MG	BA	3583	1/1	0.69	0.18	87,87,87,87	0
56	MG	DA	3091	1/1	0.69	0.40	96,96,96,96	0
56	MG	BA	2949	1/1	0.69	0.15	70,70,70,70	0
56	MG	AA	1645	1/1	0.69	0.21	82,82,82,82	0
56	MG	BA	3213	1/1	0.69	0.26	125,125,125,125	0
56	MG	CA	1886	1/1	0.69	0.20	100,100,100,100	0
56	MG	DA	3531	1/1	0.69	0.12	92,92,92,92	0
56	MG	BA	2924	1/1	0.69	0.75	64,64,64,64	0
56	MG	DA	3350	1/1	0.69	0.29	76,76,76,76	0
56	MG	BA	3006	1/1	0.69	0.30	107,107,107,107	0
56	MG	CA	1620	1/1	0.69	0.21	74,74,74,74	0
56	MG	DB	208	1/1	0.69	0.09	83,83,83,83	0
56	MG	DA	2981	1/1	0.69	0.15	105,105,105,105	0
56	MG	AA	1778	1/1	0.69	0.86	159,159,159,159	0
56	MG	CA	1675	1/1	0.69	0.13	75,75,75,75	0
56	MG	AA	1826	1/1	0.70	0.22	78,78,78,78	0
56	MG	CA	1727	1/1	0.70	0.20	112,112,112,112	0
56	MG	DA	3427	1/1	0.70	0.23	84,84,84,84	0
56	MG	CA	1887	1/1	0.70	0.14	116,116,116,116	0
56	MG	BA	3719	1/1	0.70	0.12	125,125,125,125	0
56	MG	CA	1817	1/1	0.70	0.27	111,111,111,111	0
56	MG	BA	3614	1/1	0.70	0.25	107,107,107,107	0
56	MG	BA	3650	1/1	0.70	0.24	95,95,95,95	0
56	MG	CA	1909	1/1	0.70	0.16	133,133,133,133	0
56	MG	BA	3672	1/1	0.70	0.14	88,88,88,88	0
56	MG	BA	3585	1/1	0.70	0.18	87,87,87,87	0
56	MG	DA	3108	1/1	0.70	0.09	74,74,74,74	0
56	MG	CA	1710	1/1	0.70	0.26	97,97,97,97	0
56	MG	AA	1676	1/1	0.70	0.12	152,152,152,152	0
56	MG	BA	2959	1/1	0.70	0.28	81,81,81,81	0
56	MG	DA	2903	1/1	0.70	0.13	77,77,77,77	0
56	MG	CA	1718	1/1	0.70	0.12	136,136,136,136	0
56	MG	AA	1615	1/1	0.70	0.17	87,87,87,87	0
56	MG	CA	1881	1/1	0.70	0.12	111,111,111,111	0
56	MG	CA	1790	1/1	0.70	0.15	86,86,86,86	0
56	MG	BA	3588	1/1	0.71	0.18	120,120,120,120	0
56	MG	CA	1704	1/1	0.71	0.18	88,88,88,88	0
56	MG	AC	301	1/1	0.71	0.26	98,98,98,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BA	3597	1/1	0.71	0.23	91,91,91,91	0
56	MG	DA	3421	1/1	0.71	0.14	76,76,76,76	0
56	MG	CA	1663	1/1	0.71	0.26	210,210,210,210	0
56	MG	CA	1777	1/1	0.71	0.33	98,98,98,98	0
56	MG	AA	1672	1/1	0.71	0.15	73,73,73,73	0
56	MG	CA	1793	1/1	0.71	0.15	114,114,114,114	0
56	MG	DA	3004	1/1	0.71	0.07	100,100,100,100	0
56	MG	BA	3258	1/1	0.71	0.18	67,67,67,67	0
56	MG	BA	3263	1/1	0.71	0.16	66,66,66,66	0
56	MG	BA	3032	1/1	0.71	0.25	97,97,97,97	0
56	MG	CA	1725	1/1	0.71	0.16	78,78,78,78	0
56	MG	BB	206	1/1	0.71	0.11	188,188,188,188	0
56	MG	BA	3639	1/1	0.71	0.37	79,79,79,79	0
56	MG	BA	2995	1/1	0.71	0.15	92,92,92,92	0
56	MG	CA	1845	1/1	0.71	0.11	60,60,60,60	0
56	MG	CA	1850	1/1	0.71	0.22	93,93,93,93	0
56	MG	CA	1687	1/1	0.71	0.08	58,58,58,58	0
56	MG	BA	3665	1/1	0.71	0.13	117,117,117,117	0
56	MG	BA	3155	1/1	0.71	0.21	93,93,93,93	0
56	MG	DA	3355	1/1	0.71	0.20	102,102,102,102	0
56	MG	DA	3413	1/1	0.72	0.13	79,79,79,79	0
56	MG	DA	3063	1/1	0.72	0.09	99,99,99,99	0
56	MG	DA	3081	1/1	0.72	0.15	87,87,87,87	0
56	MG	AA	1839	1/1	0.72	0.14	88,88,88,88	0
56	MG	DA	2911	1/1	0.72	0.16	84,84,84,84	0
56	MG	CA	1745	1/1	0.72	0.17	115,115,115,115	0
56	MG	BA	3004	1/1	0.72	0.09	99,99,99,99	0
56	MG	AW	110	1/1	0.72	0.39	145,145,145,145	0
56	MG	AA	1770	1/1	0.72	0.52	86,86,86,86	0
56	MG	BA	2920	1/1	0.72	0.21	70,70,70,70	0
56	MG	CA	1902	1/1	0.72	0.39	128,128,128,128	0
56	MG	BA	2922	1/1	0.72	0.20	108,108,108,108	0
56	MG	AA	1666	1/1	0.72	0.11	91,91,91,91	0
56	MG	CA	1627	1/1	0.72	0.13	85,85,85,85	0
56	MG	BA	3603	1/1	0.72	0.10	88,88,88,88	0
56	MG	DA	3375	1/1	0.72	0.11	78,78,78,78	0
56	MG	BA	2930	1/1	0.72	0.22	89,89,89,89	0
56	MG	AA	1901	1/1	0.72	0.21	71,71,71,71	0
56	MG	DA	3059	1/1	0.72	0.06	82,82,82,82	0
56	MG	DA	3409	1/1	0.72	0.43	102,102,102,102	0
56	MG	BA	3591	1/1	0.73	0.40	102,102,102,102	0
56	MG	BA	3185	1/1	0.73	0.16	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	AA	1811	1/1	0.73	0.09	91,91,91,91	0
56	MG	BA	3723	1/1	0.73	0.20	71,71,71,71	0
56	MG	BA	3212	1/1	0.73	0.37	109,109,109,109	0
56	MG	AW	116	1/1	0.73	0.09	86,86,86,86	0
56	MG	AA	1744	1/1	0.73	0.28	103,103,103,103	0
56	MG	AW	107	1/1	0.73	0.21	102,102,102,102	0
56	MG	BA	2996	1/1	0.73	0.10	209,209,209,209	0
56	MG	BA	3628	1/1	0.73	0.34	82,82,82,82	0
56	MG	DA	2985	1/1	0.73	0.18	107,107,107,107	0
56	MG	AO	101	1/1	0.73	0.11	110,110,110,110	0
56	MG	AA	1783	1/1	0.73	0.29	127,127,127,127	0
56	MG	CA	1682	1/1	0.73	0.13	152,152,152,152	0
56	MG	DA	3032	1/1	0.73	0.11	82,82,82,82	0
56	MG	CA	1684	1/1	0.73	0.18	87,87,87,87	0
56	MG	DA	3466	1/1	0.73	0.15	90,90,90,90	0
56	MG	CA	1740	1/1	0.73	0.09	101,101,101,101	0
56	MG	BA	2908	1/1	0.73	0.14	235,235,235,235	0
56	MG	BA	3063	1/1	0.73	0.15	75,75,75,75	0
56	MG	CA	1695	1/1	0.73	0.24	108,108,108,108	0
56	MG	BA	3688	1/1	0.73	0.10	59,59,59,59	0
56	MG	BA	3309	1/1	0.73	0.22	68,68,68,68	0
56	MG	DA	3106	1/1	0.73	0.09	79,79,79,79	0
56	MG	BA	2914	1/1	0.73	0.12	122,122,122,122	0
56	MG	CA	1802	1/1	0.73	0.24	61,61,61,61	0
56	MG	AA	1742	1/1	0.73	0.13	197,197,197,197	0
56	MG	CA	1626	1/1	0.73	0.09	109,109,109,109	0
56	MG	BA	3589	1/1	0.73	0.14	135,135,135,135	0
56	MG	BA	3717	1/1	0.73	0.12	100,100,100,100	0
56	MG	CA	1841	1/1	0.74	0.22	77,77,77,77	0
56	MG	BA	3173	1/1	0.74	0.33	67,67,67,67	0
56	MG	BA	3148	1/1	0.74	0.15	111,111,111,111	0
56	MG	CA	1660	1/1	0.74	0.24	94,94,94,94	0
56	MG	BA	3451	1/1	0.74	0.20	83,83,83,83	0
56	MG	CA	1794	1/1	0.74	0.15	60,60,60,60	0
56	MG	DA	3074	1/1	0.74	0.23	99,99,99,99	0
56	MG	CA	1665	1/1	0.74	0.21	94,94,94,94	0
56	MG	DA	3532	1/1	0.74	0.10	72,72,72,72	0
56	MG	CA	1628	1/1	0.74	0.09	86,86,86,86	0
56	MG	BB	213	1/1	0.74	0.08	93,93,93,93	0
56	MG	CA	1869	1/1	0.74	0.08	95,95,95,95	0
56	MG	BA	2932	1/1	0.74	0.08	78,78,78,78	0
56	MG	BA	3587	1/1	0.74	0.32	104,104,104,104	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	AT	203	1/1	0.74	0.25	99,99,99,99	0
56	MG	DA	3248	1/1	0.74	0.28	66,66,66,66	0
56	MG	CW	110	1/1	0.74	0.18	90,90,90,90	0
56	MG	CA	1800	1/1	0.75	0.14	124,124,124,124	0
56	MG	AA	1975	1/1	0.75	0.06	121,121,121,121	0
56	MG	BA	3128	1/1	0.75	0.09	111,111,111,111	0
56	MG	BA	3083	1/1	0.75	0.12	69,69,69,69	0
56	MG	BA	3138	1/1	0.75	0.07	82,82,82,82	0
56	MG	DA	3010	1/1	0.75	0.23	54,54,54,54	0
56	MG	DA	3016	1/1	0.75	0.10	99,99,99,99	0
56	MG	BA	3448	1/1	0.75	0.21	72,72,72,72	0
56	MG	CA	1693	1/1	0.75	0.12	67,67,67,67	0
56	MG	BA	3084	1/1	0.75	0.17	73,73,73,73	0
56	MG	BA	3674	1/1	0.75	0.18	55,55,55,55	0
56	MG	CA	1735	1/1	0.75	0.33	108,108,108,108	0
56	MG	DA	3073	1/1	0.75	0.14	80,80,80,80	0
56	MG	AA	1760	1/1	0.75	0.17	172,172,172,172	0
56	MG	CA	1603	1/1	0.75	0.42	255,255,255,255	0
56	MG	CA	1926	1/1	0.75	0.15	101,101,101,101	0
56	MG	CA	1852	1/1	0.75	0.14	93,93,93,93	0
56	MG	CA	1855	1/1	0.75	0.18	197,197,197,197	0
56	MG	BA	3590	1/1	0.75	0.08	90,90,90,90	0
56	MG	BA	2907	1/1	0.75	0.10	129,129,129,129	0
56	MG	BA	3470	1/1	0.75	0.26	65,65,65,65	0
56	MG	BA	3065	1/1	0.75	0.11	90,90,90,90	0
56	MG	AA	1700	1/1	0.75	0.37	158,158,158,158	0
56	MG	CA	1783	1/1	0.75	0.16	82,82,82,82	0
56	MG	BA	3298	1/1	0.75	0.08	101,101,101,101	0
56	MG	DA	2958	1/1	0.75	0.14	95,95,95,95	0
56	MG	BA	3043	1/1	0.75	0.17	155,155,155,155	0
56	MG	BA	3188	1/1	0.75	0.08	78,78,78,78	0
56	MG	CA	1792	1/1	0.76	0.16	122,122,122,122	0
56	MG	DA	2967	1/1	0.76	0.23	86,86,86,86	0
56	MG	CA	1825	1/1	0.76	0.12	80,80,80,80	0
56	MG	AA	1668	1/1	0.76	0.09	90,90,90,90	0
56	MG	DA	3095	1/1	0.76	0.09	100,100,100,100	0
56	MG	CA	1713	1/1	0.76	0.17	88,88,88,88	0
56	MG	CA	1876	1/1	0.76	0.16	127,127,127,127	0
56	MG	CA	1880	1/1	0.76	0.29	118,118,118,118	0
56	MG	CW	104	1/1	0.76	0.13	87,87,87,87	0
56	MG	AA	1836	1/1	0.76	0.08	139,139,139,139	0
56	MG	CA	1642	1/1	0.76	0.27	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	DA	3507	1/1	0.76	0.17	70,70,70,70	0
56	MG	DA	3015	1/1	0.76	0.12	91,91,91,91	0
56	MG	AA	1639	1/1	0.76	0.17	114,114,114,114	0
56	MG	BA	3535	1/1	0.76	0.23	68,68,68,68	0
56	MG	CA	1854	1/1	0.76	0.13	98,98,98,98	0
56	MG	CA	1808	1/1	0.76	0.13	74,74,74,74	0
56	MG	CA	1655	1/1	0.76	0.10	65,65,65,65	0
56	MG	CA	1812	1/1	0.76	0.13	75,75,75,75	0
56	MG	DB	206	1/1	0.76	0.14	121,121,121,121	0
56	MG	DA	3064	1/1	0.76	0.07	62,62,62,62	0
56	MG	DA	3066	1/1	0.76	0.38	90,90,90,90	0
56	MG	DA	3071	1/1	0.76	0.10	92,92,92,92	0
56	MG	AA	1607	1/1	0.76	0.16	97,97,97,97	0
56	MG	DA	3400	1/1	0.77	0.31	88,88,88,88	0
56	MG	DA	3401	1/1	0.77	0.06	81,81,81,81	0
56	MG	AA	1936	1/1	0.77	0.31	94,94,94,94	0
56	MG	BA	3036	1/1	0.77	0.09	131,131,131,131	0
56	MG	AA	1892	1/1	0.77	0.09	108,108,108,108	0
56	MG	DA	3417	1/1	0.77	0.11	145,145,145,145	0
56	MG	BA	3102	1/1	0.77	0.18	61,61,61,61	0
56	MG	DA	3080	1/1	0.77	0.12	84,84,84,84	0
56	MG	AA	1746	1/1	0.77	0.16	93,93,93,93	0
56	MG	CA	1738	1/1	0.77	0.16	123,123,123,123	0
56	MG	CA	1837	1/1	0.77	0.14	66,66,66,66	0
56	MG	AA	1956	1/1	0.77	0.12	110,110,110,110	0
56	MG	DA	3101	1/1	0.77	0.10	101,101,101,101	0
56	MG	AA	1751	1/1	0.77	0.12	108,108,108,108	0
56	MG	CA	1708	1/1	0.77	0.10	63,63,63,63	0
56	MG	AA	1792	1/1	0.77	0.23	84,84,84,84	0
56	MG	CA	1612	1/1	0.77	0.12	82,82,82,82	0
56	MG	AA	1917	1/1	0.77	0.07	86,86,86,86	0
56	MG	AA	1625	1/1	0.77	0.18	85,85,85,85	0
56	MG	BA	3081	1/1	0.77	0.25	79,79,79,79	0
56	MG	DA	3544	1/1	0.77	0.10	73,73,73,73	0
56	MG	BA	3602	1/1	0.77	0.34	117,117,117,117	0
56	MG	DA	3589	1/1	0.77	0.10	74,74,74,74	0
56	MG	BA	3273	1/1	0.77	0.26	110,110,110,110	0
56	MG	BA	3500	1/1	0.77	0.34	72,72,72,72	0
56	MG	AA	1739	1/1	0.77	0.19	88,88,88,88	0
56	MG	BA	2991	1/1	0.77	0.23	80,80,80,80	0
56	MG	BA	2928	1/1	0.77	0.09	80,80,80,80	0
56	MG	CD	302	1/1	0.77	0.29	111,111,111,111	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	DA	3382	1/1	0.77	0.34	49,49,49,49	0
56	MG	BA	3302	1/1	0.77	0.19	63,63,63,63	0
56	MG	AA	1989	1/1	0.78	0.20	70,70,70,70	0
56	MG	AA	1990	1/1	0.78	0.16	58,58,58,58	0
56	MG	BA	3193	1/1	0.78	0.08	79,79,79,79	0
56	MG	BA	3196	1/1	0.78	0.14	84,84,84,84	0
56	MG	CA	1671	1/1	0.78	0.09	92,92,92,92	0
56	MG	BA	3197	1/1	0.78	0.10	215,215,215,215	0
56	MG	BA	3576	1/1	0.78	0.15	97,97,97,97	0
56	MG	BA	3581	1/1	0.78	0.09	94,94,94,94	0
56	MG	BA	3685	1/1	0.78	0.56	79,79,79,79	0
56	MG	BA	3346	1/1	0.78	0.13	111,111,111,111	0
56	MG	BA	3201	1/1	0.78	0.18	71,71,71,71	0
56	MG	BA	3080	1/1	0.78	0.44	112,112,112,112	0
56	MG	DA	3428	1/1	0.78	0.57	71,71,71,71	0
56	MG	BA	2941	1/1	0.78	0.09	87,87,87,87	0
56	MG	BA	3442	1/1	0.78	0.36	79,79,79,79	0
56	MG	AA	1829	1/1	0.78	0.38	232,232,232,232	0
56	MG	DA	3455	1/1	0.78	0.07	72,72,72,72	0
56	MG	AA	1912	1/1	0.78	0.11	87,87,87,87	0
56	MG	CA	1848	1/1	0.78	0.13	113,113,113,113	0
56	MG	AA	1718	1/1	0.78	0.19	75,75,75,75	0
56	MG	CA	1741	1/1	0.78	0.11	104,104,104,104	0
56	MG	CR	101	1/1	0.78	0.17	182,182,182,182	0
56	MG	BA	3154	1/1	0.78	0.17	169,169,169,169	0
56	MG	AA	1799	1/1	0.78	0.25	85,85,85,85	0
56	MG	CA	1746	1/1	0.78	0.12	255,255,255,255	0
56	MG	AA	1825	1/1	0.78	0.19	138,138,138,138	0
56	MG	DA	2936	1/1	0.78	0.20	82,82,82,82	0
56	MG	CA	1748	1/1	0.78	0.18	78,78,78,78	0
56	MG	CA	1775	1/1	0.78	0.14	47,47,47,47	0
56	MG	DA	2947	1/1	0.78	0.28	192,192,192,192	0
56	MG	CA	1776	1/1	0.78	0.27	125,125,125,125	0
56	MG	BA	3606	1/1	0.78	0.20	72,72,72,72	0
56	MG	CA	1646	1/1	0.78	0.11	113,113,113,113	0
56	MG	AA	1652	1/1	0.78	0.21	98,98,98,98	0
56	MG	BA	2988	1/1	0.78	0.15	77,77,77,77	0
56	MG	DA	3356	1/1	0.78	0.08	107,107,107,107	0
56	MG	BA	3290	1/1	0.78	0.07	77,77,77,77	0
56	MG	BA	2969	1/1	0.79	0.18	79,79,79,79	0
56	MG	CA	1893	1/1	0.79	0.20	125,125,125,125	0
56	MG	CA	1622	1/1	0.79	0.12	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	AW	115	1/1	0.79	0.06	111,111,111,111	0
56	MG	BA	3278	1/1	0.79	0.11	115,115,115,115	0
56	MG	CA	1900	1/1	0.79	0.09	112,112,112,112	0
56	MG	AA	1846	1/1	0.79	0.14	118,118,118,118	0
56	MG	BA	3107	1/1	0.79	0.23	87,87,87,87	0
56	MG	DA	3033	1/1	0.79	0.18	93,93,93,93	0
56	MG	BA	2978	1/1	0.79	0.30	72,72,72,72	0
56	MG	BA	3069	1/1	0.79	0.20	69,69,69,69	0
56	MG	AA	1763	1/1	0.79	0.11	88,88,88,88	0
56	MG	CA	1703	1/1	0.79	0.07	89,89,89,89	0
56	MG	BA	2937	1/1	0.79	0.26	71,71,71,71	0
56	MG	AA	1963	1/1	0.79	0.17	80,80,80,80	0
56	MG	BA	3139	1/1	0.79	0.20	73,73,73,73	0
56	MG	BB	212	1/1	0.79	0.09	99,99,99,99	0
56	MG	BA	3548	1/1	0.79	0.16	88,88,88,88	0
56	MG	DA	3446	1/1	0.79	0.21	59,59,59,59	0
56	MG	AA	1606	1/1	0.79	0.08	77,77,77,77	0
56	MG	CA	1780	1/1	0.79	0.21	72,72,72,72	0
56	MG	BA	3236	1/1	0.79	0.12	132,132,132,132	0
56	MG	BA	3654	1/1	0.79	0.10	86,86,86,86	0
56	MG	DA	3092	1/1	0.79	0.20	200,200,200,200	0
56	MG	BA	3658	1/1	0.79	0.12	71,71,71,71	0
56	MG	BA	3664	1/1	0.79	0.07	82,82,82,82	0
56	MG	DA	3501	1/1	0.79	0.16	96,96,96,96	0
56	MG	DA	3105	1/1	0.79	0.08	94,94,94,94	0
56	MG	AA	1981	1/1	0.79	0.08	90,90,90,90	0
56	MG	CA	1795	1/1	0.79	0.18	84,84,84,84	0
56	MG	BA	3584	1/1	0.79	0.33	96,96,96,96	0
56	MG	CA	1801	1/1	0.79	0.14	76,76,76,76	0
56	MG	DA	3125	1/1	0.79	0.27	161,161,161,161	0
56	MG	DA	3146	1/1	0.79	0.40	50,50,50,50	0
56	MG	DA	2964	1/1	0.79	0.24	65,65,65,65	0
56	MG	AA	1637	1/1	0.79	0.14	67,67,67,67	0
56	MG	DA	3275	1/1	0.79	0.29	52,52,52,52	0
56	MG	DA	3287	1/1	0.79	0.30	44,44,44,44	0
56	MG	DA	3338	1/1	0.79	0.32	76,76,76,76	0
56	MG	DA	3339	1/1	0.79	0.11	63,63,63,63	0
56	MG	BA	3057	1/1	0.79	0.20	65,65,65,65	0
56	MG	AA	1622	1/1	0.79	0.17	70,70,70,70	0
56	MG	BA	3464	1/1	0.79	0.22	84,84,84,84	0
56	MG	AA	1628	1/1	0.80	0.33	213,213,213,213	0
56	MG	DA	3365	1/1	0.80	0.25	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BA	3507	1/1	0.80	0.17	56,56,56,56	0
56	MG	DA	3041	1/1	0.80	0.14	59,59,59,59	0
56	MG	BA	3510	1/1	0.80	0.20	86,86,86,86	0
56	MG	CA	1906	1/1	0.80	0.13	114,114,114,114	0
56	MG	CA	1667	1/1	0.80	0.17	118,118,118,118	0
56	MG	CA	1820	1/1	0.80	0.12	193,193,193,193	0
56	MG	BA	2999	1/1	0.80	0.15	92,92,92,92	0
56	MG	AA	1670	1/1	0.80	0.08	77,77,77,77	0
56	MG	BA	3624	1/1	0.80	0.23	83,83,83,83	0
56	MG	DA	3411	1/1	0.80	0.37	59,59,59,59	0
56	MG	BA	3114	1/1	0.80	0.09	119,119,119,119	0
56	MG	BA	3638	1/1	0.80	0.19	73,73,73,73	0
56	MG	AA	1949	1/1	0.80	0.19	60,60,60,60	0
56	MG	BA	3537	1/1	0.80	0.11	60,60,60,60	0
56	MG	BA	3540	1/1	0.80	0.29	84,84,84,84	0
56	MG	BA	3331	1/1	0.80	0.23	121,121,121,121	0
56	MG	DA	3435	1/1	0.80	0.37	68,68,68,68	0
56	MG	AA	1635	1/1	0.80	0.18	106,106,106,106	0
56	MG	BA	3555	1/1	0.80	0.12	94,94,94,94	0
56	MG	BA	3359	1/1	0.80	0.23	106,106,106,106	0
56	MG	AA	1754	1/1	0.80	0.11	72,72,72,72	0
56	MG	AA	1713	1/1	0.80	0.13	84,84,84,84	0
56	MG	CA	1772	1/1	0.80	0.23	66,66,66,66	0
56	MG	AA	1714	1/1	0.80	0.19	114,114,114,114	0
56	MG	DA	3110	1/1	0.80	0.07	63,63,63,63	0
56	MG	DA	3111	1/1	0.80	0.25	84,84,84,84	0
56	MG	CA	1700	1/1	0.80	0.24	180,180,180,180	0
56	MG	DA	3117	1/1	0.80	0.10	72,72,72,72	0
56	MG	BA	3695	1/1	0.80	0.18	95,95,95,95	0
56	MG	AA	1660	1/1	0.80	0.07	105,105,105,105	0
56	MG	AA	1977	1/1	0.80	0.15	126,126,126,126	0
56	MG	AA	1979	1/1	0.80	0.20	118,118,118,118	0
56	MG	DA	3576	1/1	0.80	0.18	102,102,102,102	0
56	MG	AA	1841	1/1	0.80	0.06	113,113,113,113	0
56	MG	DA	3278	1/1	0.80	0.08	83,83,83,83	0
56	MG	BA	2931	1/1	0.80	0.41	98,98,98,98	0
56	MG	AA	1617	1/1	0.80	0.08	108,108,108,108	0
56	MG	BA	3275	1/1	0.80	0.16	102,102,102,102	0
56	MG	DB	204	1/1	0.80	0.08	78,78,78,78	0
56	MG	BA	3720	1/1	0.80	0.08	85,85,85,85	0
56	MG	CA	1647	1/1	0.80	0.24	98,98,98,98	0
56	MG	BA	3175	1/1	0.80	0.25	109,109,109,109	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	AA	1684	1/1	0.80	0.18	62,62,62,62	0
56	MG	BA	3098	1/1	0.80	0.13	94,94,94,94	0
56	MG	DA	2930	1/1	0.81	0.31	86,86,86,86	0
56	MG	CA	1736	1/1	0.81	0.65	193,193,193,193	0
56	MG	DA	2937	1/1	0.81	0.15	104,104,104,104	0
56	MG	DA	2938	1/1	0.81	0.13	71,71,71,71	0
56	MG	DA	3320	1/1	0.81	0.12	78,78,78,78	0
56	MG	DA	3325	1/1	0.81	0.13	46,46,46,46	0
56	MG	BA	3117	1/1	0.81	0.14	92,92,92,92	0
56	MG	BA	3393	1/1	0.81	0.23	99,99,99,99	0
56	MG	BA	3398	1/1	0.81	0.23	64,64,64,64	0
56	MG	DA	2951	1/1	0.81	0.11	78,78,78,78	0
56	MG	BA	3404	1/1	0.81	0.40	82,82,82,82	0
56	MG	BB	203	1/1	0.81	0.11	78,78,78,78	0
56	MG	CA	1862	1/1	0.81	0.10	117,117,117,117	0
56	MG	BA	3118	1/1	0.81	0.17	132,132,132,132	0
56	MG	AA	1823	1/1	0.81	0.10	96,96,96,96	0
56	MG	CA	1867	1/1	0.81	0.12	82,82,82,82	0
56	MG	AA	1847	1/1	0.81	0.28	209,209,209,209	0
56	MG	BA	2962	1/1	0.81	0.35	78,78,78,78	0
56	MG	BA	3130	1/1	0.81	0.13	82,82,82,82	0
56	MG	CA	1875	1/1	0.81	0.14	267,267,267,267	0
56	MG	CA	1753	1/1	0.81	0.13	63,63,63,63	0
56	MG	BA	3134	1/1	0.81	0.25	122,122,122,122	0
56	MG	AA	1980	1/1	0.81	0.12	76,76,76,76	0
56	MG	BA	3245	1/1	0.81	0.27	185,185,185,185	0
56	MG	AA	1722	1/1	0.81	0.32	72,72,72,72	0
56	MG	BA	3254	1/1	0.81	0.07	93,93,93,93	0
56	MG	AA	1737	1/1	0.81	0.09	72,72,72,72	0
56	MG	BA	3496	1/1	0.81	0.27	63,63,63,63	0
56	MG	DA	3057	1/1	0.81	0.08	107,107,107,107	0
56	MG	BA	3141	1/1	0.81	0.28	62,62,62,62	0
56	MG	DA	3430	1/1	0.81	0.12	80,80,80,80	0
56	MG	BA	3147	1/1	0.81	0.39	88,88,88,88	0
56	MG	AA	1679	1/1	0.81	0.13	112,112,112,112	0
56	MG	AQ	201	1/1	0.81	0.26	68,68,68,68	0
56	MG	DA	3068	1/1	0.81	0.10	69,69,69,69	0
56	MG	DA	3449	1/1	0.81	0.08	53,53,53,53	0
56	MG	AA	1601	1/1	0.81	0.23	92,92,92,92	0
56	MG	BA	3655	1/1	0.81	0.22	87,87,87,87	0
56	MG	BA	3657	1/1	0.81	0.17	55,55,55,55	0
56	MG	DA	3463	1/1	0.81	0.15	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	DA	3077	1/1	0.81	0.10	77,77,77,77	0
56	MG	CA	1907	1/1	0.81	0.25	77,77,77,77	0
56	MG	BA	3037	1/1	0.81	0.07	101,101,101,101	0
56	MG	DA	3084	1/1	0.81	0.09	83,83,83,83	0
56	MG	BA	3287	1/1	0.81	0.07	55,55,55,55	0
56	MG	CA	1911	1/1	0.81	0.25	107,107,107,107	0
56	MG	BA	3160	1/1	0.81	0.10	51,51,51,51	0
56	MG	CA	1916	1/1	0.81	0.17	77,77,77,77	0
56	MG	BA	3297	1/1	0.81	0.15	122,122,122,122	0
56	MG	BA	2934	1/1	0.81	0.24	79,79,79,79	0
56	MG	DA	3560	1/1	0.81	0.23	55,55,55,55	0
56	MG	AA	1896	1/1	0.81	0.14	77,77,77,77	0
56	MG	BA	3176	1/1	0.81	0.20	52,52,52,52	0
56	MG	BA	3693	1/1	0.81	0.17	65,65,65,65	0
56	MG	AA	1653	1/1	0.81	0.16	105,105,105,105	0
56	MG	BA	3557	1/1	0.81	0.23	97,97,97,97	0
56	MG	BA	3561	1/1	0.81	0.13	58,58,58,58	0
56	MG	DB	201	1/1	0.81	0.15	62,62,62,62	0
56	MG	AA	1810	1/1	0.81	0.15	87,87,87,87	0
56	MG	AA	1840	1/1	0.81	0.41	79,79,79,79	0
56	MG	AA	1692	1/1	0.81	0.09	134,134,134,134	0
56	MG	DA	3211	1/1	0.81	0.20	33,33,33,33	0
56	MG	DA	3244	1/1	0.81	0.18	59,59,59,59	0
56	MG	BA	3194	1/1	0.81	0.19	91,91,91,91	0
56	MG	CW	111	1/1	0.82	0.21	82,82,82,82	0
56	MG	BA	3071	1/1	0.82	0.14	52,52,52,52	0
56	MG	BA	3593	1/1	0.82	0.12	57,57,57,57	0
56	MG	BA	3031	1/1	0.82	0.11	255,255,255,255	0
56	MG	BB	215	1/1	0.82	0.12	94,94,94,94	0
56	MG	BA	3468	1/1	0.82	0.28	67,67,67,67	0
56	MG	CA	1816	1/1	0.82	0.17	77,77,77,77	0
56	MG	BA	2954	1/1	0.82	0.07	77,77,77,77	0
56	MG	DA	2915	1/1	0.82	0.12	78,78,78,78	0
56	MG	CA	1818	1/1	0.82	0.14	71,71,71,71	0
56	MG	BA	3192	1/1	0.82	0.09	90,90,90,90	0
56	MG	BA	3491	1/1	0.82	0.22	85,85,85,85	0
56	MG	BA	3608	1/1	0.82	0.34	54,54,54,54	0
56	MG	BA	3289	1/1	0.82	0.20	83,83,83,83	0
56	MG	AA	1631	1/1	0.82	0.33	76,76,76,76	0
56	MG	CA	1711	1/1	0.82	0.11	88,88,88,88	0
56	MG	AA	1699	1/1	0.82	0.10	85,85,85,85	0
56	MG	DA	2949	1/1	0.82	0.17	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BA	3616	1/1	0.82	0.21	62,62,62,62	0
56	MG	AA	1855	1/1	0.82	0.10	103,103,103,103	0
56	MG	BA	3039	1/1	0.82	0.20	176,176,176,176	0
56	MG	CA	1619	1/1	0.82	0.16	128,128,128,128	0
56	MG	AA	1747	1/1	0.82	0.25	109,109,109,109	0
56	MG	BA	3304	1/1	0.82	0.26	167,167,167,167	0
56	MG	DA	2978	1/1	0.82	0.27	64,64,64,64	0
56	MG	DA	3398	1/1	0.82	0.21	107,107,107,107	0
56	MG	BA	3308	1/1	0.82	0.13	88,88,88,88	0
56	MG	BA	3529	1/1	0.82	0.06	79,79,79,79	0
56	MG	DA	2996	1/1	0.82	0.12	65,65,65,65	0
56	MG	BA	3532	1/1	0.82	0.11	58,58,58,58	0
56	MG	BA	3088	1/1	0.82	0.09	167,167,167,167	0
56	MG	DA	3001	1/1	0.82	0.34	79,79,79,79	0
56	MG	BA	3055	1/1	0.82	0.09	71,71,71,71	0
56	MG	CA	1866	1/1	0.82	0.18	85,85,85,85	0
56	MG	AA	1669	1/1	0.82	0.30	68,68,68,68	0
56	MG	BA	3221	1/1	0.82	0.11	77,77,77,77	0
56	MG	DA	3023	1/1	0.82	0.13	71,71,71,71	0
56	MG	CA	1640	1/1	0.82	0.14	78,78,78,78	0
56	MG	BA	3671	1/1	0.82	0.07	84,84,84,84	0
56	MG	BA	3222	1/1	0.82	0.20	70,70,70,70	0
56	MG	BA	3546	1/1	0.82	0.12	200,200,200,200	0
56	MG	BA	3361	1/1	0.82	0.19	106,106,106,106	0
56	MG	CA	1649	1/1	0.82	0.10	63,63,63,63	0
56	MG	BA	3550	1/1	0.82	0.17	68,68,68,68	0
56	MG	BA	3364	1/1	0.82	0.15	82,82,82,82	0
56	MG	DA	3461	1/1	0.82	0.18	73,73,73,73	0
56	MG	BA	3095	1/1	0.82	0.14	90,90,90,90	0
56	MG	CA	1658	1/1	0.82	0.20	93,93,93,93	0
56	MG	BA	3560	1/1	0.82	0.13	47,47,47,47	0
56	MG	DA	3485	1/1	0.82	0.22	120,120,120,120	0
56	MG	BA	3390	1/1	0.82	0.29	44,44,44,44	0
56	MG	DA	3072	1/1	0.82	0.31	94,94,94,94	0
56	MG	BA	3096	1/1	0.82	0.12	173,173,173,173	0
56	MG	BA	3577	1/1	0.82	0.26	88,88,88,88	0
56	MG	DA	3508	1/1	0.82	0.12	37,37,37,37	0
56	MG	CA	1773	1/1	0.82	0.14	62,62,62,62	0
56	MG	BA	3714	1/1	0.82	0.09	94,94,94,94	0
56	MG	AA	1720	1/1	0.82	0.12	86,86,86,86	0
56	MG	AA	1688	1/1	0.82	0.14	80,80,80,80	0
56	MG	BA	3019	1/1	0.82	0.17	109,109,109,109	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	AA	1711	1/1	0.82	0.14	83,83,83,83	0
56	MG	DA	3579	1/1	0.82	0.19	36,36,36,36	0
56	MG	BA	3721	1/1	0.82	0.29	86,86,86,86	0
56	MG	AA	1824	1/1	0.82	0.10	108,108,108,108	0
56	MG	AA	1657	1/1	0.82	0.20	112,112,112,112	0
56	MG	BA	3268	1/1	0.82	0.13	102,102,102,102	0
56	MG	BA	3460	1/1	0.82	0.09	51,51,51,51	0
56	MG	CA	1925	1/1	0.82	0.09	94,94,94,94	0
56	MG	DB	203	1/1	0.82	0.13	66,66,66,66	0
56	MG	BA	3178	1/1	0.82	0.17	52,52,52,52	0
56	MG	DB	205	1/1	0.82	0.27	94,94,94,94	0
56	MG	CV	101	1/1	0.82	0.14	87,87,87,87	0
56	MG	CV	102	1/1	0.82	0.35	78,78,78,78	0
56	MG	CA	1689	1/1	0.82	0.07	52,52,52,52	0
56	MG	DB	213	1/1	0.82	0.11	76,76,76,76	0
56	MG	CA	1691	1/1	0.82	0.07	161,161,161,161	0
56	MG	DA	3120	1/1	0.82	0.16	76,76,76,76	0
56	MG	DI	201	1/1	0.82	0.11	49,49,49,49	0
56	MG	DQ	201	1/1	0.82	0.19	49,49,49,49	0
56	MG	DV	201	1/1	0.82	0.09	85,85,85,85	0
56	MG	DX	101	1/1	0.82	0.28	99,99,99,99	0
56	MG	DA	3238	1/1	0.83	0.14	89,89,89,89	0
56	MG	AA	1738	1/1	0.83	0.22	71,71,71,71	0
56	MG	CA	1810	1/1	0.83	0.32	121,121,121,121	0
56	MG	DA	2906	1/1	0.83	0.28	70,70,70,70	0
56	MG	DA	3250	1/1	0.83	0.45	77,77,77,77	0
56	MG	DA	2910	1/1	0.83	0.18	90,90,90,90	0
56	MG	BA	3163	1/1	0.83	0.16	93,93,93,93	0
56	MG	DA	2913	1/1	0.83	0.34	70,70,70,70	0
56	MG	BA	3479	1/1	0.83	0.24	59,59,59,59	0
56	MG	BA	3093	1/1	0.83	0.12	55,55,55,55	0
56	MG	DA	2917	1/1	0.83	0.43	83,83,83,83	0
56	MG	BE	301	1/1	0.83	0.24	60,60,60,60	0
56	MG	CA	1602	1/1	0.83	0.10	112,112,112,112	0
56	MG	BA	3488	1/1	0.83	0.14	62,62,62,62	0
56	MG	CA	1604	1/1	0.83	0.19	99,99,99,99	0
56	MG	CA	1828	1/1	0.83	0.12	135,135,135,135	0
56	MG	BA	3280	1/1	0.83	0.08	84,84,84,84	0
56	MG	BA	3040	1/1	0.83	0.09	85,85,85,85	0
56	MG	DA	3361	1/1	0.83	0.11	73,73,73,73	0
56	MG	DA	2944	1/1	0.83	0.12	94,94,94,94	0
56	MG	DA	3366	1/1	0.83	0.09	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	DA	3370	1/1	0.83	0.29	66,66,66,66	0
56	MG	BA	3288	1/1	0.83	0.18	71,71,71,71	0
56	MG	BA	3499	1/1	0.83	0.11	40,40,40,40	0
56	MG	BA	2993	1/1	0.83	0.08	57,57,57,57	0
56	MG	BA	3049	1/1	0.83	0.07	90,90,90,90	0
56	MG	BA	3618	1/1	0.83	0.13	79,79,79,79	0
56	MG	DA	2966	1/1	0.83	0.23	42,42,42,42	0
56	MG	BA	3291	1/1	0.83	0.23	94,94,94,94	0
56	MG	BA	3052	1/1	0.83	0.34	118,118,118,118	0
56	MG	DA	2974	1/1	0.83	0.15	90,90,90,90	0
56	MG	AA	1779	1/1	0.83	0.23	74,74,74,74	0
56	MG	AA	1710	1/1	0.83	0.12	79,79,79,79	0
56	MG	BA	3523	1/1	0.83	0.17	47,47,47,47	0
56	MG	BA	3111	1/1	0.83	0.19	96,96,96,96	0
56	MG	AA	1817	1/1	0.83	0.23	175,175,175,175	0
56	MG	BA	3060	1/1	0.83	0.17	80,80,80,80	0
56	MG	BA	3534	1/1	0.83	0.14	32,32,32,32	0
56	MG	AA	1634	1/1	0.83	0.20	78,78,78,78	0
56	MG	BA	2943	1/1	0.83	0.10	98,98,98,98	0
56	MG	BA	3121	1/1	0.83	0.41	137,137,137,137	0
56	MG	CA	1643	1/1	0.83	0.12	126,126,126,126	0
56	MG	BA	2945	1/1	0.83	0.25	76,76,76,76	0
56	MG	DA	3022	1/1	0.83	0.15	80,80,80,80	0
56	MG	BA	3208	1/1	0.83	0.24	87,87,87,87	0
56	MG	BA	3126	1/1	0.83	0.54	235,235,235,235	0
56	MG	AA	1933	1/1	0.83	0.16	63,63,63,63	0
56	MG	DA	3035	1/1	0.83	0.20	71,71,71,71	0
56	MG	BA	3219	1/1	0.83	0.19	78,78,78,78	0
56	MG	CA	1651	1/1	0.83	0.28	95,95,95,95	0
56	MG	CA	1744	1/1	0.83	0.12	95,95,95,95	0
56	MG	BA	3371	1/1	0.83	0.28	55,55,55,55	0
56	MG	DA	3492	1/1	0.83	0.13	61,61,61,61	0
56	MG	AA	1640	1/1	0.83	0.07	102,102,102,102	0
56	MG	BA	3699	1/1	0.83	0.21	70,70,70,70	0
56	MG	BA	2952	1/1	0.83	0.12	55,55,55,55	0
56	MG	CA	1750	1/1	0.83	0.35	222,222,222,222	0
56	MG	BA	3569	1/1	0.83	0.24	87,87,87,87	0
56	MG	BA	3570	1/1	0.83	0.14	83,83,83,83	0
56	MG	BA	3571	1/1	0.83	0.26	68,68,68,68	0
56	MG	CA	1904	1/1	0.83	0.09	80,80,80,80	0
56	MG	BA	3573	1/1	0.83	0.09	81,81,81,81	0
56	MG	DA	3546	1/1	0.83	0.11	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	DA	3547	1/1	0.83	0.09	70,70,70,70	0
56	MG	AA	1678	1/1	0.83	0.10	101,101,101,101	0
56	MG	AA	1948	1/1	0.83	0.19	103,103,103,103	0
56	MG	BA	3239	1/1	0.83	0.12	99,99,99,99	0
56	MG	AA	1858	1/1	0.83	0.07	132,132,132,132	0
56	MG	BA	3436	1/1	0.83	0.32	86,86,86,86	0
56	MG	DA	3591	1/1	0.83	0.08	129,129,129,129	0
56	MG	CA	1913	1/1	0.83	0.21	69,69,69,69	0
56	MG	DA	3612	1/1	0.83	0.14	52,52,52,52	0
56	MG	CA	1914	1/1	0.83	0.07	96,96,96,96	0
56	MG	DA	3631	1/1	0.83	0.05	85,85,85,85	0
56	MG	CA	1791	1/1	0.83	0.25	91,91,91,91	0
56	MG	CA	1918	1/1	0.83	0.13	107,107,107,107	0
56	MG	CA	1920	1/1	0.83	0.09	138,138,138,138	0
56	MG	CA	1679	1/1	0.83	0.14	81,81,81,81	0
56	MG	CA	1680	1/1	0.83	0.18	77,77,77,77	0
56	MG	AA	1767	1/1	0.83	0.19	102,102,102,102	0
56	MG	DB	207	1/1	0.83	0.08	87,87,87,87	0
56	MG	AA	1733	1/1	0.83	0.15	94,94,94,94	0
56	MG	AA	1800	1/1	0.83	0.12	87,87,87,87	0
56	MG	CA	1685	1/1	0.83	0.10	104,104,104,104	0
56	MG	AA	1613	1/1	0.83	0.10	83,83,83,83	0
56	MG	CA	1803	1/1	0.83	0.22	146,146,146,146	0
56	MG	DB	219	1/1	0.83	0.20	66,66,66,66	0
56	MG	AA	1974	1/1	0.83	0.15	48,48,48,48	0
56	MG	BA	3157	1/1	0.83	0.20	57,57,57,57	0
56	MG	AA	1808	1/1	0.83	0.10	70,70,70,70	0
56	MG	DA	3219	1/1	0.83	0.13	42,42,42,42	0
56	MG	CA	1831	1/1	0.84	0.27	62,62,62,62	0
56	MG	DA	3060	1/1	0.84	0.06	77,77,77,77	0
56	MG	DA	3062	1/1	0.84	0.10	75,75,75,75	0
56	MG	CA	1834	1/1	0.84	0.19	108,108,108,108	0
56	MG	AA	1849	1/1	0.84	0.11	95,95,95,95	0
56	MG	BA	3617	1/1	0.84	0.13	88,88,88,88	0
56	MG	AA	1741	1/1	0.84	0.23	91,91,91,91	0
56	MG	BA	3623	1/1	0.84	0.25	79,79,79,79	0
56	MG	AG	201	1/1	0.84	0.15	78,78,78,78	0
56	MG	CA	1670	1/1	0.84	0.10	61,61,61,61	0
56	MG	BA	3627	1/1	0.84	0.21	100,100,100,100	0
56	MG	BA	3553	1/1	0.84	0.20	92,92,92,92	0
56	MG	AA	1854	1/1	0.84	0.35	187,187,187,187	0
56	MG	AA	1641	1/1	0.84	0.16	121,121,121,121	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	DA	3444	1/1	0.84	0.20	55,55,55,55	0
56	MG	AA	1856	1/1	0.84	0.13	134,134,134,134	0
56	MG	BA	3652	1/1	0.84	0.17	63,63,63,63	0
56	MG	CA	1861	1/1	0.84	0.11	79,79,79,79	0
56	MG	BA	3653	1/1	0.84	0.11	62,62,62,62	0
56	MG	AT	202	1/1	0.84	0.17	100,100,100,100	0
56	MG	AA	1833	1/1	0.84	0.08	72,72,72,72	0
56	MG	CA	1752	1/1	0.84	0.11	83,83,83,83	0
56	MG	BA	2905	1/1	0.84	0.10	54,54,54,54	0
56	MG	AA	1946	1/1	0.84	0.11	86,86,86,86	0
56	MG	BA	3663	1/1	0.84	0.26	105,105,105,105	0
56	MG	AA	1787	1/1	0.84	0.16	79,79,79,79	0
56	MG	DA	3491	1/1	0.84	0.10	71,71,71,71	0
56	MG	CA	1874	1/1	0.84	0.31	89,89,89,89	0
56	MG	AA	1701	1/1	0.84	0.07	79,79,79,79	0
56	MG	BA	3209	1/1	0.84	0.15	96,96,96,96	0
56	MG	CA	1879	1/1	0.84	0.17	53,53,53,53	0
56	MG	DA	3505	1/1	0.84	0.12	63,63,63,63	0
56	MG	AA	1730	1/1	0.84	0.19	78,78,78,78	0
56	MG	DA	3127	1/1	0.84	0.21	88,88,88,88	0
56	MG	DA	2952	1/1	0.84	0.23	68,68,68,68	0
56	MG	DA	3526	1/1	0.84	0.21	61,61,61,61	0
56	MG	AW	104	1/1	0.84	0.30	95,95,95,95	0
56	MG	CA	1787	1/1	0.84	0.23	77,77,77,77	0
56	MG	AA	1951	1/1	0.84	0.21	73,73,73,73	0
56	MG	BA	2970	1/1	0.84	0.09	93,93,93,93	0
56	MG	BA	2921	1/1	0.84	0.17	95,95,95,95	0
56	MG	AA	1955	1/1	0.84	0.19	87,87,87,87	0
56	MG	DA	3565	1/1	0.84	0.19	51,51,51,51	0
56	MG	DA	3571	1/1	0.84	0.34	70,70,70,70	0
56	MG	BA	2976	1/1	0.84	0.14	112,112,112,112	0
56	MG	BA	3332	1/1	0.84	0.39	58,58,58,58	0
56	MG	AA	1629	1/1	0.84	0.27	83,83,83,83	0
56	MG	DA	3284	1/1	0.84	0.17	53,53,53,53	0
56	MG	BA	3241	1/1	0.84	0.19	77,77,77,77	0
56	MG	DA	3311	1/1	0.84	0.12	54,54,54,54	0
56	MG	DA	3605	1/1	0.84	0.13	59,59,59,59	0
56	MG	CA	1641	1/1	0.84	0.09	135,135,135,135	0
56	MG	BA	2987	1/1	0.84	0.13	79,79,79,79	0
56	MG	DA	3630	1/1	0.84	0.09	76,76,76,76	0
56	MG	CA	1804	1/1	0.84	0.18	78,78,78,78	0
56	MG	BA	3247	1/1	0.84	0.10	105,105,105,105	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BA	3045	1/1	0.84	0.25	103,103,103,103	0
56	MG	CA	1645	1/1	0.84	0.32	113,113,113,113	0
56	MG	BA	3252	1/1	0.84	0.14	78,78,78,78	0
56	MG	AA	1716	1/1	0.84	0.19	103,103,103,103	0
56	MG	DA	3020	1/1	0.84	0.07	74,74,74,74	0
56	MG	BA	3050	1/1	0.84	0.10	60,60,60,60	0
56	MG	BA	3397	1/1	0.84	0.19	67,67,67,67	0
56	MG	AA	1706	1/1	0.84	0.12	186,186,186,186	0
56	MG	CA	1653	1/1	0.84	0.07	53,53,53,53	0
56	MG	DB	214	1/1	0.84	0.09	110,110,110,110	0
56	MG	DA	3367	1/1	0.84	0.14	74,74,74,74	0
56	MG	CA	1819	1/1	0.84	0.07	59,59,59,59	0
56	MG	CA	1654	1/1	0.84	0.16	106,106,106,106	0
56	MG	AA	1659	1/1	0.84	0.11	88,88,88,88	0
56	MG	BA	3613	1/1	0.84	0.27	76,76,76,76	0
56	MG	BA	3265	1/1	0.84	0.28	114,114,114,114	0
56	MG	DA	3058	1/1	0.84	0.06	72,72,72,72	0
56	MG	DA	3038	1/1	0.85	0.14	77,77,77,77	0
56	MG	AA	1925	1/1	0.85	0.15	63,63,63,63	0
56	MG	DA	3384	1/1	0.85	0.12	62,62,62,62	0
56	MG	BA	2936	1/1	0.85	0.07	65,65,65,65	0
56	MG	DA	3044	1/1	0.85	0.08	87,87,87,87	0
56	MG	AA	1870	1/1	0.85	0.19	73,73,73,73	0
56	MG	BA	3531	1/1	0.85	0.23	71,71,71,71	0
56	MG	CA	1676	1/1	0.85	0.12	88,88,88,88	0
56	MG	CA	1611	1/1	0.85	0.15	71,71,71,71	0
56	MG	CA	1844	1/1	0.85	0.34	104,104,104,104	0
56	MG	BA	2913	1/1	0.85	0.08	77,77,77,77	0
56	MG	BA	3210	1/1	0.85	0.08	76,76,76,76	0
56	MG	DA	3420	1/1	0.85	0.16	86,86,86,86	0
56	MG	BA	3600	1/1	0.85	0.16	73,73,73,73	0
56	MG	BA	3211	1/1	0.85	0.26	71,71,71,71	0
56	MG	DA	3067	1/1	0.85	0.15	83,83,83,83	0
56	MG	BA	3690	1/1	0.85	0.11	66,66,66,66	0
56	MG	DA	3070	1/1	0.85	0.14	69,69,69,69	0
56	MG	CY	402	1/1	0.85	0.09	44,44,44,44	0
56	MG	AA	1873	1/1	0.85	0.10	110,110,110,110	0
56	MG	BA	3074	1/1	0.85	0.11	108,108,108,108	0
56	MG	CA	1857	1/1	0.85	0.31	73,73,73,73	0
56	MG	CA	1761	1/1	0.85	0.29	49,49,49,49	0
56	MG	DA	3079	1/1	0.85	0.11	62,62,62,62	0
56	MG	BA	3218	1/1	0.85	0.24	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	AA	1620	1/1	0.85	0.06	76,76,76,76	0
56	MG	CA	1863	1/1	0.85	0.22	69,69,69,69	0
56	MG	BA	3704	1/1	0.85	0.23	43,43,43,43	0
56	MG	AA	1942	1/1	0.85	0.16	92,92,92,92	0
56	MG	DA	3470	1/1	0.85	0.06	81,81,81,81	0
56	MG	DA	3475	1/1	0.85	0.15	54,54,54,54	0
56	MG	DA	3476	1/1	0.85	0.07	73,73,73,73	0
56	MG	DA	3480	1/1	0.85	0.19	42,42,42,42	0
56	MG	DA	3483	1/1	0.85	0.19	96,96,96,96	0
56	MG	BA	3168	1/1	0.85	0.16	78,78,78,78	0
56	MG	AA	1772	1/1	0.85	0.08	94,94,94,94	0
56	MG	DA	3490	1/1	0.85	0.31	96,96,96,96	0
56	MG	DA	2927	1/1	0.85	0.12	91,91,91,91	0
56	MG	BA	3234	1/1	0.85	0.09	83,83,83,83	0
56	MG	DA	2933	1/1	0.85	0.11	35,35,35,35	0
56	MG	CA	1870	1/1	0.85	0.08	73,73,73,73	0
56	MG	CA	1786	1/1	0.85	0.09	84,84,84,84	0
56	MG	DA	3503	1/1	0.85	0.08	92,92,92,92	0
56	MG	AA	1757	1/1	0.85	0.13	74,74,74,74	0
56	MG	AA	1648	1/1	0.85	0.37	61,61,61,61	0
56	MG	BA	2923	1/1	0.85	0.38	85,85,85,85	0
56	MG	DA	3114	1/1	0.85	0.17	81,81,81,81	0
56	MG	DA	3522	1/1	0.85	0.07	77,77,77,77	0
56	MG	BA	3620	1/1	0.85	0.12	73,73,73,73	0
56	MG	DA	3530	1/1	0.85	0.08	70,70,70,70	0
56	MG	BA	3471	1/1	0.85	0.08	45,45,45,45	0
56	MG	DA	3122	1/1	0.85	0.11	67,67,67,67	0
56	MG	DA	3541	1/1	0.85	0.12	70,70,70,70	0
56	MG	DA	3542	1/1	0.85	0.41	70,70,70,70	0
56	MG	DA	3543	1/1	0.85	0.16	88,88,88,88	0
56	MG	BA	3243	1/1	0.85	0.15	149,149,149,149	0
56	MG	AA	1815	1/1	0.85	0.18	74,74,74,74	0
56	MG	CA	1882	1/1	0.85	0.24	81,81,81,81	0
56	MG	DA	2953	1/1	0.85	0.18	151,151,151,151	0
56	MG	DA	2955	1/1	0.85	0.16	30,30,30,30	0
56	MG	BA	3182	1/1	0.85	0.20	70,70,70,70	0
56	MG	CA	1648	1/1	0.85	0.30	155,155,155,155	0
56	MG	BA	3634	1/1	0.85	0.21	11,11,11,11	0
56	MG	AA	1816	1/1	0.85	0.11	69,69,69,69	0
56	MG	CA	1889	1/1	0.85	0.15	92,92,92,92	0
56	MG	DA	3251	1/1	0.85	0.11	32,32,32,32	0
56	MG	CA	1890	1/1	0.85	0.09	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BA	2963	1/1	0.85	0.13	63,63,63,63	0
56	MG	BA	3644	1/1	0.85	0.10	106,106,106,106	0
56	MG	CA	1720	1/1	0.85	0.20	84,84,84,84	0
56	MG	BA	3648	1/1	0.85	0.18	54,54,54,54	0
56	MG	DA	2991	1/1	0.85	0.28	80,80,80,80	0
56	MG	BA	3349	1/1	0.85	0.28	43,43,43,43	0
56	MG	AA	1909	1/1	0.85	0.08	65,65,65,65	0
56	MG	AA	1686	1/1	0.85	0.13	85,85,85,85	0
56	MG	DA	3340	1/1	0.85	0.18	67,67,67,67	0
56	MG	CA	1659	1/1	0.85	0.20	57,57,57,57	0
56	MG	DA	3003	1/1	0.85	0.08	59,59,59,59	0
56	MG	BB	222	1/1	0.85	0.09	206,206,206,206	0
56	MG	DA	3008	1/1	0.85	0.28	70,70,70,70	0
56	MG	AA	1618	1/1	0.85	0.10	104,104,104,104	0
56	MG	CA	1664	1/1	0.85	0.12	78,78,78,78	0
56	MG	DA	3359	1/1	0.85	0.22	57,57,57,57	0
56	MG	AA	1736	1/1	0.85	0.14	83,83,83,83	0
56	MG	CA	1822	1/1	0.85	0.09	112,112,112,112	0
56	MG	B0	102	1/1	0.85	0.20	68,68,68,68	0
56	MG	CA	1824	1/1	0.85	0.22	118,118,118,118	0
56	MG	BA	3370	1/1	0.85	0.14	50,50,50,50	0
56	MG	BA	3142	1/1	0.85	0.21	67,67,67,67	0
56	MG	CA	1917	1/1	0.85	0.17	123,123,123,123	0
56	MG	DA	2945	1/1	0.86	0.14	88,88,88,88	0
56	MG	AA	1910	1/1	0.86	0.30	68,68,68,68	0
56	MG	DA	2948	1/1	0.86	0.11	94,94,94,94	0
56	MG	DA	3434	1/1	0.86	0.12	61,61,61,61	0
56	MG	DA	3097	1/1	0.86	0.13	68,68,68,68	0
56	MG	DA	3437	1/1	0.86	0.13	59,59,59,59	0
56	MG	DA	3438	1/1	0.86	0.20	73,73,73,73	0
56	MG	BA	3072	1/1	0.86	0.10	88,88,88,88	0
56	MG	BA	3604	1/1	0.86	0.27	72,72,72,72	0
56	MG	BA	2974	1/1	0.86	0.10	85,85,85,85	0
56	MG	BA	3525	1/1	0.86	0.21	40,40,40,40	0
56	MG	DA	3451	1/1	0.86	0.24	56,56,56,56	0
56	MG	AA	1611	1/1	0.86	0.20	109,109,109,109	0
56	MG	BA	2977	1/1	0.86	0.11	72,72,72,72	0
56	MG	CA	1811	1/1	0.86	0.23	54,54,54,54	0
56	MG	BA	3133	1/1	0.86	0.14	48,48,48,48	0
56	MG	AW	106	1/1	0.86	0.04	87,87,87,87	0
56	MG	BA	2981	1/1	0.86	0.13	79,79,79,79	0
56	MG	BA	3200	1/1	0.86	0.23	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BA	3417	1/1	0.86	0.25	56,56,56,56	0
56	MG	BA	3422	1/1	0.86	0.26	42,42,42,42	0
56	MG	AA	1834	1/1	0.86	0.51	178,178,178,178	0
56	MG	BA	3202	1/1	0.86	0.07	205,205,205,205	0
56	MG	DA	3183	1/1	0.86	0.16	16,16,16,16	0
56	MG	DA	3187	1/1	0.86	0.11	32,32,32,32	0
56	MG	DA	3210	1/1	0.86	0.22	38,38,38,38	0
56	MG	CA	1908	1/1	0.86	0.13	84,84,84,84	0
56	MG	DA	2993	1/1	0.86	0.16	85,85,85,85	0
56	MG	DA	3495	1/1	0.86	0.09	63,63,63,63	0
56	MG	CA	1662	1/1	0.86	0.21	90,90,90,90	0
56	MG	AA	1920	1/1	0.86	0.09	71,71,71,71	0
56	MG	BA	3549	1/1	0.86	0.08	66,66,66,66	0
56	MG	AA	1962	1/1	0.86	0.12	55,55,55,55	0
56	MG	BA	3444	1/1	0.86	0.21	65,65,65,65	0
56	MG	CA	1836	1/1	0.86	0.17	94,94,94,94	0
56	MG	AA	1801	1/1	0.86	0.06	88,88,88,88	0
56	MG	CA	1840	1/1	0.86	0.15	101,101,101,101	0
56	MG	DA	3014	1/1	0.86	0.18	54,54,54,54	0
56	MG	DA	3524	1/1	0.86	0.10	67,67,67,67	0
56	MG	AA	1864	1/1	0.86	0.16	116,116,116,116	0
56	MG	DA	3527	1/1	0.86	0.06	77,77,77,77	0
56	MG	DA	3302	1/1	0.86	0.27	83,83,83,83	0
56	MG	BA	3454	1/1	0.86	0.25	60,60,60,60	0
56	MG	B8	101	1/1	0.86	0.12	38,38,38,38	0
56	MG	BA	3458	1/1	0.86	0.12	52,52,52,52	0
56	MG	BA	3564	1/1	0.86	0.20	28,28,28,28	0
56	MG	BA	3568	1/1	0.86	0.08	84,84,84,84	0
56	MG	AA	1819	1/1	0.86	0.30	84,84,84,84	0
56	MG	CA	1851	1/1	0.86	0.14	94,94,94,94	0
56	MG	DA	3036	1/1	0.86	0.11	80,80,80,80	0
56	MG	AA	1821	1/1	0.86	0.11	70,70,70,70	0
56	MG	DA	3039	1/1	0.86	0.31	72,72,72,72	0
56	MG	DA	3352	1/1	0.86	0.15	86,86,86,86	0
56	MG	DA	3575	1/1	0.86	0.08	49,49,49,49	0
56	MG	BA	2998	1/1	0.86	0.21	65,65,65,65	0
56	MG	AA	1784	1/1	0.86	0.09	72,72,72,72	0
56	MG	DA	3585	1/1	0.86	0.09	66,66,66,66	0
56	MG	DA	3358	1/1	0.86	0.08	141,141,141,141	0
56	MG	AA	1740	1/1	0.86	0.23	105,105,105,105	0
56	MG	AA	1762	1/1	0.86	0.12	95,95,95,95	0
56	MG	CA	1767	1/1	0.86	0.25	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BA	3580	1/1	0.86	0.08	60,60,60,60	0
56	MG	DA	2901	1/1	0.86	0.17	47,47,47,47	0
56	MG	AA	1673	1/1	0.86	0.13	104,104,104,104	0
56	MG	BA	3227	1/1	0.86	0.08	90,90,90,90	0
56	MG	BA	2964	1/1	0.86	0.06	74,74,74,74	0
56	MG	BA	3486	1/1	0.86	0.15	47,47,47,47	0
56	MG	BA	3012	1/1	0.86	0.18	91,91,91,91	0
56	MG	BA	3687	1/1	0.86	0.09	56,56,56,56	0
56	MG	BA	3064	1/1	0.86	0.12	63,63,63,63	0
56	MG	DA	3392	1/1	0.86	0.11	38,38,38,38	0
56	MG	DA	3395	1/1	0.86	0.20	95,95,95,95	0
56	MG	BA	3237	1/1	0.86	0.29	90,90,90,90	0
56	MG	AA	1828	1/1	0.86	0.07	97,97,97,97	0
56	MG	BA	3240	1/1	0.86	0.07	75,75,75,75	0
56	MG	CA	1702	1/1	0.86	0.17	75,75,75,75	0
56	MG	AA	1610	1/1	0.86	0.15	65,65,65,65	0
56	MG	BA	3242	1/1	0.86	0.17	63,63,63,63	0
56	MG	CA	1877	1/1	0.86	0.20	154,154,154,154	0
56	MG	BA	3596	1/1	0.86	0.40	140,140,140,140	0
56	MG	AA	1650	1/1	0.86	0.14	93,93,93,93	0
56	MG	CA	1709	1/1	0.86	0.15	61,61,61,61	0
56	MG	DA	3423	1/1	0.86	0.10	35,35,35,35	0
56	MG	BA	3180	1/1	0.86	0.21	113,113,113,113	0
56	MG	D0	101	1/1	0.86	0.12	42,42,42,42	0
56	MG	AA	1970	1/1	0.87	0.08	62,62,62,62	0
56	MG	AA	1683	1/1	0.87	0.07	249,249,249,249	0
56	MG	BA	3522	1/1	0.87	0.34	96,96,96,96	0
56	MG	DA	3383	1/1	0.87	0.16	51,51,51,51	0
56	MG	BA	3299	1/1	0.87	0.27	102,102,102,102	0
56	MG	BA	3097	1/1	0.87	0.21	73,73,73,73	0
56	MG	DA	3388	1/1	0.87	0.16	63,63,63,63	0
56	MG	DA	3017	1/1	0.87	0.15	60,60,60,60	0
56	MG	DA	3019	1/1	0.87	0.12	67,67,67,67	0
56	MG	AA	1698	1/1	0.87	0.10	97,97,97,97	0
56	MG	BA	3099	1/1	0.87	0.14	141,141,141,141	0
56	MG	BA	3198	1/1	0.87	0.13	66,66,66,66	0
56	MG	DA	3404	1/1	0.87	0.19	61,61,61,61	0
56	MG	AA	1765	1/1	0.87	0.09	74,74,74,74	0
56	MG	CA	1896	1/1	0.87	0.26	95,95,95,95	0
56	MG	AA	1857	1/1	0.87	0.26	45,45,45,45	0
56	MG	BA	3318	1/1	0.87	0.18	93,93,93,93	0
56	MG	BA	3536	1/1	0.87	0.22	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BA	3326	1/1	0.87	0.43	56,56,56,56	0
56	MG	BA	2910	1/1	0.87	0.11	79,79,79,79	0
56	MG	CA	1788	1/1	0.87	0.12	66,66,66,66	0
56	MG	DA	3424	1/1	0.87	0.21	52,52,52,52	0
56	MG	BA	3110	1/1	0.87	0.09	72,72,72,72	0
56	MG	BA	3343	1/1	0.87	0.13	73,73,73,73	0
56	MG	DA	3055	1/1	0.87	0.10	75,75,75,75	0
56	MG	BA	2971	1/1	0.87	0.19	89,89,89,89	0
56	MG	AA	1791	1/1	0.87	0.14	59,59,59,59	0
56	MG	AA	1924	1/1	0.87	0.30	55,55,55,55	0
56	MG	CA	1668	1/1	0.87	0.61	118,118,118,118	0
56	MG	CA	1797	1/1	0.87	0.27	61,61,61,61	0
56	MG	BA	3048	1/1	0.87	0.25	54,54,54,54	0
56	MG	AA	1859	1/1	0.87	0.13	177,177,177,177	0
56	MG	BA	3697	1/1	0.87	0.15	64,64,64,64	0
56	MG	BA	3367	1/1	0.87	0.28	84,84,84,84	0
56	MG	BA	3702	1/1	0.87	0.20	61,61,61,61	0
56	MG	AA	1987	1/1	0.87	0.12	121,121,121,121	0
56	MG	AA	1863	1/1	0.87	0.17	53,53,53,53	0
56	MG	BA	3563	1/1	0.87	0.32	83,83,83,83	0
56	MG	BA	3712	1/1	0.87	0.19	52,52,52,52	0
56	MG	BA	3125	1/1	0.87	0.10	106,106,106,106	0
56	MG	CW	102	1/1	0.87	0.22	105,105,105,105	0
56	MG	DA	3467	1/1	0.87	0.09	60,60,60,60	0
56	MG	BA	3373	1/1	0.87	0.24	39,39,39,39	0
56	MG	BA	3384	1/1	0.87	0.11	71,71,71,71	0
56	MG	CA	1815	1/1	0.87	0.16	80,80,80,80	0
56	MG	BA	3054	1/1	0.87	0.05	91,91,91,91	0
56	MG	BA	3127	1/1	0.87	0.23	102,102,102,102	0
56	MG	DA	3088	1/1	0.87	0.12	86,86,86,86	0
56	MG	AA	1835	1/1	0.87	0.29	76,76,76,76	0
56	MG	BA	3056	1/1	0.87	0.21	117,117,117,117	0
56	MG	CM	201	1/1	0.87	0.36	84,84,84,84	0
56	MG	AA	1991	1/1	0.87	0.10	96,96,96,96	0
56	MG	DA	3494	1/1	0.87	0.53	112,112,112,112	0
56	MG	AA	1992	1/1	0.87	0.32	84,84,84,84	0
56	MG	BA	3421	1/1	0.87	0.09	79,79,79,79	0
56	MG	AA	1935	1/1	0.87	0.10	39,39,39,39	0
56	MG	DA	2909	1/1	0.87	0.15	85,85,85,85	0
56	MG	BA	2989	1/1	0.87	0.40	84,84,84,84	0
56	MG	AA	1868	1/1	0.87	0.08	49,49,49,49	0
56	MG	BA	3140	1/1	0.87	0.14	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	CA	1833	1/1	0.87	0.14	65,65,65,65	0
56	MG	BA	3437	1/1	0.87	0.16	82,82,82,82	0
56	MG	BB	214	1/1	0.87	0.15	68,68,68,68	0
56	MG	DA	2918	1/1	0.87	0.13	49,49,49,49	0
56	MG	BA	2992	1/1	0.87	0.20	73,73,73,73	0
56	MG	AA	1621	1/1	0.87	0.08	74,74,74,74	0
56	MG	DA	3528	1/1	0.87	0.09	54,54,54,54	0
56	MG	BA	3446	1/1	0.87	0.11	93,93,93,93	0
56	MG	DA	3128	1/1	0.87	0.10	101,101,101,101	0
56	MG	BA	3244	1/1	0.87	0.47	67,67,67,67	0
56	MG	DA	3539	1/1	0.87	0.09	98,98,98,98	0
56	MG	AA	1685	1/1	0.87	0.11	199,199,199,199	0
56	MG	AA	1658	1/1	0.87	0.05	76,76,76,76	0
56	MG	BA	3455	1/1	0.87	0.10	64,64,64,64	0
56	MG	CA	1847	1/1	0.87	0.12	84,84,84,84	0
56	MG	BA	3599	1/1	0.87	0.19	93,93,93,93	0
56	MG	BA	3152	1/1	0.87	0.09	72,72,72,72	0
56	MG	DA	3239	1/1	0.87	0.22	43,43,43,43	0
56	MG	AA	1891	1/1	0.87	0.08	67,67,67,67	0
56	MG	AA	1798	1/1	0.87	0.07	47,47,47,47	0
56	MG	BA	3073	1/1	0.87	0.32	124,124,124,124	0
56	MG	AW	111	1/1	0.87	0.09	91,91,91,91	0
56	MG	DA	3578	1/1	0.87	0.18	57,57,57,57	0
56	MG	BA	3261	1/1	0.87	0.33	89,89,89,89	0
56	MG	DA	3582	1/1	0.87	0.15	95,95,95,95	0
56	MG	AA	1894	1/1	0.87	0.47	124,124,124,124	0
56	MG	BA	3079	1/1	0.87	0.22	48,48,48,48	0
56	MG	BA	3472	1/1	0.87	0.28	56,56,56,56	0
56	MG	BA	3612	1/1	0.87	0.18	96,96,96,96	0
56	MG	DA	3288	1/1	0.87	0.15	57,57,57,57	0
56	MG	DA	3604	1/1	0.87	0.16	58,58,58,58	0
56	MG	DA	2963	1/1	0.87	0.17	62,62,62,62	0
56	MG	DA	3610	1/1	0.87	0.13	56,56,56,56	0
56	MG	BA	3473	1/1	0.87	0.26	70,70,70,70	0
56	MG	DA	3618	1/1	0.87	0.11	69,69,69,69	0
56	MG	BA	2938	1/1	0.87	0.19	81,81,81,81	0
56	MG	DA	3627	1/1	0.87	0.22	81,81,81,81	0
56	MG	BA	3170	1/1	0.87	0.14	60,60,60,60	0
56	MG	AA	1895	1/1	0.87	0.09	33,33,33,33	0
56	MG	AA	1775	1/1	0.87	0.22	66,66,66,66	0
56	MG	AA	1667	1/1	0.87	0.17	53,53,53,53	0
56	MG	DA	3342	1/1	0.87	0.20	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BA	3279	1/1	0.87	0.08	80,80,80,80	0
56	MG	AA	1689	1/1	0.87	0.07	169,169,169,169	0
56	MG	BA	3497	1/1	0.87	0.05	78,78,78,78	0
56	MG	DA	2988	1/1	0.87	0.16	85,85,85,85	0
56	MG	AA	1958	1/1	0.87	0.25	72,72,72,72	0
56	MG	BA	3629	1/1	0.87	0.34	129,129,129,129	0
56	MG	DA	2995	1/1	0.87	0.13	65,65,65,65	0
56	MG	CA	1638	1/1	0.87	0.08	118,118,118,118	0
56	MG	AA	1761	1/1	0.87	0.31	118,118,118,118	0
56	MG	AA	1630	1/1	0.87	0.18	55,55,55,55	0
56	MG	DA	3364	1/1	0.87	0.20	80,80,80,80	0
56	MG	AA	1968	1/1	0.87	0.46	86,86,86,86	0
56	MG	DA	3002	1/1	0.87	0.29	139,139,139,139	0
56	MG	BA	3641	1/1	0.87	0.26	60,60,60,60	0
56	MG	BA	3028	1/1	0.87	0.20	70,70,70,70	0
56	MG	DA	3007	1/1	0.87	0.20	70,70,70,70	0
56	MG	AY	403	1/1	0.88	0.33	87,87,87,87	0
56	MG	CA	1798	1/1	0.88	0.15	79,79,79,79	0
56	MG	AA	1929	1/1	0.88	0.06	79,79,79,79	0
56	MG	BA	3183	1/1	0.88	0.19	79,79,79,79	0
56	MG	BA	3666	1/1	0.88	0.14	67,67,67,67	0
56	MG	BA	3668	1/1	0.88	0.18	71,71,71,71	0
56	MG	BA	3335	1/1	0.88	0.30	49,49,49,49	0
56	MG	AA	1797	1/1	0.88	0.11	60,60,60,60	0
56	MG	AA	1802	1/1	0.88	0.23	55,55,55,55	0
56	MG	DA	2977	1/1	0.88	0.15	84,84,84,84	0
56	MG	DA	3121	1/1	0.88	0.06	41,41,41,41	0
56	MG	BA	3490	1/1	0.88	0.17	45,45,45,45	0
56	MG	BA	3190	1/1	0.88	0.11	49,49,49,49	0
56	MG	CA	1901	1/1	0.88	0.13	54,54,54,54	0
56	MG	DA	3458	1/1	0.88	0.08	64,64,64,64	0
56	MG	DA	3459	1/1	0.88	0.21	76,76,76,76	0
56	MG	AA	1867	1/1	0.88	0.28	96,96,96,96	0
56	MG	BA	2965	1/1	0.88	0.37	167,167,167,167	0
56	MG	DA	3180	1/1	0.88	0.22	37,37,37,37	0
56	MG	BA	3249	1/1	0.88	0.08	84,84,84,84	0
56	MG	BA	3086	1/1	0.88	0.19	64,64,64,64	0
56	MG	DA	3473	1/1	0.88	0.09	51,51,51,51	0
56	MG	DA	3206	1/1	0.88	0.20	23,23,23,23	0
56	MG	CA	1636	1/1	0.88	0.27	56,56,56,56	0
56	MG	CA	1715	1/1	0.88	0.21	79,79,79,79	0
56	MG	CA	1637	1/1	0.88	0.15	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	DA	3229	1/1	0.88	0.25	37,37,37,37	0
56	MG	DA	3000	1/1	0.88	0.09	68,68,68,68	0
56	MG	DA	3488	1/1	0.88	0.08	70,70,70,70	0
56	MG	BA	3195	1/1	0.88	0.11	97,97,97,97	0
56	MG	AA	1813	1/1	0.88	0.13	134,134,134,134	0
56	MG	AW	101	1/1	0.88	0.14	105,105,105,105	0
56	MG	AA	1904	1/1	0.88	0.15	43,43,43,43	0
56	MG	BA	3379	1/1	0.88	0.09	23,23,23,23	0
56	MG	DA	3497	1/1	0.88	0.19	61,61,61,61	0
56	MG	BA	3515	1/1	0.88	0.25	58,58,58,58	0
56	MG	BA	2902	1/1	0.88	0.07	86,86,86,86	0
56	MG	DA	3011	1/1	0.88	0.15	47,47,47,47	0
56	MG	BA	3008	1/1	0.88	0.09	66,66,66,66	0
56	MG	DA	3286	1/1	0.88	0.12	42,42,42,42	0
56	MG	CA	1730	1/1	0.88	0.08	80,80,80,80	0
56	MG	BA	3266	1/1	0.88	0.19	73,73,73,73	0
56	MG	DA	3519	1/1	0.88	0.34	78,78,78,78	0
56	MG	DA	3293	1/1	0.88	0.19	58,58,58,58	0
56	MG	AA	1852	1/1	0.88	0.23	89,89,89,89	0
56	MG	DA	3018	1/1	0.88	0.08	83,83,83,83	0
56	MG	AA	1872	1/1	0.88	0.28	67,67,67,67	0
56	MG	CA	1839	1/1	0.88	0.09	38,38,38,38	0
56	MG	DA	3326	1/1	0.88	0.18	47,47,47,47	0
56	MG	DA	3329	1/1	0.88	0.14	46,46,46,46	0
56	MG	DA	3336	1/1	0.88	0.12	51,51,51,51	0
56	MG	BA	2975	1/1	0.88	0.12	77,77,77,77	0
56	MG	AA	1814	1/1	0.88	0.18	58,58,58,58	0
56	MG	AA	1803	1/1	0.88	0.10	77,77,77,77	0
56	MG	AA	1674	1/1	0.88	0.18	126,126,126,126	0
56	MG	DA	3343	1/1	0.88	0.15	76,76,76,76	0
56	MG	BA	3424	1/1	0.88	0.07	32,32,32,32	0
56	MG	BA	2979	1/1	0.88	0.23	77,77,77,77	0
56	MG	BA	3024	1/1	0.88	0.13	65,65,65,65	0
56	MG	BB	204	1/1	0.88	0.06	53,53,53,53	0
56	MG	CA	1849	1/1	0.88	0.05	75,75,75,75	0
56	MG	DA	3568	1/1	0.88	0.21	65,65,65,65	0
56	MG	DA	3353	1/1	0.88	0.07	66,66,66,66	0
56	MG	BA	3027	1/1	0.88	0.16	85,85,85,85	0
56	MG	AW	112	1/1	0.88	0.26	82,82,82,82	0
56	MG	BB	209	1/1	0.88	0.08	91,91,91,91	0
56	MG	DA	2905	1/1	0.88	0.16	87,87,87,87	0
56	MG	BB	210	1/1	0.88	0.08	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BA	3438	1/1	0.88	0.29	49,49,49,49	0
56	MG	CA	1666	1/1	0.88	0.10	73,73,73,73	0
56	MG	BA	3441	1/1	0.88	0.18	56,56,56,56	0
56	MG	BA	3220	1/1	0.88	0.19	58,58,58,58	0
56	MG	BA	3166	1/1	0.88	0.14	70,70,70,70	0
56	MG	BA	3293	1/1	0.88	0.06	62,62,62,62	0
56	MG	DA	3065	1/1	0.88	0.09	88,88,88,88	0
56	MG	CA	1766	1/1	0.88	0.18	49,49,49,49	0
56	MG	BA	3294	1/1	0.88	0.23	75,75,75,75	0
56	MG	DA	3614	1/1	0.88	0.16	50,50,50,50	0
56	MG	BA	3116	1/1	0.88	0.06	87,87,87,87	0
56	MG	BB	218	1/1	0.88	0.25	50,50,50,50	0
56	MG	BA	3559	1/1	0.88	0.16	76,76,76,76	0
56	MG	BA	3225	1/1	0.88	0.25	96,96,96,96	0
56	MG	DA	3389	1/1	0.88	0.19	68,68,68,68	0
56	MG	DA	3390	1/1	0.88	0.26	53,53,53,53	0
56	MG	DA	2934	1/1	0.88	0.08	76,76,76,76	0
56	MG	DA	3393	1/1	0.88	0.09	95,95,95,95	0
56	MG	BA	2985	1/1	0.88	0.12	61,61,61,61	0
56	MG	DA	3076	1/1	0.88	0.20	88,88,88,88	0
56	MG	BX	102	1/1	0.88	0.16	50,50,50,50	0
56	MG	BA	3228	1/1	0.88	0.07	83,83,83,83	0
56	MG	CA	1784	1/1	0.88	0.11	96,96,96,96	0
56	MG	BA	3229	1/1	0.88	0.20	92,92,92,92	0
56	MG	BA	3651	1/1	0.88	0.23	92,92,92,92	0
56	MG	AA	1743	1/1	0.88	0.09	81,81,81,81	0
56	MG	BA	3307	1/1	0.88	0.10	83,83,83,83	0
56	MG	DA	3090	1/1	0.88	0.08	47,47,47,47	0
56	MG	AA	1954	1/1	0.88	0.30	142,142,142,142	0
56	MG	AA	1830	1/1	0.88	0.14	179,179,179,179	0
56	MG	DA	3094	1/1	0.88	0.13	30,30,30,30	0
56	MG	BA	3122	1/1	0.88	0.10	89,89,89,89	0
56	MG	CA	1609	1/1	0.88	0.20	100,100,100,100	0
56	MG	AA	1665	1/1	0.88	0.08	59,59,59,59	0
56	MG	D5	102	1/1	0.88	0.08	68,68,68,68	0
56	MG	CA	1796	1/1	0.89	0.06	41,41,41,41	0
56	MG	BA	2951	1/1	0.89	0.07	50,50,50,50	0
56	MG	AA	1759	1/1	0.89	0.24	88,88,88,88	0
56	MG	BA	2953	1/1	0.89	0.09	56,56,56,56	0
56	MG	DA	3115	1/1	0.89	0.08	60,60,60,60	0
56	MG	DA	3436	1/1	0.89	0.05	68,68,68,68	0
56	MG	BA	3574	1/1	0.89	0.12	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	AA	1876	1/1	0.89	0.10	123,123,123,123	0
56	MG	BA	3038	1/1	0.89	0.16	58,58,58,58	0
56	MG	DA	2980	1/1	0.89	0.18	57,57,57,57	0
56	MG	CA	1617	1/1	0.89	0.13	69,69,69,69	0
56	MG	AA	1879	1/1	0.89	0.16	99,99,99,99	0
56	MG	BA	3670	1/1	0.89	0.21	79,79,79,79	0
56	MG	DA	3130	1/1	0.89	0.25	69,69,69,69	0
56	MG	AA	1919	1/1	0.89	0.20	47,47,47,47	0
56	MG	CA	1903	1/1	0.89	0.10	73,73,73,73	0
56	MG	BA	3481	1/1	0.89	0.14	59,59,59,59	0
56	MG	BA	3351	1/1	0.89	0.26	29,29,29,29	0
56	MG	DA	3200	1/1	0.89	0.16	52,52,52,52	0
56	MG	BA	3682	1/1	0.89	0.08	64,64,64,64	0
56	MG	BA	3041	1/1	0.89	0.26	68,68,68,68	0
56	MG	CA	1813	1/1	0.89	0.17	99,99,99,99	0
56	MG	BA	3253	1/1	0.89	0.15	73,73,73,73	0
56	MG	DA	3471	1/1	0.89	0.24	55,55,55,55	0
56	MG	BA	2994	1/1	0.89	0.29	71,71,71,71	0
56	MG	CA	1714	1/1	0.89	0.06	104,104,104,104	0
56	MG	BA	2960	1/1	0.89	0.31	74,74,74,74	0
56	MG	CA	1635	1/1	0.89	0.07	119,119,119,119	0
56	MG	DA	3482	1/1	0.89	0.12	50,50,50,50	0
56	MG	BA	3493	1/1	0.89	0.16	61,61,61,61	0
56	MG	DA	3009	1/1	0.89	0.35	130,130,130,130	0
56	MG	BA	2961	1/1	0.89	0.12	83,83,83,83	0
56	MG	AA	1889	1/1	0.89	0.12	81,81,81,81	0
56	MG	DA	3489	1/1	0.89	0.30	51,51,51,51	0
56	MG	DA	3253	1/1	0.89	0.19	30,30,30,30	0
56	MG	DA	3257	1/1	0.89	0.29	90,90,90,90	0
56	MG	DA	3263	1/1	0.89	0.32	61,61,61,61	0
56	MG	DA	3274	1/1	0.89	0.25	45,45,45,45	0
56	MG	DA	3012	1/1	0.89	0.36	102,102,102,102	0
56	MG	AA	1612	1/1	0.89	0.15	87,87,87,87	0
56	MG	DA	3280	1/1	0.89	0.16	59,59,59,59	0
56	MG	BA	3595	1/1	0.89	0.08	39,39,39,39	0
56	MG	BA	3146	1/1	0.89	0.22	57,57,57,57	0
56	MG	BA	3377	1/1	0.89	0.26	56,56,56,56	0
56	MG	BA	3598	1/1	0.89	0.20	62,62,62,62	0
56	MG	BA	3710	1/1	0.89	0.22	81,81,81,81	0
56	MG	DA	3294	1/1	0.89	0.26	64,64,64,64	0
56	MG	DA	3511	1/1	0.89	0.17	64,64,64,64	0
56	MG	DA	3298	1/1	0.89	0.20	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	DA	3520	1/1	0.89	0.21	93,93,93,93	0
56	MG	CW	101	1/1	0.89	0.16	96,96,96,96	0
56	MG	BA	2929	1/1	0.89	0.22	64,64,64,64	0
56	MG	AA	1705	1/1	0.89	0.34	101,101,101,101	0
56	MG	DA	3028	1/1	0.89	0.08	55,55,55,55	0
56	MG	DA	3029	1/1	0.89	0.06	73,73,73,73	0
56	MG	CA	1838	1/1	0.89	0.16	66,66,66,66	0
56	MG	BA	3388	1/1	0.89	0.20	22,22,22,22	0
56	MG	DA	3034	1/1	0.89	0.13	49,49,49,49	0
56	MG	BA	3269	1/1	0.89	0.08	66,66,66,66	0
56	MG	DA	3537	1/1	0.89	0.14	62,62,62,62	0
56	MG	BA	3391	1/1	0.89	0.18	78,78,78,78	0
56	MG	BA	3149	1/1	0.89	0.10	44,44,44,44	0
56	MG	AA	1790	1/1	0.89	0.09	53,53,53,53	0
56	MG	AA	1664	1/1	0.89	0.06	64,64,64,64	0
56	MG	BA	3007	1/1	0.89	0.17	170,170,170,170	0
56	MG	DA	3349	1/1	0.89	0.14	56,56,56,56	0
56	MG	BA	3415	1/1	0.89	0.09	47,47,47,47	0
56	MG	BA	3156	1/1	0.89	0.12	74,74,74,74	0
56	MG	BA	3217	1/1	0.89	0.20	65,65,65,65	0
56	MG	AA	1843	1/1	0.89	0.14	124,124,124,124	0
56	MG	DA	2907	1/1	0.89	0.04	75,75,75,75	0
56	MG	BA	2903	1/1	0.89	0.16	83,83,83,83	0
56	MG	BA	3430	1/1	0.89	0.09	47,47,47,47	0
56	MG	BA	3061	1/1	0.89	0.23	61,61,61,61	0
56	MG	AA	1708	1/1	0.89	0.11	103,103,103,103	0
56	MG	BA	3621	1/1	0.89	0.48	106,106,106,106	0
56	MG	AA	1681	1/1	0.89	0.10	68,68,68,68	0
56	MG	BA	3223	1/1	0.89	0.15	58,58,58,58	0
56	MG	BA	3626	1/1	0.89	0.19	62,62,62,62	0
56	MG	BA	3224	1/1	0.89	0.64	85,85,85,85	0
56	MG	DA	3592	1/1	0.89	0.05	73,73,73,73	0
56	MG	DA	2922	1/1	0.89	0.07	47,47,47,47	0
56	MG	BA	3113	1/1	0.89	0.13	109,109,109,109	0
56	MG	DA	3376	1/1	0.89	0.23	43,43,43,43	0
56	MG	DA	3378	1/1	0.89	0.18	54,54,54,54	0
56	MG	CA	1771	1/1	0.89	0.09	70,70,70,70	0
56	MG	DA	3381	1/1	0.89	0.21	43,43,43,43	0
56	MG	BA	3169	1/1	0.89	0.08	64,64,64,64	0
56	MG	AA	1899	1/1	0.89	0.06	89,89,89,89	0
56	MG	BA	3552	1/1	0.89	0.12	29,29,29,29	0
56	MG	BA	3172	1/1	0.89	0.09	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	AA	1632	1/1	0.89	0.20	87,87,87,87	0
56	MG	CA	1678	1/1	0.89	0.45	128,128,128,128	0
56	MG	CA	1781	1/1	0.89	0.06	59,59,59,59	0
56	MG	DA	3083	1/1	0.89	0.15	125,125,125,125	0
56	MG	CA	1782	1/1	0.89	0.19	56,56,56,56	0
56	MG	BA	3450	1/1	0.89	0.12	83,83,83,83	0
56	MG	BY	201	1/1	0.89	0.08	30,30,30,30	0
56	MG	AA	1832	1/1	0.89	0.08	67,67,67,67	0
56	MG	BA	3649	1/1	0.89	0.23	104,104,104,104	0
56	MG	DA	2950	1/1	0.89	0.09	61,61,61,61	0
56	MG	AA	1820	1/1	0.89	0.18	166,166,166,166	0
56	MG	DA	3407	1/1	0.89	0.06	62,62,62,62	0
56	MG	DB	215	1/1	0.89	0.12	79,79,79,79	0
56	MG	BA	2946	1/1	0.89	0.18	61,61,61,61	0
56	MG	DA	3096	1/1	0.89	0.34	82,82,82,82	0
56	MG	AA	1908	1/1	0.89	0.12	56,56,56,56	0
56	MG	BA	2982	1/1	0.89	0.22	86,86,86,86	0
56	MG	DA	3102	1/1	0.89	0.60	126,126,126,126	0
56	MG	DA	2957	1/1	0.89	0.08	64,64,64,64	0
56	MG	AA	1766	1/1	0.89	0.09	77,77,77,77	0
56	MG	CA	1690	1/1	0.89	0.14	69,69,69,69	0
56	MG	BA	3323	1/1	0.89	0.25	47,47,47,47	0
56	MG	DA	3175	1/1	0.90	0.16	38,38,38,38	0
56	MG	DA	3178	1/1	0.90	0.16	40,40,40,40	0
56	MG	AA	1729	1/1	0.90	0.26	99,99,99,99	0
56	MG	AA	1636	1/1	0.90	0.08	97,97,97,97	0
56	MG	CA	1827	1/1	0.90	0.06	45,45,45,45	0
56	MG	DA	3439	1/1	0.90	0.12	66,66,66,66	0
56	MG	CA	1924	1/1	0.90	0.11	73,73,73,73	0
56	MG	BA	3303	1/1	0.90	0.12	69,69,69,69	0
56	MG	DA	3207	1/1	0.90	0.24	41,41,41,41	0
56	MG	AA	1687	1/1	0.90	0.08	85,85,85,85	0
56	MG	BA	3305	1/1	0.90	0.20	62,62,62,62	0
56	MG	AA	1971	1/1	0.90	0.12	60,60,60,60	0
56	MG	DA	3454	1/1	0.90	0.09	62,62,62,62	0
56	MG	DA	3224	1/1	0.90	0.17	40,40,40,40	0
56	MG	DA	3228	1/1	0.90	0.23	31,31,31,31	0
56	MG	BA	3046	1/1	0.90	0.19	126,126,126,126	0
56	MG	DA	3232	1/1	0.90	0.22	48,48,48,48	0
56	MG	AA	1782	1/1	0.90	0.11	77,77,77,77	0
56	MG	AA	1663	1/1	0.90	0.20	44,44,44,44	0
56	MG	DA	3241	1/1	0.90	0.15	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	DA	3243	1/1	0.90	0.22	77,77,77,77	0
56	MG	AA	1860	1/1	0.90	0.08	62,62,62,62	0
56	MG	BA	3094	1/1	0.90	0.23	38,38,38,38	0
56	MG	BA	2967	1/1	0.90	0.32	77,77,77,77	0
56	MG	CW	113	1/1	0.90	0.21	89,89,89,89	0
56	MG	BA	3328	1/1	0.90	0.31	35,35,35,35	0
56	MG	AA	1649	1/1	0.90	0.19	110,110,110,110	0
56	MG	AA	1644	1/1	0.90	0.07	57,57,57,57	0
56	MG	DA	3030	1/1	0.90	0.38	78,78,78,78	0
56	MG	DA	3031	1/1	0.90	0.12	77,77,77,77	0
56	MG	AA	1805	1/1	0.90	0.12	71,71,71,71	0
56	MG	AA	1985	1/1	0.90	0.27	108,108,108,108	0
56	MG	BA	3259	1/1	0.90	0.15	77,77,77,77	0
56	MG	BA	3463	1/1	0.90	0.20	106,106,106,106	0
56	MG	DA	3285	1/1	0.90	0.10	63,63,63,63	0
56	MG	BA	3260	1/1	0.90	0.25	109,109,109,109	0
56	MG	DA	3037	1/1	0.90	0.30	77,77,77,77	0
56	MG	BB	220	1/1	0.90	0.09	123,123,123,123	0
56	MG	DA	3289	1/1	0.90	0.13	45,45,45,45	0
56	MG	DA	3290	1/1	0.90	0.14	38,38,38,38	0
56	MG	DA	3500	1/1	0.90	0.29	72,72,72,72	0
56	MG	DA	3292	1/1	0.90	0.07	34,34,34,34	0
56	MG	CA	1756	1/1	0.90	0.10	60,60,60,60	0
56	MG	DA	2908	1/1	0.90	0.17	60,60,60,60	0
56	MG	CA	1758	1/1	0.90	0.17	40,40,40,40	0
56	MG	AA	1806	1/1	0.90	0.18	111,111,111,111	0
56	MG	DA	3049	1/1	0.90	0.09	52,52,52,52	0
56	MG	DA	3318	1/1	0.90	0.18	42,42,42,42	0
56	MG	CA	1764	1/1	0.90	0.20	50,50,50,50	0
56	MG	DA	3321	1/1	0.90	0.19	66,66,66,66	0
56	MG	DA	2912	1/1	0.90	0.06	78,78,78,78	0
56	MG	BA	3354	1/1	0.90	0.16	38,38,38,38	0
56	MG	DA	3523	1/1	0.90	0.25	76,76,76,76	0
56	MG	DA	3327	1/1	0.90	0.11	58,58,58,58	0
56	MG	BA	3103	1/1	0.90	0.43	89,89,89,89	0
56	MG	CA	1770	1/1	0.90	0.24	39,39,39,39	0
56	MG	AA	1703	1/1	0.90	0.11	64,64,64,64	0
56	MG	DA	3061	1/1	0.90	0.14	62,62,62,62	0
56	MG	AA	1947	1/1	0.90	0.29	89,89,89,89	0
56	MG	BA	3214	1/1	0.90	0.07	85,85,85,85	0
56	MG	DA	3533	1/1	0.90	0.08	71,71,71,71	0
56	MG	CA	1774	1/1	0.90	0.12	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	DA	3538	1/1	0.90	0.09	70,70,70,70	0
56	MG	BA	3474	1/1	0.90	0.22	44,44,44,44	0
56	MG	AA	1905	1/1	0.90	0.11	59,59,59,59	0
56	MG	AA	1907	1/1	0.90	0.31	45,45,45,45	0
56	MG	CA	1779	1/1	0.90	0.20	72,72,72,72	0
56	MG	BA	3112	1/1	0.90	0.07	83,83,83,83	0
56	MG	BA	3579	1/1	0.90	0.21	65,65,65,65	0
56	MG	AA	1756	1/1	0.90	0.07	87,87,87,87	0
56	MG	DA	3548	1/1	0.90	0.25	85,85,85,85	0
56	MG	AA	1695	1/1	0.90	0.13	71,71,71,71	0
56	MG	CA	1608	1/1	0.90	0.10	86,86,86,86	0
56	MG	BA	2980	1/1	0.90	0.08	74,74,74,74	0
56	MG	BA	3380	1/1	0.90	0.15	49,49,49,49	0
56	MG	BA	3669	1/1	0.90	0.23	53,53,53,53	0
56	MG	CA	1692	1/1	0.90	0.25	62,62,62,62	0
56	MG	DA	3577	1/1	0.90	0.16	80,80,80,80	0
56	MG	BA	3492	1/1	0.90	0.25	102,102,102,102	0
56	MG	AA	1727	1/1	0.90	0.21	93,93,93,93	0
56	MG	DA	3581	1/1	0.90	0.13	69,69,69,69	0
56	MG	BA	3283	1/1	0.90	0.08	67,67,67,67	0
56	MG	DA	3583	1/1	0.90	0.12	68,68,68,68	0
56	MG	AA	1911	1/1	0.90	0.06	38,38,38,38	0
56	MG	BA	3675	1/1	0.90	0.34	145,145,145,145	0
56	MG	BA	3676	1/1	0.90	0.37	181,181,181,181	0
56	MG	DA	3590	1/1	0.90	0.24	74,74,74,74	0
56	MG	BA	2983	1/1	0.90	0.13	44,44,44,44	0
56	MG	BA	3392	1/1	0.90	0.22	63,63,63,63	0
56	MG	BA	2909	1/1	0.90	0.24	114,114,114,114	0
56	MG	CA	1894	1/1	0.90	0.14	89,89,89,89	0
56	MG	BA	3395	1/1	0.90	0.16	107,107,107,107	0
56	MG	BA	3594	1/1	0.90	0.09	88,88,88,88	0
56	MG	CA	1629	1/1	0.90	0.09	93,93,93,93	0
56	MG	DA	3385	1/1	0.90	0.13	77,77,77,77	0
56	MG	BA	3033	1/1	0.90	0.21	78,78,78,78	0
56	MG	DA	3625	1/1	0.90	0.06	82,82,82,82	0
56	MG	BA	3508	1/1	0.90	0.19	67,67,67,67	0
56	MG	BA	3077	1/1	0.90	0.06	50,50,50,50	0
56	MG	BA	3511	1/1	0.90	0.17	91,91,91,91	0
56	MG	BA	3512	1/1	0.90	0.09	42,42,42,42	0
56	MG	AW	102	1/1	0.90	0.07	94,94,94,94	0
56	MG	DA	2984	1/1	0.90	0.10	34,34,34,34	0
56	MG	CA	1905	1/1	0.90	0.12	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	DA	3113	1/1	0.90	0.11	110,110,110,110	0
56	MG	BA	3601	1/1	0.90	0.11	50,50,50,50	0
56	MG	BA	3412	1/1	0.90	0.37	58,58,58,58	0
56	MG	BA	3517	1/1	0.90	0.24	55,55,55,55	0
56	MG	DA	3118	1/1	0.90	0.07	61,61,61,61	0
56	MG	AA	1878	1/1	0.90	0.07	56,56,56,56	0
56	MG	DB	212	1/1	0.90	0.10	84,84,84,84	0
56	MG	CA	1722	1/1	0.90	0.20	168,168,168,168	0
56	MG	DA	3412	1/1	0.90	0.12	60,60,60,60	0
56	MG	BA	3296	1/1	0.90	0.24	59,59,59,59	0
56	MG	AA	1776	1/1	0.90	0.22	146,146,146,146	0
56	MG	CA	1726	1/1	0.90	0.14	80,80,80,80	0
56	MG	AA	1886	1/1	0.90	0.20	65,65,65,65	0
56	MG	BA	3716	1/1	0.90	0.07	80,80,80,80	0
56	MG	DN	201	1/1	0.90	0.12	56,56,56,56	0
56	MG	DA	3132	1/1	0.90	0.32	13,13,13,13	0
56	MG	DQ	202	1/1	0.90	0.17	31,31,31,31	0
56	MG	AA	1623	1/1	0.90	0.04	84,84,84,84	0
56	MG	DA	3159	1/1	0.90	0.16	62,62,62,62	0
56	MG	DA	3161	1/1	0.90	0.10	10,10,10,10	0
56	MG	DA	3165	1/1	0.90	0.23	25,25,25,25	0
56	MG	DA	3182	1/1	0.91	0.14	24,24,24,24	0
56	MG	DA	3431	1/1	0.91	0.06	74,74,74,74	0
56	MG	BA	3582	1/1	0.91	0.23	72,72,72,72	0
56	MG	DA	3006	1/1	0.91	0.15	66,66,66,66	0
56	MG	AA	1661	1/1	0.91	0.12	58,58,58,58	0
56	MG	CA	1723	1/1	0.91	0.06	76,76,76,76	0
56	MG	AA	1719	1/1	0.91	0.05	92,92,92,92	0
56	MG	BA	3489	1/1	0.91	0.16	54,54,54,54	0
56	MG	BA	3053	1/1	0.91	0.31	95,95,95,95	0
56	MG	DA	3440	1/1	0.91	0.10	58,58,58,58	0
56	MG	DA	3212	1/1	0.91	0.17	42,42,42,42	0
56	MG	BA	3087	1/1	0.91	0.11	82,82,82,82	0
56	MG	DA	3223	1/1	0.91	0.04	75,75,75,75	0
56	MG	BA	3389	1/1	0.91	0.15	47,47,47,47	0
56	MG	AA	1646	1/1	0.91	0.14	73,73,73,73	0
56	MG	DA	3452	1/1	0.91	0.13	73,73,73,73	0
56	MG	BA	3090	1/1	0.91	0.15	60,60,60,60	0
56	MG	CA	1830	1/1	0.91	0.12	80,80,80,80	0
56	MG	DA	3235	1/1	0.91	0.25	41,41,41,41	0
56	MG	DA	3237	1/1	0.91	0.22	42,42,42,42	0
56	MG	BA	3231	1/1	0.91	0.12	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BA	3700	1/1	0.91	0.09	60,60,60,60	0
56	MG	BA	2925	1/1	0.91	0.09	76,76,76,76	0
56	MG	CW	106	1/1	0.91	0.08	59,59,59,59	0
56	MG	BA	2927	1/1	0.91	0.07	82,82,82,82	0
56	MG	DA	3247	1/1	0.91	0.19	55,55,55,55	0
56	MG	BA	3186	1/1	0.91	0.17	98,98,98,98	0
56	MG	AA	1874	1/1	0.91	0.13	59,59,59,59	0
56	MG	BA	3504	1/1	0.91	0.07	39,39,39,39	0
56	MG	BA	3505	1/1	0.91	0.43	101,101,101,101	0
56	MG	DA	3252	1/1	0.91	0.05	42,42,42,42	0
56	MG	AA	1768	1/1	0.91	0.20	183,183,183,183	0
56	MG	BA	3405	1/1	0.91	0.18	64,64,64,64	0
56	MG	DA	3258	1/1	0.91	0.17	58,58,58,58	0
56	MG	BA	3509	1/1	0.91	0.08	75,75,75,75	0
56	MG	DA	3266	1/1	0.91	0.20	64,64,64,64	0
56	MG	BA	3407	1/1	0.91	0.22	78,78,78,78	0
56	MG	AA	1913	1/1	0.91	0.20	35,35,35,35	0
56	MG	CA	1846	1/1	0.91	0.25	101,101,101,101	0
56	MG	DA	3279	1/1	0.91	0.21	29,29,29,29	0
56	MG	DA	2904	1/1	0.91	0.40	71,71,71,71	0
56	MG	BA	2986	1/1	0.91	0.07	45,45,45,45	0
56	MG	AA	1691	1/1	0.91	0.07	84,84,84,84	0
56	MG	DA	3042	1/1	0.91	0.28	50,50,50,50	0
56	MG	BA	3418	1/1	0.91	0.18	27,27,27,27	0
56	MG	BA	3420	1/1	0.91	0.20	34,34,34,34	0
56	MG	DA	3047	1/1	0.91	0.37	69,69,69,69	0
56	MG	CA	1749	1/1	0.91	0.08	64,64,64,64	0
56	MG	AA	1964	1/1	0.91	0.13	84,84,84,84	0
56	MG	CA	1853	1/1	0.91	0.10	52,52,52,52	0
56	MG	BA	3520	1/1	0.91	0.19	51,51,51,51	0
56	MG	BA	3611	1/1	0.91	0.08	67,67,67,67	0
56	MG	CA	1754	1/1	0.91	0.52	162,162,162,162	0
56	MG	DA	3516	1/1	0.91	0.08	70,70,70,70	0
56	MG	DA	3517	1/1	0.91	0.07	62,62,62,62	0
56	MG	BA	3521	1/1	0.91	0.19	53,53,53,53	0
56	MG	DA	3317	1/1	0.91	0.12	48,48,48,48	0
56	MG	CA	1859	1/1	0.91	0.27	132,132,132,132	0
56	MG	AA	1966	1/1	0.91	0.12	51,51,51,51	0
56	MG	AW	118	1/1	0.91	0.11	69,69,69,69	0
56	MG	CA	1762	1/1	0.91	0.07	28,28,28,28	0
56	MG	DA	3525	1/1	0.91	0.09	58,58,58,58	0
56	MG	DA	2926	1/1	0.91	0.29	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BA	2912	1/1	0.91	0.25	67,67,67,67	0
56	MG	BA	3431	1/1	0.91	0.09	67,67,67,67	0
56	MG	DA	2932	1/1	0.91	0.08	59,59,59,59	0
56	MG	DA	3337	1/1	0.91	0.13	51,51,51,51	0
56	MG	BA	3104	1/1	0.91	0.12	120,120,120,120	0
56	MG	BA	2966	1/1	0.91	0.06	49,49,49,49	0
56	MG	CA	1673	1/1	0.91	0.15	73,73,73,73	0
56	MG	DA	3341	1/1	0.91	0.30	55,55,55,55	0
56	MG	BA	3153	1/1	0.91	0.06	81,81,81,81	0
56	MG	DA	3540	1/1	0.91	0.34	85,85,85,85	0
56	MG	BA	3622	1/1	0.91	0.57	68,68,68,68	0
56	MG	DA	3075	1/1	0.91	0.11	75,75,75,75	0
56	MG	BA	3322	1/1	0.91	0.27	46,46,46,46	0
56	MG	BA	3203	1/1	0.91	0.42	98,98,98,98	0
56	MG	BA	3255	1/1	0.91	0.11	66,66,66,66	0
56	MG	AA	1837	1/1	0.91	0.04	64,64,64,64	0
56	MG	BA	3539	1/1	0.91	0.22	71,71,71,71	0
56	MG	DA	3553	1/1	0.91	0.21	21,21,21,21	0
56	MG	DA	3559	1/1	0.91	0.25	51,51,51,51	0
56	MG	BA	2968	1/1	0.91	0.12	46,46,46,46	0
56	MG	AA	1795	1/1	0.91	0.14	65,65,65,65	0
56	MG	BT	201	1/1	0.91	0.23	63,63,63,63	0
56	MG	BA	3334	1/1	0.91	0.11	65,65,65,65	0
56	MG	DA	3089	1/1	0.91	0.12	70,70,70,70	0
56	MG	DA	3360	1/1	0.91	0.08	64,64,64,64	0
56	MG	BA	3547	1/1	0.91	0.20	43,43,43,43	0
56	MG	DA	3362	1/1	0.91	0.31	83,83,83,83	0
56	MG	BA	3449	1/1	0.91	0.21	49,49,49,49	0
56	MG	DA	2954	1/1	0.91	0.12	90,90,90,90	0
56	MG	AA	1865	1/1	0.91	0.12	98,98,98,98	0
56	MG	BA	3645	1/1	0.91	0.16	48,48,48,48	0
56	MG	DA	3368	1/1	0.91	0.09	83,83,83,83	0
56	MG	BA	3336	1/1	0.91	0.10	31,31,31,31	0
56	MG	DA	2960	1/1	0.91	0.23	68,68,68,68	0
56	MG	DA	3374	1/1	0.91	0.12	54,54,54,54	0
56	MG	DA	2962	1/1	0.91	0.09	59,59,59,59	0
56	MG	CA	1888	1/1	0.91	0.08	67,67,67,67	0
56	MG	BA	3341	1/1	0.91	0.12	69,69,69,69	0
56	MG	DA	2965	1/1	0.91	0.16	74,74,74,74	0
56	MG	BA	3075	1/1	0.91	0.31	73,73,73,73	0
56	MG	CA	1694	1/1	0.91	0.13	69,69,69,69	0
56	MG	BA	2917	1/1	0.91	0.49	188,188,188,188	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	DA	2973	1/1	0.91	0.15	57,57,57,57	0
56	MG	DA	3616	1/1	0.91	0.10	65,65,65,65	0
56	MG	BA	3264	1/1	0.91	0.23	89,89,89,89	0
56	MG	DA	3619	1/1	0.91	0.21	53,53,53,53	0
56	MG	BA	3161	1/1	0.91	0.16	73,73,73,73	0
56	MG	AA	1923	1/1	0.91	0.12	72,72,72,72	0
56	MG	CA	1610	1/1	0.91	0.10	78,78,78,78	0
56	MG	DA	3628	1/1	0.91	0.07	295,295,295,295	0
56	MG	DA	2979	1/1	0.91	0.21	81,81,81,81	0
56	MG	DA	3391	1/1	0.91	0.11	57,57,57,57	0
56	MG	BA	3216	1/1	0.91	0.09	48,48,48,48	0
56	MG	BA	3002	1/1	0.91	0.09	91,91,91,91	0
56	MG	DA	2983	1/1	0.91	0.31	77,77,77,77	0
56	MG	BA	3467	1/1	0.91	0.14	103,103,103,103	0
56	MG	DA	3123	1/1	0.91	0.20	72,72,72,72	0
56	MG	DA	3124	1/1	0.91	0.08	32,32,32,32	0
56	MG	DA	3402	1/1	0.91	0.14	28,28,28,28	0
56	MG	DA	3403	1/1	0.91	0.41	77,77,77,77	0
56	MG	BA	3567	1/1	0.91	0.14	75,75,75,75	0
56	MG	DB	210	1/1	0.91	0.09	82,82,82,82	0
56	MG	BA	3167	1/1	0.91	0.17	60,60,60,60	0
56	MG	BA	3469	1/1	0.91	0.05	82,82,82,82	0
56	MG	DA	3408	1/1	0.91	0.14	51,51,51,51	0
56	MG	AA	1786	1/1	0.91	0.35	71,71,71,71	0
56	MG	DB	216	1/1	0.91	0.06	51,51,51,51	0
56	MG	BA	3368	1/1	0.91	0.13	25,25,25,25	0
56	MG	DA	3139	1/1	0.91	0.13	33,33,33,33	0
56	MG	BA	2947	1/1	0.91	0.28	52,52,52,52	0
56	MG	DB	220	1/1	0.91	0.10	40,40,40,40	0
56	MG	DH	201	1/1	0.91	0.23	64,64,64,64	0
56	MG	BA	3120	1/1	0.91	0.27	62,62,62,62	0
56	MG	BA	2948	1/1	0.91	0.18	56,56,56,56	0
56	MG	BA	3477	1/1	0.91	0.09	54,54,54,54	0
56	MG	DA	3166	1/1	0.91	0.15	25,25,25,25	0
56	MG	DQ	203	1/1	0.91	0.11	67,67,67,67	0
56	MG	AA	1812	1/1	0.91	0.64	273,273,273,273	0
56	MG	DW	202	1/1	0.91	0.08	50,50,50,50	0
56	MG	DA	3426	1/1	0.91	0.19	63,63,63,63	0
56	MG	BA	3281	1/1	0.91	0.13	73,73,73,73	0
56	MG	D5	101	1/1	0.91	0.10	71,71,71,71	0
56	MG	BA	3378	1/1	0.91	0.21	30,30,30,30	0
56	MG	D5	103	1/1	0.91	0.12	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	D7	101	1/1	0.91	0.13	62,62,62,62	0
56	MG	BA	3659	1/1	0.92	0.09	46,46,46,46	0
56	MG	BA	3662	1/1	0.92	0.36	87,87,87,87	0
56	MG	BA	3498	1/1	0.92	0.12	67,67,67,67	0
56	MG	AA	1656	1/1	0.92	0.13	61,61,61,61	0
56	MG	AA	1675	1/1	0.92	0.10	96,96,96,96	0
56	MG	BA	3501	1/1	0.92	0.10	52,52,52,52	0
56	MG	DA	3481	1/1	0.92	0.17	73,73,73,73	0
56	MG	DA	3306	1/1	0.92	0.30	48,48,48,48	0
56	MG	DA	3082	1/1	0.92	0.05	67,67,67,67	0
56	MG	DA	3313	1/1	0.92	0.11	12,12,12,12	0
56	MG	DA	2959	1/1	0.92	0.29	48,48,48,48	0
56	MG	DA	3487	1/1	0.92	0.53	108,108,108,108	0
56	MG	BA	3667	1/1	0.92	0.23	52,52,52,52	0
56	MG	AA	1938	1/1	0.92	0.12	72,72,72,72	0
56	MG	AA	1939	1/1	0.92	0.05	61,61,61,61	0
56	MG	AA	1941	1/1	0.92	0.15	100,100,100,100	0
56	MG	BA	3506	1/1	0.92	0.16	53,53,53,53	0
56	MG	AA	1869	1/1	0.92	0.21	34,34,34,34	0
56	MG	DA	3328	1/1	0.92	0.24	48,48,48,48	0
56	MG	CA	1707	1/1	0.92	0.12	50,50,50,50	0
56	MG	DA	3332	1/1	0.92	0.18	45,45,45,45	0
56	MG	DA	3334	1/1	0.92	0.10	72,72,72,72	0
56	MG	AA	1745	1/1	0.92	0.14	80,80,80,80	0
56	MG	CA	1618	1/1	0.92	0.12	49,49,49,49	0
56	MG	AA	1871	1/1	0.92	0.12	29,29,29,29	0
56	MG	BA	3432	1/1	0.92	0.24	69,69,69,69	0
56	MG	DA	3098	1/1	0.92	0.11	57,57,57,57	0
56	MG	DA	3099	1/1	0.92	0.09	79,79,79,79	0
56	MG	BA	3681	1/1	0.92	0.08	42,42,42,42	0
56	MG	BA	3199	1/1	0.92	0.09	69,69,69,69	0
56	MG	BA	3144	1/1	0.92	0.06	53,53,53,53	0
56	MG	DA	3518	1/1	0.92	0.22	63,63,63,63	0
56	MG	AA	1771	1/1	0.92	0.05	55,55,55,55	0
56	MG	AA	1680	1/1	0.92	0.06	87,87,87,87	0
56	MG	BA	3689	1/1	0.92	0.32	67,67,67,67	0
56	MG	DA	3109	1/1	0.92	0.10	65,65,65,65	0
56	MG	CA	1814	1/1	0.92	0.17	156,156,156,156	0
56	MG	AA	1788	1/1	0.92	0.11	175,175,175,175	0
56	MG	BA	3691	1/1	0.92	0.07	45,45,45,45	0
56	MG	CA	1632	1/1	0.92	0.07	84,84,84,84	0
56	MG	BA	3439	1/1	0.92	0.13	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BA	3013	1/1	0.92	0.11	81,81,81,81	0
56	MG	BA	3262	1/1	0.92	0.06	75,75,75,75	0
56	MG	BA	3101	1/1	0.92	0.16	106,106,106,106	0
56	MG	DA	2998	1/1	0.92	0.26	62,62,62,62	0
56	MG	BA	2904	1/1	0.92	0.08	48,48,48,48	0
56	MG	DA	3536	1/1	0.92	0.24	50,50,50,50	0
56	MG	CA	1639	1/1	0.92	0.10	100,100,100,100	0
56	MG	AA	1853	1/1	0.92	0.10	69,69,69,69	0
56	MG	CA	1826	1/1	0.92	0.12	73,73,73,73	0
56	MG	BA	2944	1/1	0.92	0.14	62,62,62,62	0
56	MG	DA	3369	1/1	0.92	0.13	86,86,86,86	0
56	MG	BA	3355	1/1	0.92	0.14	18,18,18,18	0
56	MG	DA	3371	1/1	0.92	0.12	65,65,65,65	0
56	MG	BA	3705	1/1	0.92	0.13	62,62,62,62	0
56	MG	DA	3129	1/1	0.92	0.27	104,104,104,104	0
56	MG	AA	1616	1/1	0.92	0.12	87,87,87,87	0
56	MG	DA	3131	1/1	0.92	0.42	40,40,40,40	0
56	MG	CA	1832	1/1	0.92	0.12	65,65,65,65	0
56	MG	DA	3135	1/1	0.92	0.28	17,17,17,17	0
56	MG	AA	1818	1/1	0.92	0.11	44,44,44,44	0
56	MG	DA	3563	1/1	0.92	0.16	62,62,62,62	0
56	MG	CW	105	1/1	0.92	0.08	65,65,65,65	0
56	MG	DA	3158	1/1	0.92	0.17	18,18,18,18	0
56	MG	DA	3569	1/1	0.92	0.17	52,52,52,52	0
56	MG	DA	3570	1/1	0.92	0.13	72,72,72,72	0
56	MG	AA	1881	1/1	0.92	0.16	54,54,54,54	0
56	MG	DA	3573	1/1	0.92	0.07	34,34,34,34	0
56	MG	BA	3068	1/1	0.92	0.26	115,115,115,115	0
56	MG	BA	3459	1/1	0.92	0.12	80,80,80,80	0
56	MG	AA	1750	1/1	0.92	0.06	77,77,77,77	0
56	MG	DA	3167	1/1	0.92	0.08	13,13,13,13	0
56	MG	DA	3174	1/1	0.92	0.23	49,49,49,49	0
56	MG	AA	1693	1/1	0.92	0.12	74,74,74,74	0
56	MG	CW	116	1/1	0.92	0.04	70,70,70,70	0
56	MG	BA	3030	1/1	0.92	0.22	64,64,64,64	0
56	MG	DA	3394	1/1	0.92	0.21	49,49,49,49	0
56	MG	BA	3115	1/1	0.92	0.10	62,62,62,62	0
56	MG	DA	3587	1/1	0.92	0.18	90,90,90,90	0
56	MG	AA	1793	1/1	0.92	0.33	127,127,127,127	0
56	MG	BA	3376	1/1	0.92	0.07	59,59,59,59	0
56	MG	DA	3188	1/1	0.92	0.27	50,50,50,50	0
56	MG	AA	1961	1/1	0.92	0.05	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	DA	3594	1/1	0.92	0.07	50,50,50,50	0
56	MG	DA	3025	1/1	0.92	0.09	30,30,30,30	0
56	MG	DA	3601	1/1	0.92	0.12	61,61,61,61	0
56	MG	DA	3026	1/1	0.92	0.18	78,78,78,78	0
56	MG	DA	3027	1/1	0.92	0.07	94,94,94,94	0
56	MG	BA	3286	1/1	0.92	0.27	63,63,63,63	0
56	MG	AA	1822	1/1	0.92	0.07	69,69,69,69	0
56	MG	DA	3215	1/1	0.92	0.34	46,46,46,46	0
56	MG	BB	202	1/1	0.92	0.06	98,98,98,98	0
56	MG	AA	1922	1/1	0.92	0.13	86,86,86,86	0
56	MG	AA	1677	1/1	0.92	0.17	65,65,65,65	0
56	MG	CA	1751	1/1	0.92	0.41	163,163,163,163	0
56	MG	DA	3418	1/1	0.92	0.12	11,11,11,11	0
56	MG	DA	3419	1/1	0.92	0.14	54,54,54,54	0
56	MG	BA	3174	1/1	0.92	0.14	69,69,69,69	0
56	MG	DA	3629	1/1	0.92	0.20	67,67,67,67	0
56	MG	BB	207	1/1	0.92	0.13	84,84,84,84	0
56	MG	BA	2957	1/1	0.92	0.16	71,71,71,71	0
56	MG	AA	1893	1/1	0.92	0.33	48,48,48,48	0
56	MG	CA	1757	1/1	0.92	0.27	43,43,43,43	0
56	MG	BA	3630	1/1	0.92	0.12	19,19,19,19	0
56	MG	CA	1760	1/1	0.92	0.19	67,67,67,67	0
56	MG	BA	3177	1/1	0.92	0.05	78,78,78,78	0
56	MG	BA	3480	1/1	0.92	0.06	77,77,77,77	0
56	MG	AA	1753	1/1	0.92	0.07	72,72,72,72	0
56	MG	BA	3124	1/1	0.92	0.15	79,79,79,79	0
56	MG	BA	3643	1/1	0.92	0.25	57,57,57,57	0
56	MG	BA	3565	1/1	0.92	0.14	63,63,63,63	0
56	MG	DB	211	1/1	0.92	0.12	35,35,35,35	0
56	MG	BA	3485	1/1	0.92	0.23	53,53,53,53	0
56	MG	DA	2929	1/1	0.92	0.11	77,77,77,77	0
56	MG	BA	3647	1/1	0.92	0.14	88,88,88,88	0
56	MG	DA	3254	1/1	0.92	0.22	50,50,50,50	0
56	MG	BA	3394	1/1	0.92	0.22	56,56,56,56	0
56	MG	BA	3235	1/1	0.92	0.13	63,63,63,63	0
56	MG	AA	1842	1/1	0.92	0.14	98,98,98,98	0
56	MG	CA	1871	1/1	0.92	0.09	56,56,56,56	0
56	MG	DA	3450	1/1	0.92	0.06	64,64,64,64	0
56	MG	DD	301	1/1	0.92	0.07	62,62,62,62	0
56	MG	AA	1734	1/1	0.92	0.08	66,66,66,66	0
56	MG	BA	3400	1/1	0.92	0.10	37,37,37,37	0
56	MG	BA	3042	1/1	0.92	0.12	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	AW	117	1/1	0.92	0.12	68,68,68,68	0
56	MG	AA	1866	1/1	0.92	0.07	118,118,118,118	0
56	MG	DA	3281	1/1	0.92	0.13	48,48,48,48	0
56	MG	B5	101	1/1	0.92	0.09	34,34,34,34	0
56	MG	BA	3656	1/1	0.92	0.10	31,31,31,31	0
56	MG	DA	3460	1/1	0.92	0.06	67,67,67,67	0
56	MG	B8	102	1/1	0.92	0.11	39,39,39,39	0
56	MG	CA	1785	1/1	0.92	0.11	63,63,63,63	0
56	MG	DA	3465	1/1	0.92	0.18	60,60,60,60	0
56	MG	BA	3131	1/1	0.92	0.06	65,65,65,65	0
56	MG	BA	3189	1/1	0.92	0.33	105,105,105,105	0
56	MG	DA	3297	1/1	0.93	0.23	64,64,64,64	0
56	MG	BA	3706	1/1	0.93	0.34	102,102,102,102	0
56	MG	DA	3477	1/1	0.93	0.29	56,56,56,56	0
56	MG	AA	1785	1/1	0.93	0.18	62,62,62,62	0
56	MG	DA	2968	1/1	0.93	0.07	54,54,54,54	0
56	MG	DA	3309	1/1	0.93	0.14	81,81,81,81	0
56	MG	AA	1898	1/1	0.93	0.10	70,70,70,70	0
56	MG	AA	1984	1/1	0.93	0.05	42,42,42,42	0
56	MG	DA	3316	1/1	0.93	0.14	49,49,49,49	0
56	MG	DA	3486	1/1	0.93	0.17	62,62,62,62	0
56	MG	BA	3615	1/1	0.93	0.14	73,73,73,73	0
56	MG	BA	3023	1/1	0.93	0.15	58,58,58,58	0
56	MG	AA	1827	1/1	0.93	0.09	98,98,98,98	0
56	MG	BA	3538	1/1	0.93	0.13	82,82,82,82	0
56	MG	AA	1608	1/1	0.93	0.69	108,108,108,108	0
56	MG	BA	2956	1/1	0.93	0.07	42,42,42,42	0
56	MG	DA	3493	1/1	0.93	0.08	57,57,57,57	0
56	MG	AA	1712	1/1	0.93	0.18	166,166,166,166	0
56	MG	DA	2982	1/1	0.93	0.06	44,44,44,44	0
56	MG	DA	3496	1/1	0.93	0.10	40,40,40,40	0
56	MG	BA	3544	1/1	0.93	0.17	55,55,55,55	0
56	MG	DA	3330	1/1	0.93	0.23	36,36,36,36	0
56	MG	BA	3385	1/1	0.93	0.23	50,50,50,50	0
56	MG	BA	3387	1/1	0.93	0.17	49,49,49,49	0
56	MG	DA	2987	1/1	0.93	0.13	63,63,63,63	0
56	MG	AA	1988	1/1	0.93	0.08	53,53,53,53	0
56	MG	CA	1922	1/1	0.93	0.14	67,67,67,67	0
56	MG	BA	3070	1/1	0.93	0.23	159,159,159,159	0
56	MG	DA	2994	1/1	0.93	0.10	62,62,62,62	0
56	MG	AA	1903	1/1	0.93	0.13	51,51,51,51	0
56	MG	DA	3513	1/1	0.93	0.12	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	DA	3515	1/1	0.93	0.06	76,76,76,76	0
56	MG	BA	3301	1/1	0.93	0.07	64,64,64,64	0
56	MG	AA	1774	1/1	0.93	0.16	68,68,68,68	0
56	MG	AA	1882	1/1	0.93	0.23	32,32,32,32	0
56	MG	CA	1742	1/1	0.93	0.16	61,61,61,61	0
56	MG	BA	3251	1/1	0.93	0.16	55,55,55,55	0
56	MG	BA	3558	1/1	0.93	0.16	71,71,71,71	0
56	MG	AA	1934	1/1	0.93	0.12	96,96,96,96	0
56	MG	BA	3396	1/1	0.93	0.17	43,43,43,43	0
56	MG	DA	3126	1/1	0.93	0.20	65,65,65,65	0
56	MG	CW	107	1/1	0.93	0.06	50,50,50,50	0
56	MG	CW	109	1/1	0.93	0.08	49,49,49,49	0
56	MG	DA	3357	1/1	0.93	0.24	78,78,78,78	0
56	MG	AA	1671	1/1	0.93	0.19	87,87,87,87	0
56	MG	BA	3076	1/1	0.93	0.09	48,48,48,48	0
56	MG	BA	3484	1/1	0.93	0.20	104,104,104,104	0
56	MG	AA	1887	1/1	0.93	0.10	70,70,70,70	0
56	MG	DA	3133	1/1	0.93	0.16	20,20,20,20	0
56	MG	CW	115	1/1	0.93	0.15	81,81,81,81	0
56	MG	BA	3403	1/1	0.93	0.32	79,79,79,79	0
56	MG	DA	3013	1/1	0.93	0.12	55,55,55,55	0
56	MG	DA	3149	1/1	0.93	0.14	22,22,22,22	0
56	MG	DA	3153	1/1	0.93	0.29	22,22,22,22	0
56	MG	BA	3487	1/1	0.93	0.14	51,51,51,51	0
56	MG	BA	3162	1/1	0.93	0.25	60,60,60,60	0
56	MG	DA	3160	1/1	0.93	0.31	45,45,45,45	0
56	MG	BA	3316	1/1	0.93	0.09	26,26,26,26	0
56	MG	DA	3545	1/1	0.93	0.07	91,91,91,91	0
56	MG	CA	1755	1/1	0.93	0.58	120,120,120,120	0
56	MG	BA	3317	1/1	0.93	0.12	16,16,16,16	0
56	MG	BA	3409	1/1	0.93	0.07	115,115,115,115	0
56	MG	DA	3549	1/1	0.93	0.16	16,16,16,16	0
56	MG	DA	3377	1/1	0.93	0.09	58,58,58,58	0
56	MG	DA	3554	1/1	0.93	0.25	13,13,13,13	0
56	MG	BA	3257	1/1	0.93	0.15	69,69,69,69	0
56	MG	DA	3379	1/1	0.93	0.10	54,54,54,54	0
56	MG	BF	1901	1/1	0.93	0.15	74,74,74,74	0
56	MG	BP	201	1/1	0.93	0.10	54,54,54,54	0
56	MG	BA	3414	1/1	0.93	0.23	47,47,47,47	0
56	MG	CA	1763	1/1	0.93	0.15	46,46,46,46	0
56	MG	BA	2901	1/1	0.93	0.29	123,123,123,123	0
56	MG	DA	3186	1/1	0.93	0.20	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	AA	1626	1/1	0.93	0.16	91,91,91,91	0
56	MG	BA	3661	1/1	0.93	0.18	56,56,56,56	0
56	MG	DA	3195	1/1	0.93	0.14	20,20,20,20	0
56	MG	DA	3196	1/1	0.93	0.16	30,30,30,30	0
56	MG	CA	1768	1/1	0.93	0.06	55,55,55,55	0
56	MG	DA	3202	1/1	0.93	0.19	25,25,25,25	0
56	MG	DA	3203	1/1	0.93	0.21	51,51,51,51	0
56	MG	DA	3205	1/1	0.93	0.13	36,36,36,36	0
56	MG	AA	1603	1/1	0.93	0.06	64,64,64,64	0
56	MG	AA	1940	1/1	0.93	0.14	82,82,82,82	0
56	MG	DA	3399	1/1	0.93	0.09	85,85,85,85	0
56	MG	BA	3215	1/1	0.93	0.05	88,88,88,88	0
56	MG	BA	3001	1/1	0.93	0.11	86,86,86,86	0
56	MG	AW	105	1/1	0.93	0.04	55,55,55,55	0
56	MG	BA	3428	1/1	0.93	0.13	51,51,51,51	0
56	MG	DA	3217	1/1	0.93	0.16	24,24,24,24	0
56	MG	DA	2919	1/1	0.93	0.23	50,50,50,50	0
56	MG	DA	3406	1/1	0.93	0.05	62,62,62,62	0
56	MG	CA	1688	1/1	0.93	0.08	45,45,45,45	0
56	MG	BA	3429	1/1	0.93	0.21	43,43,43,43	0
56	MG	DA	2924	1/1	0.93	0.14	43,43,43,43	0
56	MG	DA	2925	1/1	0.93	0.25	80,80,80,80	0
56	MG	DA	3230	1/1	0.93	0.18	41,41,41,41	0
56	MG	DA	3613	1/1	0.93	0.07	49,49,49,49	0
56	MG	BA	2906	1/1	0.93	0.22	84,84,84,84	0
56	MG	DA	3416	1/1	0.93	0.07	60,60,60,60	0
56	MG	AA	1614	1/1	0.93	0.18	51,51,51,51	0
56	MG	BA	2942	1/1	0.93	0.18	37,37,37,37	0
56	MG	AA	1707	1/1	0.93	0.13	67,67,67,67	0
56	MG	DA	2931	1/1	0.93	0.17	87,87,87,87	0
56	MG	BA	3272	1/1	0.93	0.09	49,49,49,49	0
56	MG	BA	3051	1/1	0.93	0.15	32,32,32,32	0
56	MG	BA	3129	1/1	0.93	0.22	72,72,72,72	0
56	MG	DA	2935	1/1	0.93	0.16	89,89,89,89	0
56	MG	AW	108	1/1	0.93	0.12	72,72,72,72	0
56	MG	BA	3009	1/1	0.93	0.13	86,86,86,86	0
56	MG	BA	3440	1/1	0.93	0.23	37,37,37,37	0
56	MG	DA	2939	1/1	0.93	0.21	66,66,66,66	0
56	MG	BA	3358	1/1	0.93	0.12	150,150,150,150	0
56	MG	AA	1655	1/1	0.93	0.15	80,80,80,80	0
56	MG	BA	3443	1/1	0.93	0.20	18,18,18,18	0
56	MG	DA	3255	1/1	0.93	0.18	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	DA	3256	1/1	0.93	0.07	41,41,41,41	0
56	MG	CA	1705	1/1	0.93	0.09	94,94,94,94	0
56	MG	DA	2946	1/1	0.93	0.13	55,55,55,55	0
56	MG	DA	3261	1/1	0.93	0.11	32,32,32,32	0
56	MG	DA	3442	1/1	0.93	0.21	64,64,64,64	0
56	MG	AA	1755	1/1	0.93	0.05	123,123,123,123	0
56	MG	BA	3362	1/1	0.93	0.13	26,26,26,26	0
56	MG	DA	3267	1/1	0.93	0.09	32,32,32,32	0
56	MG	DA	3268	1/1	0.93	0.27	52,52,52,52	0
56	MG	CA	1624	1/1	0.93	0.08	98,98,98,98	0
56	MG	BA	3135	1/1	0.93	0.27	55,55,55,55	0
56	MG	DA	3276	1/1	0.93	0.07	26,26,26,26	0
56	MG	DA	3277	1/1	0.93	0.14	45,45,45,45	0
56	MG	AA	1976	1/1	0.93	0.08	60,60,60,60	0
56	MG	DF	301	1/1	0.93	0.14	37,37,37,37	0
56	MG	BA	3605	1/1	0.93	0.10	72,72,72,72	0
56	MG	BA	3526	1/1	0.93	0.11	65,65,65,65	0
56	MG	BA	3698	1/1	0.93	0.12	55,55,55,55	0
56	MG	DA	3078	1/1	0.93	0.08	75,75,75,75	0
56	MG	BA	3527	1/1	0.93	0.07	31,31,31,31	0
56	MG	BA	3284	1/1	0.93	0.10	82,82,82,82	0
56	MG	CA	1805	1/1	0.93	0.25	63,63,63,63	0
56	MG	CA	1716	1/1	0.93	0.09	86,86,86,86	0
56	MG	BA	3530	1/1	0.93	0.10	57,57,57,57	0
56	MG	BA	3703	1/1	0.93	0.44	70,70,70,70	0
56	MG	DA	3469	1/1	0.93	0.09	55,55,55,55	0
56	MG	AA	1709	1/1	0.93	0.15	71,71,71,71	0
56	MG	AA	1602	1/1	0.93	0.15	163,163,163,163	0
56	MG	CA	1721	1/1	0.93	0.09	74,74,74,74	0
56	MG	DA	3172	1/1	0.94	0.28	24,24,24,24	0
56	MG	BA	3365	1/1	0.94	0.15	14,14,14,14	0
56	MG	DA	2916	1/1	0.94	0.15	57,57,57,57	0
56	MG	BA	3366	1/1	0.94	0.23	31,31,31,31	0
56	MG	DA	3179	1/1	0.94	0.08	13,13,13,13	0
56	MG	BA	3586	1/1	0.94	0.07	17,17,17,17	0
56	MG	AA	1916	1/1	0.94	0.10	49,49,49,49	0
56	MG	DA	3504	1/1	0.94	0.09	68,68,68,68	0
56	MG	BA	3295	1/1	0.94	0.21	97,97,97,97	0
56	MG	B0	101	1/1	0.94	0.10	33,33,33,33	0
56	MG	BA	2926	1/1	0.94	0.27	80,80,80,80	0
56	MG	B1	101	1/1	0.94	0.14	75,75,75,75	0
56	MG	DA	3191	1/1	0.94	0.14	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	DA	3192	1/1	0.94	0.12	38,38,38,38	0
56	MG	AA	1884	1/1	0.94	0.21	47,47,47,47	0
56	MG	AA	1696	1/1	0.94	0.17	96,96,96,96	0
56	MG	DA	3198	1/1	0.94	0.24	41,41,41,41	0
56	MG	DA	3199	1/1	0.94	0.21	36,36,36,36	0
56	MG	DA	2928	1/1	0.94	0.10	55,55,55,55	0
56	MG	DA	3201	1/1	0.94	0.15	25,25,25,25	0
56	MG	AA	1609	1/1	0.94	0.18	46,46,46,46	0
56	MG	CA	1601	1/1	0.94	0.08	34,34,34,34	0
56	MG	BA	3447	1/1	0.94	0.17	64,64,64,64	0
56	MG	AA	1959	1/1	0.94	0.13	63,63,63,63	0
56	MG	DA	3048	1/1	0.94	0.24	49,49,49,49	0
56	MG	AA	1982	1/1	0.94	0.08	73,73,73,73	0
56	MG	DA	3051	1/1	0.94	0.07	64,64,64,64	0
56	MG	DA	3529	1/1	0.94	0.20	70,70,70,70	0
56	MG	BA	3143	1/1	0.94	0.25	81,81,81,81	0
56	MG	BA	3047	1/1	0.94	0.16	50,50,50,50	0
56	MG	DA	3056	1/1	0.94	0.10	77,77,77,77	0
56	MG	CA	1696	1/1	0.94	0.12	66,66,66,66	0
56	MG	BA	2984	1/1	0.94	0.11	40,40,40,40	0
56	MG	BA	3382	1/1	0.94	0.25	51,51,51,51	0
56	MG	CA	1883	1/1	0.94	0.12	78,78,78,78	0
56	MG	CA	1789	1/1	0.94	0.31	184,184,184,184	0
56	MG	BA	3679	1/1	0.94	0.15	27,27,27,27	0
56	MG	BA	3456	1/1	0.94	0.13	65,65,65,65	0
56	MG	DA	3233	1/1	0.94	0.23	62,62,62,62	0
56	MG	BA	3383	1/1	0.94	0.26	39,39,39,39	0
56	MG	BA	3684	1/1	0.94	0.15	47,47,47,47	0
56	MG	AA	1960	1/1	0.94	0.10	48,48,48,48	0
56	MG	BA	3306	1/1	0.94	0.09	68,68,68,68	0
56	MG	DA	3396	1/1	0.94	0.12	18,18,18,18	0
56	MG	BA	3017	1/1	0.94	0.19	27,27,27,27	0
56	MG	DA	3242	1/1	0.94	0.16	40,40,40,40	0
56	MG	DA	3552	1/1	0.94	0.30	19,19,19,19	0
56	MG	AA	1715	1/1	0.94	0.10	86,86,86,86	0
56	MG	AA	1731	1/1	0.94	0.07	57,57,57,57	0
56	MG	CA	1799	1/1	0.94	0.19	51,51,51,51	0
56	MG	AW	114	1/1	0.94	0.13	82,82,82,82	0
56	MG	DA	3562	1/1	0.94	0.12	45,45,45,45	0
56	MG	BA	3312	1/1	0.94	0.25	20,20,20,20	0
56	MG	BA	3313	1/1	0.94	0.13	63,63,63,63	0
56	MG	DA	3566	1/1	0.94	0.09	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	DA	2956	1/1	0.94	0.20	59,59,59,59	0
56	MG	AA	1732	1/1	0.94	0.16	60,60,60,60	0
56	MG	BA	3267	1/1	0.94	0.21	123,123,123,123	0
56	MG	BA	3541	1/1	0.94	0.05	44,44,44,44	0
56	MG	BA	2911	1/1	0.94	0.25	91,91,91,91	0
56	MG	DA	3574	1/1	0.94	0.11	67,67,67,67	0
56	MG	BA	3543	1/1	0.94	0.07	53,53,53,53	0
56	MG	BA	3701	1/1	0.94	0.12	74,74,74,74	0
56	MG	AA	1807	1/1	0.94	0.06	45,45,45,45	0
56	MG	DA	3259	1/1	0.94	0.14	49,49,49,49	0
56	MG	BA	3270	1/1	0.94	0.08	70,70,70,70	0
56	MG	BA	3271	1/1	0.94	0.11	68,68,68,68	0
56	MG	BA	3232	1/1	0.94	0.15	65,65,65,65	0
56	MG	CA	1634	1/1	0.94	0.07	74,74,74,74	0
56	MG	BA	3619	1/1	0.94	0.14	53,53,53,53	0
56	MG	BA	3708	1/1	0.94	0.17	61,61,61,61	0
56	MG	BA	3402	1/1	0.94	0.13	37,37,37,37	0
56	MG	BA	3329	1/1	0.94	0.27	19,19,19,19	0
56	MG	BA	3233	1/1	0.94	0.23	55,55,55,55	0
56	MG	DA	3429	1/1	0.94	0.20	59,59,59,59	0
56	MG	BA	3274	1/1	0.94	0.08	105,105,105,105	0
56	MG	BA	3554	1/1	0.94	0.06	62,62,62,62	0
56	MG	CA	1821	1/1	0.94	0.13	56,56,56,56	0
56	MG	BA	3406	1/1	0.94	0.17	28,28,28,28	0
56	MG	BA	3715	1/1	0.94	0.09	75,75,75,75	0
56	MG	CA	1923	1/1	0.94	0.13	77,77,77,77	0
56	MG	DA	3606	1/1	0.94	0.07	54,54,54,54	0
56	MG	DA	3607	1/1	0.94	0.08	30,30,30,30	0
56	MG	DA	3609	1/1	0.94	0.05	27,27,27,27	0
56	MG	BA	3556	1/1	0.94	0.23	54,54,54,54	0
56	MG	DA	3611	1/1	0.94	0.26	60,60,60,60	0
56	MG	BA	3025	1/1	0.94	0.16	66,66,66,66	0
56	MG	BA	3158	1/1	0.94	0.36	150,150,150,150	0
56	MG	AA	1875	1/1	0.94	0.15	37,37,37,37	0
56	MG	DA	2989	1/1	0.94	0.07	53,53,53,53	0
56	MG	BA	3338	1/1	0.94	0.12	28,28,28,28	0
56	MG	CA	1829	1/1	0.94	0.16	49,49,49,49	0
56	MG	DA	3621	1/1	0.94	0.17	77,77,77,77	0
56	MG	DA	3624	1/1	0.94	0.10	35,35,35,35	0
56	MG	BA	3635	1/1	0.94	0.20	37,37,37,37	0
56	MG	DA	3448	1/1	0.94	0.16	43,43,43,43	0
56	MG	DA	3296	1/1	0.94	0.15	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BA	3636	1/1	0.94	0.18	28,28,28,28	0
56	MG	BA	3637	1/1	0.94	0.09	20,20,20,20	0
56	MG	DA	3301	1/1	0.94	0.12	52,52,52,52	0
56	MG	CA	1652	1/1	0.94	0.17	193,193,193,193	0
56	MG	DA	3303	1/1	0.94	0.15	53,53,53,53	0
56	MG	BB	201	1/1	0.94	0.06	59,59,59,59	0
56	MG	CW	108	1/1	0.94	0.22	26,26,26,26	0
56	MG	DA	3310	1/1	0.94	0.14	52,52,52,52	0
56	MG	CA	1835	1/1	0.94	0.32	61,61,61,61	0
56	MG	AA	1967	1/1	0.94	0.06	61,61,61,61	0
56	MG	DA	3314	1/1	0.94	0.32	65,65,65,65	0
56	MG	BA	3238	1/1	0.94	0.13	61,61,61,61	0
56	MG	CA	1656	1/1	0.94	0.18	52,52,52,52	0
56	MG	BA	3640	1/1	0.94	0.26	60,60,60,60	0
56	MG	DA	3319	1/1	0.94	0.13	34,34,34,34	0
56	MG	DA	3468	1/1	0.94	0.15	33,33,33,33	0
56	MG	BB	205	1/1	0.94	0.11	64,64,64,64	0
56	MG	BA	3029	1/1	0.94	0.15	44,44,44,44	0
56	MG	BA	3642	1/1	0.94	0.15	34,34,34,34	0
56	MG	AA	1851	1/1	0.94	0.19	111,111,111,111	0
56	MG	BA	3350	1/1	0.94	0.19	28,28,28,28	0
56	MG	AA	1748	1/1	0.94	0.13	54,54,54,54	0
56	MG	BA	3423	1/1	0.94	0.13	38,38,38,38	0
56	MG	DA	3478	1/1	0.94	0.15	67,67,67,67	0
56	MG	BA	3353	1/1	0.94	0.13	54,54,54,54	0
56	MG	DA	3331	1/1	0.94	0.18	93,93,93,93	0
56	MG	DA	2902	1/1	0.94	0.15	65,65,65,65	0
56	MG	AA	1749	1/1	0.94	0.10	114,114,114,114	0
56	MG	AA	1972	1/1	0.94	0.16	56,56,56,56	0
56	MG	BA	3356	1/1	0.94	0.24	43,43,43,43	0
56	MG	AA	1973	1/1	0.94	0.30	65,65,65,65	0
56	MG	AA	1633	1/1	0.94	0.15	45,45,45,45	0
56	MG	CA	1759	1/1	0.94	0.18	65,65,65,65	0
56	MG	DW	201	1/1	0.94	0.27	76,76,76,76	0
56	MG	BA	3132	1/1	0.94	0.28	53,53,53,53	0
56	MG	BA	3434	1/1	0.94	0.35	55,55,55,55	0
56	MG	BB	221	1/1	0.94	0.05	65,65,65,65	0
56	MG	D1	101	1/1	0.94	0.05	66,66,66,66	0
56	MG	DA	3164	1/1	0.94	0.10	30,30,30,30	0
56	MG	AW	103	1/1	0.94	0.04	70,70,70,70	0
56	MG	BA	3363	1/1	0.94	0.13	19,19,19,19	0
56	MG	AA	1624	1/1	0.94	0.08	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	DA	3100	1/1	0.95	0.29	97,97,97,97	0
56	MG	CA	1616	1/1	0.95	0.13	61,61,61,61	0
56	MG	BA	3342	1/1	0.95	0.15	25,25,25,25	0
56	MG	BA	3452	1/1	0.95	0.33	53,53,53,53	0
56	MG	BA	3453	1/1	0.95	0.19	40,40,40,40	0
56	MG	BA	3100	1/1	0.95	0.09	70,70,70,70	0
56	MG	DA	3246	1/1	0.95	0.28	51,51,51,51	0
56	MG	CA	1621	1/1	0.95	0.12	48,48,48,48	0
56	MG	BA	3344	1/1	0.95	0.28	39,39,39,39	0
56	MG	AA	1926	1/1	0.95	0.10	37,37,37,37	0
56	MG	BA	3399	1/1	0.95	0.22	38,38,38,38	0
56	MG	BA	3292	1/1	0.95	0.18	40,40,40,40	0
56	MG	AA	1978	1/1	0.95	0.13	129,129,129,129	0
56	MG	BA	3136	1/1	0.95	0.33	205,205,205,205	0
56	MG	BA	3044	1/1	0.95	0.07	53,53,53,53	0
56	MG	BA	2916	1/1	0.95	0.17	37,37,37,37	0
56	MG	BA	3724	1/1	0.95	0.12	119,119,119,119	0
56	MG	DA	3119	1/1	0.95	0.09	82,82,82,82	0
56	MG	BA	3528	1/1	0.95	0.25	53,53,53,53	0
56	MG	AA	1928	1/1	0.95	0.13	67,67,67,67	0
56	MG	DA	3260	1/1	0.95	0.14	58,58,58,58	0
56	MG	DA	2943	1/1	0.95	0.05	25,25,25,25	0
56	MG	DA	3262	1/1	0.95	0.15	65,65,65,65	0
56	MG	AA	1844	1/1	0.95	0.15	78,78,78,78	0
56	MG	DA	3265	1/1	0.95	0.11	40,40,40,40	0
56	MG	BA	3408	1/1	0.95	0.20	50,50,50,50	0
56	MG	BA	3108	1/1	0.95	0.28	61,61,61,61	0
56	MG	BA	3411	1/1	0.95	0.12	31,31,31,31	0
56	MG	DA	3270	1/1	0.95	0.32	69,69,69,69	0
56	MG	BA	3109	1/1	0.95	0.06	63,63,63,63	0
56	MG	CA	1778	1/1	0.95	0.13	36,36,36,36	0
56	MG	BA	2919	1/1	0.95	0.07	127,127,127,127	0
56	MG	BA	3184	1/1	0.95	0.06	37,37,37,37	0
56	MG	AA	1930	1/1	0.95	0.34	198,198,198,198	0
56	MG	BA	3476	1/1	0.95	0.32	52,52,52,52	0
56	MG	DA	3556	1/1	0.95	0.09	19,19,19,19	0
56	MG	BA	3226	1/1	0.95	0.15	58,58,58,58	0
56	MG	DA	3134	1/1	0.95	0.17	18,18,18,18	0
56	MG	DA	3282	1/1	0.95	0.14	42,42,42,42	0
56	MG	BA	3419	1/1	0.95	0.04	57,57,57,57	0
56	MG	DA	3136	1/1	0.95	0.20	12,12,12,12	0
56	MG	AA	1845	1/1	0.95	0.08	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	DA	3567	1/1	0.95	0.10	74,74,74,74	0
56	MG	DA	3141	1/1	0.95	0.18	15,15,15,15	0
56	MG	DA	3422	1/1	0.95	0.32	77,77,77,77	0
56	MG	AA	1983	1/1	0.95	0.28	76,76,76,76	0
56	MG	DA	3147	1/1	0.95	0.14	20,20,20,20	0
56	MG	AA	1965	1/1	0.95	0.04	37,37,37,37	0
56	MG	DA	3151	1/1	0.95	0.04	12,12,12,12	0
56	MG	CW	103	1/1	0.95	0.10	57,57,57,57	0
56	MG	DA	3154	1/1	0.95	0.12	12,12,12,12	0
56	MG	DA	3155	1/1	0.95	0.15	18,18,18,18	0
56	MG	DA	3156	1/1	0.95	0.17	33,33,33,33	0
56	MG	AA	1918	1/1	0.95	0.10	51,51,51,51	0
56	MG	DA	3580	1/1	0.95	0.17	79,79,79,79	0
56	MG	DA	3300	1/1	0.95	0.17	69,69,69,69	0
56	MG	DA	2961	1/1	0.95	0.26	143,143,143,143	0
56	MG	BA	3150	1/1	0.95	0.17	79,79,79,79	0
56	MG	DA	3053	1/1	0.95	0.07	61,61,61,61	0
56	MG	DA	3304	1/1	0.95	0.07	41,41,41,41	0
56	MG	DA	3305	1/1	0.95	0.26	46,46,46,46	0
56	MG	CA	1858	1/1	0.95	0.09	97,97,97,97	0
56	MG	DA	3441	1/1	0.95	0.22	46,46,46,46	0
56	MG	DA	3307	1/1	0.95	0.12	82,82,82,82	0
56	MG	BA	3425	1/1	0.95	0.36	202,202,202,202	0
56	MG	BA	3426	1/1	0.95	0.19	28,28,28,28	0
56	MG	BA	3677	1/1	0.95	0.15	18,18,18,18	0
56	MG	DA	3597	1/1	0.95	0.15	22,22,22,22	0
56	MG	DA	3600	1/1	0.95	0.07	23,23,23,23	0
56	MG	DA	3312	1/1	0.95	0.06	61,61,61,61	0
56	MG	DA	3168	1/1	0.95	0.24	33,33,33,33	0
56	MG	DA	3171	1/1	0.95	0.08	25,25,25,25	0
56	MG	BA	3026	1/1	0.95	0.16	114,114,114,114	0
56	MG	BD	301	1/1	0.95	0.10	15,15,15,15	0
56	MG	DA	2970	1/1	0.95	0.15	69,69,69,69	0
56	MG	DA	3177	1/1	0.95	0.14	21,21,21,21	0
56	MG	DA	2971	1/1	0.95	0.08	132,132,132,132	0
56	MG	BA	3311	1/1	0.95	0.26	17,17,17,17	0
56	MG	DA	3457	1/1	0.95	0.17	64,64,64,64	0
56	MG	DA	3322	1/1	0.95	0.06	46,46,46,46	0
56	MG	BA	3372	1/1	0.95	0.16	27,27,27,27	0
56	MG	DA	3181	1/1	0.95	0.22	13,13,13,13	0
56	MG	CW	114	1/1	0.95	0.09	61,61,61,61	0
56	MG	DA	3462	1/1	0.95	0.20	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	AA	1604	1/1	0.95	0.09	91,91,91,91	0
56	MG	DA	3464	1/1	0.95	0.20	42,42,42,42	0
56	MG	BA	3375	1/1	0.95	0.17	30,30,30,30	0
56	MG	CA	1868	1/1	0.95	0.11	69,69,69,69	0
56	MG	BX	101	1/1	0.95	0.08	55,55,55,55	0
56	MG	DA	3189	1/1	0.95	0.21	27,27,27,27	0
56	MG	DA	3190	1/1	0.95	0.14	25,25,25,25	0
56	MG	AA	1789	1/1	0.95	0.12	63,63,63,63	0
56	MG	AA	1969	1/1	0.95	0.20	63,63,63,63	0
56	MG	BA	3495	1/1	0.95	0.07	51,51,51,51	0
56	MG	BA	3058	1/1	0.95	0.16	60,60,60,60	0
56	MG	AA	1953	1/1	0.95	0.18	51,51,51,51	0
56	MG	B3	101	1/1	0.95	0.20	26,26,26,26	0
56	MG	DA	2986	1/1	0.95	0.21	110,110,110,110	0
56	MG	BA	3089	1/1	0.95	0.10	72,72,72,72	0
56	MG	DA	3344	1/1	0.95	0.14	29,29,29,29	0
56	MG	DA	3345	1/1	0.95	0.19	68,68,68,68	0
56	MG	BA	3694	1/1	0.95	0.16	35,35,35,35	0
56	MG	CA	1878	1/1	0.95	0.16	66,66,66,66	0
56	MG	AA	1838	1/1	0.95	0.04	56,56,56,56	0
56	MG	BA	3325	1/1	0.95	0.24	39,39,39,39	0
56	MG	BA	2955	1/1	0.95	0.10	45,45,45,45	0
56	MG	BA	3502	1/1	0.95	0.10	26,26,26,26	0
56	MG	BA	3566	1/1	0.95	0.12	63,63,63,63	0
56	MG	DA	3085	1/1	0.95	0.07	49,49,49,49	0
56	MG	DA	3213	1/1	0.95	0.20	60,60,60,60	0
56	MG	DA	3214	1/1	0.95	0.18	22,22,22,22	0
56	MG	AA	1937	1/1	0.95	0.23	51,51,51,51	0
56	MG	DA	3216	1/1	0.95	0.13	23,23,23,23	0
56	MG	BA	3005	1/1	0.95	0.12	45,45,45,45	0
56	MG	BA	3282	1/1	0.95	0.20	78,78,78,78	0
56	MG	DA	3221	1/1	0.95	0.07	38,38,38,38	0
56	MG	DA	3363	1/1	0.95	0.08	42,42,42,42	0
56	MG	AA	1883	1/1	0.95	0.22	50,50,50,50	0
56	MG	AA	1735	1/1	0.95	0.05	52,52,52,52	0
56	MG	BA	3572	1/1	0.95	0.18	62,62,62,62	0
56	MG	DQ	204	1/1	0.95	0.09	41,41,41,41	0
56	MG	AA	1902	1/1	0.95	0.12	33,33,33,33	0
56	MG	AY	402	1/1	0.95	0.07	40,40,40,40	0
56	MG	DA	3231	1/1	0.95	0.14	32,32,32,32	0
56	MG	DA	3005	1/1	0.95	0.21	89,89,89,89	0
56	MG	BA	3575	1/1	0.95	0.07	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	DA	3510	1/1	0.95	0.25	69,69,69,69	0
56	MG	DA	3372	1/1	0.95	0.08	40,40,40,40	0
56	MG	BA	3010	1/1	0.95	0.07	93,93,93,93	0
56	MG	DA	3514	1/1	0.95	0.11	48,48,48,48	0
56	MG	AA	1885	1/1	0.95	0.13	61,61,61,61	0
56	MG	DA	3162	1/1	0.96	0.12	23,23,23,23	0
56	MG	DA	3555	1/1	0.96	0.15	14,14,14,14	0
56	MG	DA	3354	1/1	0.96	0.16	33,33,33,33	0
56	MG	DA	3557	1/1	0.96	0.12	16,16,16,16	0
56	MG	BA	3692	1/1	0.96	0.15	56,56,56,56	0
56	MG	AA	1651	1/1	0.96	0.08	84,84,84,84	0
56	MG	BA	3151	1/1	0.96	0.27	80,80,80,80	0
56	MG	BB	219	1/1	0.96	0.13	33,33,33,33	0
56	MG	CA	1891	1/1	0.96	0.07	63,63,63,63	0
56	MG	DA	3264	1/1	0.96	0.18	44,44,44,44	0
56	MG	AA	1914	1/1	0.96	0.05	53,53,53,53	0
56	MG	BA	3357	1/1	0.96	0.08	64,64,64,64	0
56	MG	DA	3173	1/1	0.96	0.21	46,46,46,46	0
56	MG	BA	3206	1/1	0.96	0.04	176,176,176,176	0
56	MG	DA	3024	1/1	0.96	0.14	65,65,65,65	0
56	MG	DA	3273	1/1	0.96	0.18	30,30,30,30	0
56	MG	DA	3176	1/1	0.96	0.13	13,13,13,13	0
56	MG	BA	3513	1/1	0.96	0.09	40,40,40,40	0
56	MG	DA	3093	1/1	0.96	0.07	76,76,76,76	0
56	MG	AA	1662	1/1	0.96	0.14	108,108,108,108	0
56	MG	BA	3475	1/1	0.96	0.20	55,55,55,55	0
56	MG	BA	3516	1/1	0.96	0.10	29,29,29,29	0
56	MG	CA	1899	1/1	0.96	0.21	41,41,41,41	0
56	MG	DA	3472	1/1	0.96	0.16	52,52,52,52	0
56	MG	AA	1952	1/1	0.96	0.08	53,53,53,53	0
56	MG	BA	3320	1/1	0.96	0.20	23,23,23,23	0
56	MG	DA	3584	1/1	0.96	0.14	49,49,49,49	0
56	MG	BA	3478	1/1	0.96	0.11	63,63,63,63	0
56	MG	DA	2969	1/1	0.96	0.04	68,68,68,68	0
56	MG	BA	3321	1/1	0.96	0.07	50,50,50,50	0
56	MG	DA	3588	1/1	0.96	0.14	24,24,24,24	0
56	MG	DA	3103	1/1	0.96	0.08	65,65,65,65	0
56	MG	DA	3104	1/1	0.96	0.26	70,70,70,70	0
56	MG	AA	1927	1/1	0.96	0.07	48,48,48,48	0
56	MG	DA	3194	1/1	0.96	0.05	28,28,28,28	0
56	MG	DA	3593	1/1	0.96	0.14	70,70,70,70	0
56	MG	BA	3707	1/1	0.96	0.10	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	AA	1906	1/1	0.96	0.21	38,38,38,38	0
56	MG	CA	1697	1/1	0.96	0.25	50,50,50,50	0
56	MG	DA	3599	1/1	0.96	0.11	14,14,14,14	0
56	MG	DA	3295	1/1	0.96	0.26	48,48,48,48	0
56	MG	DA	3387	1/1	0.96	0.12	39,39,39,39	0
56	MG	DA	3602	1/1	0.96	0.10	22,22,22,22	0
56	MG	DA	3603	1/1	0.96	0.04	17,17,17,17	0
56	MG	BA	3524	1/1	0.96	0.09	95,95,95,95	0
56	MG	DA	3040	1/1	0.96	0.15	102,102,102,102	0
56	MG	BA	3014	1/1	0.96	0.06	44,44,44,44	0
56	MG	DA	3299	1/1	0.96	0.06	38,38,38,38	0
56	MG	DA	3608	1/1	0.96	0.23	50,50,50,50	0
56	MG	BA	3034	1/1	0.96	0.04	36,36,36,36	0
56	MG	BA	3327	1/1	0.96	0.09	28,28,28,28	0
56	MG	DA	3204	1/1	0.96	0.10	35,35,35,35	0
56	MG	BA	3015	1/1	0.96	0.21	71,71,71,71	0
56	MG	DA	3045	1/1	0.96	0.09	62,62,62,62	0
56	MG	DA	3397	1/1	0.96	0.16	54,54,54,54	0
56	MG	DA	3615	1/1	0.96	0.12	57,57,57,57	0
56	MG	DA	3116	1/1	0.96	0.05	124,124,124,124	0
56	MG	DA	3617	1/1	0.96	0.07	46,46,46,46	0
56	MG	DA	3046	1/1	0.96	0.12	48,48,48,48	0
56	MG	DA	2920	1/1	0.96	0.11	83,83,83,83	0
56	MG	DA	3308	1/1	0.96	0.35	72,72,72,72	0
56	MG	DA	3622	1/1	0.96	0.08	50,50,50,50	0
56	MG	AA	1758	1/1	0.96	0.05	48,48,48,48	0
56	MG	AA	1627	1/1	0.96	0.15	64,64,64,64	0
56	MG	CA	1915	1/1	0.96	0.20	67,67,67,67	0
56	MG	DA	3052	1/1	0.96	0.10	76,76,76,76	0
56	MG	BA	3018	1/1	0.96	0.03	59,59,59,59	0
56	MG	AA	1943	1/1	0.96	0.12	45,45,45,45	0
56	MG	DA	3512	1/1	0.96	0.07	33,33,33,33	0
56	MG	BA	3164	1/1	0.96	0.06	62,62,62,62	0
56	MG	DA	3220	1/1	0.96	0.29	43,43,43,43	0
56	MG	CA	1919	1/1	0.96	0.11	39,39,39,39	0
56	MG	BA	3413	1/1	0.96	0.04	21,21,21,21	0
56	MG	BA	3165	1/1	0.96	0.10	59,59,59,59	0
56	MG	BA	3337	1/1	0.96	0.19	20,20,20,20	0
56	MG	BA	3246	1/1	0.96	0.15	47,47,47,47	0
56	MG	DA	3323	1/1	0.96	0.04	42,42,42,42	0
56	MG	BA	3673	1/1	0.96	0.09	133,133,133,133	0
56	MG	CA	1661	1/1	0.96	0.15	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	CA	1765	1/1	0.96	0.15	38,38,38,38	0
56	MG	AA	1944	1/1	0.96	0.24	67,67,67,67	0
56	MG	AA	1643	1/1	0.96	0.14	114,114,114,114	0
56	MG	BA	3381	1/1	0.96	0.21	17,17,17,17	0
56	MG	DA	3425	1/1	0.96	0.31	52,52,52,52	0
56	MG	AA	1694	1/1	0.96	0.23	165,165,165,165	0
56	MG	DA	3140	1/1	0.96	0.20	11,11,11,11	0
56	MG	DA	3333	1/1	0.96	0.10	47,47,47,47	0
56	MG	DA	3240	1/1	0.96	0.09	35,35,35,35	0
56	MG	DA	3335	1/1	0.96	0.08	38,38,38,38	0
56	MG	BA	3678	1/1	0.96	0.26	20,20,20,20	0
56	MG	DA	3534	1/1	0.96	0.15	70,70,70,70	0
56	MG	DA	3535	1/1	0.96	0.11	67,67,67,67	0
56	MG	DA	3143	1/1	0.96	0.17	19,19,19,19	0
56	MG	DA	3144	1/1	0.96	0.21	14,14,14,14	0
56	MG	BA	3277	1/1	0.96	0.06	51,51,51,51	0
56	MG	DA	2942	1/1	0.96	0.18	69,69,69,69	0
56	MG	DA	3148	1/1	0.96	0.28	34,34,34,34	0
56	MG	BA	3633	1/1	0.96	0.24	12,12,12,12	0
56	MG	BA	3145	1/1	0.96	0.18	53,53,53,53	0
56	MG	BA	3683	1/1	0.96	0.27	55,55,55,55	0
56	MG	AA	1861	1/1	0.96	0.19	42,42,42,42	0
56	MG	BA	2939	1/1	0.96	0.17	79,79,79,79	0
56	MG	DA	3347	1/1	0.96	0.07	23,23,23,23	0
56	MG	BA	2940	1/1	0.96	0.04	67,67,67,67	0
56	MG	BA	3466	1/1	0.96	0.10	39,39,39,39	0
56	MG	BA	3352	1/1	0.96	0.10	17,17,17,17	0
56	MG	DA	3550	1/1	0.96	0.17	18,18,18,18	0
56	MG	AA	1877	1/1	0.96	0.16	37,37,37,37	0
56	MG	BA	3551	1/1	0.96	0.08	52,52,52,52	0
57	ZN	CD	301	1/1	0.96	0.27	109,109,109,109	0
56	MG	BA	3631	1/1	0.97	0.08	8,8,8,8	0
56	MG	DA	3509	1/1	0.97	0.17	142,142,142,142	0
56	MG	DA	3291	1/1	0.97	0.16	44,44,44,44	0
56	MG	AA	1690	1/1	0.97	0.22	174,174,174,174	0
56	MG	BA	3416	1/1	0.97	0.16	42,42,42,42	0
56	MG	DA	3225	1/1	0.97	0.23	59,59,59,59	0
56	MG	DA	3226	1/1	0.97	0.11	20,20,20,20	0
56	MG	DA	3227	1/1	0.97	0.07	45,45,45,45	0
56	MG	DA	3598	1/1	0.97	0.18	12,12,12,12	0
56	MG	DA	3163	1/1	0.97	0.22	31,31,31,31	0
56	MG	BA	3106	1/1	0.97	0.18	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	AA	1915	1/1	0.97	0.12	50,50,50,50	0
56	MG	DA	2976	1/1	0.97	0.13	71,71,71,71	0
56	MG	DA	3021	1/1	0.97	0.39	66,66,66,66	0
56	MG	DA	3443	1/1	0.97	0.09	45,45,45,45	0
56	MG	BA	3445	1/1	0.97	0.07	19,19,19,19	0
56	MG	DA	3445	1/1	0.97	0.13	46,46,46,46	0
56	MG	DA	3234	1/1	0.97	0.06	31,31,31,31	0
56	MG	DA	3169	1/1	0.97	0.12	33,33,33,33	0
56	MG	BA	3345	1/1	0.97	0.15	20,20,20,20	0
56	MG	DA	3069	1/1	0.97	0.13	32,32,32,32	0
56	MG	AA	1769	1/1	0.97	0.09	79,79,79,79	0
56	MG	BA	3348	1/1	0.97	0.17	25,25,25,25	0
56	MG	AA	1654	1/1	0.97	0.14	61,61,61,61	0
56	MG	AA	1704	1/1	0.97	0.39	186,186,186,186	0
56	MG	BA	3680	1/1	0.97	0.05	35,35,35,35	0
56	MG	BA	3066	1/1	0.97	0.15	61,61,61,61	0
56	MG	DA	3245	1/1	0.97	0.23	45,45,45,45	0
56	MG	BA	3374	1/1	0.97	0.17	30,30,30,30	0
56	MG	AA	1888	1/1	0.97	0.17	49,49,49,49	0
56	MG	DA	3620	1/1	0.97	0.12	50,50,50,50	0
56	MG	BA	3646	1/1	0.97	0.09	52,52,52,52	0
56	MG	BA	3483	1/1	0.97	0.04	23,23,23,23	0
56	MG	BA	3686	1/1	0.97	0.22	28,28,28,28	0
56	MG	DA	3184	1/1	0.97	0.15	14,14,14,14	0
56	MG	BA	3578	1/1	0.97	0.13	32,32,32,32	0
56	MG	DA	2992	1/1	0.97	0.12	63,63,63,63	0
56	MG	BA	3427	1/1	0.97	0.17	35,35,35,35	0
56	MG	DA	3324	1/1	0.97	0.11	13,13,13,13	0
56	MG	BA	3330	1/1	0.97	0.20	27,27,27,27	0
56	MG	BA	3187	1/1	0.97	0.16	56,56,56,56	0
56	MG	BA	3457	1/1	0.97	0.12	68,68,68,68	0
56	MG	CA	1683	1/1	0.97	0.18	62,62,62,62	0
56	MG	DA	3193	1/1	0.97	0.07	34,34,34,34	0
56	MG	BA	3518	1/1	0.97	0.09	27,27,27,27	0
56	MG	AA	1781	1/1	0.97	0.07	42,42,42,42	0
56	MG	DA	3474	1/1	0.97	0.19	55,55,55,55	0
56	MG	BA	3333	1/1	0.97	0.18	12,12,12,12	0
56	MG	DA	3197	1/1	0.97	0.12	21,21,21,21	0
56	MG	BA	2933	1/1	0.97	0.04	69,69,69,69	0
56	MG	BA	3461	1/1	0.97	0.10	23,23,23,23	0
56	MG	DA	3558	1/1	0.97	0.17	14,14,14,14	0
56	MG	DA	3142	1/1	0.97	0.17	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BA	3204	1/1	0.97	0.12	65,65,65,65	0
56	MG	DA	3561	1/1	0.97	0.06	16,16,16,16	0
56	MG	BA	2990	1/1	0.97	0.12	47,47,47,47	0
56	MG	DA	3269	1/1	0.97	0.18	42,42,42,42	0
56	MG	DA	3564	1/1	0.97	0.18	25,25,25,25	0
56	MG	DA	3145	1/1	0.97	0.19	39,39,39,39	0
56	MG	DA	3271	1/1	0.97	0.07	65,65,65,65	0
56	MG	DA	3410	1/1	0.97	0.04	22,22,22,22	0
56	MG	CA	1769	1/1	0.97	0.22	58,58,58,58	0
56	MG	DE	301	1/1	0.97	0.25	29,29,29,29	0
56	MG	DA	3050	1/1	0.97	0.11	56,56,56,56	0
56	MG	BA	3360	1/1	0.97	0.18	24,24,24,24	0
56	MG	DA	3414	1/1	0.97	0.19	48,48,48,48	0
56	MG	DA	3415	1/1	0.97	0.15	46,46,46,46	0
56	MG	DP	201	1/1	0.97	0.10	43,43,43,43	0
56	MG	DP	202	1/1	0.97	0.18	73,73,73,73	0
56	MG	BA	3191	1/1	0.97	0.12	64,64,64,64	0
56	MG	DA	3208	1/1	0.97	0.18	29,29,29,29	0
56	MG	DA	3209	1/1	0.97	0.12	17,17,17,17	0
56	MG	DA	3150	1/1	0.97	0.12	17,17,17,17	0
56	MG	DA	2923	1/1	0.97	0.07	28,28,28,28	0
56	MG	DA	3152	1/1	0.97	0.18	23,23,23,23	0
56	MG	DA	3498	1/1	0.97	0.14	80,80,80,80	0
56	MG	BA	3625	1/1	0.97	0.17	117,117,117,117	0
56	MG	DA	3283	1/1	0.97	0.09	26,26,26,26	0
56	MG	BA	3000	1/1	0.97	0.04	64,64,64,64	0
56	MG	BA	3386	1/1	0.97	0.06	39,39,39,39	0
56	MG	BA	3340	1/1	0.97	0.15	31,31,31,31	0
56	MG	DA	3157	1/1	0.97	0.15	23,23,23,23	0
56	MG	BA	3562	1/1	0.97	0.04	45,45,45,45	0
56	MG	D7	102	1/1	0.97	0.07	32,32,32,32	0
57	ZN	AD	301	1/1	0.97	0.20	71,71,71,71	0
56	MG	BA	3285	1/1	0.97	0.14	66,66,66,66	0
56	MG	BA	3181	1/1	0.98	0.16	56,56,56,56	0
56	MG	DA	3137	1/1	0.98	0.18	23,23,23,23	0
56	MG	DA	3272	1/1	0.98	0.05	53,53,53,53	0
56	MG	DA	3138	1/1	0.98	0.11	12,12,12,12	0
56	MG	DA	2990	1/1	0.98	0.24	61,61,61,61	0
56	MG	BA	3401	1/1	0.98	0.21	28,28,28,28	0
56	MG	BA	3632	1/1	0.98	0.15	15,15,15,15	0
56	MG	AA	1773	1/1	0.98	0.27	281,281,281,281	0
56	MG	DA	3506	1/1	0.98	0.07	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	DA	3623	1/1	0.98	0.06	52,52,52,52	0
56	MG	DA	3479	1/1	0.98	0.07	55,55,55,55	0
56	MG	AA	1932	1/1	0.98	0.17	159,159,159,159	0
56	MG	DI	202	1/1	0.98	0.20	54,54,54,54	0
56	MG	BA	3319	1/1	0.98	0.18	19,19,19,19	0
56	MG	DA	3596	1/1	0.98	0.32	15,15,15,15	0
56	MG	BA	3545	1/1	0.98	0.13	245,245,245,245	0
56	MG	DA	3087	1/1	0.98	0.29	52,52,52,52	0
56	MG	BA	3171	1/1	0.98	0.07	43,43,43,43	0
56	MG	DA	3236	1/1	0.98	0.34	30,30,30,30	0
56	MG	DA	3433	1/1	0.98	0.07	27,27,27,27	0
56	MG	DA	3572	1/1	0.98	0.04	51,51,51,51	0
56	MG	DB	202	1/1	0.98	0.03	51,51,51,51	0
56	MG	AA	1880	1/1	0.98	0.17	43,43,43,43	0
56	MG	BA	3207	1/1	0.98	0.18	65,65,65,65	0
56	MG	CA	1623	1/1	0.98	0.04	43,43,43,43	0
56	MG	BA	3347	1/1	0.98	0.05	27,27,27,27	0
56	MG	AA	1862	1/1	0.98	0.35	212,212,212,212	0
56	MG	DA	3218	1/1	0.98	0.04	29,29,29,29	0
56	MG	BA	3410	1/1	0.98	0.04	25,25,25,25	0
56	MG	DA	3315	1/1	0.98	0.25	60,60,60,60	0
56	MG	AA	1647	1/1	0.98	0.16	34,34,34,34	0
56	MG	BA	3250	1/1	0.98	0.16	269,269,269,269	0
56	MG	BA	3315	1/1	0.98	0.12	17,17,17,17	0
57	ZN	CN	101	1/1	0.98	0.07	111,111,111,111	0
56	MG	DA	3551	1/1	0.99	0.15	13,13,13,13	0
56	MG	BA	3339	1/1	0.99	0.11	26,26,26,26	0
56	MG	DA	3222	1/1	0.99	0.13	17,17,17,17	0
56	MG	DF	302	1/1	0.99	0.09	25,25,25,25	0
56	MG	BA	3660	1/1	0.99	0.05	45,45,45,45	0
57	ZN	AN	101	1/1	0.99	0.09	115,115,115,115	0
56	MG	DA	3170	1/1	0.99	0.05	12,12,12,12	0
56	MG	BA	3324	1/1	0.99	0.09	15,15,15,15	0
56	MG	BA	3314	1/1	1.00	0.29	13,13,13,13	0
56	MG	DA	3185	1/1	1.00	0.07	12,12,12,12	0

6.5 Other polymers

There are no such residues in this entry.