wwPDB X-ray Structure Validation Summary Report (i)

Sep 14, 2023 – 03:40 AM EDT

PDB ID	:	4V63
Title	:	Structural basis for translation termination on the 70S ribosome.
Authors	:	Laurberg, M.; Asahara, H.; Korostelev, A.; Zhu, J.; Trakhanov, S.; Noller, H.F.
Deposited on	:	2008-05-16
Resolution	:	3.21 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 (i) 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 (1)) were used in the production of this report:

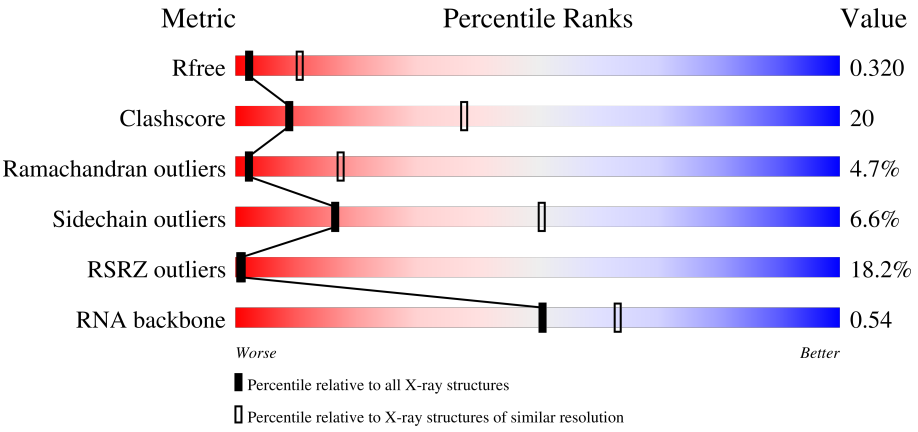
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.21 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)
RNA backbone	3102	1010 (3.50-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	1525	5% 41% 48% 9% ··
1	CA	1525	8% 42% 47% 9% ··
2	AY	77	47% 44% 8% ·
2	AZ	77	12% 43% 49% 8%

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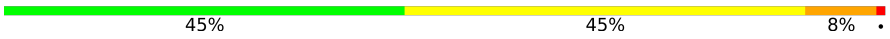
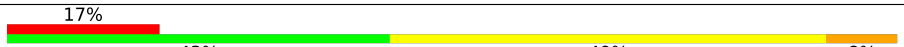
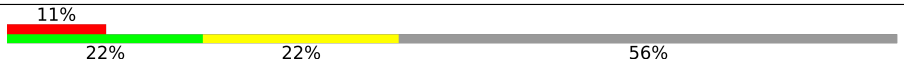
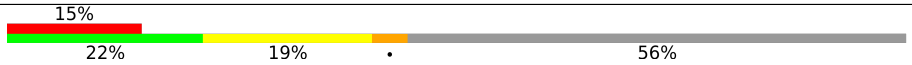
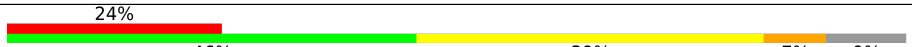
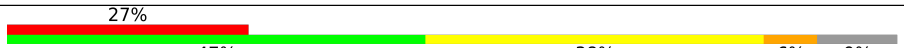
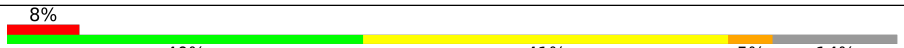
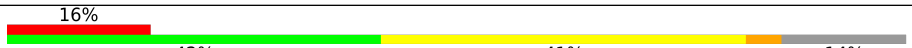
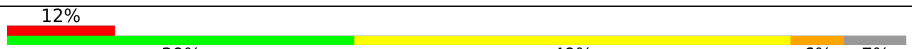
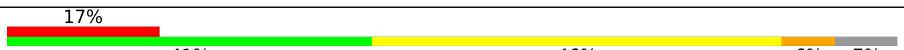
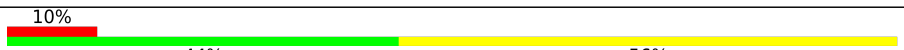
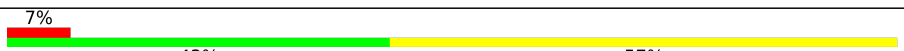
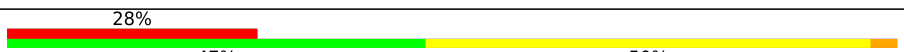
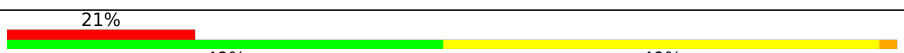
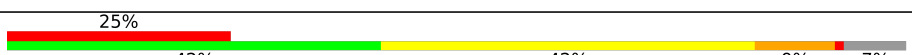
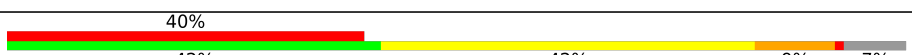
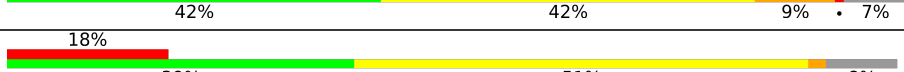
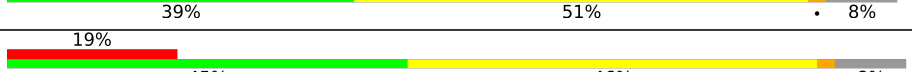
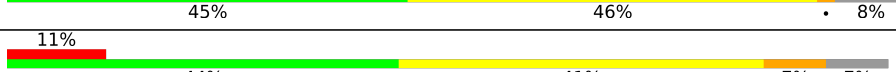
Mol	Chain	Length	Quality of chain
2	CY	77	
2	CZ	77	
3	AV	27	
3	CV	27	
4	AB	256	
4	CB	256	
5	AC	239	
5	CC	239	
6	AD	209	
6	CD	209	
7	AE	162	
7	CE	162	
8	AF	101	
8	CF	101	
9	AG	156	
9	CG	156	
10	AH	138	
10	CH	138	
11	AI	128	
11	CI	128	
12	AJ	105	
12	CJ	105	
13	AK	129	
13	CK	129	
14	AL	134	

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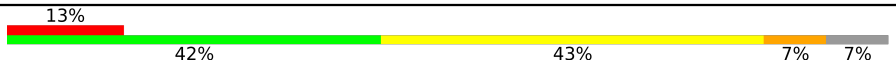
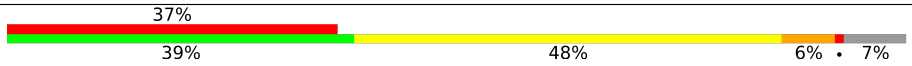
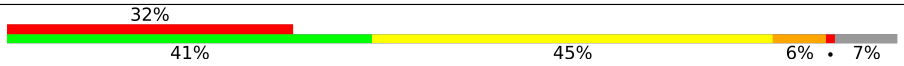
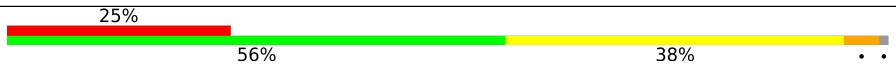
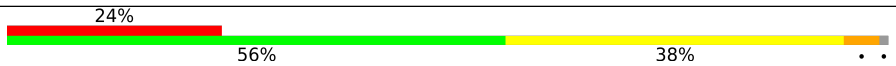
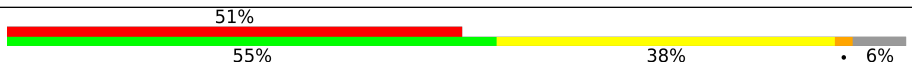
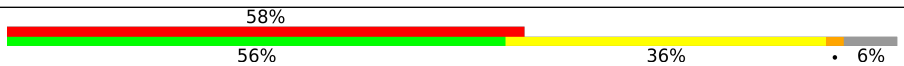
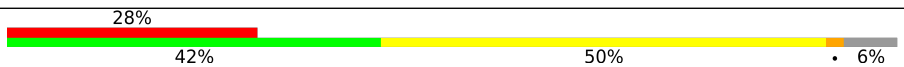
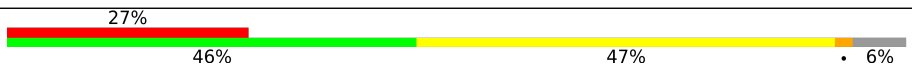
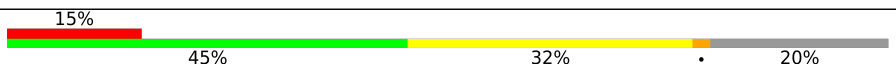
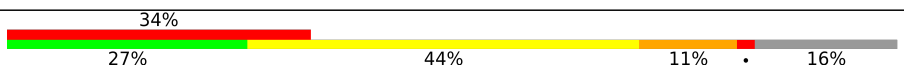
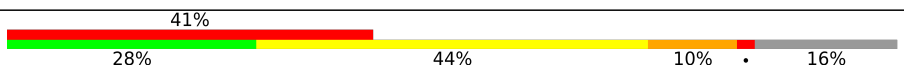
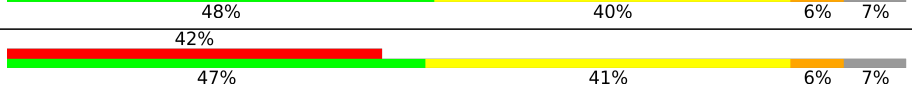
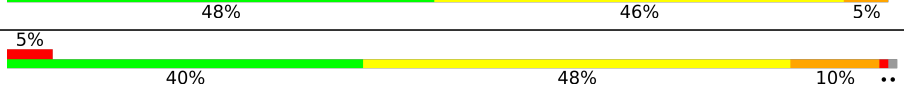
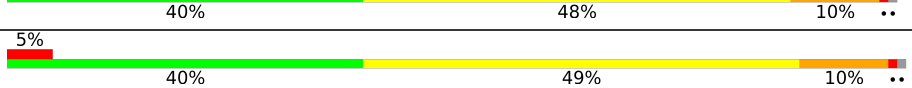
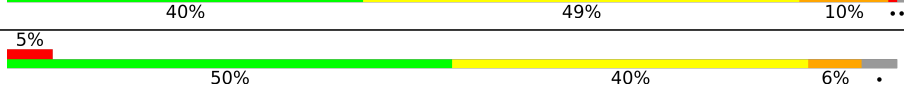
Mol	Chain	Length	Quality of chain
14	CL	134	
15	AM	126	
15	CM	126	
16	AN	61	
16	CN	61	
17	AO	89	
17	CO	89	
18	AP	88	
18	CP	88	
19	AQ	105	
19	CQ	105	
20	AR	88	
20	CR	88	
21	AS	93	
21	CS	93	
22	AT	106	
22	CT	106	
23	AU	27	
23	CU	27	
24	AX	354	
24	CX	354	
25	BA	2894	
25	DA	2894	
26	BB	124	
26	DB	124	

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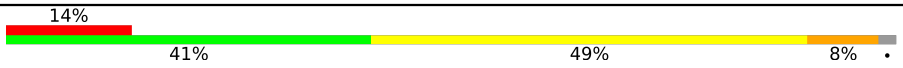
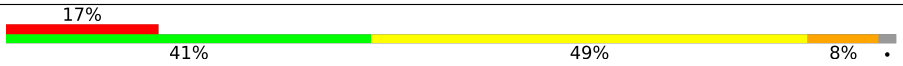
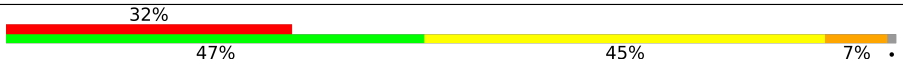
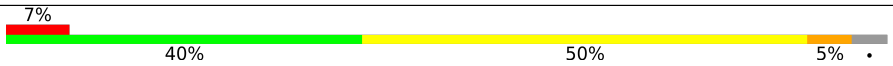
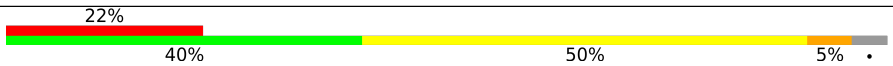
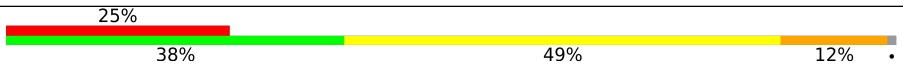
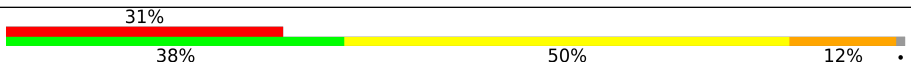
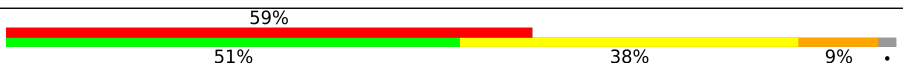
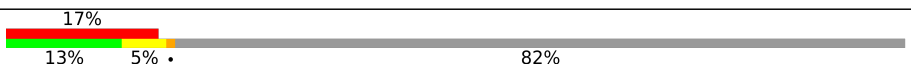
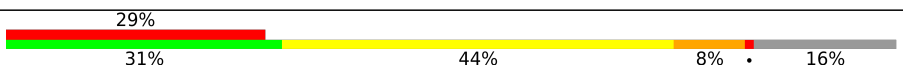
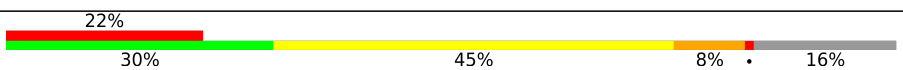
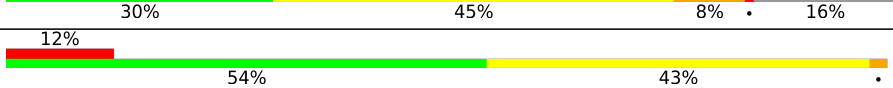
Mol	Chain	Length	Quality of chain
27	BD	276	
27	DD	276	
28	BE	206	
28	DE	206	
29	BF	210	
29	DF	210	
30	BG	182	
30	DG	182	
31	BH	180	
31	DH	180	
32	BI	148	
32	DI	148	
33	BJ	173	
33	DJ	173	
34	BN	163	
34	DN	163	
35	BO	122	
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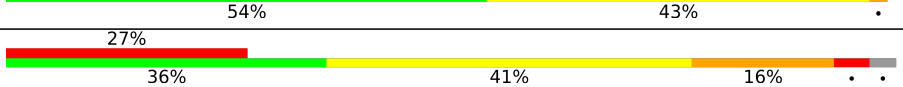
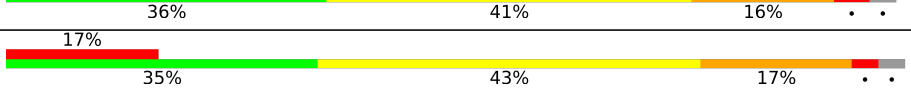
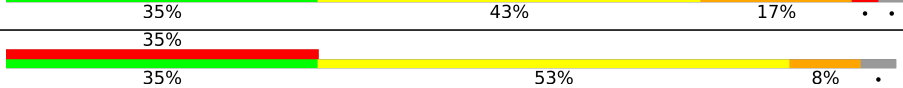
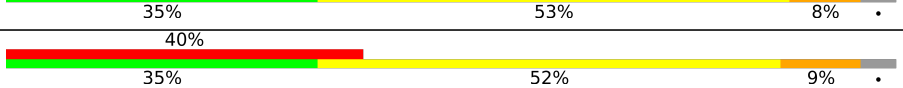
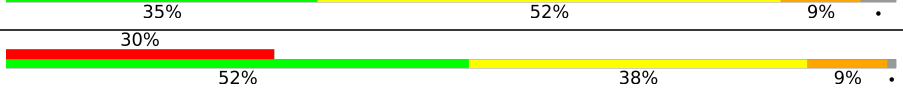
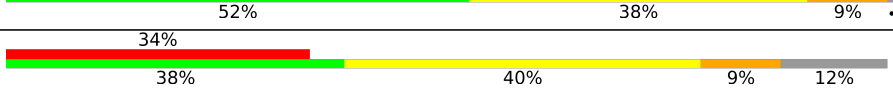
36	BP	150	
36	DP	150	
37	BQ	141	
37	DQ	141	
38	BR	118	
38	DR	118	
39	BS	112	

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Mol	Chain	Length	Quality of chain
39	DS	112	27% 38% 40% 9% 12%
40	BT	146	11% 45% 38% 9% 6%
40	DT	146	27% 42% 41% 9% 6%
41	BU	118	21% 41% 53% 5%
41	DU	118	31% 42% 51% 6%
42	BV	101	18% 47% 42% 12%
42	DV	101	20% 48% 41% 12%
43	BW	113	12% 52% 44%
43	DW	113	10% 51% 45%
44	BX	96	27% 35% 55% 5%
44	DX	96	23% 35% 55% 5%
45	BY	110	52% 34% 45% 12% 9%
45	DY	110	41% 35% 44% 11% 9%
46	BZ	206	28% 49% 38% 9%
46	DZ	206	16% 46% 41% 9%
47	B0	85	40% 45% 41% 11%
47	D0	85	46% 44% 41% 5% 11%
48	B1	98	15% 37% 44% 9% 10%
48	D1	98	17% 38% 44% 8% 10%
49	B2	72	21% 33% 56% 11%
49	D2	72	25% 33% 56% 11%
50	B3	60	37% 53% 40%
50	D3	60	23% 57% 37%
51	B4	97	11% 9% 21% 69%
51	D4	97	8% 8% 22% 69%

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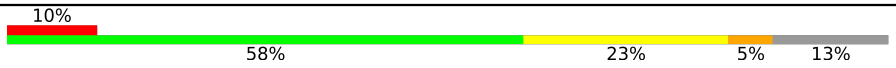
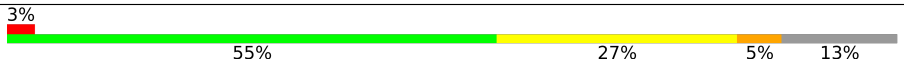
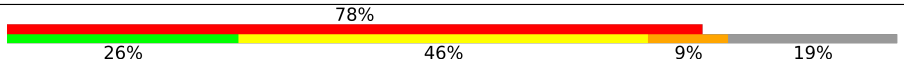
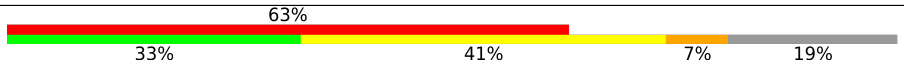
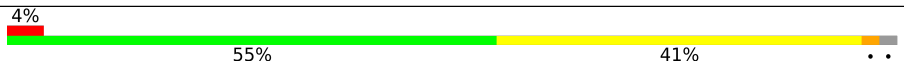
Mol	Chain	Length	Quality of chain
52	B5	60	
52	D5	60	
53	B6	54	
53	D6	54	
54	B7	49	
54	D7	49	
55	B8	65	
55	D8	65	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	BA	3677	-	-	-	X
56	MG	BR	202	-	-	-	X
56	MG	CA	1905	-	-	-	X
56	MG	CA	1930	-	-	-	X
56	MG	DA	3546	-	-	-	X
56	MG	DA	3661	-	-	-	X
56	MG	DA	3673	-	-	-	X

2 Entry composition (i)

There are 57 unique types of molecules in this entry. The entry contains 299961 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.

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			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AA	466	G	C	conflict	GB 155076
CA	466	G	C	conflict	GB 155076

- Molecule 2 is a RNA chain called P and E-site tRNA(fMet).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AZ	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			
2	AY	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			
2	CZ	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			
2	CY	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			

- Molecule 3 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AV	12	Total	C	N	O	P	0	0	0
			258	118	54	75	11			
3	CV	12	Total	C	N	O	P	0	0	0
			258	118	54	75	11			

- Molecule 4 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AB	234	Total	C	N	O	S	0	0	0
			1900	1213	341	341	5			
4	CB	234	Total	C	N	O	S	0	0	0
			1900	1213	341	341	5			

- Molecule 5 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AC	206	Total	C	N	O	S	0	0	0
			1612	1016	314	281	1			
5	CC	206	Total	C	N	O	S	0	0	0
			1612	1016	314	281	1			

- Molecule 6 is a protein called 30S ribosomal protein S4.

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

- Molecule 7 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AE	151	Total	C	N	O	S	0	0	0
			1155	729	218	204	4			
7	CE	151	Total	C	N	O	S	0	0	0
			1155	729	218	204	4			

- Molecule 8 is a protein called 30S ribosomal protein S6.

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

- Molecule 9 is a protein called 30S ribosomal protein S7.

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

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

- Molecule 10 is a protein called 30S ribosomal protein S8.

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

- Molecule 11 is a protein called 30S ribosomal protein S9.

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

- Molecule 12 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AJ	98	Total	C	N	O	S	0	0	0
			794	499	156	138	1			
12	CJ	98	Total	C	N	O	S	0	0	0
			794	499	156	138	1			

- Molecule 13 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AK	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			
13	CK	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			

- Molecule 14 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AL	124	Total	C	N	O	S	0	0	0
			970	611	195	163	1			
14	CL	124	Total	C	N	O	S	0	0	0
			970	611	195	163	1			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AL	2	ALA	-	insertion	UNP P61941
AL	3	LEU	-	insertion	UNP P61941
CL	2	ALA	-	insertion	UNP P61941
CL	3	LEU	-	insertion	UNP P61941

- Molecule 15 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AM	117	Total	C	N	O	S	0	0	0
			933	577	192	162	2			
15	CM	117	Total	C	N	O	S	0	0	0
			933	577	192	162	2			

- Molecule 16 is a protein called 30S ribosomal protein S14.

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

- Molecule 17 is a protein called 30S ribosomal protein S15.

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

- Molecule 18 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	AP	83	Total	C	N	O	S	0	0	0
			700	443	139	117	1			
18	CP	83	Total	C	N	O	S	0	0	0
			700	443	139	117	1			

- Molecule 19 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AQ	99	Total	C	N	O	S	0	0	0
			823	528	152	141	2			
19	CQ	99	Total	C	N	O	S	0	0	0
			823	528	152	141	2			

- Molecule 20 is a protein called 30S ribosomal protein S18.

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

- Molecule 21 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	AS	78	Total	C	N	O	S	0	0	0
			629	403	114	110	2			
21	CS	78	Total	C	N	O	S	0	0	0
			629	403	114	110	2			

- Molecule 22 is a protein called 30S ribosomal protein S20.

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
23	AU	24	Total	C	N	O	0	0	0
			208	128	50	30			
23	CU	24	Total	C	N	O	0	0	0
			208	128	50	30			

- Molecule 24 is a protein called Peptide chain release factor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	AX	354	Total	C	N	O	S	0	0	0
			2813	1743	509	549	12			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	CX	354	Total	C	N	O	S	0	0	0
			2813	1743	509	549	12			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	BA	2879	Total	C	N	O	P	0	0	0
			61997	27594	11582	19943	2878			
25	DA	2879	Total	C	N	O	P	0	0	0
			61997	27594	11582	19943	2878			

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

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			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BB	-1	A	-	insertion	GB 48271
BB	120	U	-	insertion	GB 48271
BB	121	U	-	insertion	GB 48271
DB	-1	A	-	insertion	GB 48271
DB	120	U	-	insertion	GB 48271
DB	121	U	-	insertion	GB 48271

- 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
			2104	1329	416	356	3			
27	DD	271	Total	C	N	O	S	0	0	0
			2104	1329	416	356	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
			1563	988	299	270	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	DE	204	Total	C	N	O	S	0	0	0
			1563	988	299	270	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
			1586	1011	297	275	3			
29	DF	202	Total	C	N	O	S	0	0	0
			1586	1011	297	275	3			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BF	1	MET	-	insertion	UNP Q72I05
BF	2	LYS	-	insertion	UNP Q72I05
BF	3	GLU	-	insertion	UNP Q72I05
BF	4	VAL	-	insertion	UNP Q72I05
BF	5	ALA	-	insertion	UNP Q72I05
DF	1	MET	-	insertion	UNP Q72I05
DF	2	LYS	-	insertion	UNP Q72I05
DF	3	GLU	-	insertion	UNP Q72I05
DF	4	VAL	-	insertion	UNP Q72I05
DF	5	ALA	-	insertion	UNP Q72I05

- 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
			1222	773	228	220	1			
31	DH	159	Total	C	N	O	S	0	0	0
			1222	773	228	220	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
			1132	724	200	207	1			
32	DI	145	Total	C	N	O	S	0	0	0
			1132	724	200	207	1			

- Molecule 33 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
33	BJ	32	Total	C	N	O	0	0	0
			253	157	49	47			
33	DJ	32	Total	C	N	O	0	0	0
			253	157	49	47			

- 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
			1096	707	205	181	3			
34	DN	137	Total	C	N	O	S	0	0	0
			1096	707	205	181	3			

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BN	2	VAL	-	insertion	UNP Q72IN1
BN	3	LYS	-	insertion	UNP Q72IN1
BN	4	SER	-	insertion	UNP Q72IN1
BN	5	SER	-	insertion	UNP Q72IN1
BN	6	LEU	-	insertion	UNP Q72IN1
BN	7	ALA	-	insertion	UNP Q72IN1
BN	8	PHE	-	insertion	UNP Q72IN1
BN	9	LEU	-	insertion	UNP Q72IN1
BN	10	ARG	-	insertion	UNP Q72IN1
BN	11	GLY	-	insertion	UNP Q72IN1
BN	12	PRO	-	insertion	UNP Q72IN1
BN	13	PRO	-	insertion	UNP Q72IN1
BN	14	ILE	-	insertion	UNP Q72IN1
BN	15	PRO	-	insertion	UNP Q72IN1
BN	16	ARG	-	insertion	UNP Q72IN1
BN	17	GLN	-	insertion	UNP Q72IN1
BN	18	GLU	-	insertion	UNP Q72IN1
BN	19	GLN	-	insertion	UNP Q72IN1
BN	20	ARG	-	insertion	UNP Q72IN1

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Chain	Residue	Modelled	Actual	Comment	Reference
BN	21	ARG	-	insertion	UNP Q72IN1
BN	22	ALA	-	insertion	UNP Q72IN1
BN	23	LEU	-	insertion	UNP Q72IN1
BN	24	VAL	-	insertion	UNP Q72IN1
DN	2	VAL	-	insertion	UNP Q72IN1
DN	3	LYS	-	insertion	UNP Q72IN1
DN	4	SER	-	insertion	UNP Q72IN1
DN	5	SER	-	insertion	UNP Q72IN1
DN	6	LEU	-	insertion	UNP Q72IN1
DN	7	ALA	-	insertion	UNP Q72IN1
DN	8	PHE	-	insertion	UNP Q72IN1
DN	9	LEU	-	insertion	UNP Q72IN1
DN	10	ARG	-	insertion	UNP Q72IN1
DN	11	GLY	-	insertion	UNP Q72IN1
DN	12	PRO	-	insertion	UNP Q72IN1
DN	13	PRO	-	insertion	UNP Q72IN1
DN	14	ILE	-	insertion	UNP Q72IN1
DN	15	PRO	-	insertion	UNP Q72IN1
DN	16	ARG	-	insertion	UNP Q72IN1
DN	17	GLN	-	insertion	UNP Q72IN1
DN	18	GLU	-	insertion	UNP Q72IN1
DN	19	GLN	-	insertion	UNP Q72IN1
DN	20	ARG	-	insertion	UNP Q72IN1
DN	21	ARG	-	insertion	UNP Q72IN1
DN	22	ALA	-	insertion	UNP Q72IN1
DN	23	LEU	-	insertion	UNP Q72IN1
DN	24	VAL	-	insertion	UNP Q72IN1

- 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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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	136	Total	C	N	O	S	0	0	0
			1079	688	204	182	5			
37	DQ	136	Total	C	N	O	S	0	0	0
			1079	688	204	182	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
			770	486	154	130			
39	DS	98	Total	C	N	O	0	0	0
			770	486	154	130			

- 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
			1143	713	234	195	1			
40	DT	137	Total	C	N	O	S	0	0	0
			1143	713	234	195	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
			890	560	175	153	2			
43	DW	112	Total	C	N	O	S	0	0	0
			890	560	175	153	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
			725	471	131	123			
44	DX	92	Total	C	N	O	0	0	0
			725	471	131	123			

- 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
			775	500	148	123	4			
45	DY	100	Total	C	N	O	S	0	0	0
			775	500	148	123	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	BZ	188	Total	C	N	O	S	0	0	0
			1491	950	265	274	2			
46	DZ	188	Total	C	N	O	S	0	0	0
			1491	950	265	274	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
			694	435	141	118			
48	D1	88	Total	C	N	O	0	0	0
			694	435	141	118			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	B2	72	Total	C	N	O	S	0	0	0
			605	375	122	106	2			
49	D2	72	Total	C	N	O	S	0	0	0
			605	375	122	106	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
			467	298	90	78	1			
50	D3	59	Total	C	N	O	S	0	0	0
			467	298	90	78	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
			225	142	36	43	4			
51	D4	30	Total	C	N	O	S	0	0	0
			225	142	36	43	4			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B4	2	PRO	-	insertion	UNP Q72JR0
B4	3	LEU	-	insertion	UNP Q72JR0
B4	4	GLY	-	insertion	UNP Q72JR0

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Chain	Residue	Modelled	Actual	Comment	Reference
B4	5	VAL	-	insertion	UNP Q72JR0
B4	6	HIS	-	insertion	UNP Q72JR0
B4	7	PRO	-	insertion	UNP Q72JR0
B4	8	LEU	-	insertion	UNP Q72JR0
B4	9	TYR	-	insertion	UNP Q72JR0
B4	10	THR	-	insertion	UNP Q72JR0
B4	11	LYS	-	insertion	UNP Q72JR0
B4	12	ARG	-	insertion	UNP Q72JR0
B4	13	TRP	-	insertion	UNP Q72JR0
B4	14	LEU	-	insertion	UNP Q72JR0
B4	15	ALA	-	insertion	UNP Q72JR0
B4	16	HIS	-	insertion	UNP Q72JR0
B4	17	GLY	-	insertion	UNP Q72JR0
B4	18	GLN	-	insertion	UNP Q72JR0
B4	19	ASP	-	insertion	UNP Q72JR0
B4	20	ARG	-	insertion	UNP Q72JR0
B4	21	ALA	-	insertion	UNP Q72JR0
B4	22	LYS	-	insertion	UNP Q72JR0
B4	23	LYS	-	insertion	UNP Q72JR0
B4	24	GLU	-	insertion	UNP Q72JR0
B4	25	ALA	-	insertion	UNP Q72JR0
B4	26	ASN	-	insertion	UNP Q72JR0
B4	27	VAL	-	insertion	UNP Q72JR0
D4	2	PRO	-	insertion	UNP Q72JR0
D4	3	LEU	-	insertion	UNP Q72JR0
D4	4	GLY	-	insertion	UNP Q72JR0
D4	5	VAL	-	insertion	UNP Q72JR0
D4	6	HIS	-	insertion	UNP Q72JR0
D4	7	PRO	-	insertion	UNP Q72JR0
D4	8	LEU	-	insertion	UNP Q72JR0
D4	9	TYR	-	insertion	UNP Q72JR0
D4	10	THR	-	insertion	UNP Q72JR0
D4	11	LYS	-	insertion	UNP Q72JR0
D4	12	ARG	-	insertion	UNP Q72JR0
D4	13	TRP	-	insertion	UNP Q72JR0
D4	14	LEU	-	insertion	UNP Q72JR0
D4	15	ALA	-	insertion	UNP Q72JR0
D4	16	HIS	-	insertion	UNP Q72JR0
D4	17	GLY	-	insertion	UNP Q72JR0
D4	18	GLN	-	insertion	UNP Q72JR0
D4	19	ASP	-	insertion	UNP Q72JR0
D4	20	ARG	-	insertion	UNP Q72JR0

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Chain	Residue	Modelled	Actual	Comment	Reference
D4	21	ALA	-	insertion	UNP Q72JR0
D4	22	LYS	-	insertion	UNP Q72JR0
D4	23	LYS	-	insertion	UNP Q72JR0
D4	24	GLU	-	insertion	UNP Q72JR0
D4	25	ALA	-	insertion	UNP Q72JR0
D4	26	ASN	-	insertion	UNP Q72JR0
D4	27	VAL	-	insertion	UNP Q72JR0

- 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
			404	255	79	65	5			
52	D5	52	Total	C	N	O	S	0	0	0
			404	255	79	65	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
			380	235	77	64	4			
53	D6	44	Total	C	N	O	S	0	0	0
			380	235	77	64	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
			418	257	104	55	2			
54	D7	48	Total	C	N	O	S	0	0	0
			418	257	104	55	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
			507	326	101	78	2			
55	D8	63	Total	C	N	O	S	0	0	0
			507	326	101	78	2			

- Molecule 56 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	AA	310	Total Mg 310 310	0	0
56	AZ	6	Total Mg 6 6	0	0
56	AV	1	Total Mg 1 1	0	0
56	AY	25	Total Mg 25 25	0	0
56	AB	2	Total Mg 2 2	0	0
56	AC	6	Total Mg 6 6	0	0
56	AD	8	Total Mg 8 8	0	0
56	AE	1	Total Mg 1 1	0	0
56	AF	2	Total Mg 2 2	0	0
56	AG	1	Total Mg 1 1	0	0
56	AH	2	Total Mg 2 2	0	0
56	AI	2	Total Mg 2 2	0	0
56	AJ	1	Total Mg 1 1	0	0
56	AK	1	Total Mg 1 1	0	0
56	AL	2	Total Mg 2 2	0	0
56	AM	1	Total Mg 1 1	0	0
56	AO	3	Total Mg 3 3	0	0
56	AP	1	Total Mg 1 1	0	0
56	AQ	1	Total Mg 1 1	0	0
56	AX	6	Total Mg 6 6	0	0
56	BA	806	Total Mg 806 806	0	0
56	BB	26	Total Mg 26 26	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	BD	2	Total Mg 2 2	0	0
56	BE	1	Total Mg 1 1	0	0
56	BF	5	Total Mg 5 5	0	0
56	BG	3	Total Mg 3 3	0	0
56	BH	2	Total Mg 2 2	0	0
56	BI	3	Total Mg 3 3	0	0
56	BJ	1	Total Mg 1 1	0	0
56	BN	2	Total Mg 2 2	0	0
56	BO	3	Total Mg 3 3	0	0
56	BP	1	Total Mg 1 1	0	0
56	BQ	3	Total Mg 3 3	0	0
56	BR	3	Total Mg 3 3	0	0
56	BT	2	Total Mg 2 2	0	0
56	BU	1	Total Mg 1 1	0	0
56	BV	1	Total Mg 1 1	0	0
56	BW	2	Total Mg 2 2	0	0
56	BY	1	Total Mg 1 1	0	0
56	BZ	1	Total Mg 1 1	0	0
56	B1	2	Total Mg 2 2	0	0
56	B2	3	Total Mg 3 3	0	0
56	B5	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	B7	3	Total Mg 3 3	0	0
56	CA	414	Total Mg 414 414	0	0
56	CZ	19	Total Mg 19 19	0	0
56	CV	4	Total Mg 4 4	0	0
56	CY	21	Total Mg 21 21	0	0
56	CB	2	Total Mg 2 2	0	0
56	CC	7	Total Mg 7 7	0	0
56	CD	2	Total Mg 2 2	0	0
56	CE	1	Total Mg 1 1	0	0
56	CF	1	Total Mg 1 1	0	0
56	CG	1	Total Mg 1 1	0	0
56	CH	1	Total Mg 1 1	0	0
56	CI	2	Total Mg 2 2	0	0
56	CJ	1	Total Mg 1 1	0	0
56	CK	2	Total Mg 2 2	0	0
56	CL	1	Total Mg 1 1	0	0
56	CO	2	Total Mg 2 2	0	0
56	CP	1	Total Mg 1 1	0	0
56	CX	9	Total Mg 9 9	0	0
56	DD	1	Total Mg 1 1	0	0
56	DF	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	DG	1	Total Mg 1 1	0	0
56	DH	4	Total Mg 4 4	0	0
56	DI	2	Total Mg 2 2	0	0
56	DN	1	Total Mg 1 1	0	0
56	DO	2	Total Mg 2 2	0	0
56	DP	6	Total Mg 6 6	0	0
56	DQ	1	Total Mg 1 1	0	0
56	DR	1	Total Mg 1 1	0	0
56	DT	1	Total Mg 1 1	0	0
56	DV	1	Total Mg 1 1	0	0
56	DW	3	Total Mg 3 3	0	0
56	DX	1	Total Mg 1 1	0	0
56	DZ	4	Total Mg 4 4	0	0
56	D2	2	Total Mg 2 2	0	0
56	D3	1	Total Mg 1 1	0	0
56	D4	3	Total Mg 3 3	0	0
56	D5	1	Total Mg 1 1	0	0
56	D7	2	Total Mg 2 2	0	0
56	D8	1	Total Mg 1 1	0	0
56	DA	758	Total Mg 758 758	0	0
56	DB	28	Total Mg 28 28	0	0

- Molecule 57 is ZINC ION (three-letter code: ZN) (formula: Zn).

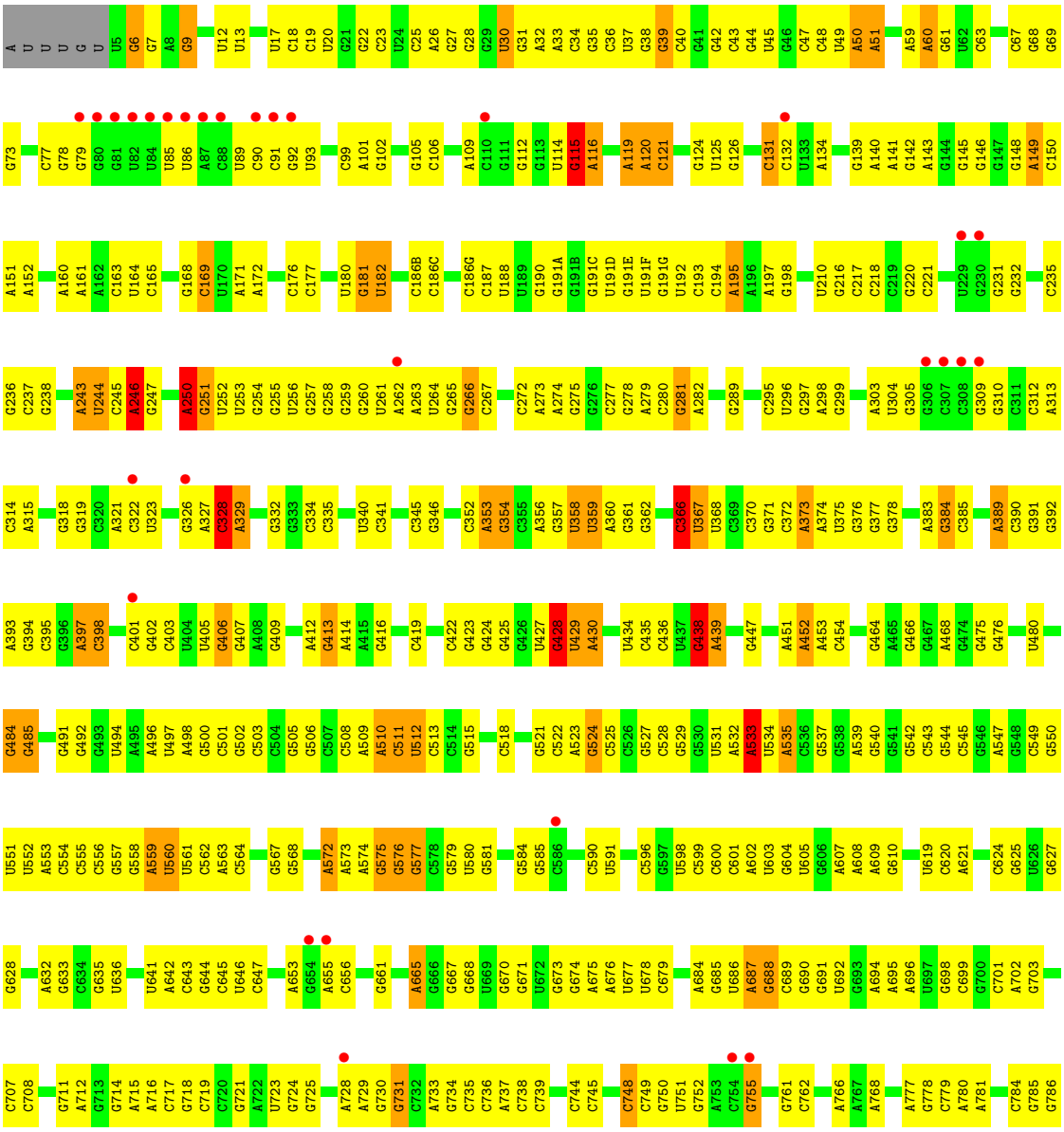
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	AD	1	Total Zn 1 1	0	0
57	AN	1	Total Zn 1 1	0	0
57	CD	1	Total Zn 1 1	0	0
57	CN	1	Total Zn 1 1	0	0

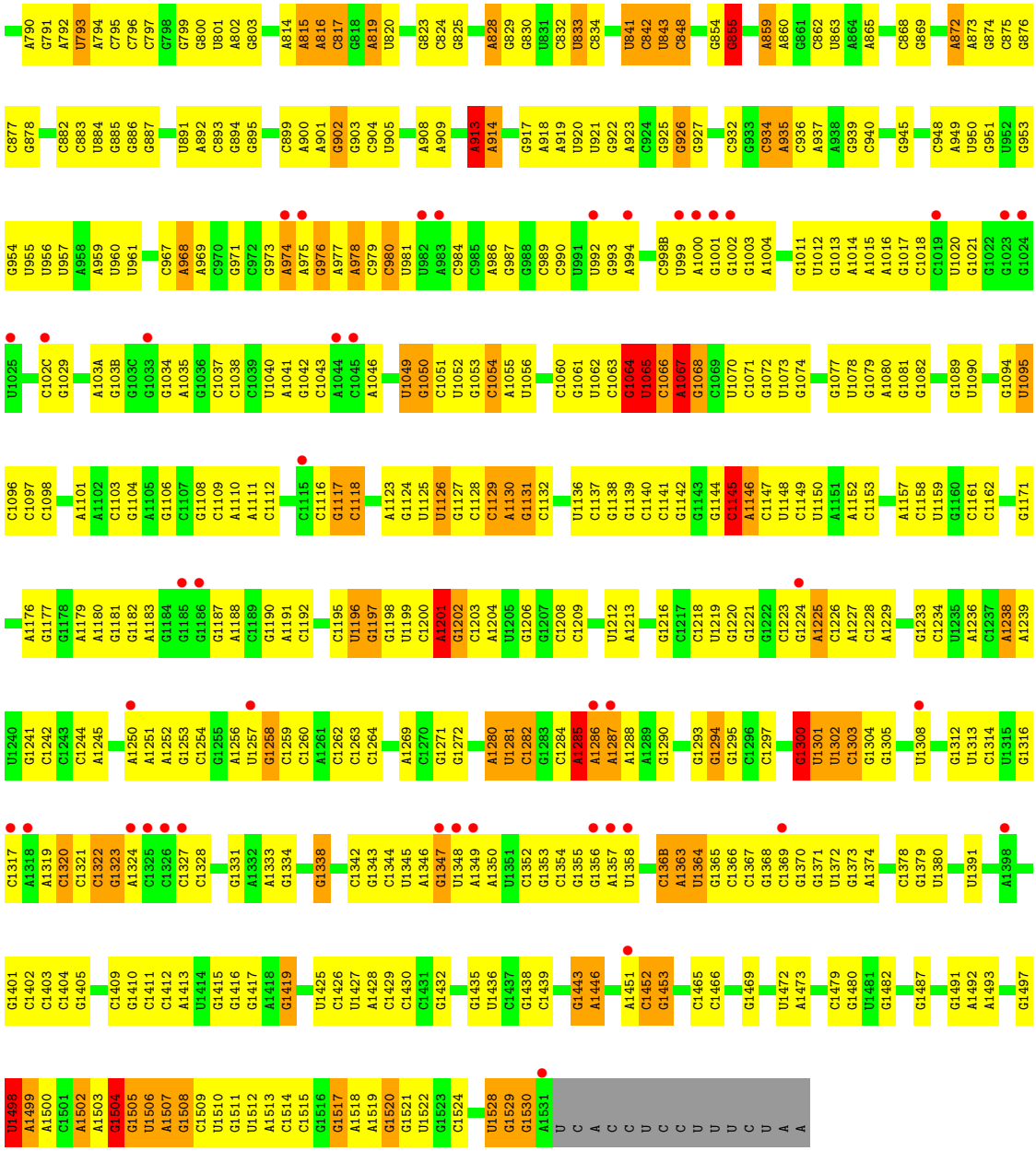
3 Residue-property plots (i)

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

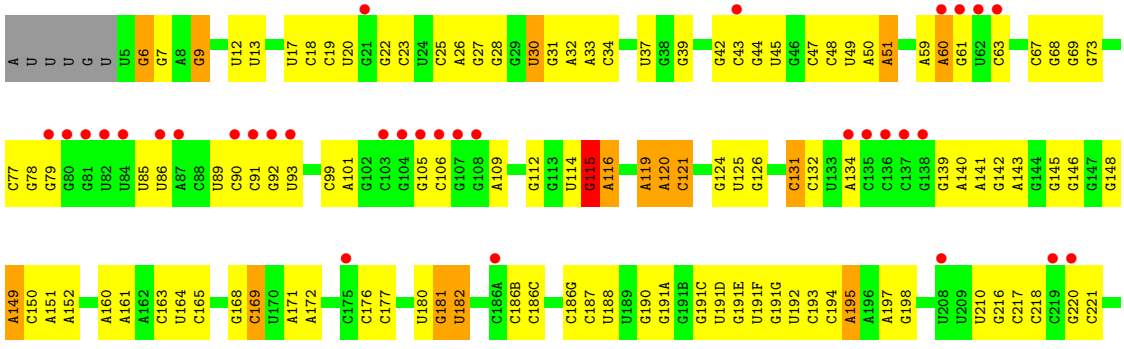
Chain AA:

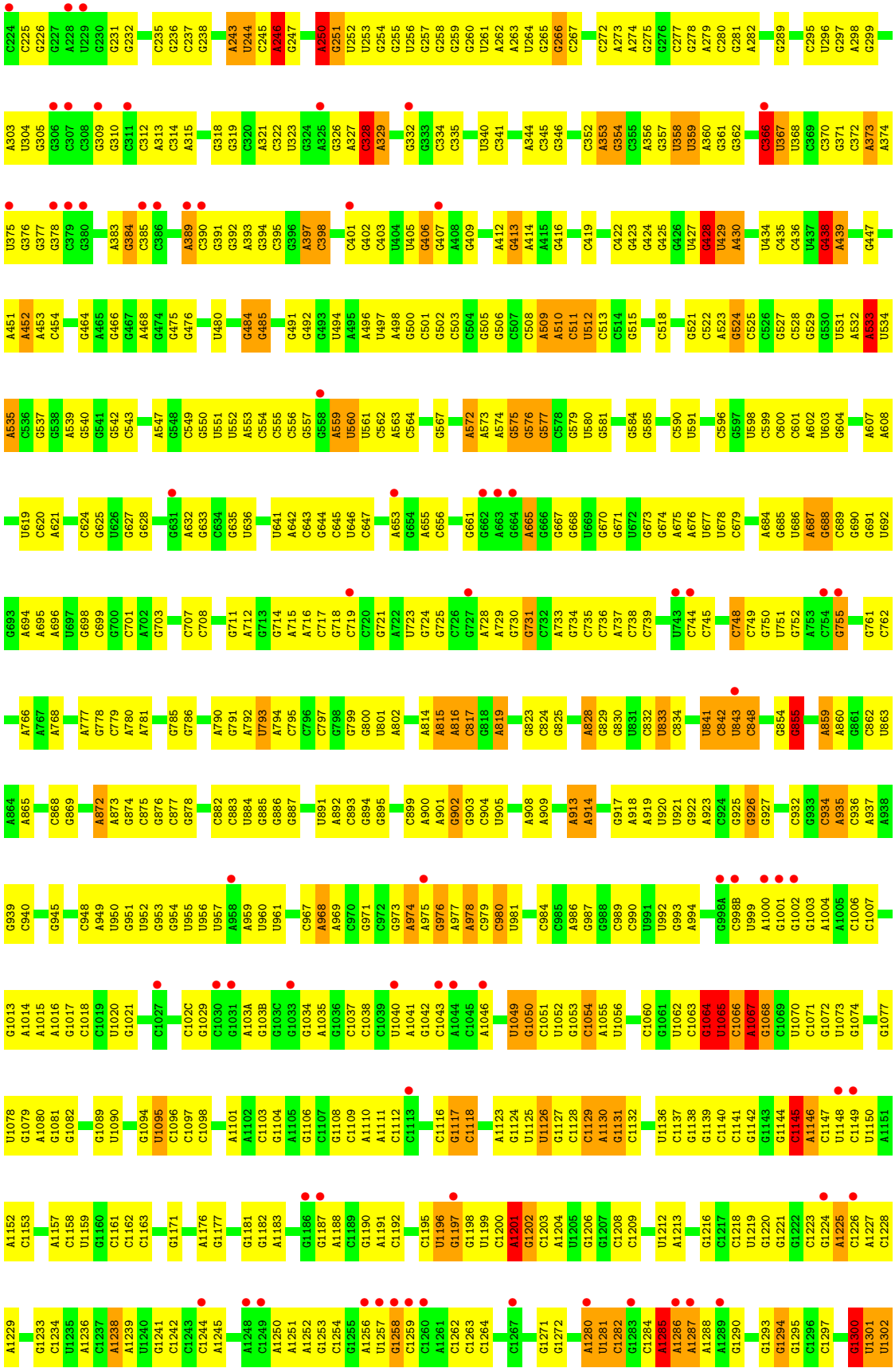


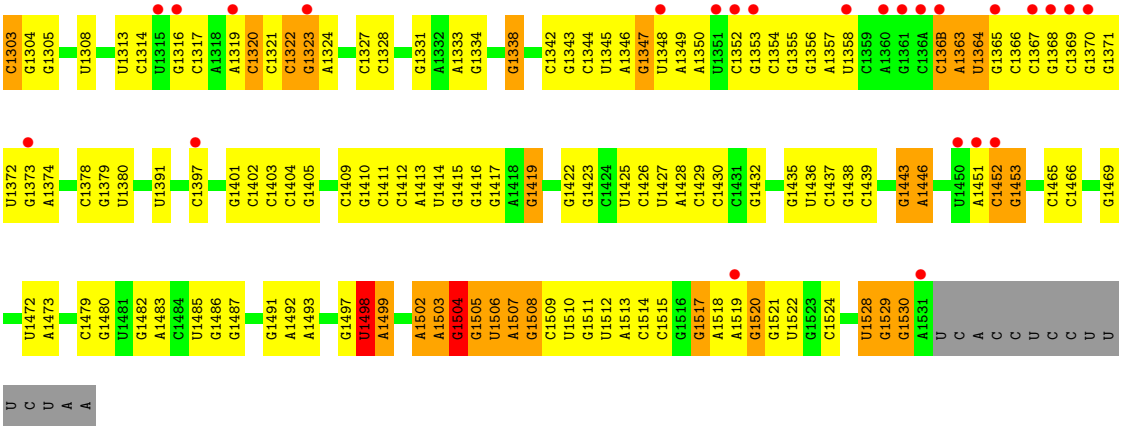


• Molecule 1: 16S RRNA

Chain CA:

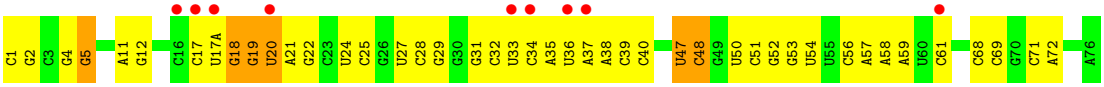






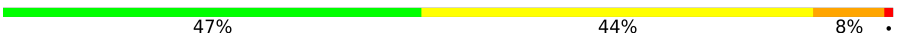
• Molecule 2: P and E-site tRNA(fMet)

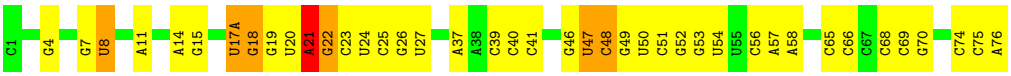
Chain AZ:



• Molecule 2: P and E-site tRNA(fMet)

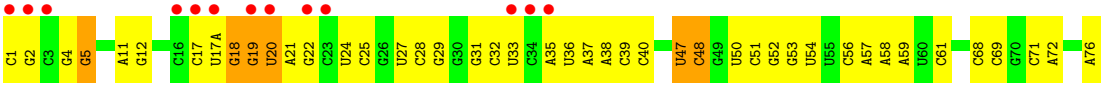
Chain AY:





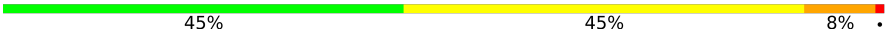
• Molecule 2: P and E-site tRNA(fMet)

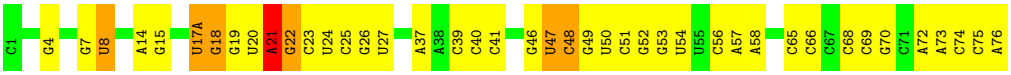
Chain CZ:



• Molecule 2: P and E-site tRNA(fMet)

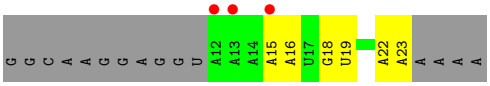
Chain CY:





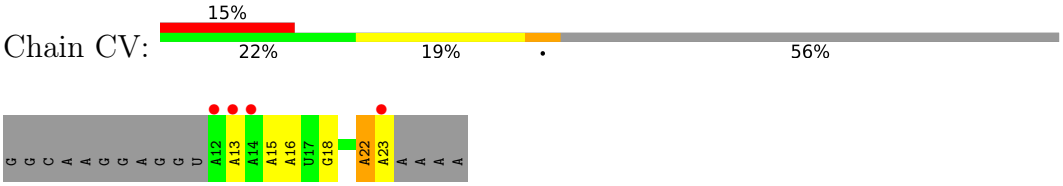
• Molecule 3: mRNA

Chain AV:



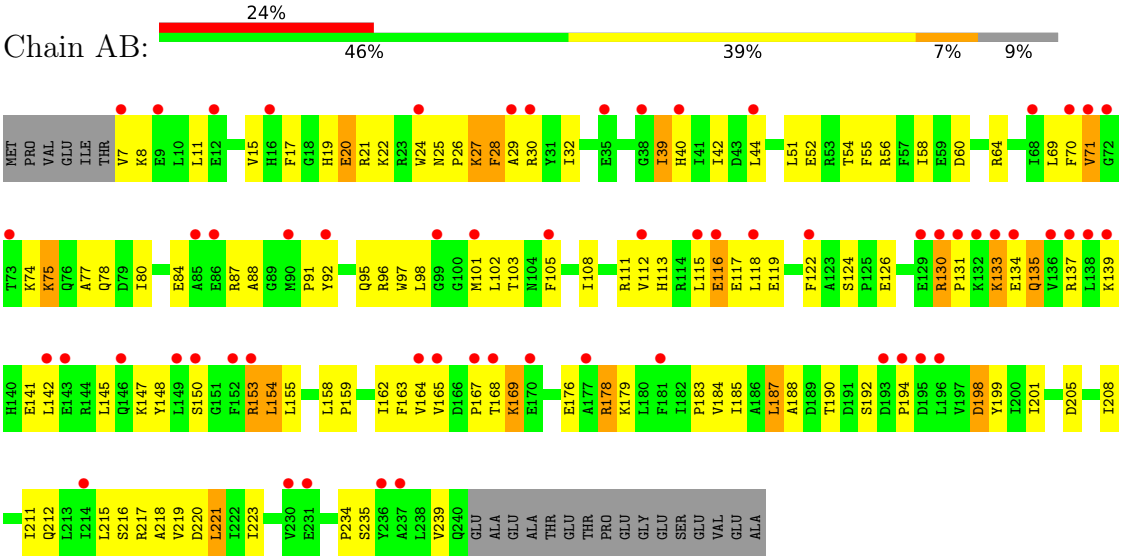
• Molecule 3: mRNA

Chain CV:



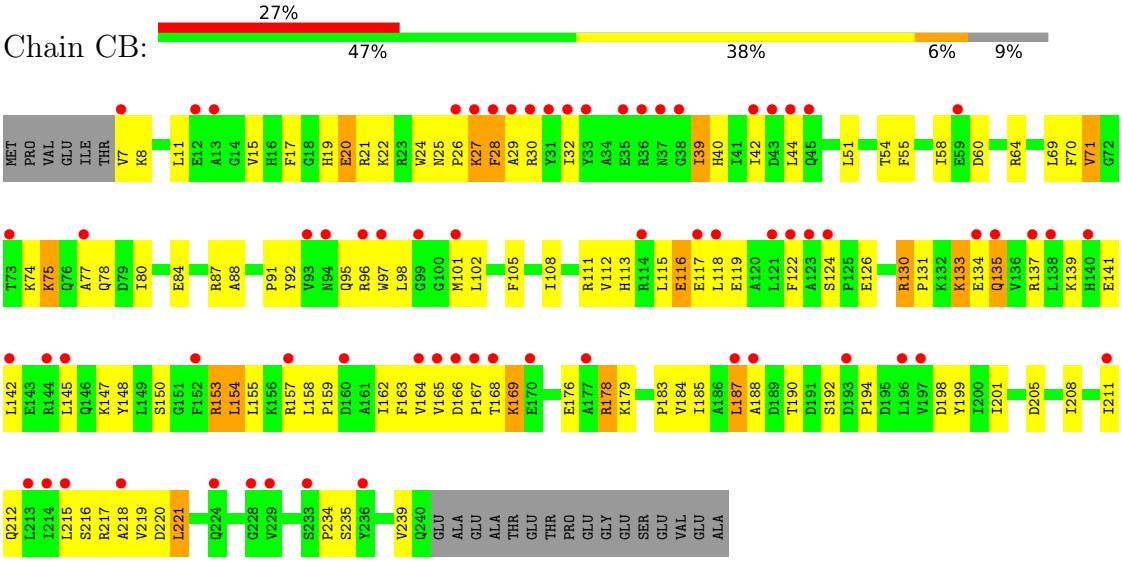
• Molecule 4: 30S ribosomal protein S2

Chain AB:



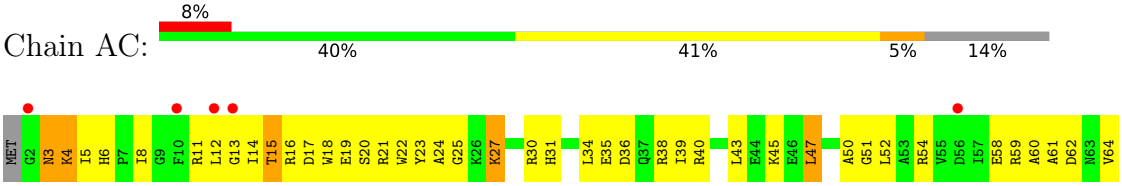
• Molecule 4: 30S ribosomal protein S2

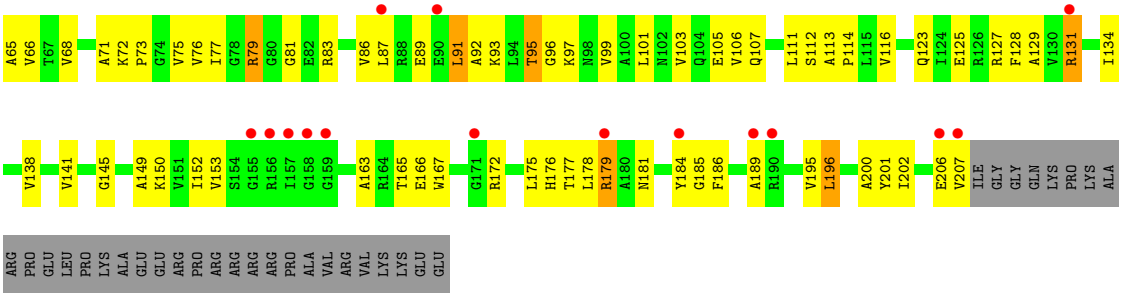
Chain CB:



• Molecule 5: 30S ribosomal protein S3

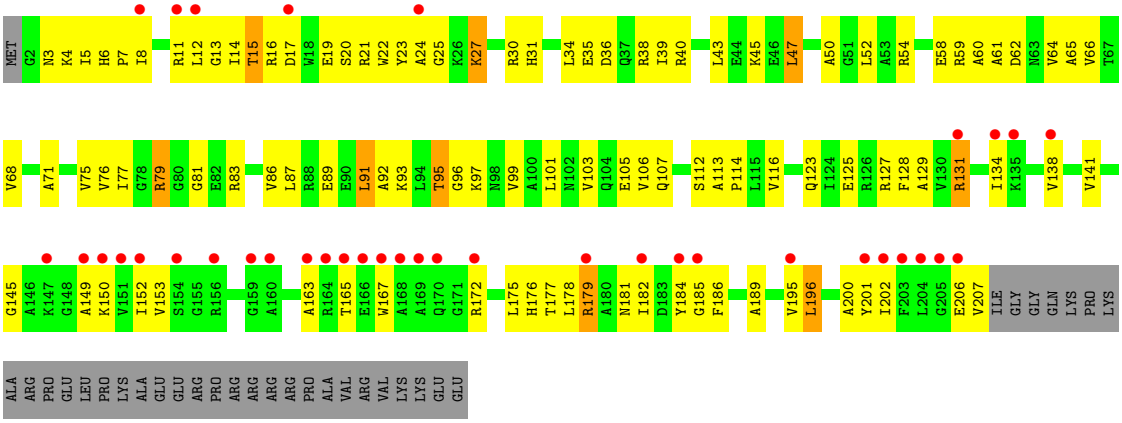
Chain AC:





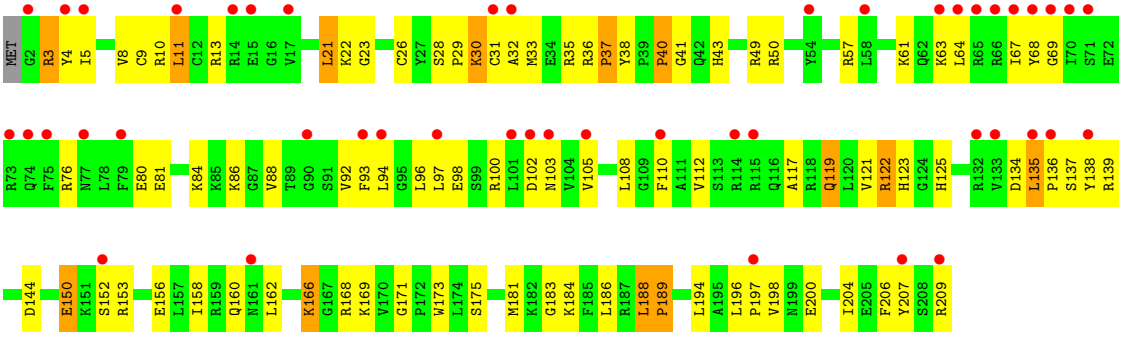
• Molecule 5: 30S ribosomal protein S3

Chain CC:



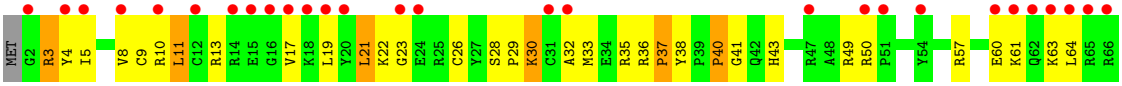
• Molecule 6: 30S ribosomal protein S4

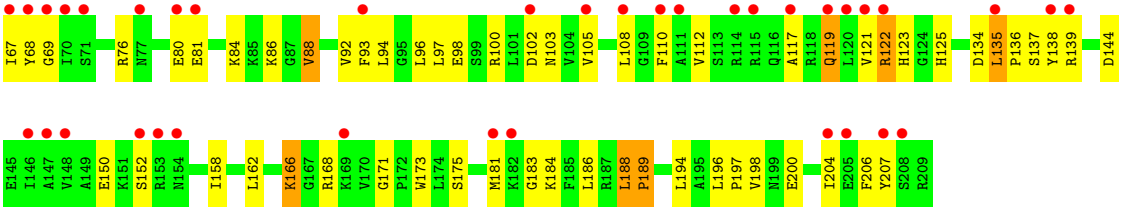
Chain AD:



• Molecule 6: 30S ribosomal protein S4

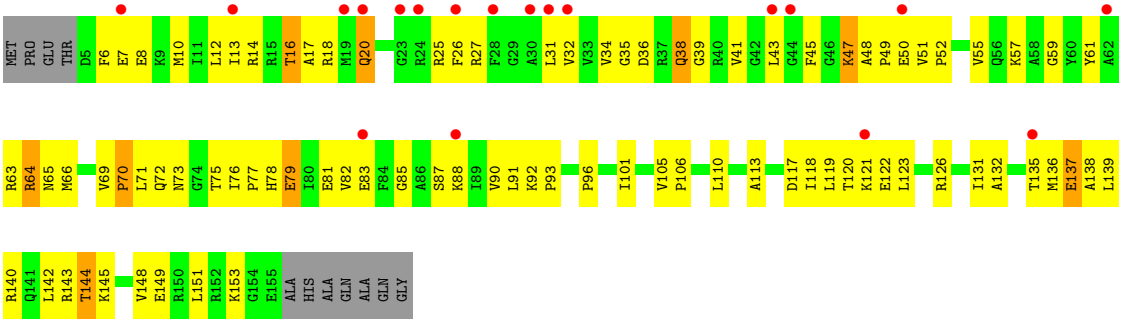
Chain CD:





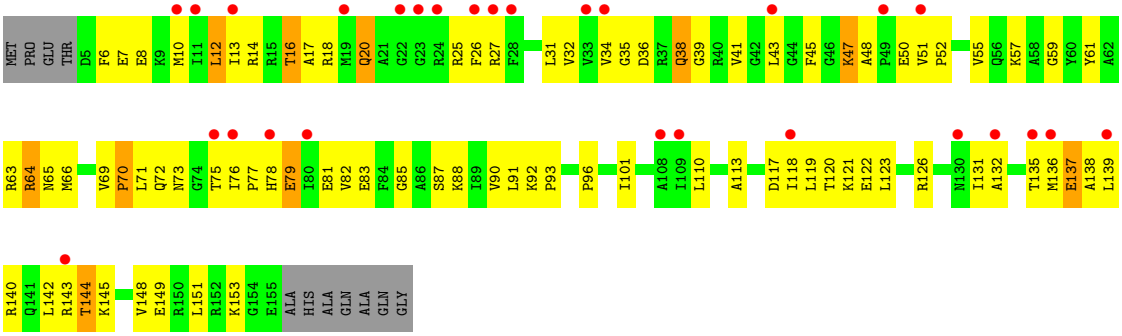
• Molecule 7: 30S ribosomal protein S5

Chain AE:



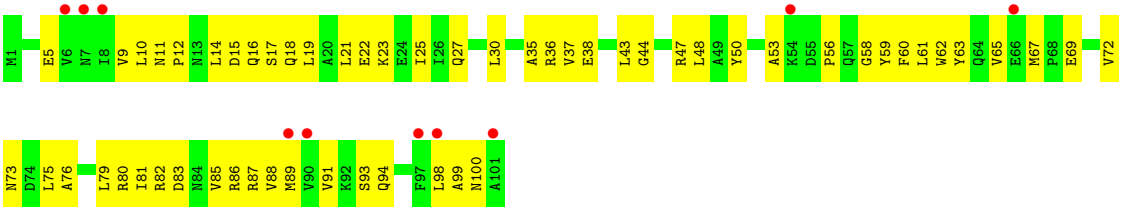
• Molecule 7: 30S ribosomal protein S5

Chain CE:



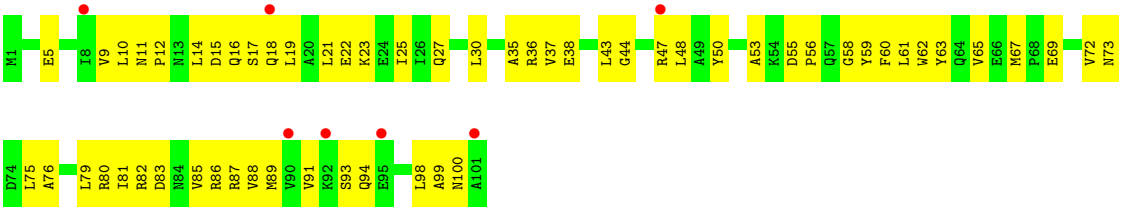
• Molecule 8: 30S ribosomal protein S6

Chain AF:

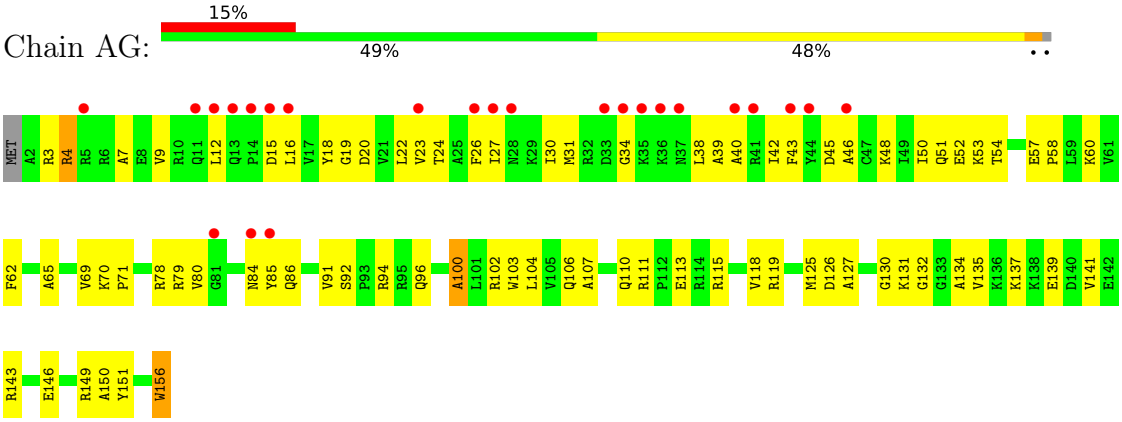


• Molecule 8: 30S ribosomal protein S6

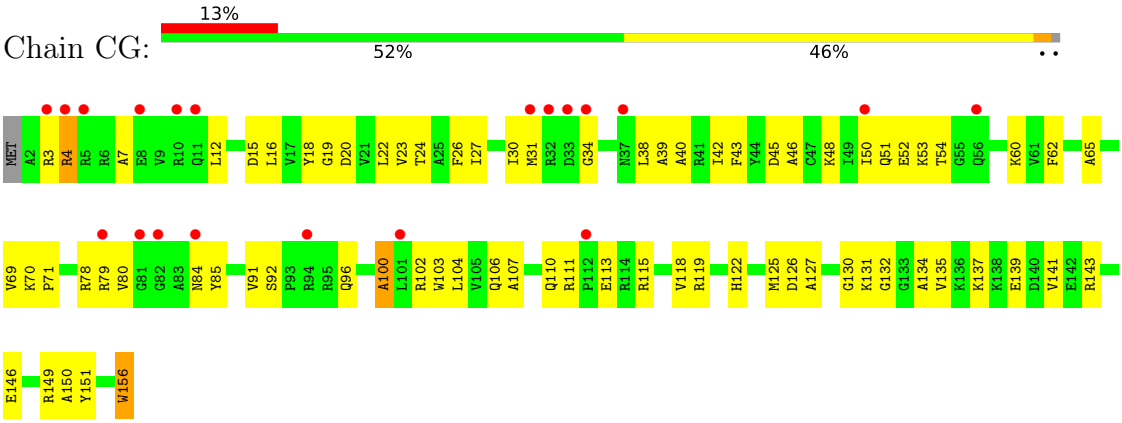
Chain CF:



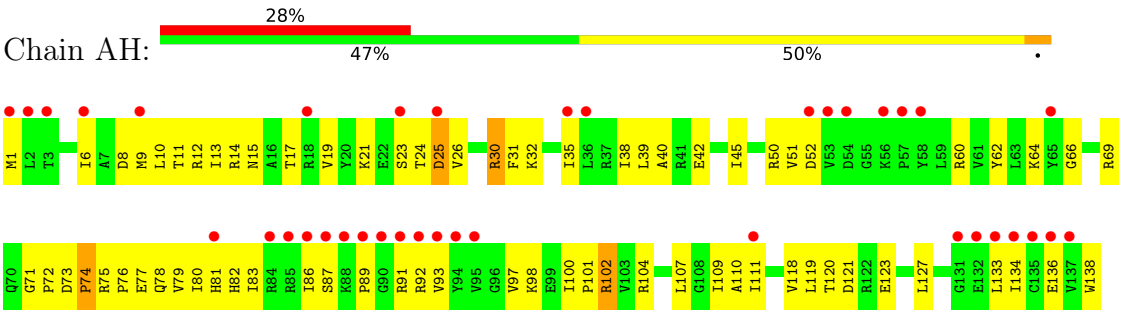
• Molecule 9: 30S ribosomal protein S7



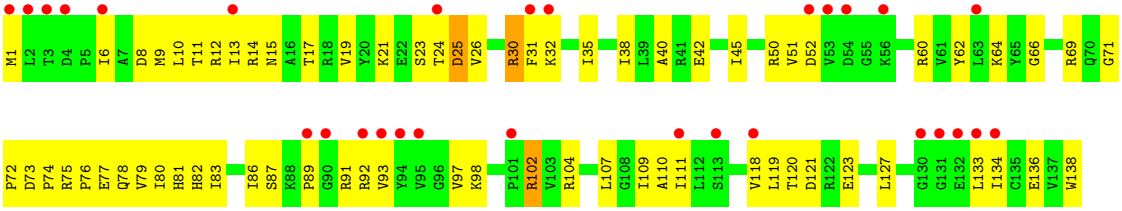
• Molecule 9: 30S ribosomal protein S7



• Molecule 10: 30S ribosomal protein S8

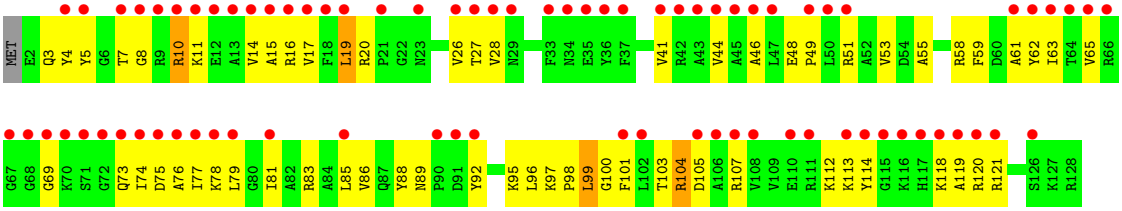


• Molecule 10: 30S ribosomal protein S8



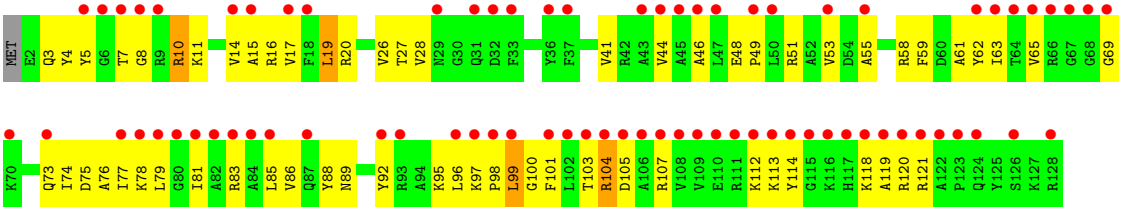
• Molecule 11: 30S ribosomal protein S9

Chain AI:



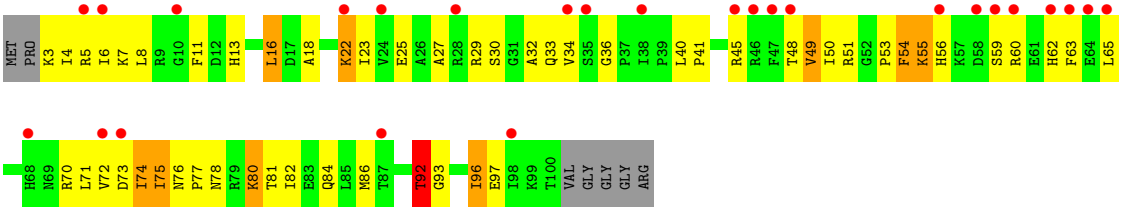
• Molecule 11: 30S ribosomal protein S9

Chain CI:



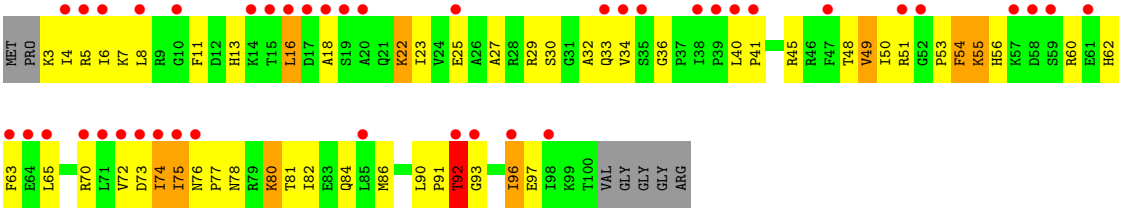
• Molecule 12: 30S ribosomal protein S10

Chain AJ:



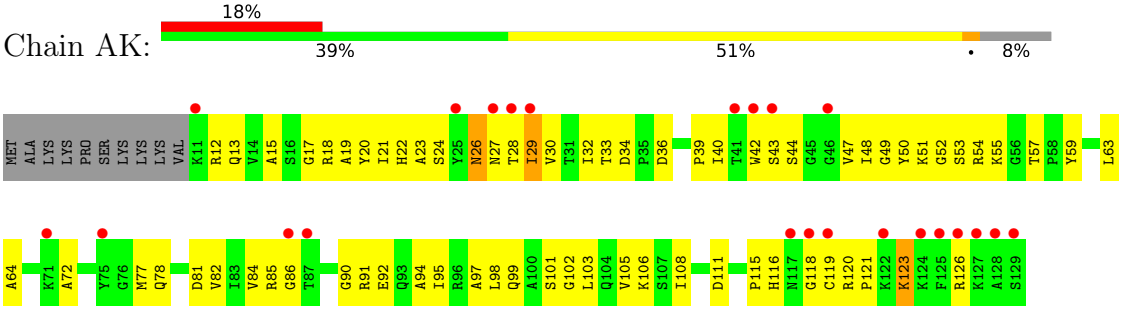
• Molecule 12: 30S ribosomal protein S10

Chain CJ:



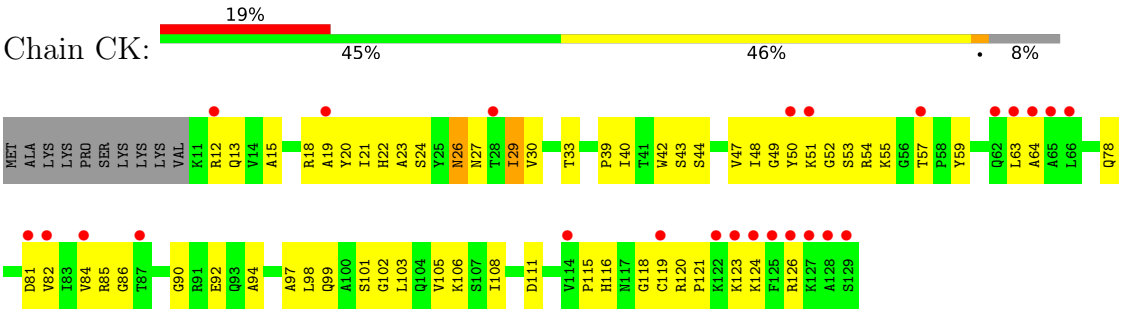
• Molecule 13: 30S ribosomal protein S11

Chain AK:



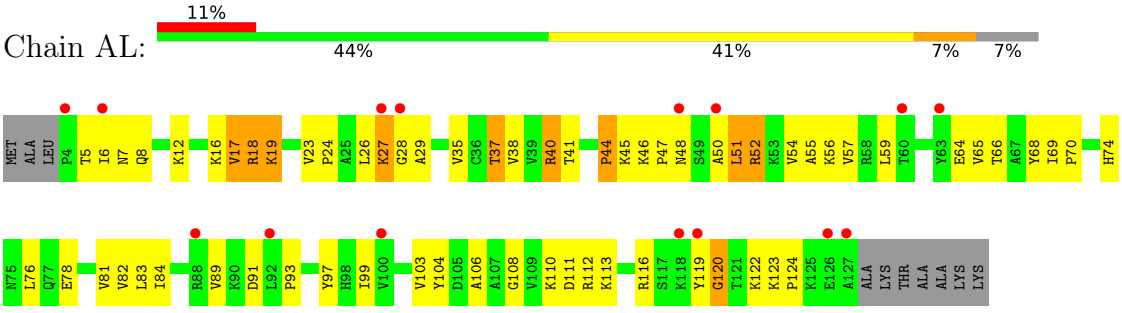
• Molecule 13: 30S ribosomal protein S11

Chain CK:



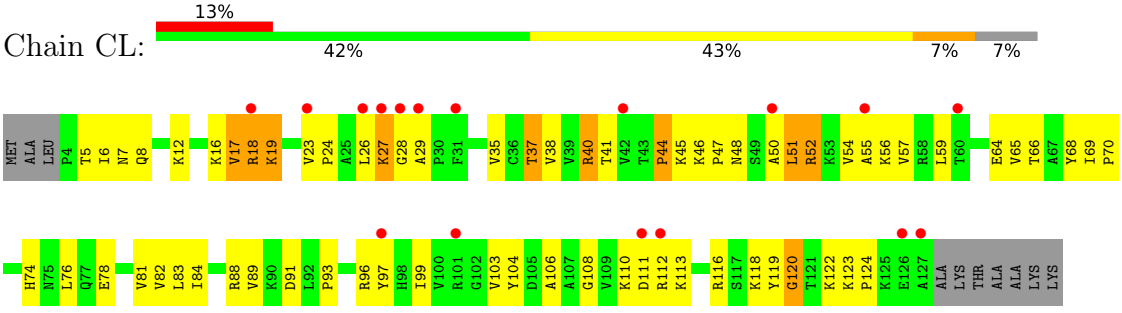
• Molecule 14: 30S ribosomal protein S12

Chain AL:



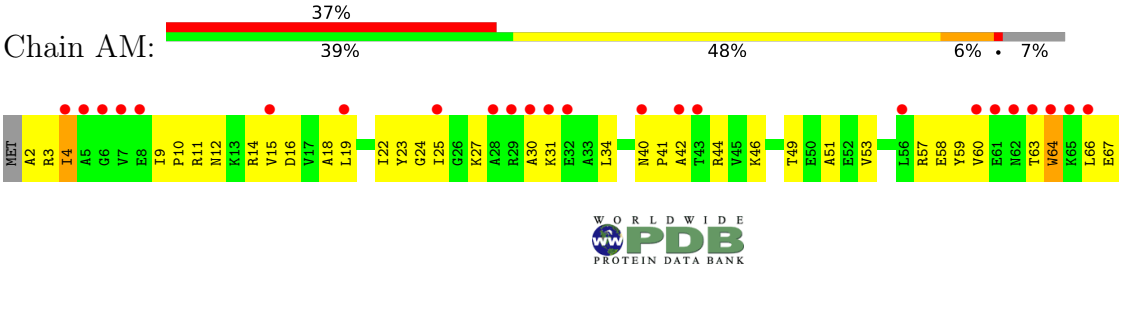
• Molecule 14: 30S ribosomal protein S12

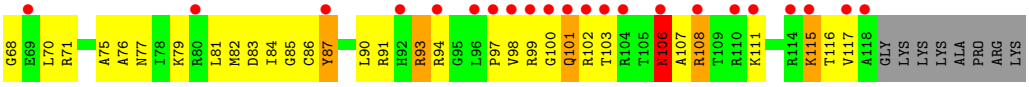
Chain CL:



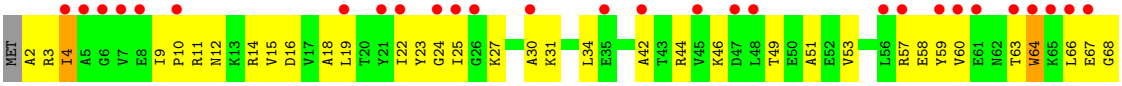
• Molecule 15: 30S ribosomal protein S13

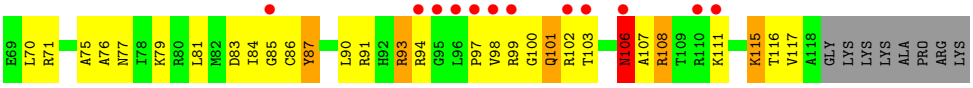
Chain AM:



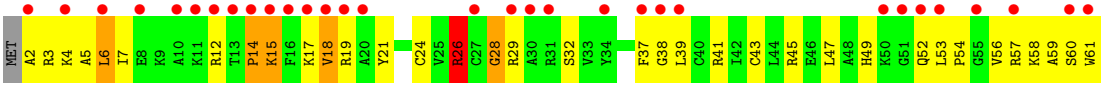


• Molecule 15: 30S ribosomal protein S13

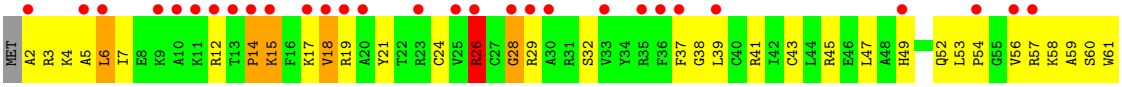




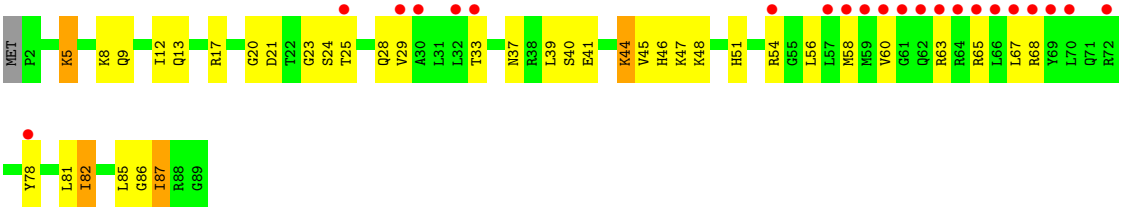
• Molecule 16: 30S ribosomal protein S14



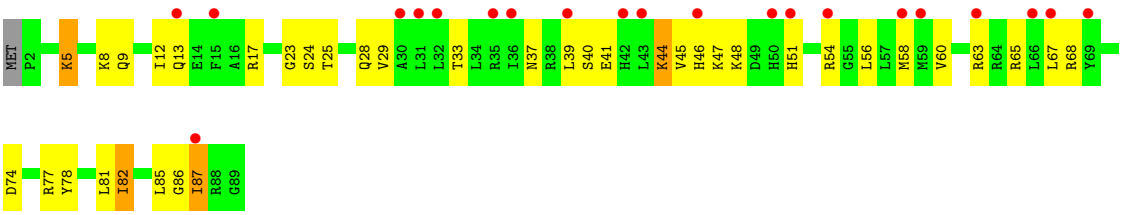
• Molecule 16: 30S ribosomal protein S14



• Molecule 17: 30S ribosomal protein S15

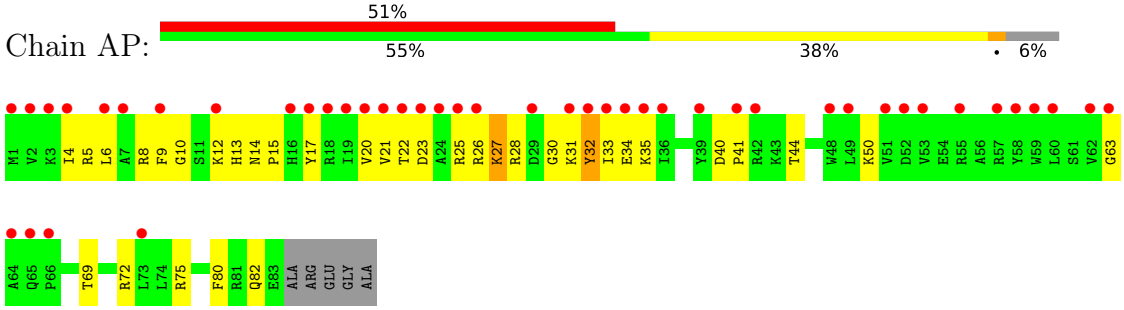


• Molecule 17: 30S ribosomal protein S15



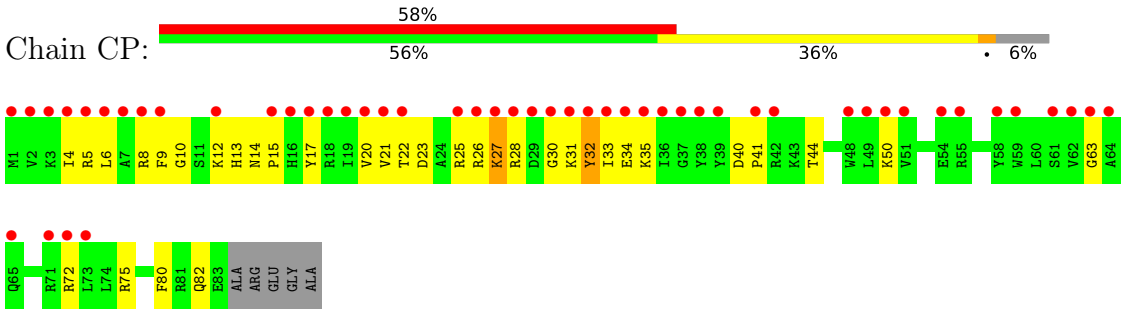
• Molecule 18: 30S ribosomal protein S16

Chain AP:



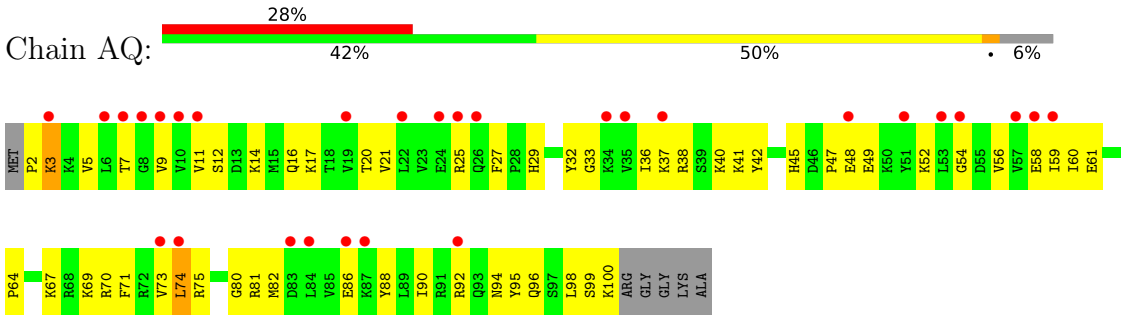
• Molecule 18: 30S ribosomal protein S16

Chain CP:



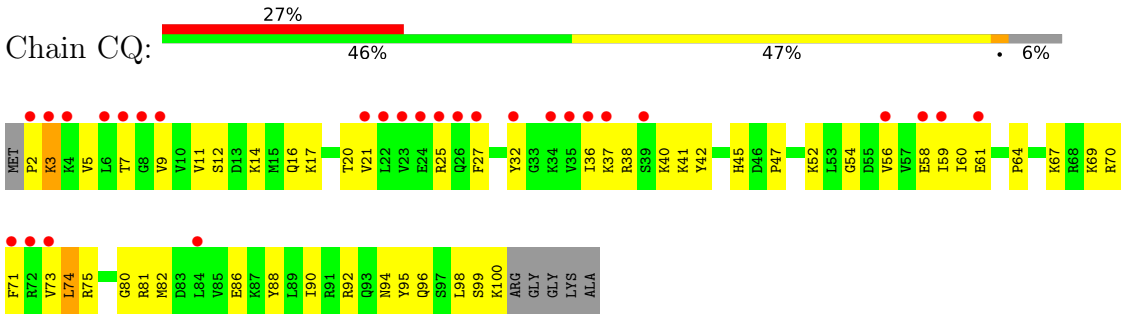
• Molecule 19: 30S ribosomal protein S17

Chain AQ:



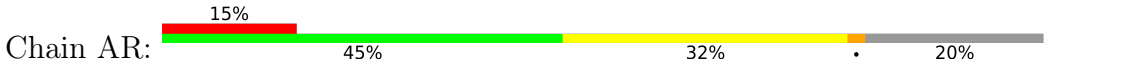
• Molecule 19: 30S ribosomal protein S17

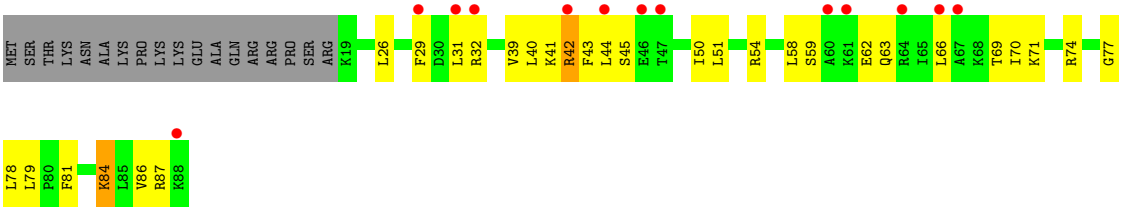
Chain CQ:



• Molecule 20: 30S ribosomal protein S18

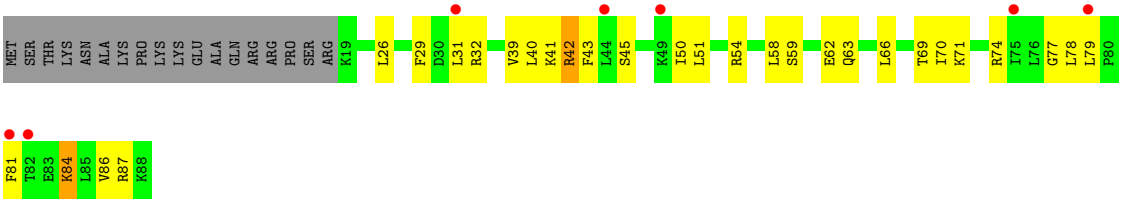
Chain AR:





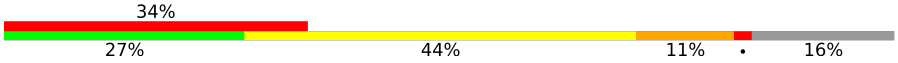
• Molecule 20: 30S ribosomal protein S18

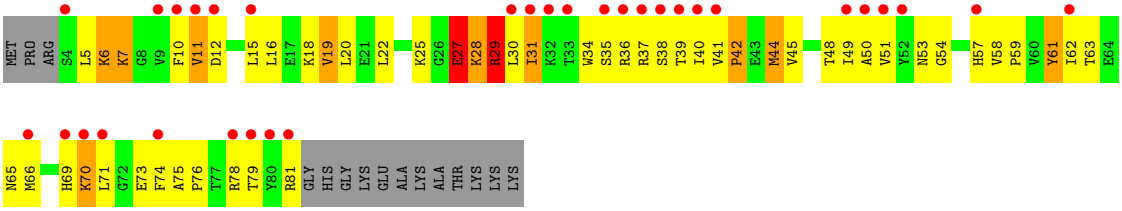
Chain CR:



• Molecule 21: 30S ribosomal protein S19

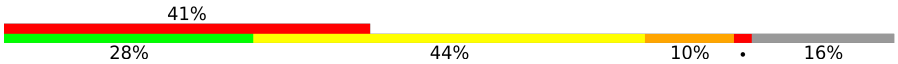
Chain AS:

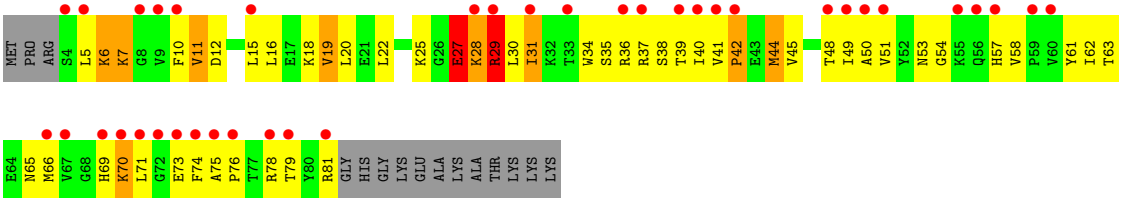




• Molecule 21: 30S ribosomal protein S19

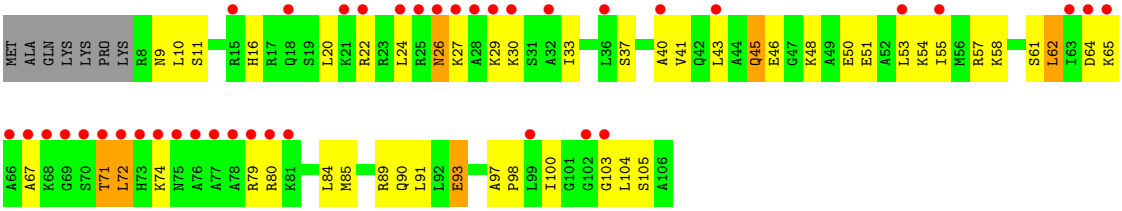
Chain CS:





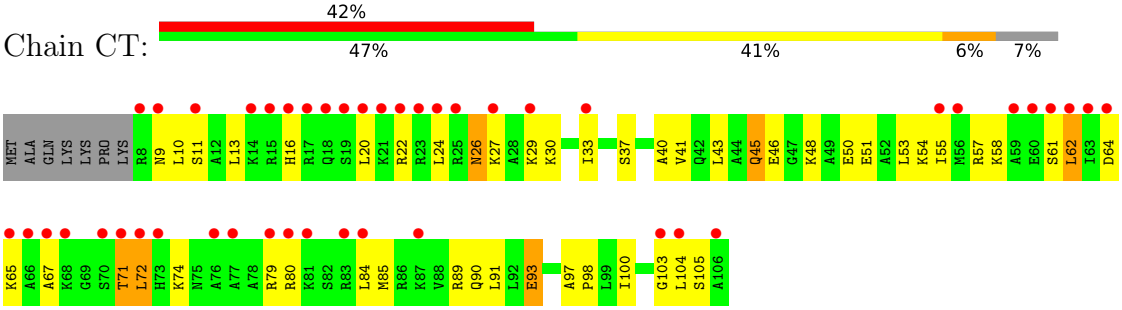
• Molecule 22: 30S ribosomal protein S20

Chain AT:



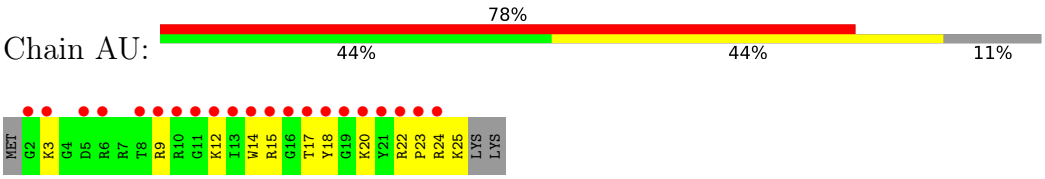
• Molecule 22: 30S ribosomal protein S20

Chain CT:



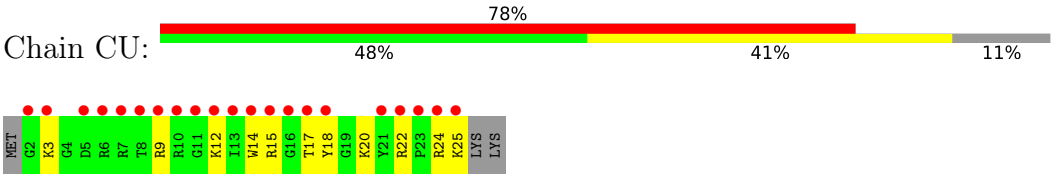
• Molecule 23: 30S ribosomal protein Thx

Chain AU:



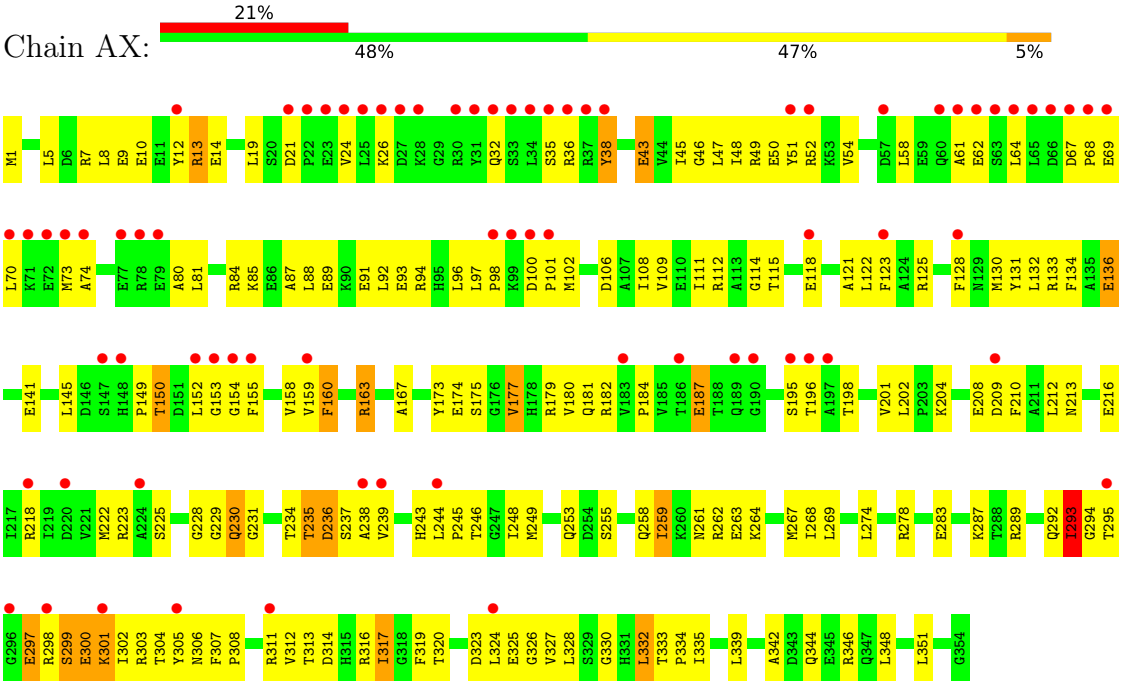
• Molecule 23: 30S ribosomal protein Thx

Chain CU:



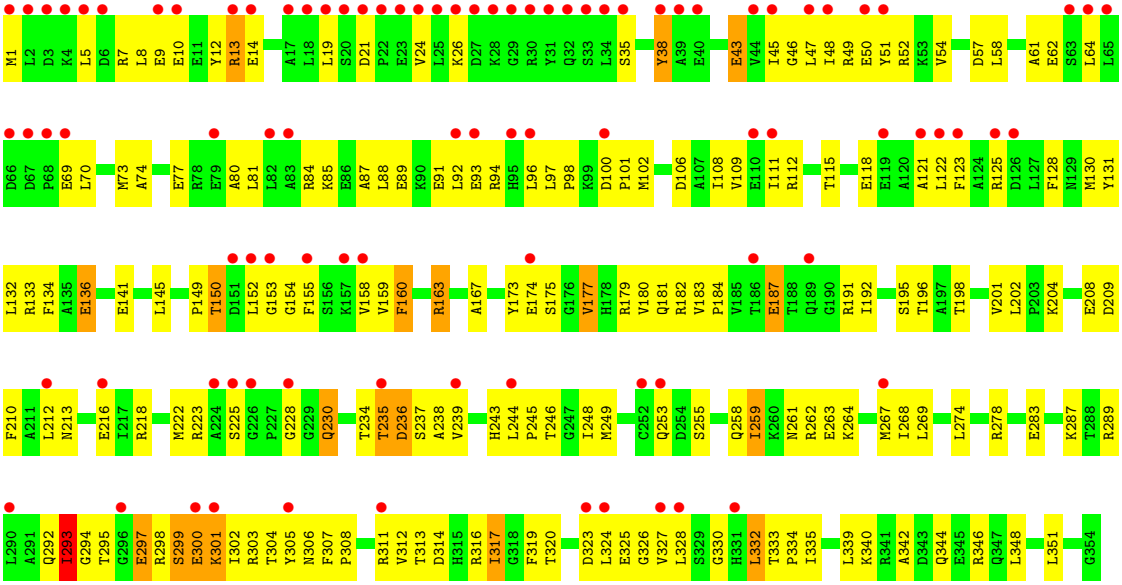
• Molecule 24: Peptide chain release factor 1

Chain AX:



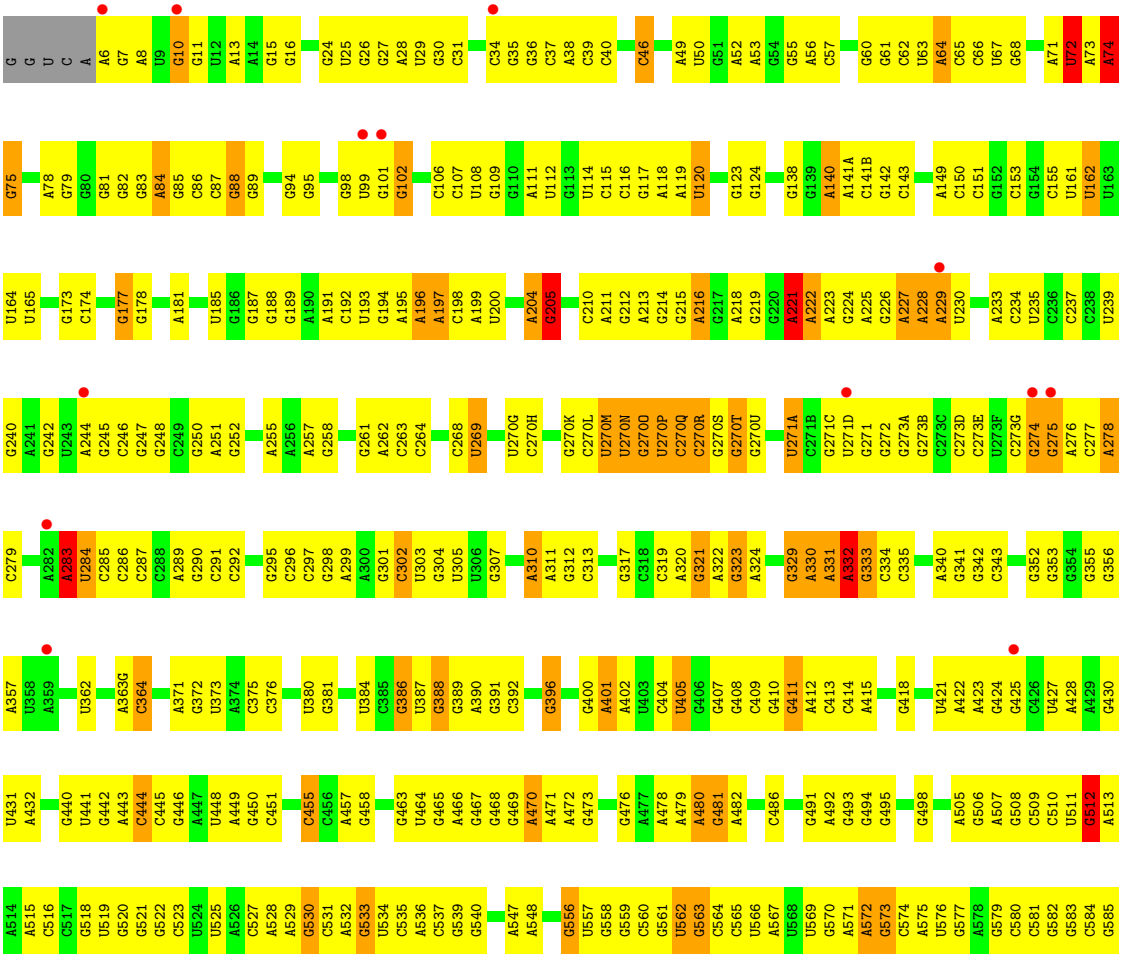
• Molecule 24: Peptide chain release factor 1

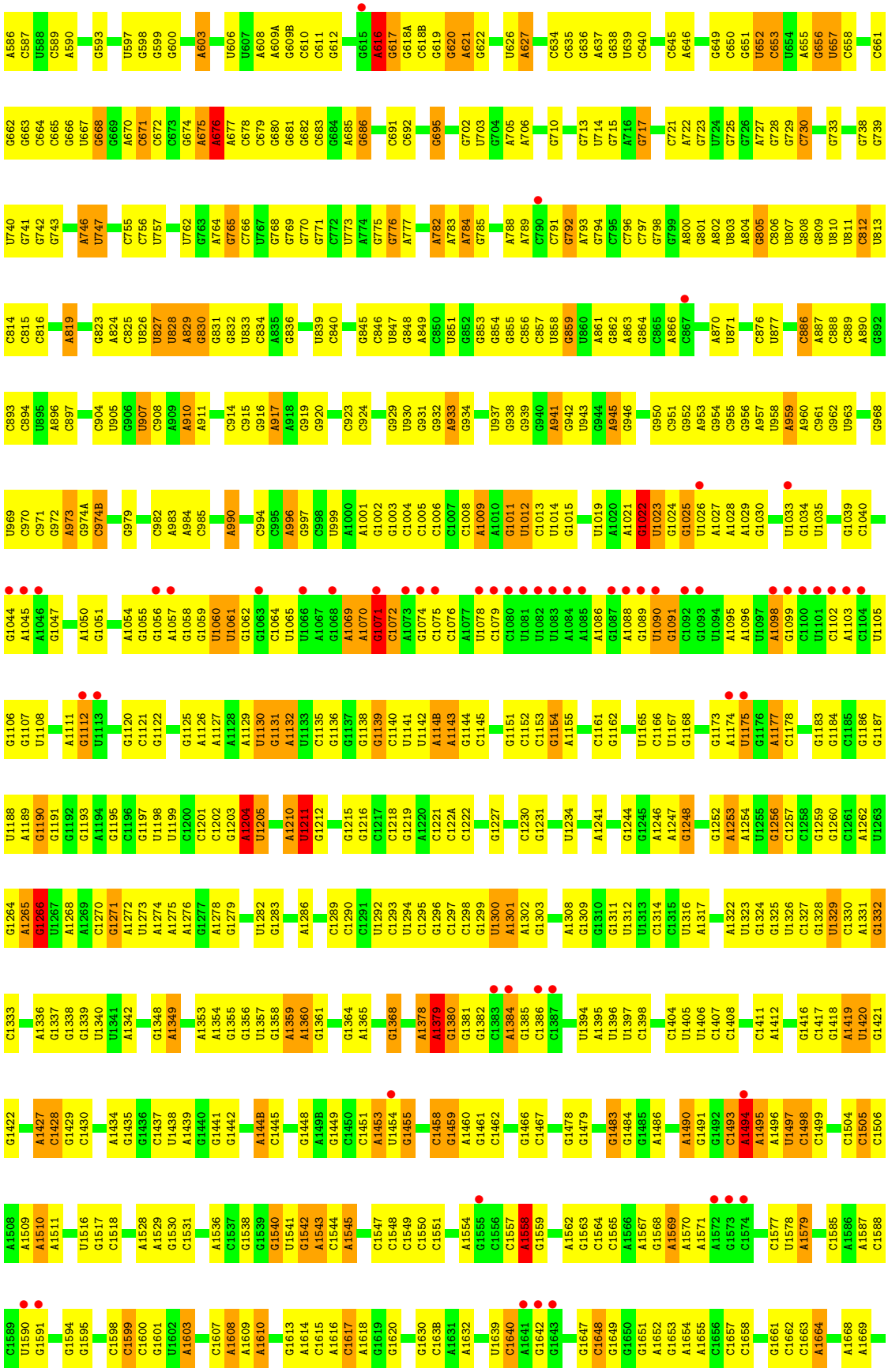
Chain CX:

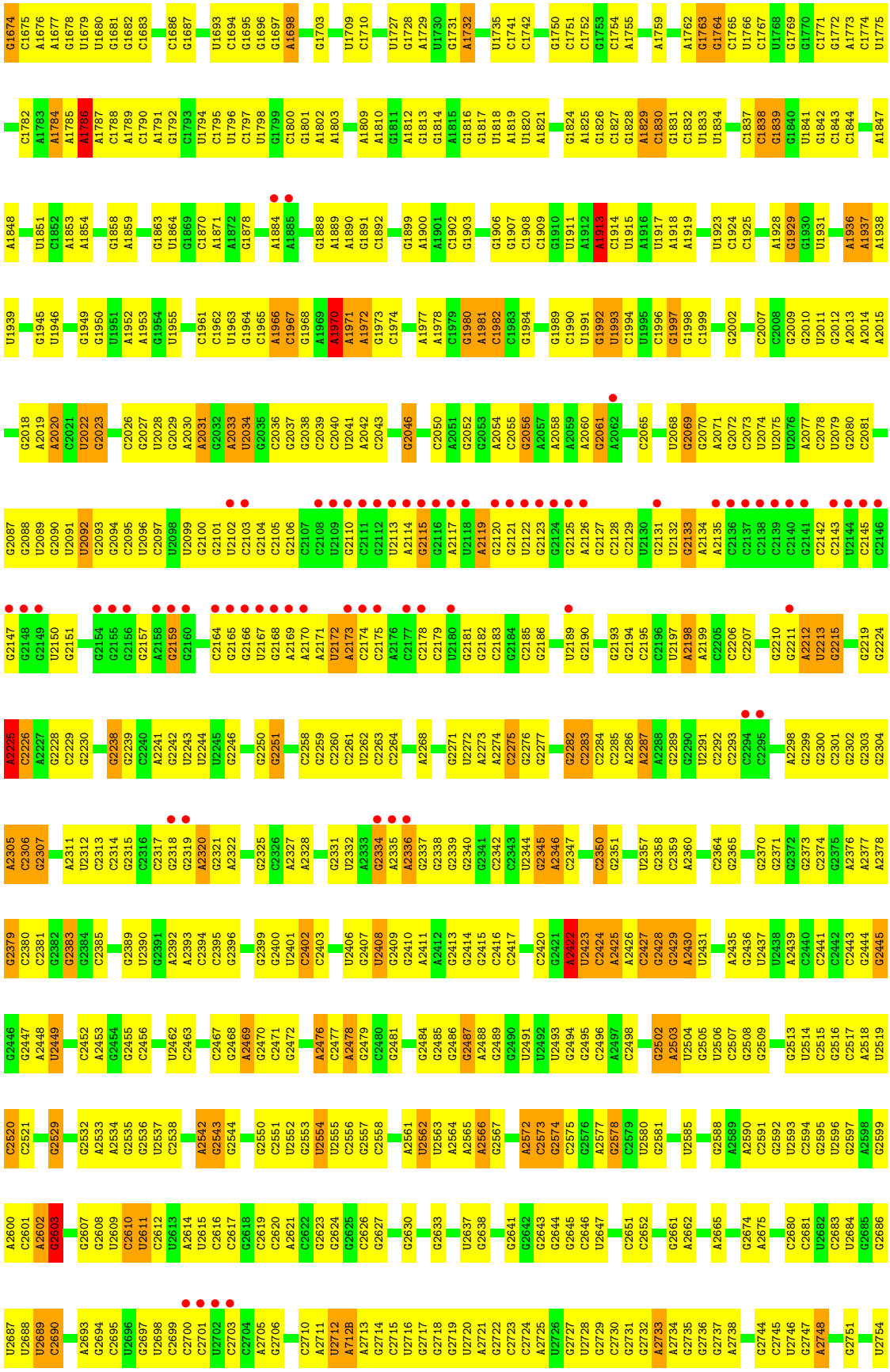


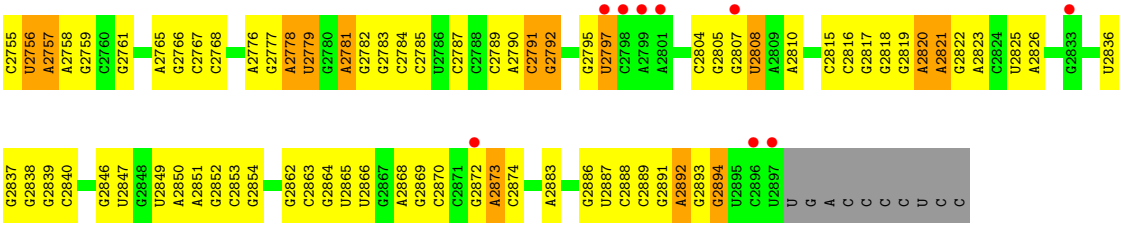
• Molecule 25: 23S RRNA

Chain BA:



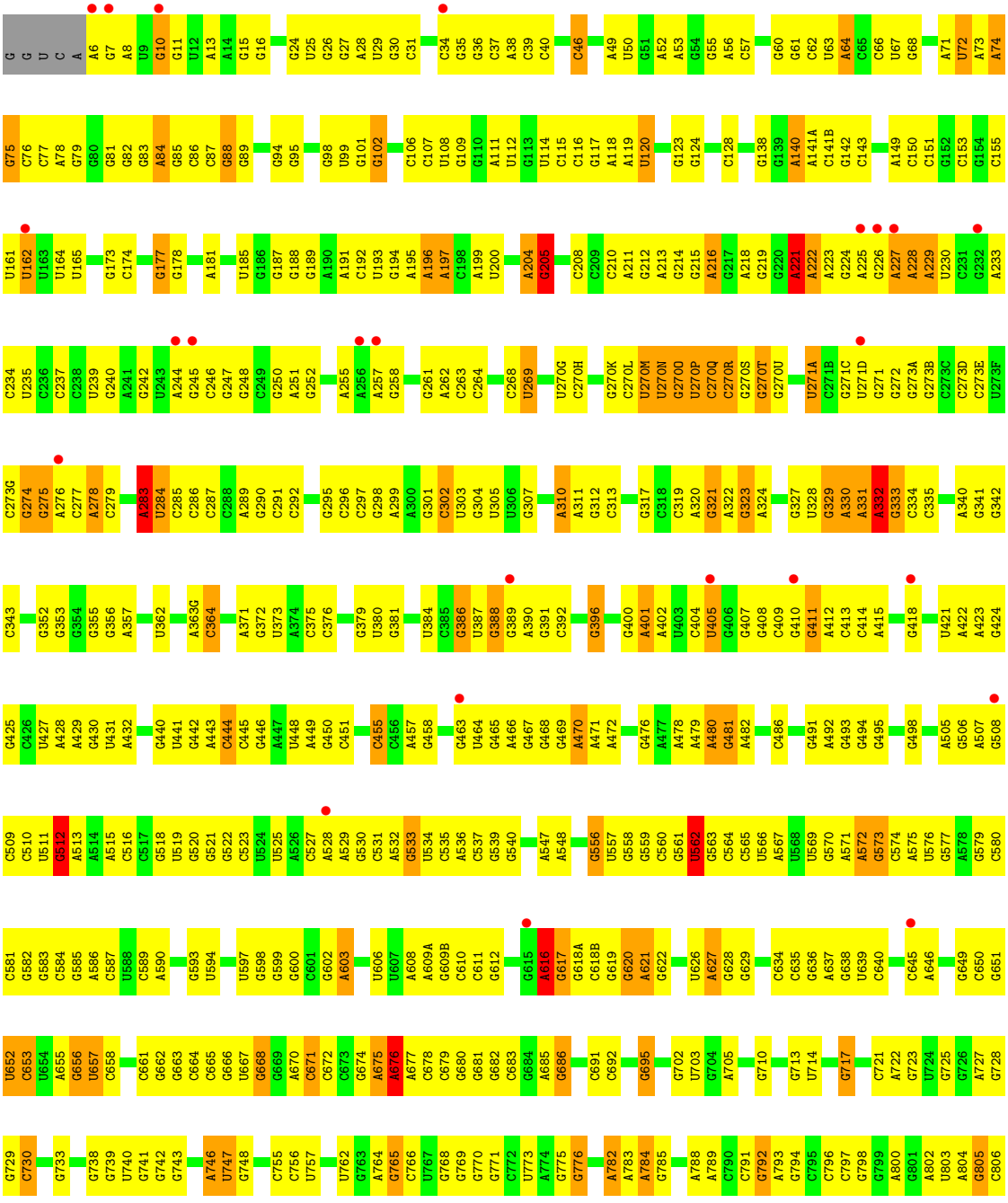


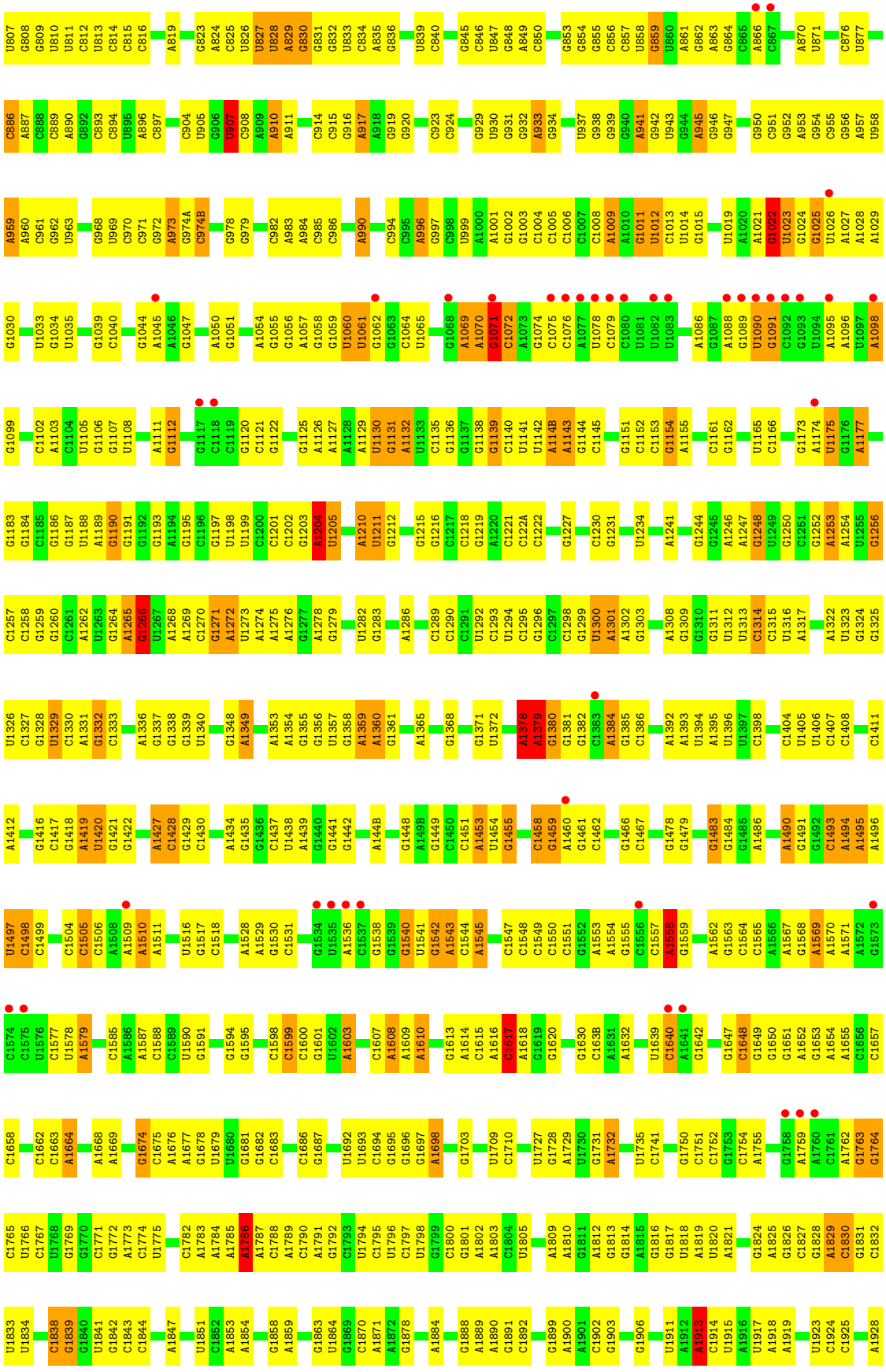


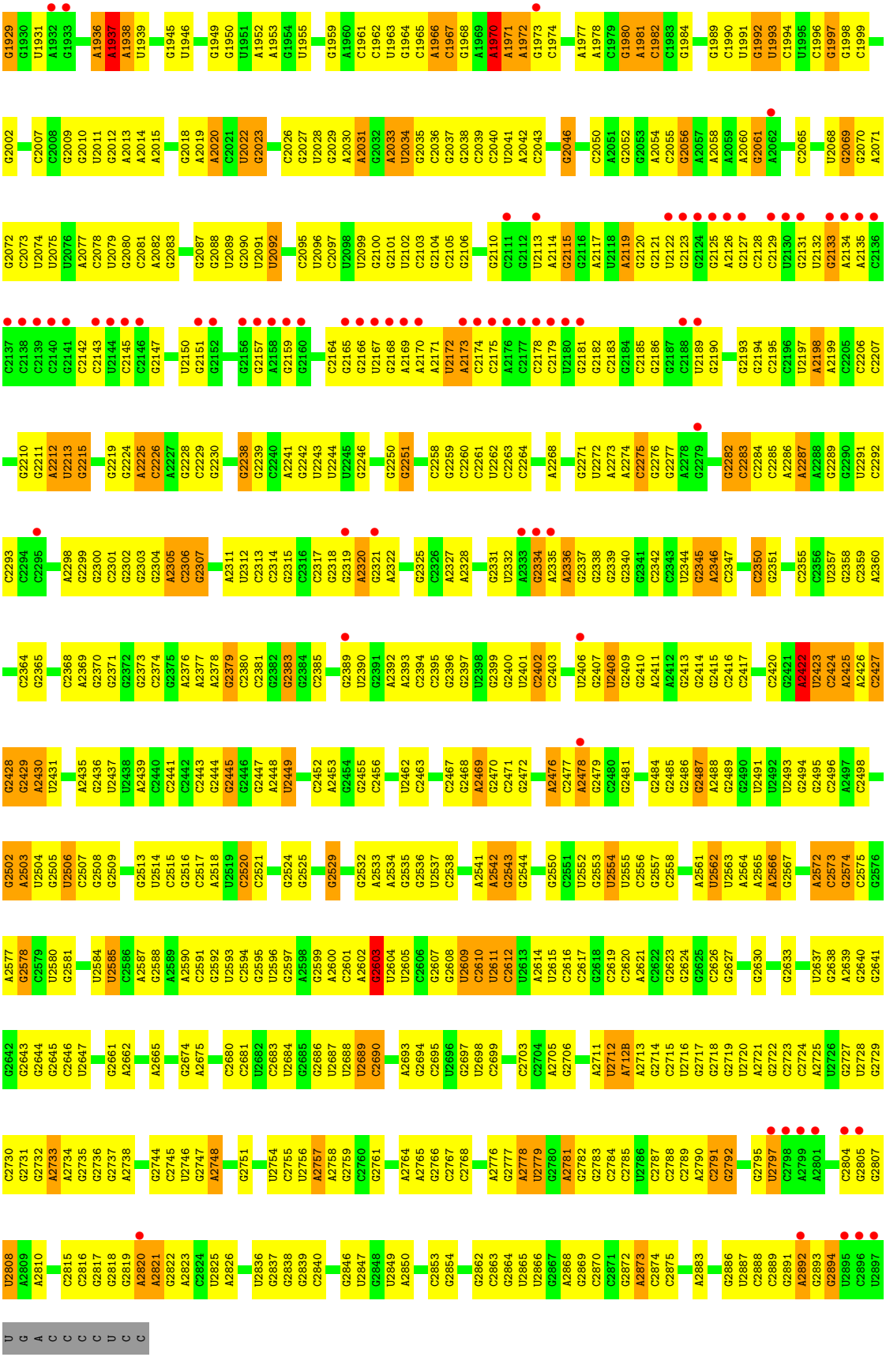


• Molecule 25: 23S RRNA

Chain DA:

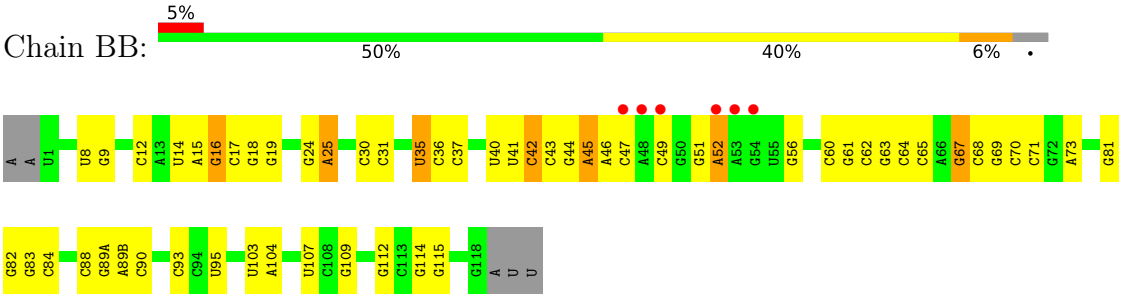






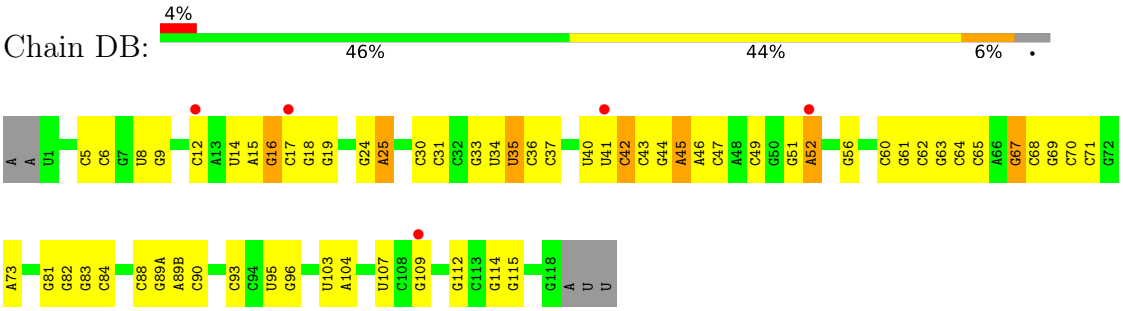
• Molecule 26: 5S RRNA

Chain BB:



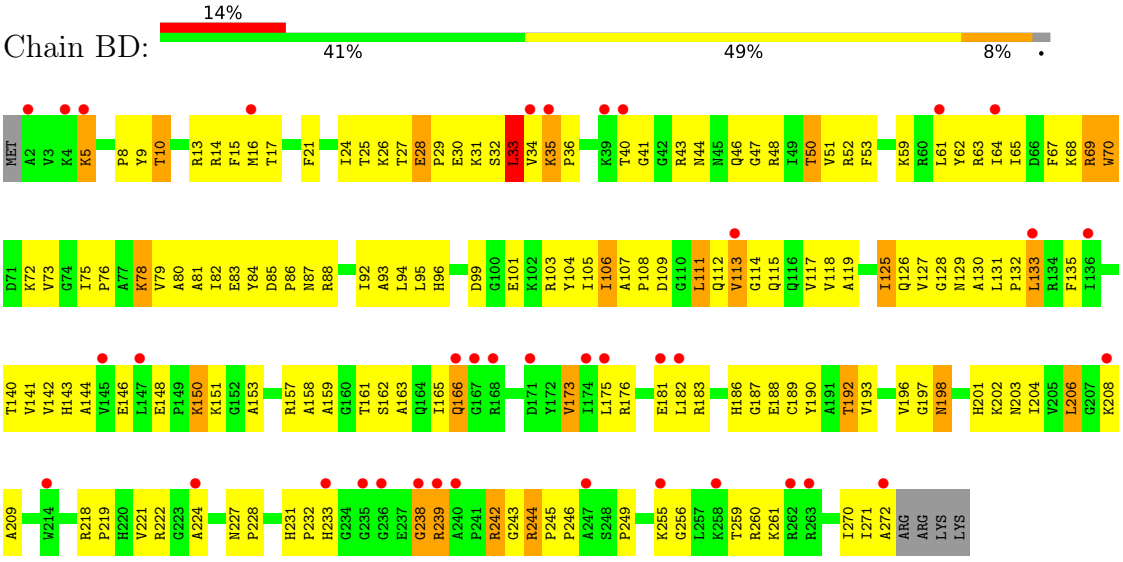
• Molecule 26: 5S RRNA

Chain DB:



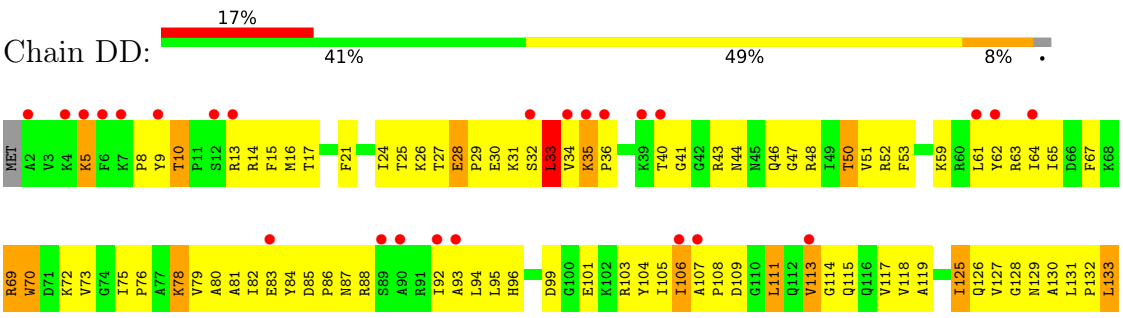
• Molecule 27: 50S ribosomal protein L2

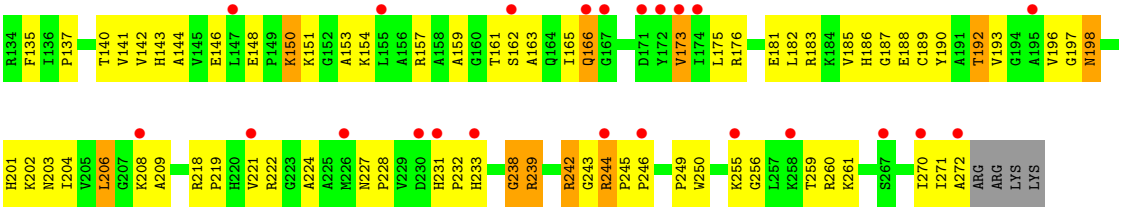
Chain BD:

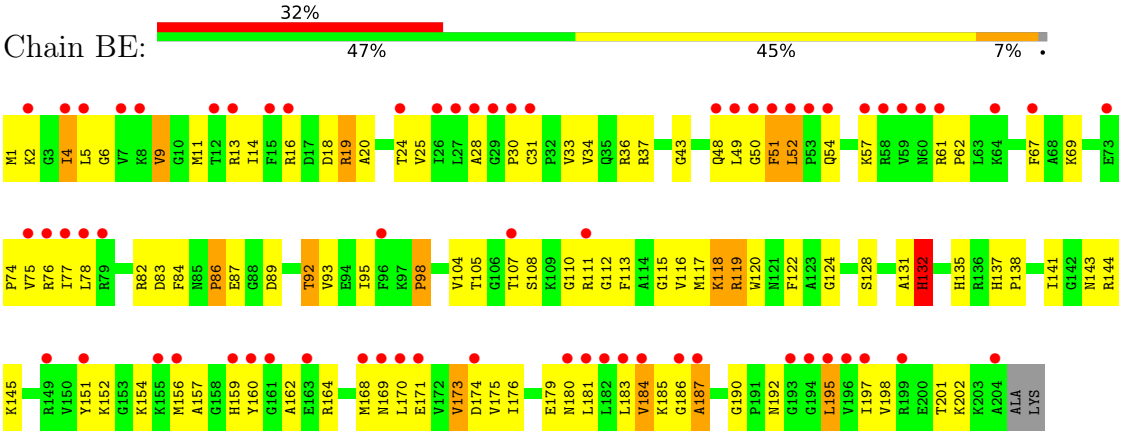


• Molecule 27: 50S ribosomal protein L2

Chain DD:





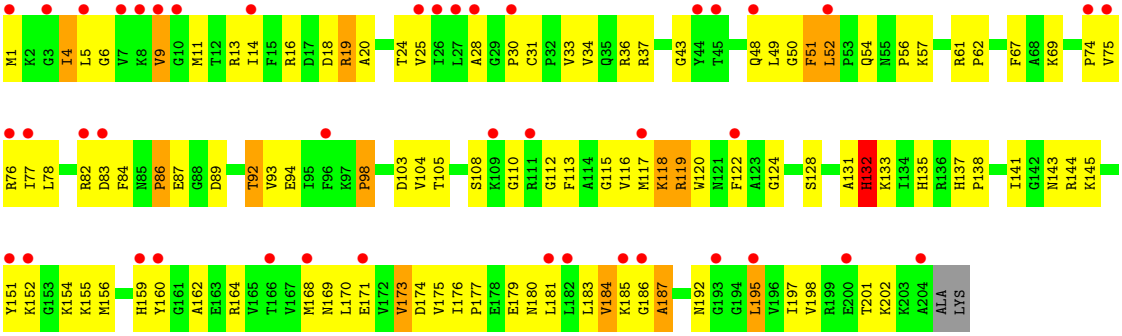


• Molecule 28: 50S ribosomal protein L3

Chain BE:

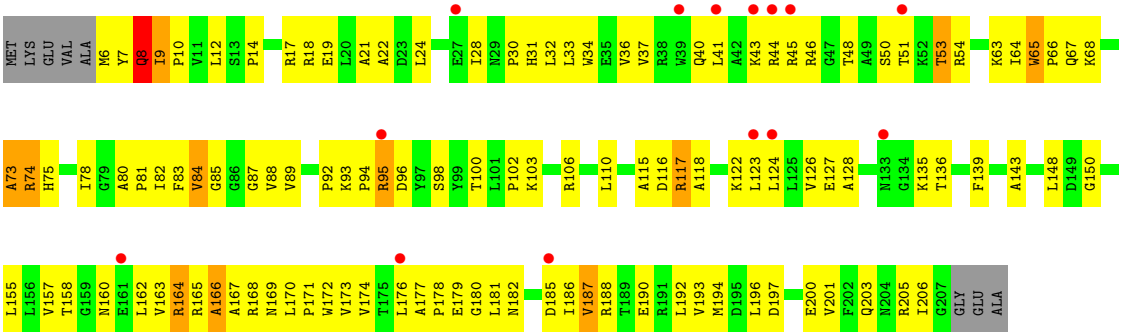
• Molecule 28: 50S ribosomal protein L3

Chain DE:



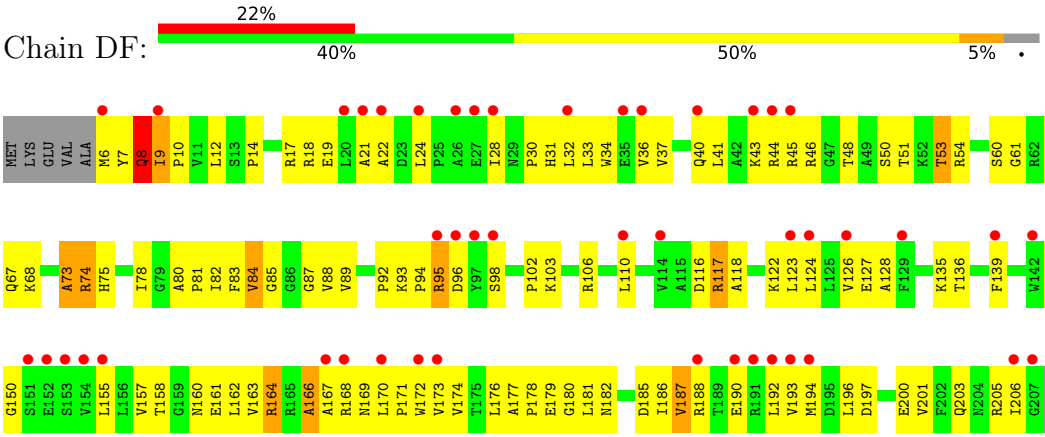
• Molecule 29: 50S ribosomal protein L4

Chain BF:



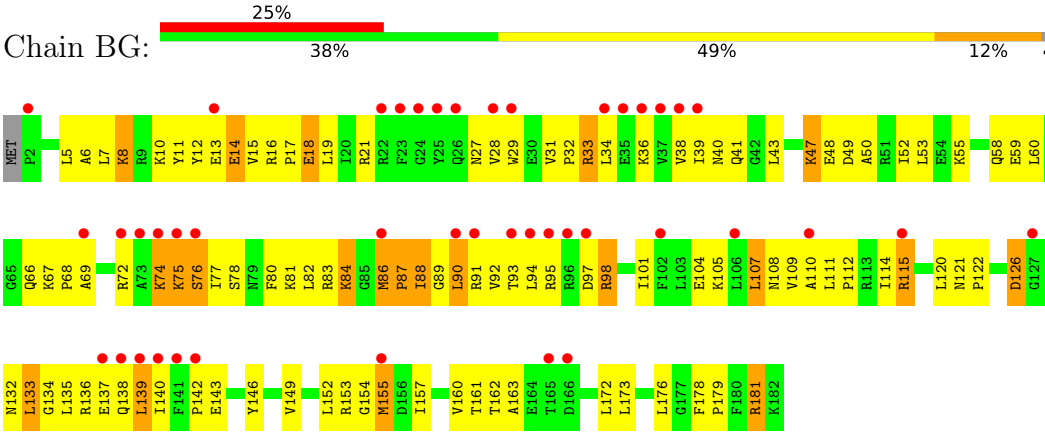
• Molecule 29: 50S ribosomal protein L4

Chain DF:



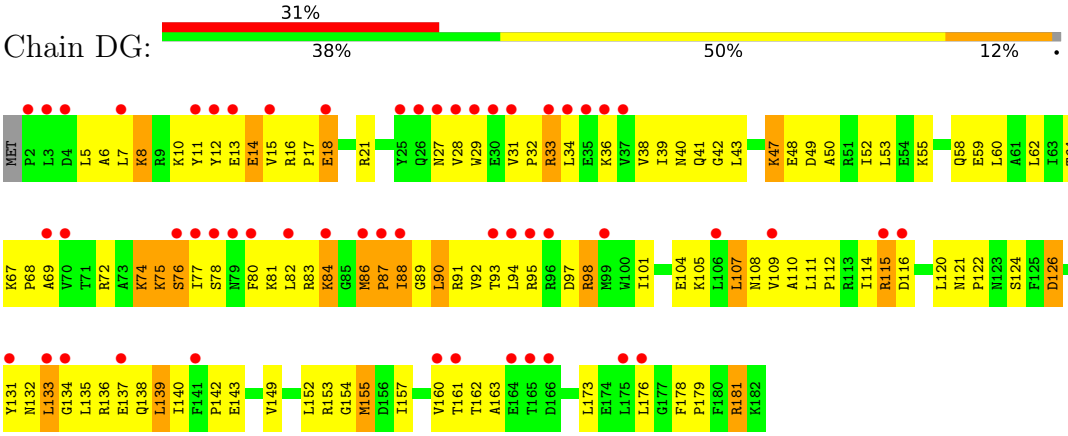
• Molecule 30: 50S ribosomal protein L5

Chain BG:



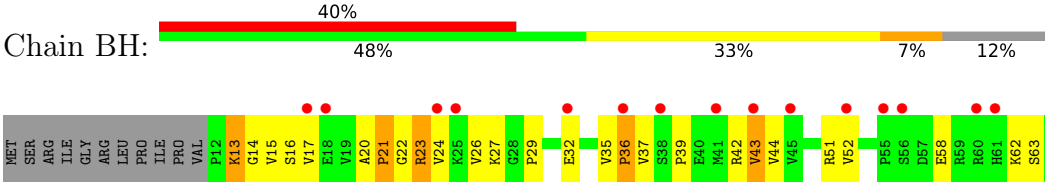
• Molecule 30: 50S ribosomal protein L5

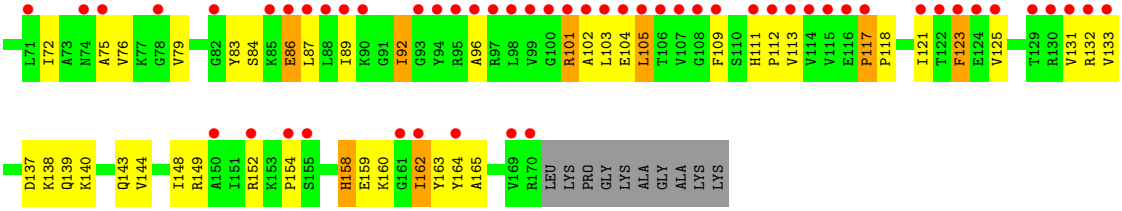
Chain DG:



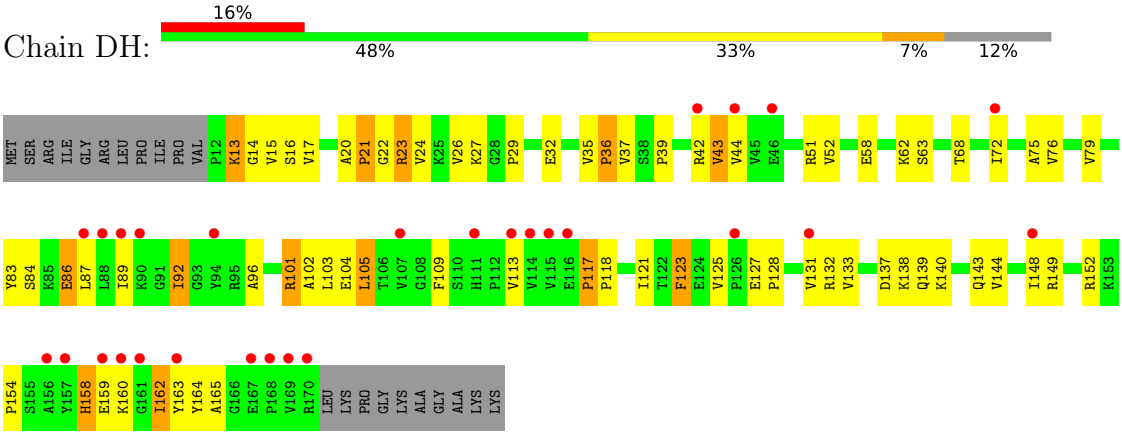
• Molecule 31: 50S ribosomal protein L6

Chain BH:

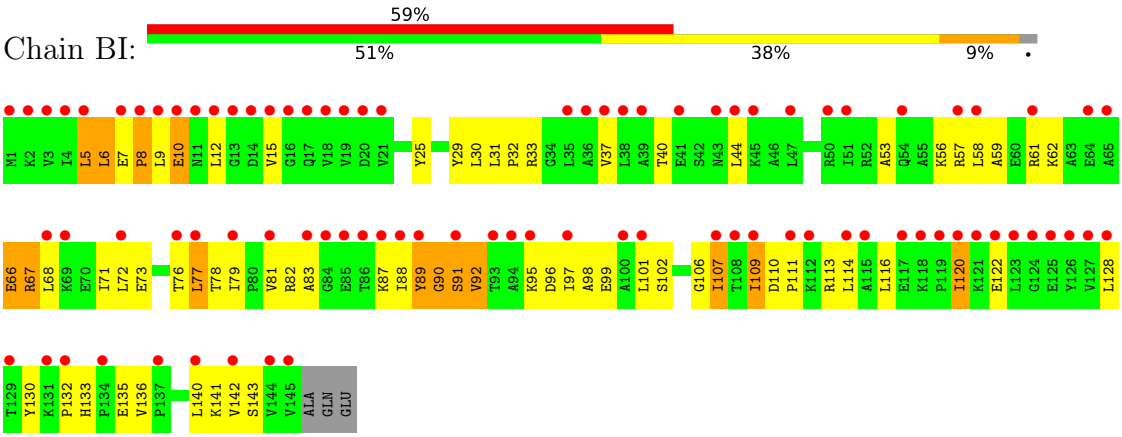




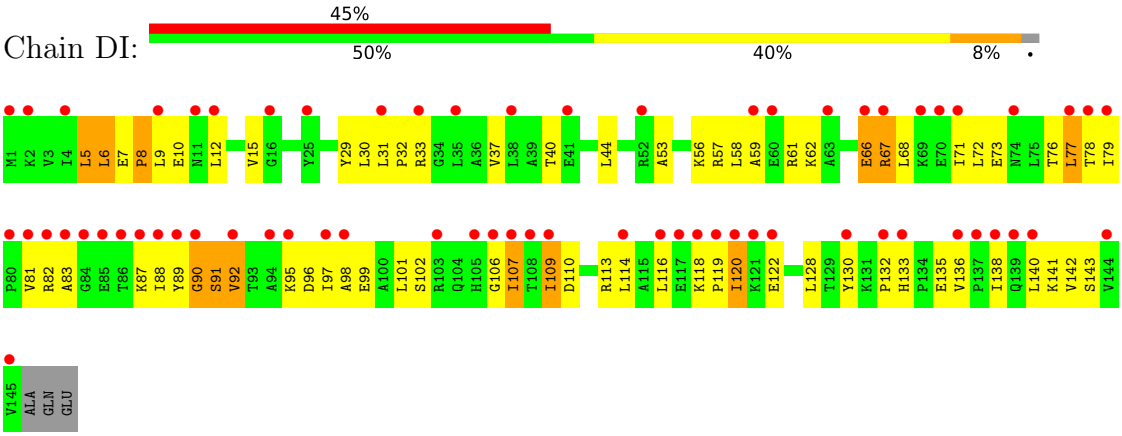
• Molecule 31: 50S ribosomal protein L6



• Molecule 32: 50S ribosomal protein L9

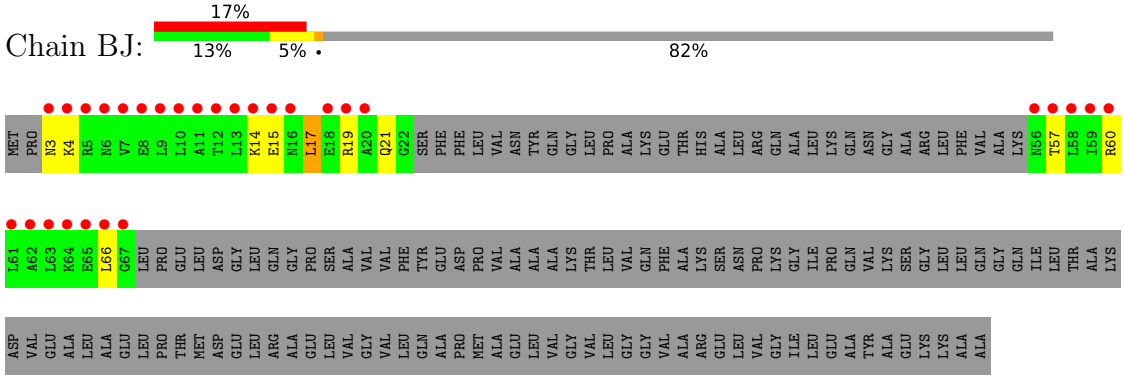


• Molecule 32: 50S ribosomal protein L9



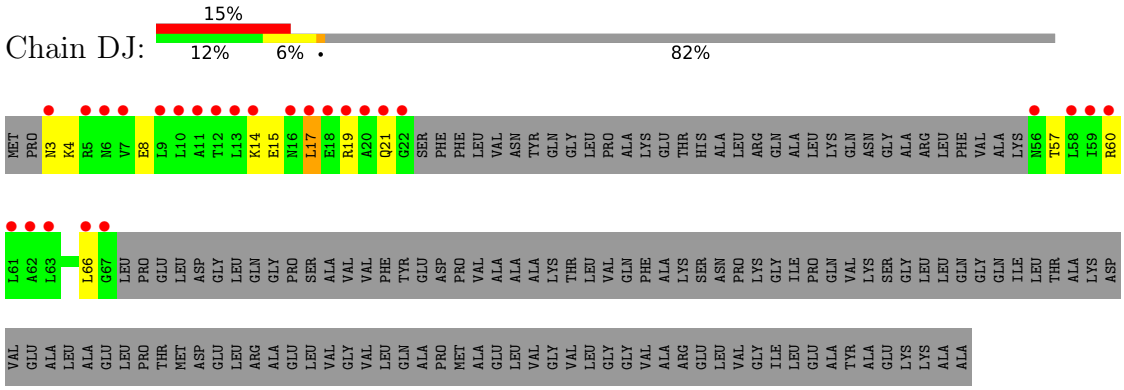
• Molecule 33: 50S ribosomal protein L10

Chain BJ:



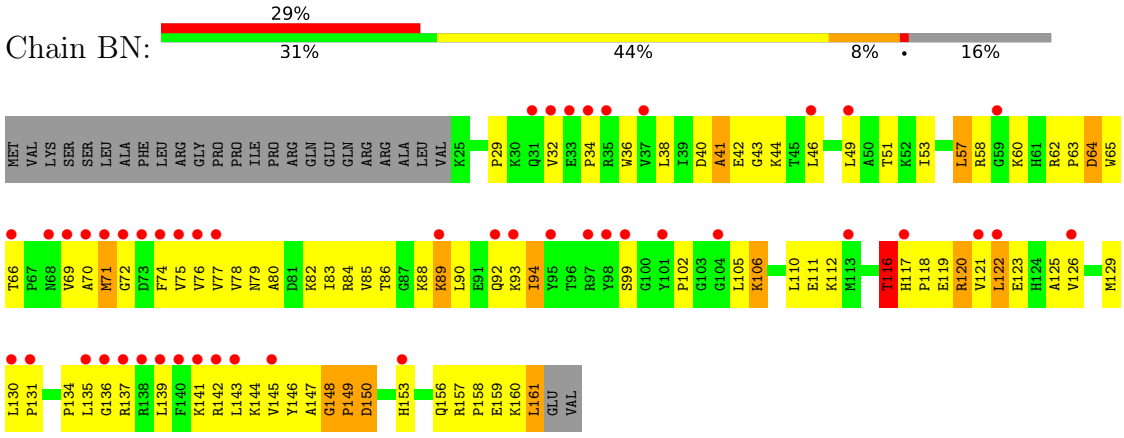
• Molecule 33: 50S ribosomal protein L10

Chain DJ:



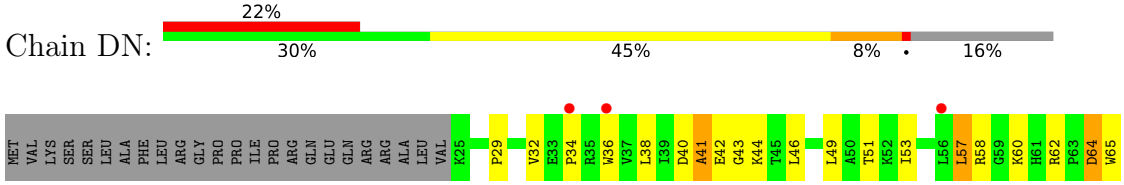
• Molecule 34: 50S ribosomal protein L13

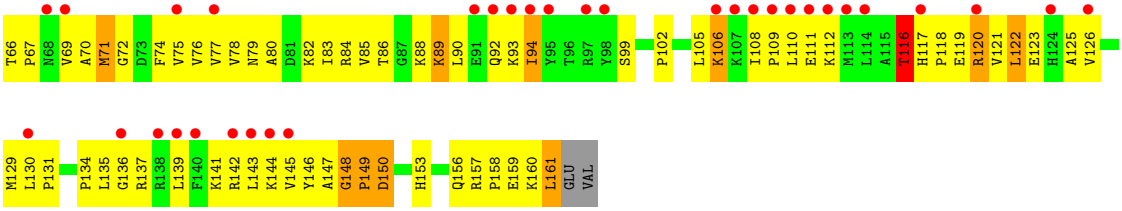
Chain BN:



• Molecule 34: 50S ribosomal protein L13

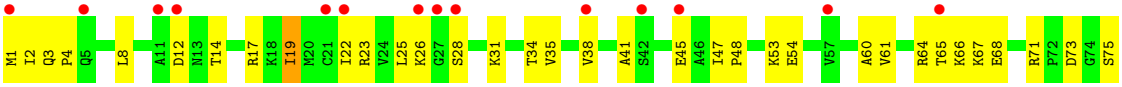
Chain DN:

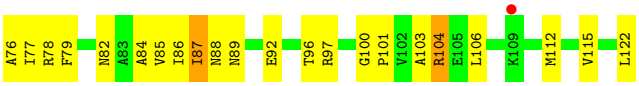




• Molecule 35: 50S ribosomal protein L14

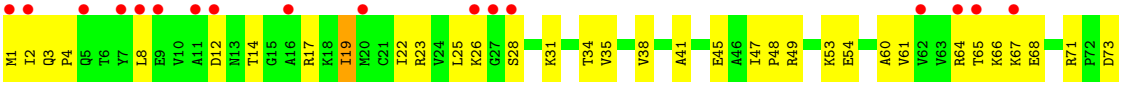
Chain BO:

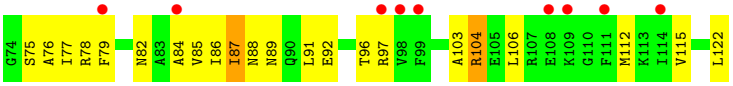




• Molecule 35: 50S ribosomal protein L14

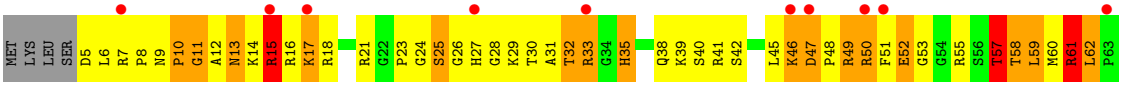
Chain DO:

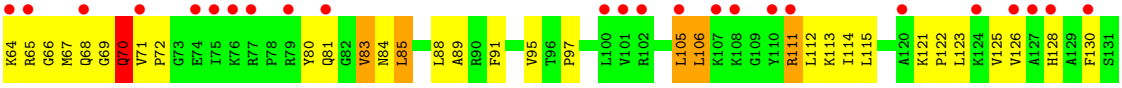


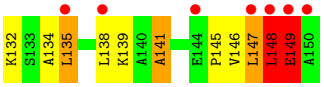


• Molecule 36: 50S ribosomal protein L15

Chain BP:

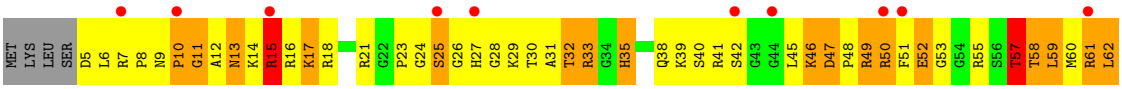


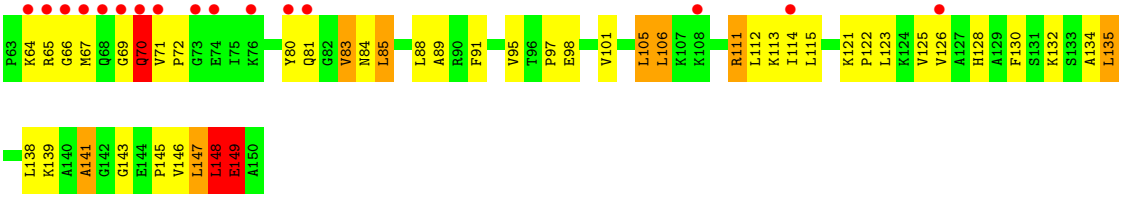




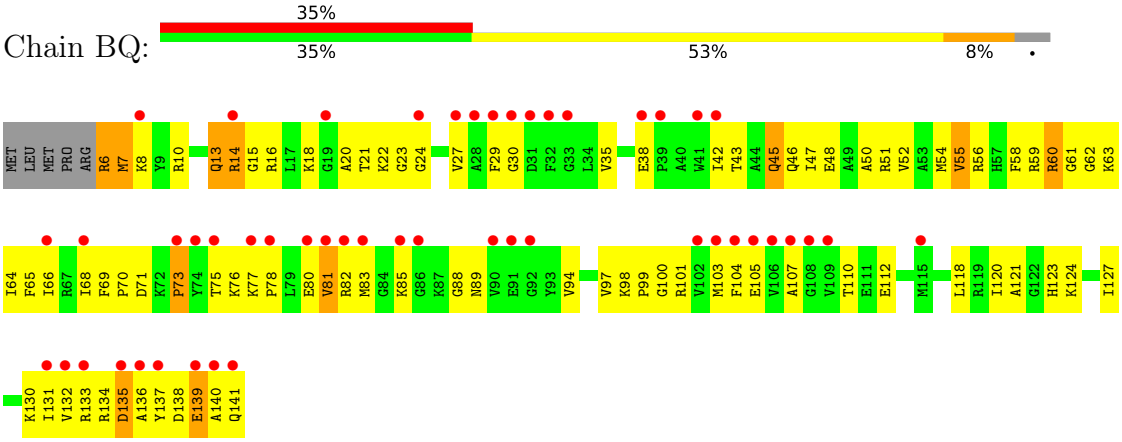
• Molecule 36: 50S ribosomal protein L15

Chain DP:

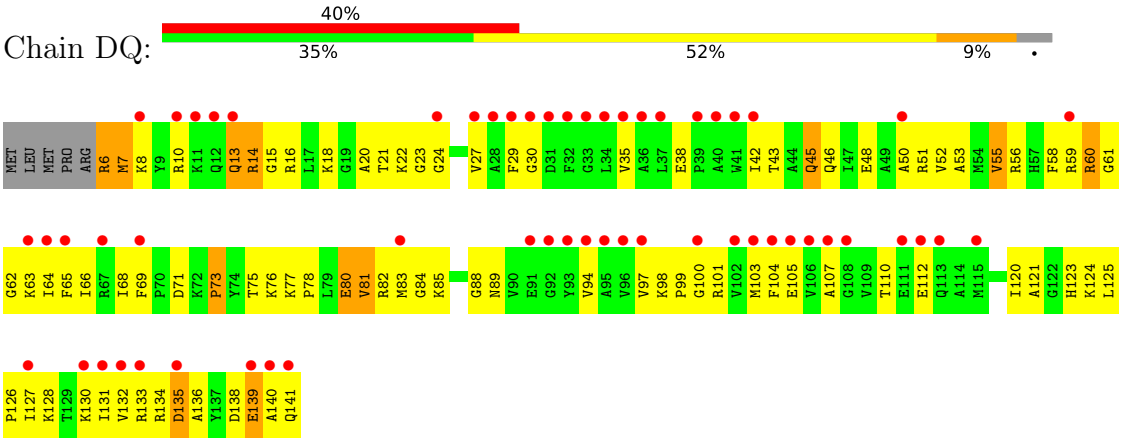




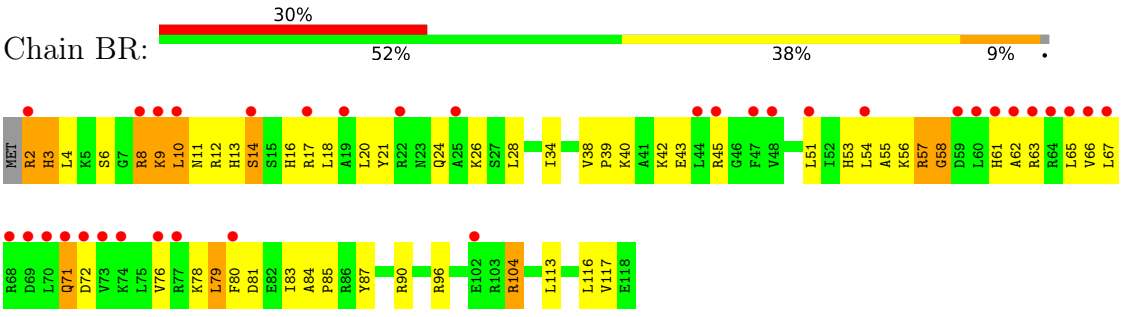
• Molecule 37: 50S ribosomal protein L16



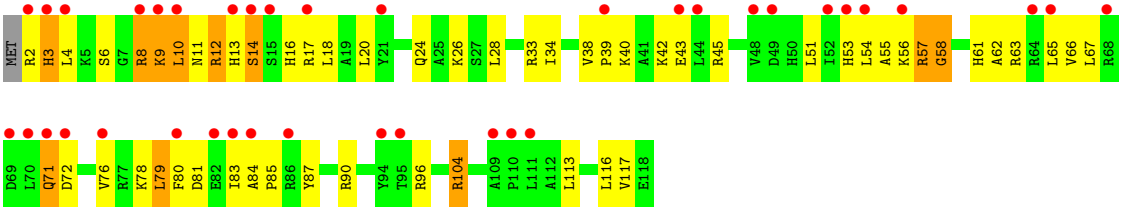
• Molecule 37: 50S ribosomal protein L16



• Molecule 38: 50S ribosomal protein L17

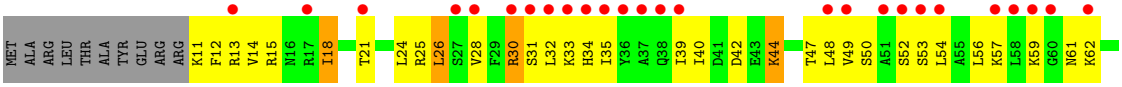


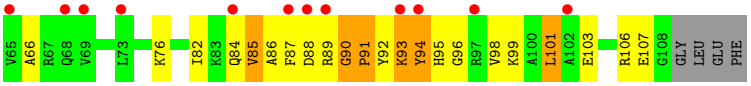
• Molecule 38: 50S ribosomal protein L17



• Molecule 39: 50S ribosomal protein L18

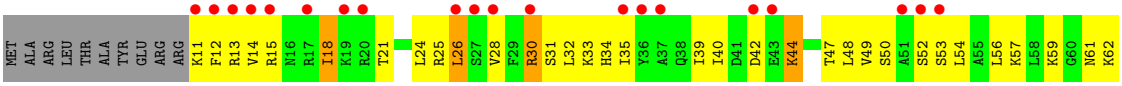
Chain BS:

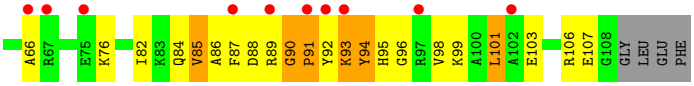




• Molecule 39: 50S ribosomal protein L18

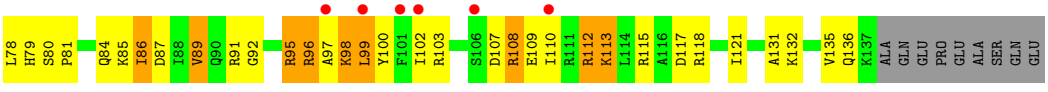
Chain DS:





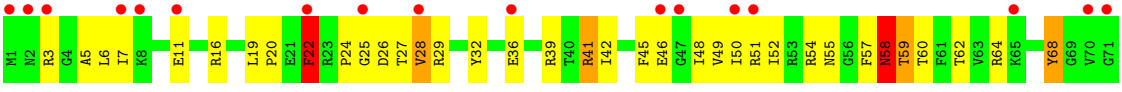
• Molecule 40: 50S ribosomal protein L19

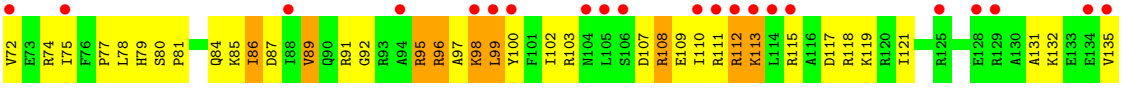
Chain BT:

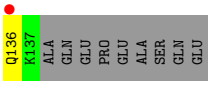


• Molecule 40: 50S ribosomal protein L19

Chain DT:

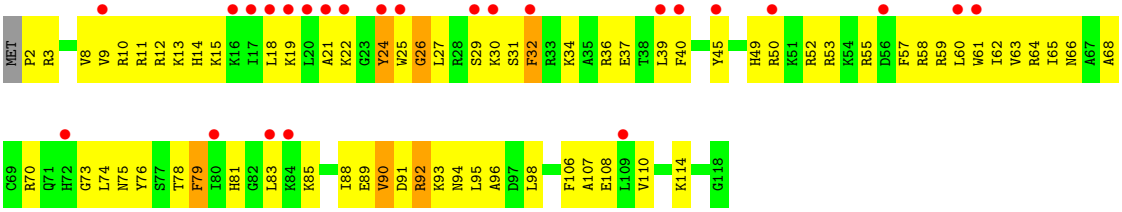






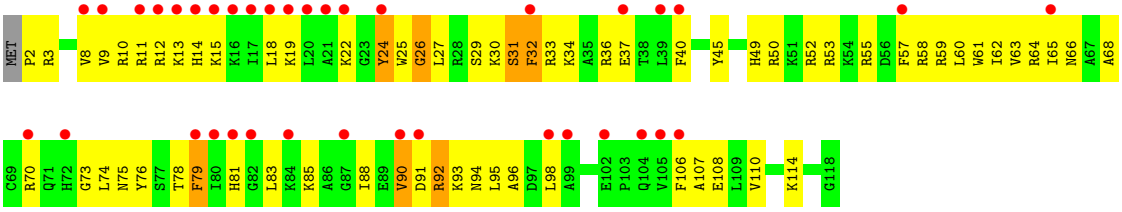
• Molecule 41: 50S ribosomal protein L20

Chain BU:



• Molecule 41: 50S ribosomal protein L20

Chain DU:

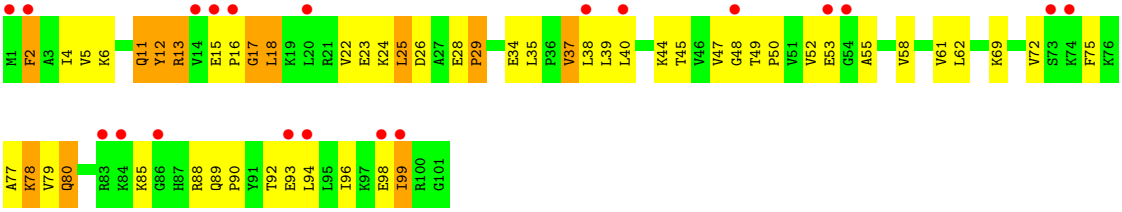


• Molecule 42: 50S ribosomal protein L21

Chain BV:

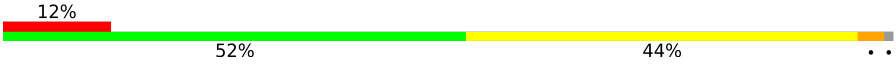
• Molecule 42: 50S ribosomal protein L21

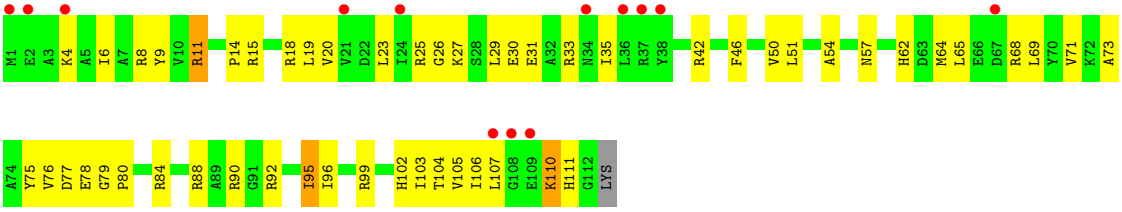
Chain DV:



• Molecule 43: 50S ribosomal protein L22

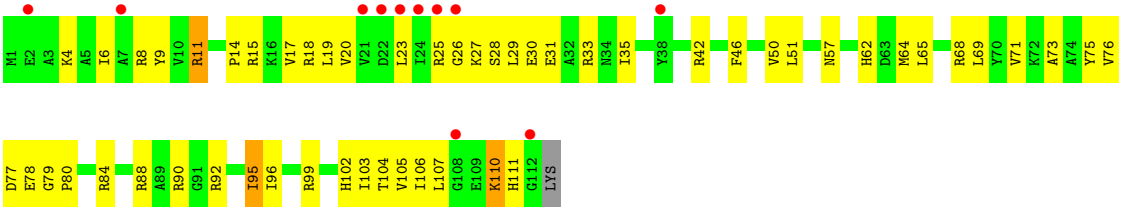
Chain BW:





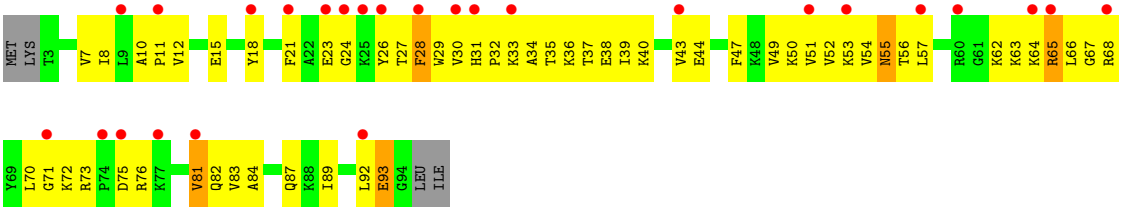
• Molecule 43: 50S ribosomal protein L22

Chain DW:



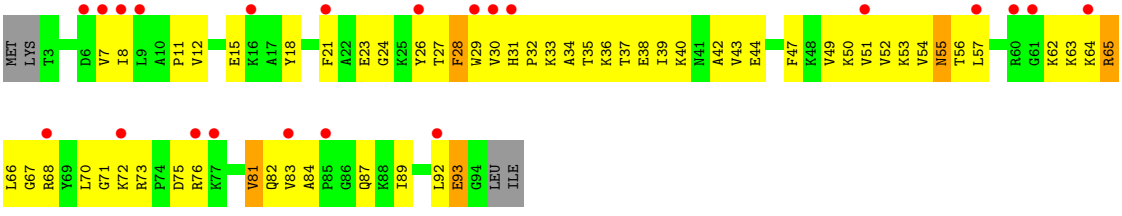
• Molecule 44: 50S ribosomal protein L23

Chain BX:



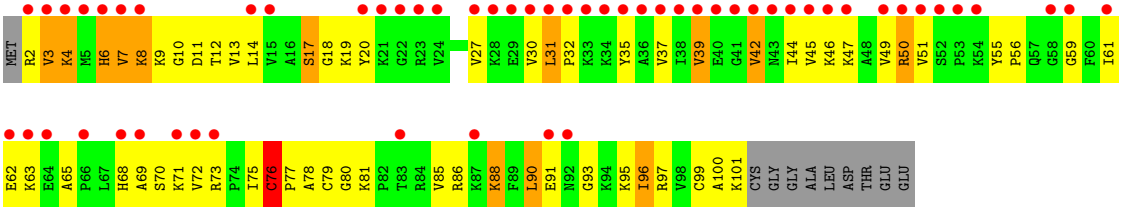
• Molecule 44: 50S ribosomal protein L23

Chain DX:



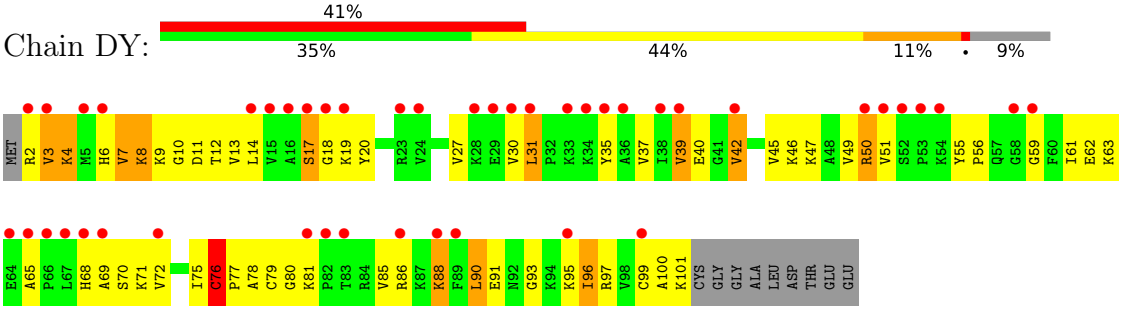
• Molecule 45: 50S ribosomal protein L24

Chain BY:



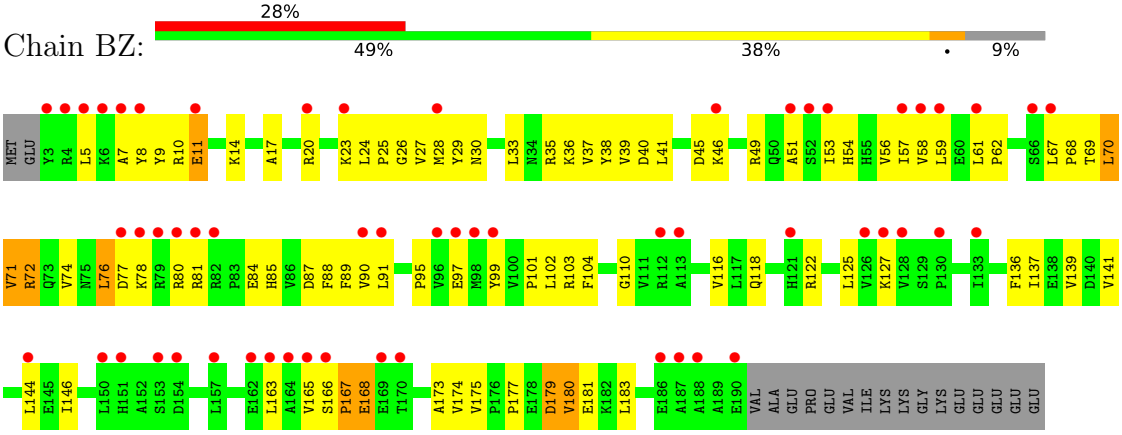
• Molecule 45: 50S ribosomal protein L24

Chain DY:



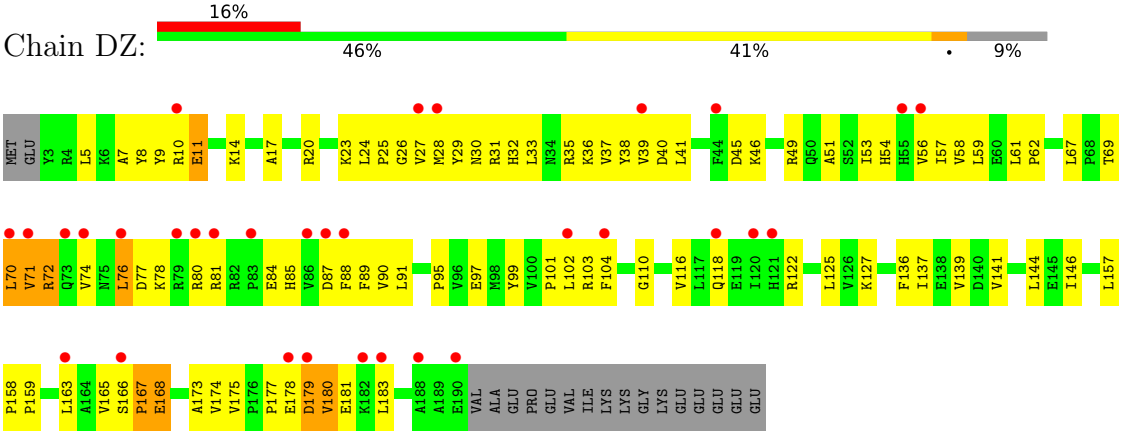
• Molecule 46: 50S ribosomal protein L25

Chain BZ:



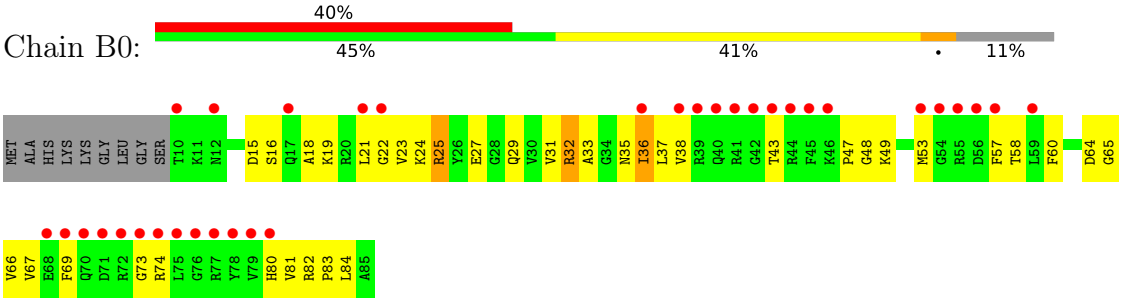
• Molecule 46: 50S ribosomal protein L25

Chain DZ:



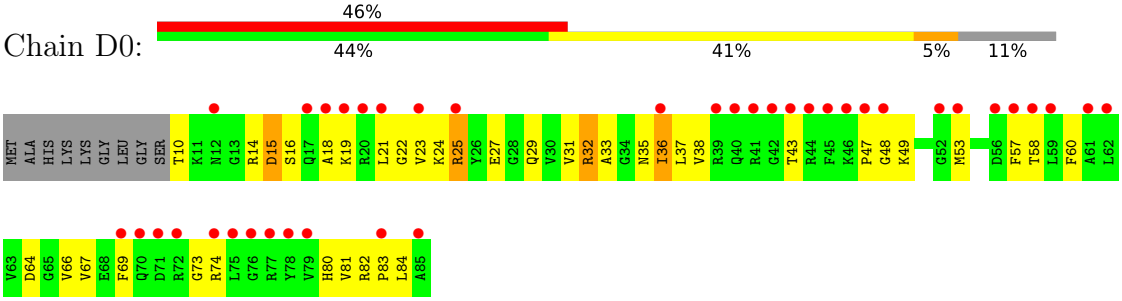
• Molecule 47: 50S ribosomal protein L27

Chain B0:



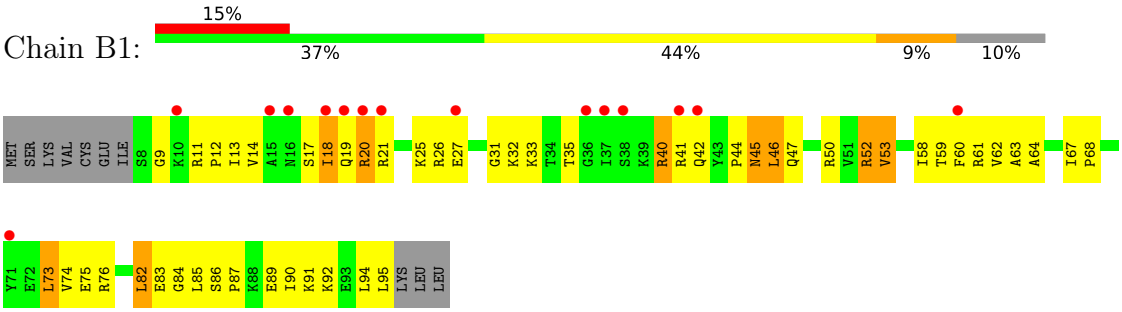
• Molecule 47: 50S ribosomal protein L27

Chain D0:



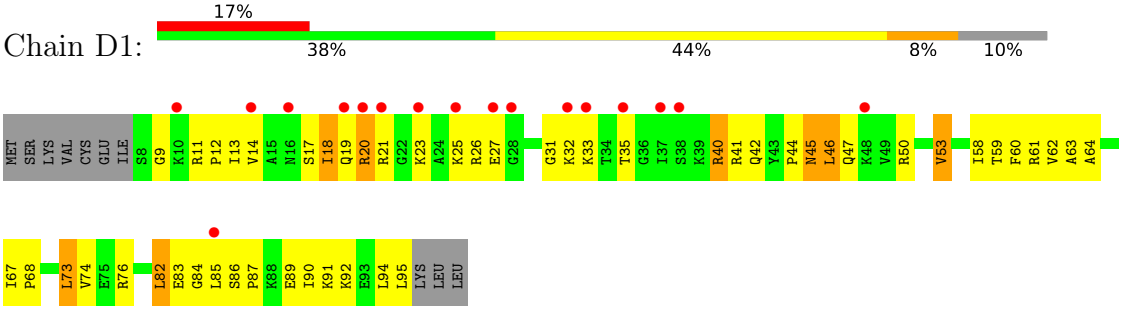
• Molecule 48: 50S ribosomal protein L28

Chain B1:



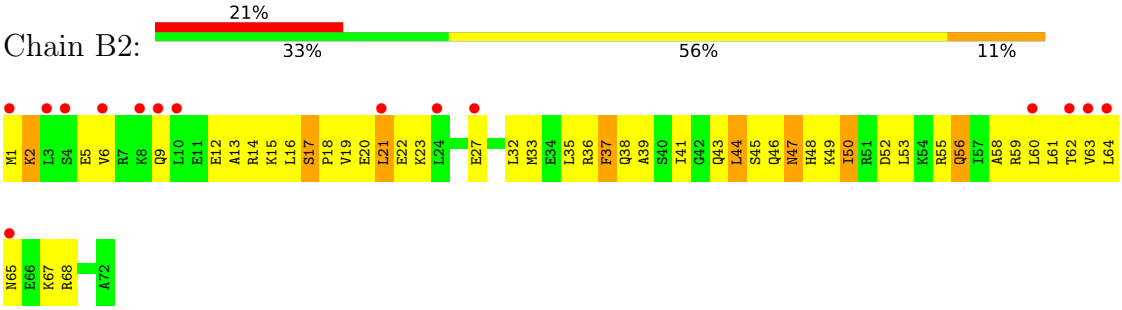
• Molecule 48: 50S ribosomal protein L28

Chain D1:



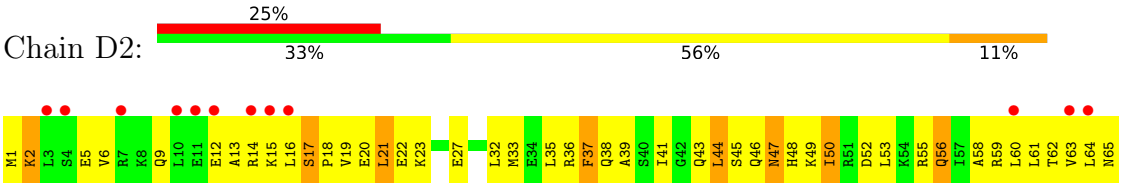
• Molecule 49: 50S ribosomal protein L29

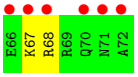
Chain B2:



• Molecule 49: 50S ribosomal protein L29

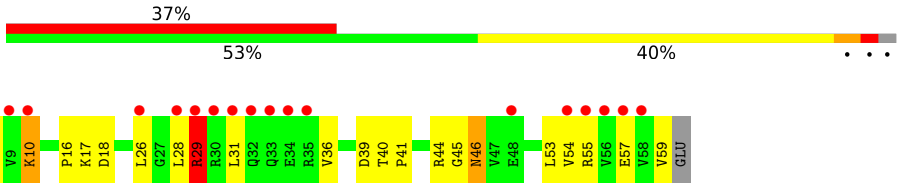
Chain D2:





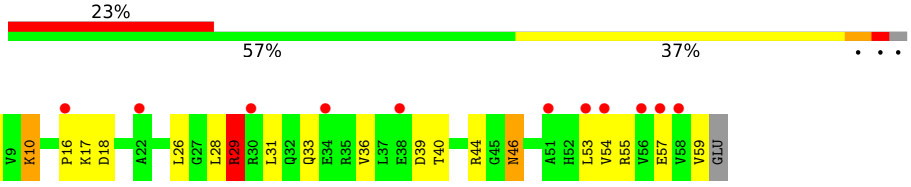
• Molecule 50: 50S ribosomal protein L30

Chain B3:



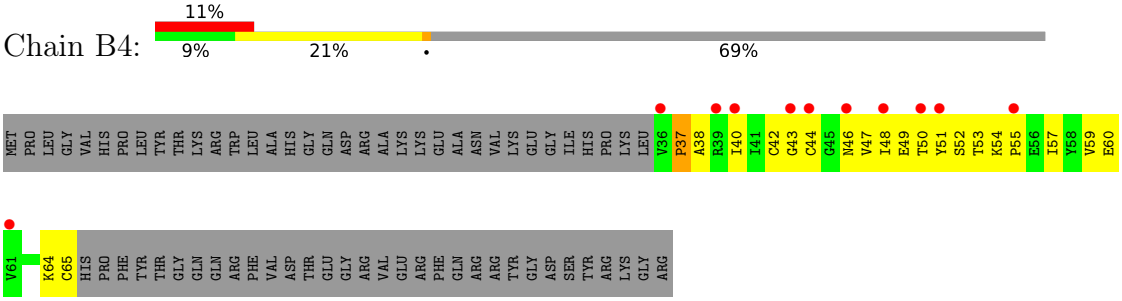
• Molecule 50: 50S ribosomal protein L30

Chain D3:



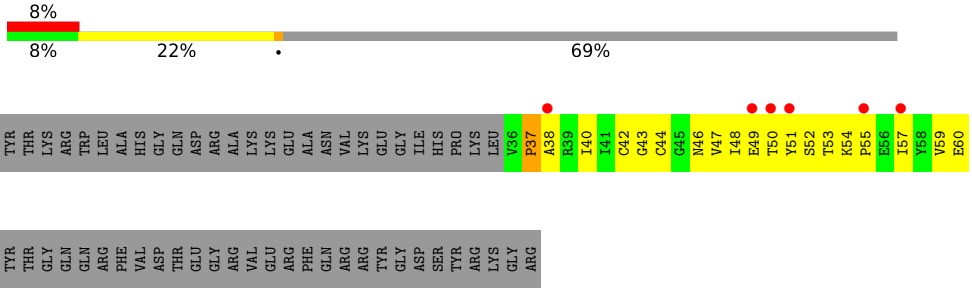
• Molecule 51: 50S ribosomal protein L31

Chain B4:



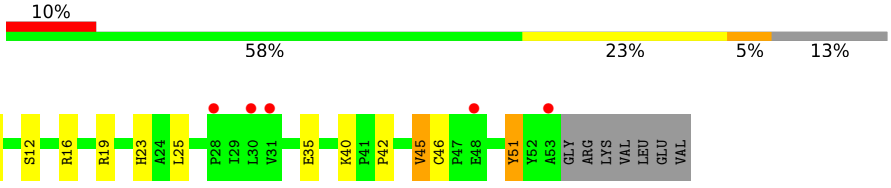
• Molecule 51: 50S ribosomal protein L31

Chain D4:



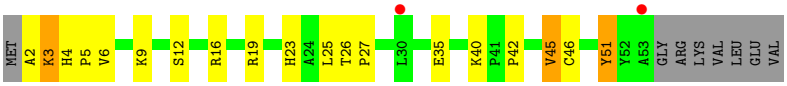
• Molecule 52: 50S ribosomal protein L32

Chain B5:



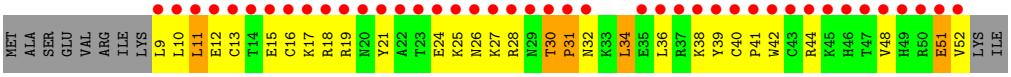
• Molecule 52: 50S ribosomal protein L32

Chain D5:



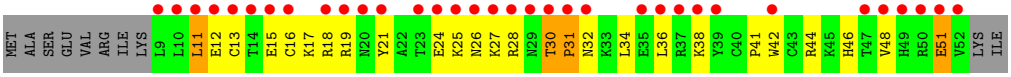
• Molecule 53: 50S ribosomal protein L33

Chain B6:



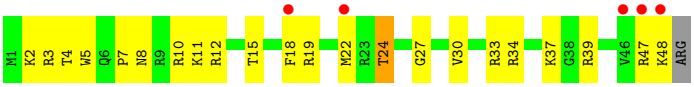
• Molecule 53: 50S ribosomal protein L33

Chain D6:



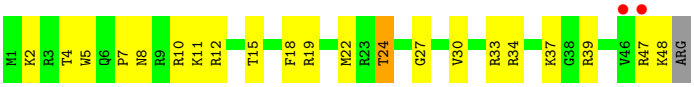
• Molecule 54: 50S ribosomal protein L34

Chain B7:



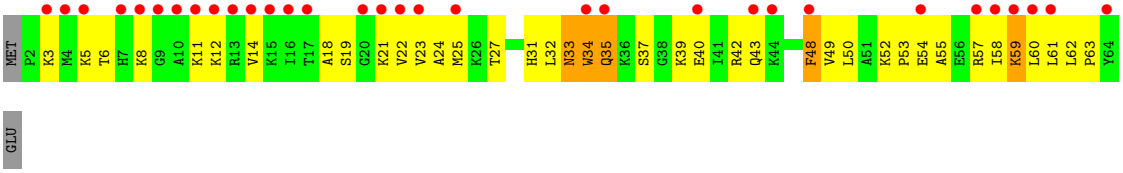
• Molecule 54: 50S ribosomal protein L34

Chain D7:



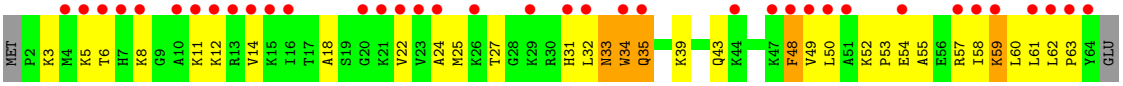
• Molecule 55: 50S ribosomal protein L35

Chain B8:



• Molecule 55: 50S ribosomal protein L35

Chain D8:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	210.13Å 454.39Å 616.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.90 – 3.21 87.17 – 3.20	Depositor EDS
% Data completeness (in resolution range)	95.1 (49.90-3.21) 95.1 (87.17-3.20)	Depositor EDS
R_{merge}	0.27	Depositor
R_{sym}	0.27	Depositor
$< I/\sigma(I) >$ [1]	2.69 (at 3.19Å)	Xtriage
Refinement program	PHENIX (phenix.refine), CNS 1.2	Depositor
R, R_{free}	0.292 , 0.319 0.290 , 0.320	Depositor DCC
R_{free} test set	8774 reflections (0.92%)	wwPDB-VP
Wilson B-factor (Å^2)	54.0	Xtriage
Anisotropy	0.069	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.17 , 71.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.26$, $< L^2 > = 0.11$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.82	EDS
Total number of atoms	299961	wwPDB-VP
Average B, all atoms (Å^2)	143.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.17% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.42	0/36194	0.85	27/56493 (0.0%)
1	CA	0.41	0/36194	0.85	24/56493 (0.0%)
2	AY	0.42	0/1832	0.81	1/2855 (0.0%)
2	AZ	0.39	0/1832	0.80	0/2855
2	CY	0.43	0/1832	0.82	1/2855 (0.0%)
2	CZ	0.40	0/1832	0.80	0/2855
3	AV	0.43	0/291	0.81	0/452
3	CV	0.42	0/291	0.82	0/452
4	AB	0.21	0/1935	0.38	0/2609
4	CB	0.21	0/1935	0.38	0/2609
5	AC	0.21	0/1636	0.36	0/2205
5	CC	0.21	0/1636	0.36	0/2205
6	AD	0.22	0/1733	0.38	0/2318
6	CD	0.22	0/1733	0.37	0/2318
7	AE	0.22	0/1171	0.39	0/1576
7	CE	0.22	0/1171	0.39	0/1576
8	AF	0.22	0/856	0.39	0/1154
8	CF	0.23	0/856	0.40	0/1154
9	AG	0.21	0/1276	0.36	0/1709
9	CG	0.21	0/1276	0.36	0/1709
10	AH	0.22	0/1136	0.40	0/1527
10	CH	0.21	0/1136	0.40	0/1527
11	AI	0.21	0/1029	0.37	0/1378
11	CI	0.21	0/1029	0.37	0/1378
12	AJ	0.21	0/807	0.39	0/1085
12	CJ	0.21	0/807	0.39	0/1085
13	AK	0.21	0/900	0.39	0/1213
13	CK	0.22	0/900	0.39	0/1213
14	AL	0.23	0/986	0.42	0/1320
14	CL	0.23	0/986	0.42	0/1320
15	AM	0.19	0/943	0.39	0/1265
15	CM	0.19	0/943	0.39	0/1265

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
16	AN	0.22	0/501	0.36	0/664
16	CN	0.22	0/501	0.36	0/664
17	AO	0.22	0/745	0.36	0/992
17	CO	0.21	0/745	0.36	0/992
18	AP	0.22	0/716	0.40	0/963
18	CP	0.21	0/716	0.39	0/963
19	AQ	0.22	0/836	0.38	0/1117
19	CQ	0.23	0/836	0.38	0/1117
20	AR	0.22	0/579	0.39	0/768
20	CR	0.22	0/579	0.39	0/768
21	AS	0.21	0/642	0.38	0/865
21	CS	0.21	0/642	0.38	0/865
22	AT	0.22	0/764	0.36	0/1006
22	CT	0.21	0/764	0.36	0/1006
23	AU	0.20	0/212	0.36	0/277
23	CU	0.19	0/212	0.36	0/277
24	AX	0.23	0/2850	0.40	0/3829
24	CX	0.22	0/2850	0.40	0/3829
25	BA	0.44	0/69437	0.88	51/108401 (0.0%)
25	DA	0.44	0/69437	0.89	55/108401 (0.1%)
26	BB	0.41	0/2853	0.85	1/4451 (0.0%)
26	DB	0.41	0/2853	0.84	1/4451 (0.0%)
27	BD	0.25	0/2154	0.44	0/2905
27	DD	0.26	0/2154	0.44	0/2905
28	BE	0.24	0/1596	0.44	0/2153
28	DE	0.23	0/1596	0.44	0/2153
29	BF	0.23	0/1621	0.40	0/2194
29	DF	0.23	0/1621	0.40	0/2194
30	BG	0.21	0/1500	0.40	0/2017
30	DG	0.21	0/1500	0.40	0/2017
31	BH	0.20	0/1245	0.40	0/1682
31	DH	0.20	0/1245	0.40	0/1682
32	BI	0.21	0/1147	0.41	0/1552
32	DI	0.21	0/1147	0.41	0/1552
33	BJ	0.21	0/251	0.38	0/333
33	DJ	0.21	0/251	0.38	0/333
34	BN	0.22	0/1123	0.44	0/1515
34	DN	0.22	0/1123	0.44	0/1515
35	BO	0.25	0/942	0.42	0/1268
35	DO	0.24	0/942	0.42	0/1268
36	BP	0.24	0/1131	0.45	0/1504
36	DP	0.24	0/1131	0.46	0/1504
37	BQ	0.24	0/1099	0.44	0/1468

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
37	DQ	0.24	0/1099	0.44	0/1468
38	BR	0.23	0/974	0.45	1/1302 (0.1%)
38	DR	0.22	0/974	0.41	0/1302
39	BS	0.21	0/778	0.38	0/1036
39	DS	0.21	0/778	0.38	0/1036
40	BT	0.23	0/1157	0.40	0/1544
40	DT	0.22	0/1157	0.39	0/1544
41	BU	0.26	0/982	0.41	0/1306
41	DU	0.28	0/982	0.42	0/1306
42	BV	0.23	0/790	0.40	0/1057
42	DV	0.23	0/790	0.40	0/1057
43	BW	0.23	0/901	0.40	0/1209
43	DW	0.24	0/901	0.39	0/1209
44	BX	0.24	0/739	0.41	0/993
44	DX	0.24	0/739	0.41	0/993
45	BY	0.24	0/788	0.44	0/1051
45	DY	0.24	0/788	0.43	0/1051
46	BZ	0.22	0/1523	0.42	0/2068
46	DZ	0.22	0/1523	0.42	0/2068
47	B0	0.22	0/613	0.39	0/816
47	D0	0.22	0/613	0.39	0/816
48	B1	0.25	0/701	0.47	0/932
48	D1	0.25	0/701	0.47	0/932
49	B2	0.24	0/607	0.48	0/803
49	D2	0.24	0/607	0.48	0/803
50	B3	0.22	0/472	0.40	0/634
50	D3	0.22	0/472	0.40	0/634
51	B4	0.20	0/228	0.41	0/309
51	D4	0.21	0/228	0.41	0/309
52	B5	0.22	0/418	0.43	0/567
52	D5	0.22	0/418	0.43	0/567
53	B6	0.23	0/387	0.43	0/518
53	D6	0.23	0/387	0.43	0/518
54	B7	0.23	0/426	0.41	0/561
54	D7	0.25	0/426	0.41	0/561
55	B8	0.24	0/515	0.41	0/679
55	D8	0.24	0/515	0.41	0/679
All	All	0.38	0/323000	0.77	162/482646 (0.0%)

There are no bond length outliers.

The worst 5 of 162 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	DA	1379	A	C1'-O4'-C4'	-11.90	100.38	109.90
25	BA	1379	A	C1'-O4'-C4'	-11.49	100.71	109.90
25	DA	1091	G	P-O3'-C3'	10.71	132.56	119.70
25	BA	1091	G	P-O3'-C3'	10.65	132.48	119.70
25	DA	1786	A	C1'-O4'-C4'	-9.82	102.04	109.90

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32332	0	16318	788	0
1	CA	32332	0	16318	782	0
2	AY	1640	0	837	31	0
2	AZ	1640	0	837	34	0
2	CY	1640	0	837	32	0
2	CZ	1640	0	837	32	0
3	AV	258	0	132	4	0
3	CV	258	0	132	6	0
4	AB	1900	0	1951	109	0
4	CB	1900	0	1951	109	0
5	AC	1612	0	1677	92	0
5	CC	1612	0	1677	88	0
6	AD	1703	0	1765	74	0
6	CD	1703	0	1765	72	0
7	AE	1155	0	1213	74	0
7	CE	1155	0	1213	70	0
8	AF	843	0	857	44	0
8	CF	843	0	857	45	0
9	AG	1257	0	1296	64	0
9	CG	1257	0	1296	59	0
10	AH	1116	0	1177	64	0
10	CH	1116	0	1177	62	0
11	AI	1011	0	1043	62	0
11	CI	1011	0	1043	60	0
12	AJ	794	0	840	61	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	CJ	794	0	840	61	0
13	AK	885	0	904	60	0
13	CK	885	0	904	55	0
14	AL	970	0	1057	74	0
14	CL	970	0	1057	78	0
15	AM	933	0	992	55	0
15	CM	933	0	992	56	0
16	AN	492	0	531	42	0
16	CN	492	0	532	40	0
17	AO	734	0	771	33	0
17	CO	734	0	771	31	0
18	AP	700	0	720	36	0
18	CP	700	0	720	36	0
19	AQ	823	0	893	44	0
19	CQ	823	0	893	43	0
20	AR	574	0	644	28	0
20	CR	574	0	644	27	0
21	AS	629	0	652	61	0
21	CS	629	0	652	59	0
22	AT	762	0	859	39	0
22	CT	762	0	859	40	0
23	AU	208	0	221	8	0
23	CU	208	0	221	7	0
24	AX	2813	0	2823	159	0
24	CX	2813	0	2823	155	0
25	BA	61997	0	31250	1569	0
25	DA	61997	0	31250	1579	0
26	BB	2551	0	1295	54	0
26	DB	2551	0	1295	58	0
27	BD	2104	0	2182	166	0
27	DD	2104	0	2182	170	0
28	BE	1563	0	1629	110	0
28	DE	1563	0	1629	111	0
29	BF	1586	0	1632	128	0
29	DF	1586	0	1632	124	0
30	BG	1475	0	1537	115	0
30	DG	1475	0	1537	114	0
31	BH	1222	0	1282	59	0
31	DH	1222	0	1282	58	0
32	BI	1132	0	1220	60	0
32	DI	1132	0	1220	57	0
33	BJ	253	0	275	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	DJ	253	0	275	10	0
34	BN	1096	0	1168	83	0
34	DN	1096	0	1168	85	0
35	BO	932	0	994	52	0
35	DO	932	0	994	56	0
36	BP	1114	0	1187	148	0
36	DP	1114	0	1187	150	0
37	BQ	1079	0	1127	85	0
37	DQ	1079	0	1127	89	0
38	BR	960	0	1021	60	0
38	DR	960	0	1021	57	0
39	BS	770	0	832	57	0
39	DS	770	0	832	57	0
40	BT	1143	0	1211	77	0
40	DT	1143	0	1211	82	0
41	BU	964	0	1022	84	0
41	DU	964	0	1022	80	0
42	BV	779	0	852	57	0
42	DV	779	0	852	57	0
43	BW	890	0	951	51	0
43	DW	890	0	951	55	0
44	BX	725	0	778	68	0
44	DX	725	0	778	68	0
45	BY	775	0	870	76	0
45	DY	775	0	870	71	0
46	BZ	1491	0	1513	79	0
46	DZ	1491	0	1513	83	0
47	B0	605	0	628	31	0
47	D0	605	0	628	34	0
48	B1	694	0	764	64	0
48	D1	694	0	764	66	0
49	B2	605	0	665	61	0
49	D2	605	0	665	62	0
50	B3	467	0	523	20	0
50	D3	467	0	523	18	0
51	B4	225	0	225	18	0
51	D4	225	0	225	20	0
52	B5	404	0	420	27	0
52	D5	404	0	420	28	0
53	B6	380	0	391	32	0
53	D6	380	0	391	28	0
54	B7	418	0	467	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	D7	418	0	467	17	0
55	B8	507	0	576	39	0
55	D8	507	0	576	38	0
56	AA	310	0	0	0	0
56	AB	2	0	0	0	0
56	AC	6	0	0	0	0
56	AD	8	0	0	0	0
56	AE	1	0	0	0	0
56	AF	2	0	0	0	0
56	AG	1	0	0	0	0
56	AH	2	0	0	0	0
56	AI	2	0	0	0	0
56	AJ	1	0	0	0	0
56	AK	1	0	0	0	0
56	AL	2	0	0	0	0
56	AM	1	0	0	0	0
56	AO	3	0	0	0	0
56	AP	1	0	0	0	0
56	AQ	1	0	0	0	0
56	AV	1	0	0	0	0
56	AX	6	0	0	0	0
56	AY	25	0	0	0	0
56	AZ	6	0	0	0	0
56	B1	2	0	0	0	0
56	B2	3	0	0	0	0
56	B5	1	0	0	0	0
56	B7	3	0	0	0	0
56	BA	806	0	0	0	0
56	BB	26	0	0	0	0
56	BD	2	0	0	0	0
56	BE	1	0	0	0	0
56	BF	5	0	0	0	0
56	BG	3	0	0	0	0
56	BH	2	0	0	0	0
56	BI	3	0	0	0	0
56	BJ	1	0	0	0	0
56	BN	2	0	0	0	0
56	BO	3	0	0	0	0
56	BP	1	0	0	0	0
56	BQ	3	0	0	0	0
56	BR	3	0	0	0	0
56	BT	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	BU	1	0	0	0	0
56	BV	1	0	0	0	0
56	BW	2	0	0	0	0
56	BY	1	0	0	0	0
56	BZ	1	0	0	0	0
56	CA	414	0	0	0	0
56	CB	2	0	0	0	0
56	CC	7	0	0	0	0
56	CD	2	0	0	0	0
56	CE	1	0	0	0	0
56	CF	1	0	0	0	0
56	CG	1	0	0	0	0
56	CH	1	0	0	0	0
56	CI	2	0	0	0	0
56	CJ	1	0	0	0	0
56	CK	2	0	0	0	0
56	CL	1	0	0	0	0
56	CO	2	0	0	0	0
56	CP	1	0	0	0	0
56	CV	4	0	0	0	0
56	CX	9	0	0	0	0
56	CY	21	0	0	0	0
56	CZ	19	0	0	0	0
56	D2	2	0	0	0	0
56	D3	1	0	0	0	0
56	D4	3	0	0	0	0
56	D5	1	0	0	0	0
56	D7	2	0	0	0	0
56	D8	1	0	0	0	0
56	DA	758	0	0	0	0
56	DB	28	0	0	0	0
56	DD	1	0	0	0	0
56	DF	1	0	0	0	0
56	DG	1	0	0	0	0
56	DH	4	0	0	0	0
56	DI	2	0	0	0	0
56	DN	1	0	0	0	0
56	DO	2	0	0	0	0
56	DP	6	0	0	0	0
56	DQ	1	0	0	0	0
56	DR	1	0	0	0	0
56	DT	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	DV	1	0	0	0	0
56	DW	3	0	0	0	0
56	DX	1	0	0	0	0
56	DZ	4	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	299961	0	202995	10201	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 20.

The worst 5 of 10201 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)
29:DF:40:GLN:HE22	29:DF:182:ASN:HB2	1.10	1.14
37:DQ:23:GLY:HA3	37:DQ:98:LYS:HG3	1.31	1.13
37:BQ:23:GLY:HA3	37:BQ:98:LYS:HG3	1.31	1.12
29:BF:40:GLN:HE22	29:BF:182:ASN:HB2	1.10	1.07
37:BQ:14:ARG:HG2	37:BQ:14:ARG:HH11	1.20	1.06

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
4	AB	232/256 (91%)	186 (80%)	37 (16%)	9 (4%)	3 22
4	CB	232/256 (91%)	188 (81%)	37 (16%)	7 (3%)	4 28
5	AC	204/239 (85%)	156 (76%)	36 (18%)	12 (6%)	1 12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
5	CC	204/239 (85%)	155 (76%)	38 (19%)	11 (5%)	2 14
6	AD	206/209 (99%)	163 (79%)	31 (15%)	12 (6%)	1 13
6	CD	206/209 (99%)	163 (79%)	30 (15%)	13 (6%)	1 10
7	AE	149/162 (92%)	122 (82%)	24 (16%)	3 (2%)	7 38
7	CE	149/162 (92%)	122 (82%)	24 (16%)	3 (2%)	7 38
8	AF	99/101 (98%)	85 (86%)	13 (13%)	1 (1%)	15 54
8	CF	99/101 (98%)	85 (86%)	13 (13%)	1 (1%)	15 54
9	AG	153/156 (98%)	125 (82%)	24 (16%)	4 (3%)	5 31
9	CG	153/156 (98%)	127 (83%)	22 (14%)	4 (3%)	5 31
10	AH	136/138 (99%)	118 (87%)	17 (12%)	1 (1%)	22 61
10	CH	136/138 (99%)	118 (87%)	18 (13%)	0	100 100
11	AI	125/128 (98%)	100 (80%)	23 (18%)	2 (2%)	9 43
11	CI	125/128 (98%)	101 (81%)	22 (18%)	2 (2%)	9 43
12	AJ	96/105 (91%)	73 (76%)	18 (19%)	5 (5%)	2 15
12	CJ	96/105 (91%)	73 (76%)	18 (19%)	5 (5%)	2 15
13	AK	117/129 (91%)	97 (83%)	18 (15%)	2 (2%)	9 42
13	CK	117/129 (91%)	96 (82%)	19 (16%)	2 (2%)	9 42
14	AL	122/134 (91%)	88 (72%)	26 (21%)	8 (7%)	1 9
14	CL	122/134 (91%)	88 (72%)	26 (21%)	8 (7%)	1 9
15	AM	115/126 (91%)	92 (80%)	16 (14%)	7 (6%)	1 12
15	CM	115/126 (91%)	92 (80%)	16 (14%)	7 (6%)	1 12
16	AN	58/61 (95%)	45 (78%)	8 (14%)	5 (9%)	1 4
16	CN	58/61 (95%)	45 (78%)	8 (14%)	5 (9%)	1 4
17	AO	86/89 (97%)	70 (81%)	15 (17%)	1 (1%)	13 49
17	CO	86/89 (97%)	69 (80%)	16 (19%)	1 (1%)	13 49
18	AP	81/88 (92%)	65 (80%)	14 (17%)	2 (2%)	5 32
18	CP	81/88 (92%)	65 (80%)	14 (17%)	2 (2%)	5 32
19	AQ	97/105 (92%)	87 (90%)	8 (8%)	2 (2%)	7 37
19	CQ	97/105 (92%)	86 (89%)	9 (9%)	2 (2%)	7 37
20	AR	68/88 (77%)	53 (78%)	13 (19%)	2 (3%)	4 28
20	CR	68/88 (77%)	52 (76%)	14 (21%)	2 (3%)	4 28

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
21	AS	76/93 (82%)	53 (70%)	16 (21%)	7 (9%)	1 3
21	CS	76/93 (82%)	53 (70%)	16 (21%)	7 (9%)	1 3
22	AT	97/106 (92%)	79 (81%)	14 (14%)	4 (4%)	3 21
22	CT	97/106 (92%)	79 (81%)	14 (14%)	4 (4%)	3 21
23	AU	22/27 (82%)	18 (82%)	3 (14%)	1 (4%)	2 18
23	CU	22/27 (82%)	18 (82%)	3 (14%)	1 (4%)	2 18
24	AX	352/354 (99%)	297 (84%)	44 (12%)	11 (3%)	4 26
24	CX	352/354 (99%)	296 (84%)	45 (13%)	11 (3%)	4 26
27	BD	269/276 (98%)	213 (79%)	40 (15%)	16 (6%)	1 12
27	DD	269/276 (98%)	213 (79%)	40 (15%)	16 (6%)	1 12
28	BE	202/206 (98%)	151 (75%)	41 (20%)	10 (5%)	2 16
28	DE	202/206 (98%)	151 (75%)	42 (21%)	9 (4%)	2 18
29	BF	200/210 (95%)	158 (79%)	35 (18%)	7 (4%)	3 24
29	DF	200/210 (95%)	158 (79%)	35 (18%)	7 (4%)	3 24
30	BG	179/182 (98%)	127 (71%)	42 (24%)	10 (6%)	2 14
30	DG	179/182 (98%)	124 (69%)	44 (25%)	11 (6%)	1 12
31	BH	157/180 (87%)	126 (80%)	24 (15%)	7 (4%)	2 18
31	DH	157/180 (87%)	126 (80%)	24 (15%)	7 (4%)	2 18
32	BI	143/148 (97%)	111 (78%)	25 (18%)	7 (5%)	2 17
32	DI	143/148 (97%)	112 (78%)	24 (17%)	7 (5%)	2 17
33	BJ	28/173 (16%)	27 (96%)	1 (4%)	0	100 100
33	DJ	28/173 (16%)	27 (96%)	1 (4%)	0	100 100
34	BN	135/163 (83%)	100 (74%)	27 (20%)	8 (6%)	1 12
34	DN	135/163 (83%)	100 (74%)	27 (20%)	8 (6%)	1 12
35	BO	120/122 (98%)	101 (84%)	18 (15%)	1 (1%)	19 58
35	DO	120/122 (98%)	101 (84%)	18 (15%)	1 (1%)	19 58
36	BP	144/150 (96%)	82 (57%)	44 (31%)	18 (12%)	0 1
36	DP	144/150 (96%)	82 (57%)	45 (31%)	17 (12%)	0 2
37	BQ	134/141 (95%)	86 (64%)	36 (27%)	12 (9%)	1 4
37	DQ	134/141 (95%)	87 (65%)	35 (26%)	12 (9%)	1 4
38	BR	115/118 (98%)	92 (80%)	18 (16%)	5 (4%)	2 20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
38	DR	115/118 (98%)	91 (79%)	18 (16%)	6 (5%)	2 15
39	BS	96/112 (86%)	62 (65%)	24 (25%)	10 (10%)	0 3
39	DS	96/112 (86%)	61 (64%)	25 (26%)	10 (10%)	0 3
40	BT	135/146 (92%)	102 (76%)	29 (22%)	4 (3%)	4 28
40	DT	135/146 (92%)	103 (76%)	28 (21%)	4 (3%)	4 28
41	BU	115/118 (98%)	90 (78%)	21 (18%)	4 (4%)	3 24
41	DU	115/118 (98%)	89 (77%)	22 (19%)	4 (4%)	3 24
42	BV	99/101 (98%)	69 (70%)	21 (21%)	9 (9%)	1 3
42	DV	99/101 (98%)	69 (70%)	21 (21%)	9 (9%)	1 3
43	BW	110/113 (97%)	91 (83%)	17 (16%)	2 (2%)	8 41
43	DW	110/113 (97%)	91 (83%)	17 (16%)	2 (2%)	8 41
44	BX	90/96 (94%)	69 (77%)	20 (22%)	1 (1%)	14 51
44	DX	90/96 (94%)	69 (77%)	20 (22%)	1 (1%)	14 51
45	BY	98/110 (89%)	65 (66%)	21 (21%)	12 (12%)	0 2
45	DY	98/110 (89%)	65 (66%)	21 (21%)	12 (12%)	0 2
46	BZ	186/206 (90%)	142 (76%)	34 (18%)	10 (5%)	2 14
46	DZ	186/206 (90%)	142 (76%)	34 (18%)	10 (5%)	2 14
47	B0	74/85 (87%)	55 (74%)	14 (19%)	5 (7%)	1 9
47	D0	74/85 (87%)	55 (74%)	14 (19%)	5 (7%)	1 9
48	B1	86/98 (88%)	53 (62%)	27 (31%)	6 (7%)	1 8
48	D1	86/98 (88%)	53 (62%)	28 (33%)	5 (6%)	1 13
49	B2	70/72 (97%)	48 (69%)	16 (23%)	6 (9%)	1 4
49	D2	70/72 (97%)	48 (69%)	16 (23%)	6 (9%)	1 4
50	B3	57/60 (95%)	43 (75%)	13 (23%)	1 (2%)	8 41
50	D3	57/60 (95%)	44 (77%)	12 (21%)	1 (2%)	8 41
51	B4	28/97 (29%)	14 (50%)	11 (39%)	3 (11%)	0 2
51	D4	28/97 (29%)	14 (50%)	11 (39%)	3 (11%)	0 2
52	B5	50/60 (83%)	36 (72%)	12 (24%)	2 (4%)	3 21
52	D5	50/60 (83%)	36 (72%)	12 (24%)	2 (4%)	3 21
53	B6	42/54 (78%)	31 (74%)	8 (19%)	3 (7%)	1 8
53	D6	42/54 (78%)	31 (74%)	8 (19%)	3 (7%)	1 8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
54	B7	46/49 (94%)	39 (85%)	7 (15%)	0	100 100
54	D7	46/49 (94%)	39 (85%)	7 (15%)	0	100 100
55	B8	61/65 (94%)	42 (69%)	15 (25%)	4 (7%)	1 9
55	D8	61/65 (94%)	42 (69%)	15 (25%)	4 (7%)	1 9
All	All	11920/13210 (90%)	9191 (77%)	2165 (18%)	564 (5%)	2 17

5 of 564 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	AC	47	LEU
12	AJ	75	ILE
15	AM	4	ILE
15	AM	106	ASN
15	AM	117	VAL

5.3.2 Protein sidechains (i)

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	AB	202/220 (92%)	189 (94%)	13 (6%)	17 52
4	CB	202/220 (92%)	189 (94%)	13 (6%)	17 52
5	AC	160/188 (85%)	151 (94%)	9 (6%)	21 57
5	CC	160/188 (85%)	151 (94%)	9 (6%)	21 57
6	AD	180/181 (99%)	171 (95%)	9 (5%)	24 60
6	CD	180/181 (99%)	171 (95%)	9 (5%)	24 60
7	AE	116/123 (94%)	105 (90%)	11 (10%)	8 32
7	CE	116/123 (94%)	105 (90%)	11 (10%)	8 32
8	AF	90/90 (100%)	86 (96%)	4 (4%)	28 64
8	CF	90/90 (100%)	86 (96%)	4 (4%)	28 64
9	AG	126/127 (99%)	125 (99%)	1 (1%)	81 93
9	CG	126/127 (99%)	125 (99%)	1 (1%)	81 93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	AH	119/119 (100%)	114 (96%)	5 (4%)	30	65
10	CH	119/119 (100%)	114 (96%)	5 (4%)	30	65
11	AI	98/99 (99%)	92 (94%)	6 (6%)	18	54
11	CI	98/99 (99%)	92 (94%)	6 (6%)	18	54
12	AJ	88/92 (96%)	80 (91%)	8 (9%)	9	34
12	CJ	88/92 (96%)	80 (91%)	8 (9%)	9	34
13	AK	90/99 (91%)	86 (96%)	4 (4%)	28	64
13	CK	90/99 (91%)	86 (96%)	4 (4%)	28	64
14	AL	104/110 (94%)	98 (94%)	6 (6%)	20	55
14	CL	104/110 (94%)	98 (94%)	6 (6%)	20	55
15	AM	94/101 (93%)	87 (93%)	7 (7%)	13	46
15	CM	94/101 (93%)	87 (93%)	7 (7%)	13	46
16	AN	49/50 (98%)	47 (96%)	2 (4%)	30	66
16	CN	49/50 (98%)	47 (96%)	2 (4%)	30	66
17	AO	79/80 (99%)	74 (94%)	5 (6%)	18	52
17	CO	79/80 (99%)	74 (94%)	5 (6%)	18	52
18	AP	72/74 (97%)	68 (94%)	4 (6%)	21	57
18	CP	72/74 (97%)	68 (94%)	4 (6%)	21	57
19	AQ	94/97 (97%)	91 (97%)	3 (3%)	39	71
19	CQ	94/97 (97%)	91 (97%)	3 (3%)	39	71
20	AR	61/77 (79%)	59 (97%)	2 (3%)	38	71
20	CR	61/77 (79%)	59 (97%)	2 (3%)	38	71
21	AS	69/80 (86%)	59 (86%)	10 (14%)	3	15
21	CS	69/80 (86%)	59 (86%)	10 (14%)	3	15
22	AT	76/82 (93%)	71 (93%)	5 (7%)	16	51
22	CT	76/82 (93%)	71 (93%)	5 (7%)	16	51
23	AU	19/22 (86%)	19 (100%)	0	100	100
23	CU	19/22 (86%)	19 (100%)	0	100	100
24	AX	299/299 (100%)	278 (93%)	21 (7%)	15	48
24	CX	299/299 (100%)	278 (93%)	21 (7%)	15	48
27	BD	213/218 (98%)	196 (92%)	17 (8%)	12	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
27	DD	213/218 (98%)	196 (92%)	17 (8%)	12 42
28	BE	165/166 (99%)	153 (93%)	12 (7%)	14 46
28	DE	165/166 (99%)	153 (93%)	12 (7%)	14 46
29	BF	161/166 (97%)	154 (96%)	7 (4%)	29 64
29	DF	161/166 (97%)	154 (96%)	7 (4%)	29 64
30	BG	155/156 (99%)	142 (92%)	13 (8%)	11 39
30	DG	155/156 (99%)	142 (92%)	13 (8%)	11 39
31	BH	132/148 (89%)	123 (93%)	9 (7%)	16 49
31	DH	132/148 (89%)	123 (93%)	9 (7%)	16 49
32	BI	122/124 (98%)	113 (93%)	9 (7%)	13 46
32	DI	122/124 (98%)	113 (93%)	9 (7%)	13 46
33	BJ	27/135 (20%)	26 (96%)	1 (4%)	34 68
33	DJ	27/135 (20%)	26 (96%)	1 (4%)	34 68
34	BN	116/139 (84%)	106 (91%)	10 (9%)	10 38
34	DN	116/139 (84%)	106 (91%)	10 (9%)	10 38
35	BO	100/100 (100%)	95 (95%)	5 (5%)	24 60
35	DO	100/100 (100%)	95 (95%)	5 (5%)	24 60
36	BP	112/116 (97%)	92 (82%)	20 (18%)	2 9
36	DP	112/116 (97%)	92 (82%)	20 (18%)	2 9
37	BQ	106/111 (96%)	95 (90%)	11 (10%)	7 28
37	DQ	106/111 (96%)	95 (90%)	11 (10%)	7 28
38	BR	100/101 (99%)	95 (95%)	5 (5%)	24 60
38	DR	100/101 (99%)	95 (95%)	5 (5%)	24 60
39	BS	77/88 (88%)	70 (91%)	7 (9%)	9 34
39	DS	77/88 (88%)	70 (91%)	7 (9%)	9 34
40	BT	121/128 (94%)	106 (88%)	15 (12%)	4 21
40	DT	121/128 (94%)	106 (88%)	15 (12%)	4 21
41	BU	93/94 (99%)	90 (97%)	3 (3%)	39 71
41	DU	93/94 (99%)	89 (96%)	4 (4%)	29 64
42	BV	82/82 (100%)	73 (89%)	9 (11%)	6 26
42	DV	82/82 (100%)	73 (89%)	9 (11%)	6 26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
43	BW	91/92 (99%)	89 (98%)	2 (2%)	52 79
43	DW	91/92 (99%)	89 (98%)	2 (2%)	52 79
44	BX	74/78 (95%)	68 (92%)	6 (8%)	11 42
44	DX	74/78 (95%)	68 (92%)	6 (8%)	11 42
45	BY	84/91 (92%)	79 (94%)	5 (6%)	19 54
45	DY	84/91 (92%)	79 (94%)	5 (6%)	19 54
46	BZ	163/179 (91%)	160 (98%)	3 (2%)	59 82
46	DZ	163/179 (91%)	160 (98%)	3 (2%)	59 82
47	B0	61/67 (91%)	59 (97%)	2 (3%)	38 71
47	D0	61/67 (91%)	59 (97%)	2 (3%)	38 71
48	B1	73/83 (88%)	63 (86%)	10 (14%)	3 17
48	D1	73/83 (88%)	64 (88%)	9 (12%)	4 21
49	B2	67/67 (100%)	64 (96%)	3 (4%)	27 63
49	D2	67/67 (100%)	64 (96%)	3 (4%)	27 63
50	B3	51/52 (98%)	47 (92%)	4 (8%)	12 43
50	D3	51/52 (98%)	48 (94%)	3 (6%)	19 54
51	B4	27/84 (32%)	25 (93%)	2 (7%)	13 46
51	D4	27/84 (32%)	25 (93%)	2 (7%)	13 46
52	B5	45/52 (86%)	43 (96%)	2 (4%)	28 64
52	D5	45/52 (86%)	43 (96%)	2 (4%)	28 64
53	B6	43/52 (83%)	40 (93%)	3 (7%)	15 48
53	D6	43/52 (83%)	40 (93%)	3 (7%)	15 48
54	B7	41/42 (98%)	38 (93%)	3 (7%)	14 46
54	D7	41/42 (98%)	38 (93%)	3 (7%)	14 46
55	B8	53/55 (96%)	51 (96%)	2 (4%)	33 67
55	D8	53/55 (96%)	51 (96%)	2 (4%)	33 67
All	All	10080/10952 (92%)	9411 (93%)	669 (7%)	16 51

5 of 669 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
24	CX	259	ILE
37	DQ	6	ARG

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Mol	Chain	Res	Type
27	DD	95	LEU
24	CX	249	MET
31	DH	23	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 231 such sidechains are listed below:

Mol	Chain	Res	Type
55	B8	33	ASN
48	D1	66	HIS
13	CK	38	ASN
48	D1	45	ASN
40	DT	79	HIS

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1503/1525 (98%)	211 (14%)	56 (3%)
1	CA	1503/1525 (98%)	211 (14%)	56 (3%)
2	AY	76/77 (98%)	11 (14%)	2 (2%)
2	AZ	76/77 (98%)	8 (10%)	1 (1%)
2	CY	76/77 (98%)	11 (14%)	2 (2%)
2	CZ	76/77 (98%)	8 (10%)	1 (1%)
25	BA	2878/2894 (99%)	448 (15%)	101 (3%)
25	DA	2878/2894 (99%)	445 (15%)	102 (3%)
26	BB	118/124 (95%)	12 (10%)	1 (0%)
26	DB	118/124 (95%)	12 (10%)	1 (0%)
3	AV	11/27 (40%)	2 (18%)	1 (9%)
3	CV	11/27 (40%)	2 (18%)	1 (9%)
All	All	9324/9448 (98%)	1381 (14%)	325 (3%)

5 of 1381 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	6	G
1	AA	9	G
1	AA	31	G
1	AA	39	G
1	AA	47	C

5 of 325 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	DA	221	A
25	DA	1816	G
25	DA	331	A
25	DA	1069	A
25	DA	2172	U

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2581 ligands modelled in this entry, 2581 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, 95^{th} 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	1504/1525 (98%)	0.23	73 (4%) 29 17	85, 138, 234, 323	0
1	CA	1504/1525 (98%)	0.47	128 (8%) 10 6	93, 155, 241, 322	0
2	AY	77/77 (100%)	-0.23	0 100 100	97, 129, 164, 212	0
2	AZ	77/77 (100%)	0.97	9 (11%) 4 2	216, 256, 275, 295	0
2	CY	77/77 (100%)	-0.17	0 100 100	86, 127, 171, 213	0
2	CZ	77/77 (100%)	0.87	13 (16%) 1 1	219, 254, 280, 289	0
3	AV	12/27 (44%)	1.15	3 (25%) 0 0	120, 129, 207, 226	0
3	CV	12/27 (44%)	1.99	4 (33%) 0 0	118, 127, 212, 221	0
4	AB	234/256 (91%)	1.21	61 (26%) 0 0	155, 190, 223, 247	0
4	CB	234/256 (91%)	1.31	68 (29%) 0 0	158, 188, 218, 246	0
5	AC	206/239 (86%)	0.45	20 (9%) 7 4	160, 191, 220, 245	0
5	CC	206/239 (86%)	0.90	38 (18%) 1 1	157, 174, 194, 224	0
6	AD	208/209 (99%)	1.05	46 (22%) 0 0	125, 146, 174, 188	0
6	CD	208/209 (99%)	1.37	65 (31%) 0 0	146, 177, 205, 230	0
7	AE	151/162 (93%)	0.69	19 (12%) 3 2	124, 145, 174, 198	0
7	CE	151/162 (93%)	0.91	28 (18%) 1 1	133, 154, 184, 220	0
8	AF	101/101 (100%)	0.21	10 (9%) 7 4	128, 148, 172, 192	0
8	CF	101/101 (100%)	0.32	7 (6%) 16 9	133, 151, 182, 195	0
9	AG	155/156 (99%)	0.65	24 (15%) 2 1	150, 170, 198, 213	0
9	CG	155/156 (99%)	0.50	20 (12%) 3 2	149, 171, 195, 210	0
10	AH	138/138 (100%)	1.45	38 (27%) 0 0	121, 147, 175, 193	0
10	CH	138/138 (100%)	1.20	29 (21%) 1 1	138, 162, 187, 202	0
11	AI	127/128 (99%)	3.26	78 (61%) 0 0	150, 194, 216, 233	0
11	CI	127/128 (99%)	3.17	76 (59%) 0 0	154, 183, 205, 227	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å^2)	Q<0.9
12	AJ	98/105 (93%)	1.27	26 (26%)	0	161, 211, 241, 252	0
12	CJ	98/105 (93%)	2.16	42 (42%)	0	159, 190, 217, 226	0
13	AK	119/129 (92%)	0.82	23 (19%)	1	117, 147, 176, 185	0
13	CK	119/129 (92%)	1.09	25 (21%)	1	114, 136, 169, 204	0
14	AL	124/134 (92%)	0.59	15 (12%)	4	106, 118, 143, 171	0
14	CL	124/134 (92%)	0.93	17 (13%)	3	122, 134, 161, 208	0
15	AM	117/126 (92%)	1.90	46 (39%)	0	152, 182, 203, 216	0
15	CM	117/126 (92%)	1.71	40 (34%)	0	164, 193, 219, 240	0
16	AN	60/61 (98%)	2.48	31 (51%)	0	171, 185, 211, 230	0
16	CN	60/61 (98%)	2.58	29 (48%)	0	163, 173, 205, 214	0
17	AO	88/89 (98%)	1.01	22 (25%)	0	114, 134, 161, 176	0
17	CO	88/89 (98%)	1.14	21 (23%)	0	121, 148, 175, 193	0
18	AP	83/88 (94%)	2.27	45 (54%)	0	120, 133, 162, 173	0
18	CP	83/88 (94%)	3.46	51 (61%)	0	154, 178, 202, 235	0
19	AQ	99/105 (94%)	1.30	29 (29%)	0	115, 126, 154, 159	0
19	CQ	99/105 (94%)	1.71	28 (28%)	0	122, 151, 171, 188	0
20	AR	70/88 (79%)	0.81	13 (18%)	1	134, 151, 184, 198	0
20	CR	70/88 (79%)	0.62	7 (10%)	4	131, 147, 174, 191	0
21	AS	78/93 (83%)	2.05	32 (41%)	0	163, 192, 214, 226	0
21	CS	78/93 (83%)	1.88	38 (48%)	0	171, 196, 216, 232	0
22	AT	99/106 (93%)	1.81	39 (39%)	0	126, 144, 174, 200	0
22	CT	99/106 (93%)	2.39	45 (45%)	0	155, 177, 205, 234	0
23	AU	24/27 (88%)	5.84	21 (87%)	0	195, 213, 232, 241	0
23	CU	24/27 (88%)	5.54	21 (87%)	0	180, 201, 227, 248	0
24	AX	354/354 (100%)	1.07	74 (20%)	1	98, 137, 242, 255	0
24	CX	354/354 (100%)	1.50	93 (26%)	0	105, 134, 292, 310	0
25	BA	2879/2894 (99%)	0.16	149 (5%)	27	65, 112, 248, 354	0
25	DA	2879/2894 (99%)	0.13	139 (4%)	30	59, 110, 238, 321	0
26	BB	119/124 (95%)	0.18	6 (5%)	28	138, 171, 208, 265	0
26	DB	119/124 (95%)	0.16	5 (4%)	36	132, 181, 215, 265	0
27	BD	271/276 (98%)	0.73	38 (14%)	2	98, 122, 149, 167	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
27	DD	271/276 (98%)	0.83	48 (17%)	1	1	93, 115, 140, 163	0
28	BE	204/206 (99%)	1.39	66 (32%)	0	0	95, 126, 164, 180	0
28	DE	204/206 (99%)	1.05	43 (21%)	1	1	99, 141, 171, 194	0
29	BF	202/210 (96%)	0.50	14 (6%)	16	9	97, 142, 175, 194	0
29	DF	202/210 (96%)	1.11	47 (23%)	0	0	92, 132, 163, 183	0
30	BG	181/182 (99%)	1.05	45 (24%)	0	0	147, 198, 223, 252	0
30	DG	181/182 (99%)	1.54	57 (31%)	0	0	146, 197, 233, 251	0
31	BH	159/180 (88%)	2.26	72 (45%)	0	0	141, 172, 206, 222	0
31	DH	159/180 (88%)	0.79	28 (17%)	1	1	148, 172, 202, 215	0
32	BI	145/148 (97%)	3.70	87 (60%)	0	0	134, 211, 264, 286	0
32	DI	145/148 (97%)	2.42	66 (45%)	0	0	125, 203, 254, 286	0
33	BJ	32/173 (18%)	5.26	29 (90%)	0	0	203, 228, 245, 262	0
33	DJ	32/173 (18%)	4.23	26 (81%)	0	0	188, 222, 247, 258	0
34	BN	137/163 (84%)	1.61	47 (34%)	0	0	110, 142, 167, 219	0
34	DN	137/163 (84%)	1.20	36 (26%)	0	0	112, 140, 165, 184	0
35	BO	122/122 (100%)	0.70	15 (12%)	4	2	104, 113, 133, 184	0
35	DO	122/122 (100%)	1.13	26 (21%)	0	1	111, 128, 146, 175	0
36	BP	146/150 (97%)	1.33	41 (28%)	0	0	105, 145, 182, 203	0
36	DP	146/150 (97%)	0.84	26 (17%)	1	1	100, 143, 178, 198	0
37	BQ	136/141 (96%)	1.76	49 (36%)	0	0	109, 142, 172, 226	0
37	DQ	136/141 (96%)	2.45	57 (41%)	0	0	105, 140, 174, 226	0
38	BR	117/118 (99%)	1.57	35 (29%)	0	0	102, 116, 153, 180	0
38	DR	117/118 (99%)	1.62	38 (32%)	0	0	108, 129, 167, 183	0
39	BS	98/112 (87%)	1.99	38 (38%)	0	0	164, 192, 215, 232	0
39	DS	98/112 (87%)	1.31	30 (30%)	0	0	164, 197, 225, 240	0
40	BT	137/146 (93%)	0.52	16 (11%)	4	2	107, 120, 163, 190	0
40	DT	137/146 (93%)	1.14	39 (28%)	0	0	121, 145, 189, 205	0
41	BU	117/118 (99%)	0.95	25 (21%)	0	1	109, 144, 175, 196	0
41	DU	117/118 (99%)	1.42	37 (31%)	0	0	102, 136, 170, 183	0
42	BV	101/101 (100%)	0.71	18 (17%)	1	1	110, 160, 187, 202	0
42	DV	101/101 (100%)	0.96	20 (19%)	1	1	104, 150, 183, 202	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
43	BW	112/113 (99%)	0.85	13 (11%) 4 3	95, 118, 156, 181	0
43	DW	112/113 (99%)	0.68	11 (9%) 7 4	92, 116, 145, 172	0
44	BX	92/96 (95%)	1.27	26 (28%) 0 0	111, 129, 161, 179	0
44	DX	92/96 (95%)	1.15	22 (23%) 0 0	101, 120, 145, 174	0
45	BY	100/110 (90%)	2.98	57 (57%) 0 0	131, 150, 181, 216	0
45	DY	100/110 (90%)	2.26	45 (45%) 0 0	115, 135, 172, 199	0
46	BZ	188/206 (91%)	1.45	57 (30%) 0 0	138, 180, 207, 229	0
46	DZ	188/206 (91%)	0.71	32 (17%) 1 1	134, 173, 200, 215	0
47	B0	76/85 (89%)	2.45	34 (44%) 0 0	116, 147, 174, 187	0
47	D0	76/85 (89%)	2.39	39 (51%) 0 0	115, 148, 175, 193	0
48	B1	88/98 (89%)	1.06	15 (17%) 1 1	107, 128, 162, 180	0
48	D1	88/98 (89%)	0.96	17 (19%) 1 1	102, 121, 165, 187	0
49	B2	72/72 (100%)	0.97	15 (20%) 1 1	128, 148, 181, 208	0
49	D2	72/72 (100%)	1.12	18 (25%) 0 0	115, 129, 183, 197	0
50	B3	59/60 (98%)	1.97	22 (37%) 0 0	127, 147, 180, 210	0
50	D3	59/60 (98%)	1.25	14 (23%) 0 0	121, 143, 172, 212	0
51	B4	30/97 (30%)	1.93	11 (36%) 0 0	204, 221, 244, 244	0
51	D4	30/97 (30%)	1.42	8 (26%) 0 0	208, 226, 243, 245	0
52	B5	52/60 (86%)	0.68	6 (11%) 4 3	98, 120, 159, 188	0
52	D5	52/60 (86%)	0.25	2 (3%) 40 26	96, 126, 177, 192	0
53	B6	44/54 (81%)	6.11	42 (95%) 0 0	132, 166, 195, 199	0
53	D6	44/54 (81%)	6.65	34 (77%) 0 0	134, 165, 193, 200	0
54	B7	48/49 (97%)	0.70	5 (10%) 6 4	98, 105, 132, 171	0
54	D7	48/49 (97%)	0.44	2 (4%) 36 23	92, 97, 120, 175	0
55	B8	63/65 (96%)	2.19	32 (50%) 0 0	115, 125, 158, 176	0
55	D8	63/65 (96%)	2.30	37 (58%) 0 0	109, 124, 151, 190	0
All	All	21460/22658 (94%)	0.89	3904 (18%) 1 1	59, 143, 230, 354	0

The worst 5 of 3904 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AA	80	G	42.4
1	AA	81	G	35.6

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Mol	Chain	Res	Type	RSRZ
32	BI	85	GLU	26.8
53	B6	13	CYS	22.4
37	DQ	140	ALA	22.1

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 monosaccharides 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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	CE	201	1/1	0.40	0.25	70,70,70,70	0
56	MG	DA	3661	1/1	0.51	1.22	80,80,80,80	0
56	MG	DA	3659	1/1	0.57	0.33	66,66,66,66	0
56	MG	DA	3546	1/1	0.57	0.70	82,82,82,82	0
56	MG	AX	404	1/1	0.58	0.18	68,68,68,68	0
56	MG	DA	3492	1/1	0.59	0.16	37,37,37,37	0
56	MG	BB	206	1/1	0.59	0.21	65,65,65,65	0
56	MG	CA	1614	1/1	0.62	0.35	39,39,39,39	0
56	MG	BA	3595	1/1	0.66	0.12	61,61,61,61	0
56	MG	CA	1826	1/1	0.67	0.24	65,65,65,65	0
56	MG	BA	3572	1/1	0.67	0.17	72,72,72,72	0
56	MG	BA	3780	1/1	0.69	0.25	56,56,56,56	0
56	MG	CA	1615	1/1	0.69	0.34	55,55,55,55	0
56	MG	DA	3192	1/1	0.70	0.11	67,67,67,67	0
56	MG	DA	3673	1/1	0.72	1.06	65,65,65,65	0
56	MG	CA	1985	1/1	0.73	0.14	52,52,52,52	0
56	MG	BA	3693	1/1	0.73	0.09	51,51,51,51	0
56	MG	AE	201	1/1	0.73	0.37	60,60,60,60	0
56	MG	BA	3529	1/1	0.73	0.17	32,32,32,32	0
56	MG	CA	1974	1/1	0.74	0.21	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	AA	1631	1/1	0.74	0.19	58,58,58,58	0
56	MG	BA	3677	1/1	0.74	0.45	63,63,63,63	0
56	MG	CA	1936	1/1	0.75	0.24	63,63,63,63	0
56	MG	CA	1930	1/1	0.76	0.59	57,57,57,57	0
56	MG	AA	1764	1/1	0.76	0.28	61,61,61,61	0
56	MG	DA	3594	1/1	0.76	0.22	83,83,83,83	0
56	MG	DA	3683	1/1	0.76	0.08	89,89,89,89	0
56	MG	DA	3189	1/1	0.77	0.18	40,40,40,40	0
56	MG	CY	109	1/1	0.77	0.20	68,68,68,68	0
56	MG	BA	3415	1/1	0.77	0.27	52,52,52,52	0
56	MG	CA	1737	1/1	0.78	0.15	58,58,58,58	0
56	MG	CA	1819	1/1	0.78	0.19	46,46,46,46	0
56	MG	BA	3708	1/1	0.78	0.32	60,60,60,60	0
56	MG	CA	1981	1/1	0.78	0.11	77,77,77,77	0
56	MG	DA	3351	1/1	0.78	0.20	38,38,38,38	0
56	MG	CA	1905	1/1	0.78	0.41	64,64,64,64	0
56	MG	AA	1795	1/1	0.79	0.24	65,65,65,65	0
56	MG	DA	3178	1/1	0.79	0.14	47,47,47,47	0
56	MG	BA	3754	1/1	0.79	0.14	70,70,70,70	0
56	MG	BR	202	1/1	0.79	0.55	61,61,61,61	0
56	MG	CA	1818	1/1	0.80	0.20	64,64,64,64	0
56	MG	BA	3555	1/1	0.80	0.11	54,54,54,54	0
56	MG	CA	1825	1/1	0.80	0.18	26,26,26,26	0
56	MG	BA	3766	1/1	0.80	0.19	44,44,44,44	0
56	MG	CV	104	1/1	0.80	0.43	54,54,54,54	0
56	MG	CA	1830	1/1	0.80	0.24	36,36,36,36	0
56	MG	AY	109	1/1	0.80	0.15	63,63,63,63	0
56	MG	CH	201	1/1	0.80	0.72	51,51,51,51	0
56	MG	DA	3134	1/1	0.80	0.11	61,61,61,61	0
56	MG	AX	405	1/1	0.80	0.23	58,58,58,58	0
56	MG	DA	3698	1/1	0.80	0.67	73,73,73,73	0
56	MG	DA	3757	1/1	0.80	0.41	43,43,43,43	0
56	MG	DA	3184	1/1	0.81	0.21	22,22,22,22	0
56	MG	AA	1654	1/1	0.81	0.21	80,80,80,80	0
56	MG	CA	1932	1/1	0.81	0.27	54,54,54,54	0
56	MG	AY	113	1/1	0.81	0.13	41,41,41,41	0
56	MG	DA	3354	1/1	0.81	0.28	43,43,43,43	0
56	MG	DA	3437	1/1	0.81	0.26	41,41,41,41	0
56	MG	AA	1840	1/1	0.81	0.26	49,49,49,49	0
56	MG	DA	3516	1/1	0.81	0.47	62,62,62,62	0
56	MG	CA	1862	1/1	0.82	0.28	71,71,71,71	0
56	MG	DA	3548	1/1	0.82	0.18	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DA	3583	1/1	0.82	0.37	43,43,43,43	0
56	MG	CA	1873	1/1	0.82	0.18	62,62,62,62	0
56	MG	BA	3593	1/1	0.82	0.37	55,55,55,55	0
56	MG	BA	3747	1/1	0.82	0.28	63,63,63,63	0
56	MG	AA	1884	1/1	0.82	0.35	55,55,55,55	0
56	MG	AD	304	1/1	0.82	0.57	50,50,50,50	0
56	MG	CA	1950	1/1	0.82	0.25	67,67,67,67	0
56	MG	BA	3517	1/1	0.82	0.12	40,40,40,40	0
56	MG	AA	1844	1/1	0.83	0.37	38,38,38,38	0
56	MG	CA	1749	1/1	0.83	0.15	41,41,41,41	0
56	MG	CA	1754	1/1	0.83	0.24	59,59,59,59	0
56	MG	CA	1768	1/1	0.83	0.11	39,39,39,39	0
56	MG	BA	3453	1/1	0.83	0.39	43,43,43,43	0
56	MG	BA	3465	1/1	0.83	0.42	37,37,37,37	0
56	MG	CA	2014	1/1	0.83	0.44	52,52,52,52	0
56	MG	BA	3665	1/1	0.83	0.30	46,46,46,46	0
56	MG	BA	3806	1/1	0.83	0.15	54,54,54,54	0
56	MG	DA	3575	1/1	0.83	0.27	53,53,53,53	0
56	MG	BA	3184	1/1	0.83	0.11	64,64,64,64	0
56	MG	BA	3315	1/1	0.83	0.37	64,64,64,64	0
56	MG	CX	406	1/1	0.83	1.60	71,71,71,71	0
56	MG	DH	202	1/1	0.83	0.16	64,64,64,64	0
56	MG	BA	3345	1/1	0.83	0.13	37,37,37,37	0
56	MG	DA	3176	1/1	0.83	0.21	46,46,46,46	0
56	MG	BA	3719	1/1	0.83	0.34	51,51,51,51	0
56	MG	CA	1666	1/1	0.83	0.19	50,50,50,50	0
56	MG	BA	3613	1/1	0.84	0.14	45,45,45,45	0
56	MG	DA	3646	1/1	0.84	0.16	55,55,55,55	0
56	MG	BA	3725	1/1	0.84	0.22	52,52,52,52	0
56	MG	CX	402	1/1	0.84	0.14	38,38,38,38	0
56	MG	CA	1883	1/1	0.84	0.13	41,41,41,41	0
56	MG	DA	3679	1/1	0.84	0.45	62,62,62,62	0
56	MG	CX	407	1/1	0.84	0.31	70,70,70,70	0
56	MG	CA	1689	1/1	0.84	0.21	59,59,59,59	0
56	MG	DA	3718	1/1	0.84	0.45	60,60,60,60	0
56	MG	DA	3754	1/1	0.84	0.27	59,59,59,59	0
56	MG	CA	1924	1/1	0.84	0.24	45,45,45,45	0
56	MG	BA	3582	1/1	0.85	0.21	53,53,53,53	0
56	MG	BA	3039	1/1	0.85	0.21	33,33,33,33	0
56	MG	DP	205	1/1	0.85	0.24	42,42,42,42	0
56	MG	DA	3554	1/1	0.85	0.14	71,71,71,71	0
56	MG	DA	3055	1/1	0.85	0.15	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DA	3116	1/1	0.85	0.25	41,41,41,41	0
56	MG	AA	1890	1/1	0.85	0.16	39,39,39,39	0
56	MG	CA	2012	1/1	0.85	0.19	59,59,59,59	0
56	MG	CA	1917	1/1	0.85	0.15	70,70,70,70	0
56	MG	AA	1688	1/1	0.85	0.10	52,52,52,52	0
56	MG	BA	3639	1/1	0.85	0.31	54,54,54,54	0
56	MG	AY	110	1/1	0.85	0.10	53,53,53,53	0
56	MG	BA	3380	1/1	0.85	0.28	56,56,56,56	0
56	MG	CP	101	1/1	0.85	0.45	57,57,57,57	0
56	MG	DA	3379	1/1	0.85	0.52	51,51,51,51	0
56	MG	DA	3724	1/1	0.85	0.84	62,62,62,62	0
56	MG	AA	1677	1/1	0.85	0.10	49,49,49,49	0
56	MG	CA	1970	1/1	0.85	0.16	63,63,63,63	0
56	MG	DB	222	1/1	0.85	0.10	59,59,59,59	0
56	MG	DA	3440	1/1	0.86	0.16	71,71,71,71	0
56	MG	DA	3468	1/1	0.86	0.12	30,30,30,30	0
56	MG	BA	3187	1/1	0.86	0.17	65,65,65,65	0
56	MG	BA	3746	1/1	0.86	0.41	65,65,65,65	0
56	MG	DA	3532	1/1	0.86	0.13	65,65,65,65	0
56	MG	DA	3541	1/1	0.86	0.14	53,53,53,53	0
56	MG	CA	1964	1/1	0.86	0.46	39,39,39,39	0
56	MG	DA	3547	1/1	0.86	0.16	48,48,48,48	0
56	MG	CA	1625	1/1	0.86	0.13	60,60,60,60	0
56	MG	CA	1651	1/1	0.86	0.14	54,54,54,54	0
56	MG	CA	1831	1/1	0.86	0.12	66,66,66,66	0
56	MG	CA	1982	1/1	0.86	0.58	63,63,63,63	0
56	MG	BA	3672	1/1	0.86	0.14	45,45,45,45	0
56	MG	DA	3609	1/1	0.86	0.29	62,62,62,62	0
56	MG	CA	1682	1/1	0.86	0.12	46,46,46,46	0
56	MG	DA	3654	1/1	0.86	0.32	41,41,41,41	0
56	MG	CA	1881	1/1	0.86	0.46	47,47,47,47	0
56	MG	BA	3674	1/1	0.86	0.26	52,52,52,52	0
56	MG	AA	1876	1/1	0.86	0.29	57,57,57,57	0
56	MG	DA	3198	1/1	0.86	0.47	51,51,51,51	0
56	MG	DA	3244	1/1	0.86	0.30	57,57,57,57	0
56	MG	BA	3330	1/1	0.86	0.10	45,45,45,45	0
56	MG	BA	3694	1/1	0.86	0.15	50,50,50,50	0
56	MG	DA	3375	1/1	0.86	0.30	42,42,42,42	0
56	MG	BA	3562	1/1	0.86	0.20	29,29,29,29	0
56	MG	DA	3432	1/1	0.86	0.21	51,51,51,51	0
56	MG	DA	3758	1/1	0.86	0.52	63,63,63,63	0
56	MG	DB	210	1/1	0.86	0.14	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	AA	1693	1/1	0.86	0.14	45,45,45,45	0
56	MG	AA	1891	1/1	0.87	0.36	68,68,68,68	0
56	MG	BA	3655	1/1	0.87	0.17	47,47,47,47	0
56	MG	DA	3559	1/1	0.87	0.23	44,44,44,44	0
56	MG	DA	3567	1/1	0.87	0.12	74,74,74,74	0
56	MG	CC	304	1/1	0.87	0.19	93,93,93,93	0
56	MG	CA	1824	1/1	0.87	0.12	31,31,31,31	0
56	MG	BA	3656	1/1	0.87	0.40	52,52,52,52	0
56	MG	CA	1937	1/1	0.87	0.50	56,56,56,56	0
56	MG	BA	3151	1/1	0.87	0.26	52,52,52,52	0
56	MG	BA	3178	1/1	0.87	0.21	39,39,39,39	0
56	MG	AA	1779	1/1	0.87	0.40	51,51,51,51	0
56	MG	AF	202	1/1	0.87	0.12	58,58,58,58	0
56	MG	AA	1762	1/1	0.87	0.12	52,52,52,52	0
56	MG	DQ	201	1/1	0.87	0.10	53,53,53,53	0
56	MG	DA	3466	1/1	0.87	0.25	47,47,47,47	0
56	MG	AA	1848	1/1	0.87	0.09	45,45,45,45	0
56	MG	DA	3093	1/1	0.87	0.24	23,23,23,23	0
56	MG	BB	225	1/1	0.87	0.13	50,50,50,50	0
56	MG	CA	1988	1/1	0.87	0.17	48,48,48,48	0
56	MG	DA	3138	1/1	0.87	0.21	52,52,52,52	0
56	MG	DA	3545	1/1	0.87	0.08	50,50,50,50	0
56	MG	BA	3629	1/1	0.87	0.09	53,53,53,53	0
56	MG	DB	212	1/1	0.87	0.20	45,45,45,45	0
56	MG	CA	1781	1/1	0.87	0.49	57,57,57,57	0
56	MG	DB	228	1/1	0.87	0.21	46,46,46,46	0
56	MG	CA	1789	1/1	0.88	0.54	53,53,53,53	0
56	MG	DA	3227	1/1	0.88	0.13	37,37,37,37	0
56	MG	BJ	201	1/1	0.88	0.10	59,59,59,59	0
56	MG	DA	3570	1/1	0.88	0.07	36,36,36,36	0
56	MG	DA	3263	1/1	0.88	0.19	22,22,22,22	0
56	MG	DA	3302	1/1	0.88	0.25	31,31,31,31	0
56	MG	BA	3400	1/1	0.88	0.18	35,35,35,35	0
56	MG	BA	3697	1/1	0.88	0.28	40,40,40,40	0
56	MG	CA	1947	1/1	0.88	0.31	44,44,44,44	0
56	MG	BA	3087	1/1	0.88	0.17	30,30,30,30	0
56	MG	DA	3658	1/1	0.88	0.22	61,61,61,61	0
56	MG	DA	3390	1/1	0.88	0.24	36,36,36,36	0
56	MG	DA	3412	1/1	0.88	0.29	50,50,50,50	0
56	MG	BA	3438	1/1	0.88	0.24	52,52,52,52	0
56	MG	CA	1827	1/1	0.88	0.12	48,48,48,48	0
56	MG	BA	3197	1/1	0.88	0.16	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	BA	3214	1/1	0.88	0.16	62,62,62,62	0
56	MG	BA	3469	1/1	0.88	0.11	28,28,28,28	0
56	MG	CA	1868	1/1	0.88	0.25	54,54,54,54	0
56	MG	DA	3738	1/1	0.88	0.21	58,58,58,58	0
56	MG	BA	3270	1/1	0.88	0.13	8,8,8,8	0
56	MG	BA	3100	1/1	0.88	0.17	42,42,42,42	0
56	MG	AA	1731	1/1	0.88	0.13	48,48,48,48	0
56	MG	DB	204	1/1	0.88	0.13	48,48,48,48	0
56	MG	AA	1625	1/1	0.88	0.15	27,27,27,27	0
56	MG	AA	1892	1/1	0.88	0.12	48,48,48,48	0
56	MG	CY	118	1/1	0.88	0.14	56,56,56,56	0
56	MG	BA	3396	1/1	0.88	0.21	57,57,57,57	0
56	MG	BA	3673	1/1	0.89	0.40	46,46,46,46	0
56	MG	AA	1901	1/1	0.89	0.20	43,43,43,43	0
56	MG	CA	1899	1/1	0.89	0.25	49,49,49,49	0
56	MG	DA	3482	1/1	0.89	0.26	42,42,42,42	0
56	MG	CA	1690	1/1	0.89	0.17	30,30,30,30	0
56	MG	CA	1911	1/1	0.89	0.12	62,62,62,62	0
56	MG	CA	1702	1/1	0.89	0.06	56,56,56,56	0
56	MG	CA	1719	1/1	0.89	0.20	58,58,58,58	0
56	MG	CA	1925	1/1	0.89	0.32	45,45,45,45	0
56	MG	BA	3757	1/1	0.89	0.21	45,45,45,45	0
56	MG	BA	3489	1/1	0.89	0.12	46,46,46,46	0
56	MG	DA	3004	1/1	0.89	0.79	42,42,42,42	0
56	MG	BA	3772	1/1	0.89	0.48	57,57,57,57	0
56	MG	BA	3224	1/1	0.89	0.14	52,52,52,52	0
56	MG	DA	3101	1/1	0.89	0.09	33,33,33,33	0
56	MG	AA	1842	1/1	0.89	0.11	49,49,49,49	0
56	MG	BA	3536	1/1	0.89	0.11	34,34,34,34	0
56	MG	CA	1955	1/1	0.89	0.15	29,29,29,29	0
56	MG	BB	221	1/1	0.89	0.25	37,37,37,37	0
56	MG	CA	1967	1/1	0.89	0.21	60,60,60,60	0
56	MG	CA	1969	1/1	0.89	0.10	43,43,43,43	0
56	MG	BA	3706	1/1	0.89	0.08	38,38,38,38	0
56	MG	BG	203	1/1	0.89	0.35	54,54,54,54	0
56	MG	CA	1979	1/1	0.89	0.16	59,59,59,59	0
56	MG	DA	3218	1/1	0.89	0.27	46,46,46,46	0
56	MG	BA	3092	1/1	0.89	0.19	40,40,40,40	0
56	MG	BA	3711	1/1	0.89	0.22	28,28,28,28	0
56	MG	BA	3712	1/1	0.89	0.22	37,37,37,37	0
56	MG	DA	3271	1/1	0.89	0.14	17,17,17,17	0
56	MG	AA	1803	1/1	0.89	0.15	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	CA	1994	1/1	0.89	0.17	58,58,58,58	0
56	MG	CA	2000	1/1	0.89	0.13	45,45,45,45	0
56	MG	BA	3122	1/1	0.89	0.16	50,50,50,50	0
56	MG	CA	1833	1/1	0.89	0.10	37,37,37,37	0
56	MG	BA	3730	1/1	0.89	0.22	40,40,40,40	0
56	MG	CA	1653	1/1	0.89	0.14	49,49,49,49	0
56	MG	DA	3428	1/1	0.89	0.12	61,61,61,61	0
56	MG	CY	112	1/1	0.89	0.09	20,20,20,20	0
56	MG	DA	3435	1/1	0.89	0.21	41,41,41,41	0
56	MG	BA	3372	1/1	0.89	0.12	38,38,38,38	0
56	MG	CA	1720	1/1	0.90	0.10	51,51,51,51	0
56	MG	CA	1926	1/1	0.90	0.15	61,61,61,61	0
56	MG	DA	3458	1/1	0.90	0.21	44,44,44,44	0
56	MG	BA	3669	1/1	0.90	0.41	33,33,33,33	0
56	MG	CA	1931	1/1	0.90	0.32	59,59,59,59	0
56	MG	CA	1747	1/1	0.90	0.15	31,31,31,31	0
56	MG	DP	201	1/1	0.90	0.08	45,45,45,45	0
56	MG	CA	1748	1/1	0.90	0.14	60,60,60,60	0
56	MG	AY	125	1/1	0.90	0.11	51,51,51,51	0
56	MG	D2	102	1/1	0.90	0.56	49,49,49,49	0
56	MG	BA	3484	1/1	0.90	0.16	23,23,23,23	0
56	MG	BA	3781	1/1	0.90	0.35	54,54,54,54	0
56	MG	AA	1822	1/1	0.90	0.16	39,39,39,39	0
56	MG	BA	3327	1/1	0.90	0.08	43,43,43,43	0
56	MG	AA	1669	1/1	0.90	0.15	40,40,40,40	0
56	MG	BB	223	1/1	0.90	0.24	52,52,52,52	0
56	MG	BA	3340	1/1	0.90	0.13	49,49,49,49	0
56	MG	DA	3169	1/1	0.90	0.15	42,42,42,42	0
56	MG	BA	3344	1/1	0.90	0.16	42,42,42,42	0
56	MG	BA	3700	1/1	0.90	0.28	67,67,67,67	0
56	MG	BA	3133	1/1	0.90	0.29	48,48,48,48	0
56	MG	DA	3601	1/1	0.90	0.12	45,45,45,45	0
56	MG	CA	1607	1/1	0.90	0.08	38,38,38,38	0
56	MG	DA	3615	1/1	0.90	0.19	40,40,40,40	0
56	MG	AA	1789	1/1	0.90	0.15	33,33,33,33	0
56	MG	AA	1792	1/1	0.90	0.06	58,58,58,58	0
56	MG	AA	1691	1/1	0.90	0.21	52,52,52,52	0
56	MG	BA	3012	1/1	0.90	0.09	36,36,36,36	0
56	MG	AA	1799	1/1	0.90	0.24	49,49,49,49	0
56	MG	BA	3425	1/1	0.90	0.31	48,48,48,48	0
56	MG	CA	1678	1/1	0.90	0.18	65,65,65,65	0
56	MG	DA	3287	1/1	0.90	0.14	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DA	3690	1/1	0.90	0.11	41,41,41,41	0
56	MG	DA	3695	1/1	0.90	0.23	52,52,52,52	0
56	MG	CY	105	1/1	0.90	0.14	58,58,58,58	0
56	MG	DA	3708	1/1	0.90	0.29	60,60,60,60	0
56	MG	DA	3343	1/1	0.90	0.12	35,35,35,35	0
56	MG	BA	3432	1/1	0.90	0.09	53,53,53,53	0
56	MG	CA	1902	1/1	0.90	0.12	50,50,50,50	0
56	MG	DA	3745	1/1	0.90	0.21	39,39,39,39	0
56	MG	BA	3048	1/1	0.90	0.26	64,64,64,64	0
56	MG	CC	302	1/1	0.90	0.14	56,56,56,56	0
56	MG	BA	3749	1/1	0.90	0.18	30,30,30,30	0
56	MG	DA	3403	1/1	0.90	0.30	42,42,42,42	0
56	MG	AA	1644	1/1	0.90	0.08	31,31,31,31	0
56	MG	BA	3229	1/1	0.90	0.11	27,27,27,27	0
56	MG	DB	219	1/1	0.90	0.09	55,55,55,55	0
56	MG	CK	201	1/1	0.90	0.14	51,51,51,51	0
56	MG	CO	102	1/1	0.90	0.33	73,73,73,73	0
56	MG	DA	3253	1/1	0.91	0.19	48,48,48,48	0
56	MG	BA	3413	1/1	0.91	0.07	62,62,62,62	0
56	MG	BA	3181	1/1	0.91	0.18	51,51,51,51	0
56	MG	BA	3671	1/1	0.91	0.18	57,57,57,57	0
56	MG	BA	3423	1/1	0.91	0.16	22,22,22,22	0
56	MG	DA	3322	1/1	0.91	0.12	46,46,46,46	0
56	MG	AA	1868	1/1	0.91	0.37	41,41,41,41	0
56	MG	CA	1671	1/1	0.91	0.13	40,40,40,40	0
56	MG	BA	3004	1/1	0.91	0.49	57,57,57,57	0
56	MG	AA	1638	1/1	0.91	0.14	22,22,22,22	0
56	MG	BA	3691	1/1	0.91	0.14	44,44,44,44	0
56	MG	DA	3381	1/1	0.91	0.38	36,36,36,36	0
56	MG	AA	1757	1/1	0.91	0.06	26,26,26,26	0
56	MG	CA	1701	1/1	0.91	0.09	40,40,40,40	0
56	MG	BA	3462	1/1	0.91	0.27	39,39,39,39	0
56	MG	CA	1713	1/1	0.91	0.14	21,21,21,21	0
56	MG	CA	1715	1/1	0.91	0.12	39,39,39,39	0
56	MG	BA	3695	1/1	0.91	0.17	50,50,50,50	0
56	MG	BA	3463	1/1	0.91	0.15	27,27,27,27	0
56	MG	CA	1728	1/1	0.91	0.22	28,28,28,28	0
56	MG	CA	2009	1/1	0.91	0.30	41,41,41,41	0
56	MG	BA	3220	1/1	0.91	0.31	55,55,55,55	0
56	MG	BA	3703	1/1	0.91	0.11	29,29,29,29	0
56	MG	CZ	109	1/1	0.91	0.16	51,51,51,51	0
56	MG	BA	3467	1/1	0.91	0.23	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	BA	3043	1/1	0.91	0.22	30,30,30,30	0
56	MG	BA	3472	1/1	0.91	0.22	44,44,44,44	0
56	MG	BA	3476	1/1	0.91	0.27	39,39,39,39	0
56	MG	AA	1885	1/1	0.91	0.11	33,33,33,33	0
56	MG	BA	3255	1/1	0.91	0.07	43,43,43,43	0
56	MG	CA	1815	1/1	0.91	0.12	12,12,12,12	0
56	MG	BA	3728	1/1	0.91	0.17	28,28,28,28	0
56	MG	BA	3499	1/1	0.91	0.11	18,18,18,18	0
56	MG	BA	3512	1/1	0.91	0.12	16,16,16,16	0
56	MG	AA	1888	1/1	0.91	0.11	53,53,53,53	0
56	MG	BA	3289	1/1	0.91	0.23	46,46,46,46	0
56	MG	BA	3311	1/1	0.91	0.14	43,43,43,43	0
56	MG	BA	3544	1/1	0.91	0.41	38,38,38,38	0
56	MG	BA	3091	1/1	0.91	0.23	39,39,39,39	0
56	MG	DH	201	1/1	0.91	0.14	46,46,46,46	0
56	MG	AC	302	1/1	0.91	0.24	57,57,57,57	0
56	MG	CA	1841	1/1	0.91	0.06	63,63,63,63	0
56	MG	DA	3620	1/1	0.91	0.16	49,49,49,49	0
56	MG	DA	3624	1/1	0.91	0.18	39,39,39,39	0
56	MG	DA	3634	1/1	0.91	0.17	58,58,58,58	0
56	MG	CA	1847	1/1	0.91	0.14	22,22,22,22	0
56	MG	CA	1856	1/1	0.91	0.28	78,78,78,78	0
56	MG	AA	1633	1/1	0.91	0.12	49,49,49,49	0
56	MG	BA	3119	1/1	0.91	0.20	39,39,39,39	0
56	MG	BA	3790	1/1	0.91	0.13	75,75,75,75	0
56	MG	DA	3664	1/1	0.91	0.26	39,39,39,39	0
56	MG	DA	3066	1/1	0.91	0.16	47,47,47,47	0
56	MG	BA	3803	1/1	0.91	0.43	55,55,55,55	0
56	MG	BA	3805	1/1	0.91	0.14	39,39,39,39	0
56	MG	DA	3110	1/1	0.91	0.18	43,43,43,43	0
56	MG	DA	3692	1/1	0.91	0.18	46,46,46,46	0
56	MG	CA	1886	1/1	0.91	0.30	62,62,62,62	0
56	MG	AA	1650	1/1	0.91	0.27	50,50,50,50	0
56	MG	BA	3130	1/1	0.91	0.11	36,36,36,36	0
56	MG	DA	3151	1/1	0.91	0.18	58,58,58,58	0
56	MG	AA	1708	1/1	0.91	0.08	48,48,48,48	0
56	MG	DA	3731	1/1	0.91	0.15	60,60,60,60	0
56	MG	BA	3374	1/1	0.91	0.15	25,25,25,25	0
56	MG	CA	1915	1/1	0.91	0.27	56,56,56,56	0
56	MG	BA	3631	1/1	0.91	0.18	34,34,34,34	0
56	MG	DA	3756	1/1	0.91	0.09	53,53,53,53	0
56	MG	AO	103	1/1	0.91	0.26	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	BA	3651	1/1	0.91	0.16	34,34,34,34	0
56	MG	BA	3156	1/1	0.91	0.12	48,48,48,48	0
56	MG	DA	3208	1/1	0.91	0.34	42,42,42,42	0
56	MG	BR	203	1/1	0.91	0.74	49,49,49,49	0
56	MG	AA	1895	1/1	0.91	0.11	50,50,50,50	0
56	MG	DA	3243	1/1	0.91	0.17	41,41,41,41	0
56	MG	BA	3661	1/1	0.91	0.35	67,67,67,67	0
56	MG	AJ	201	1/1	0.92	0.10	36,36,36,36	0
56	MG	BA	3621	1/1	0.92	0.06	57,57,57,57	0
56	MG	AL	201	1/1	0.92	0.10	29,29,29,29	0
56	MG	DA	3179	1/1	0.92	0.13	50,50,50,50	0
56	MG	BB	217	1/1	0.92	0.10	63,63,63,63	0
56	MG	CA	1885	1/1	0.92	0.19	72,72,72,72	0
56	MG	AO	102	1/1	0.92	0.35	36,36,36,36	0
56	MG	CA	1891	1/1	0.92	0.10	30,30,30,30	0
56	MG	BA	3632	1/1	0.92	0.17	50,50,50,50	0
56	MG	DA	3214	1/1	0.92	0.10	46,46,46,46	0
56	MG	BA	3633	1/1	0.92	0.18	20,20,20,20	0
56	MG	BF	301	1/1	0.92	0.13	39,39,39,39	0
56	MG	BA	3637	1/1	0.92	0.11	14,14,14,14	0
56	MG	AA	1831	1/1	0.92	0.09	44,44,44,44	0
56	MG	BA	3649	1/1	0.92	0.12	29,29,29,29	0
56	MG	BA	3170	1/1	0.92	0.14	18,18,18,18	0
56	MG	BA	3407	1/1	0.92	0.08	15,15,15,15	0
56	MG	AA	1832	1/1	0.92	0.18	49,49,49,49	0
56	MG	AA	1893	1/1	0.92	0.09	40,40,40,40	0
56	MG	CA	1616	1/1	0.92	0.10	54,54,54,54	0
56	MG	BA	3664	1/1	0.92	0.10	41,41,41,41	0
56	MG	CA	1934	1/1	0.92	0.22	56,56,56,56	0
56	MG	CA	1650	1/1	0.92	0.21	49,49,49,49	0
56	MG	DA	3355	1/1	0.92	0.18	39,39,39,39	0
56	MG	AA	1630	1/1	0.92	0.15	58,58,58,58	0
56	MG	CA	1946	1/1	0.92	0.25	41,41,41,41	0
56	MG	BA	3668	1/1	0.92	0.12	50,50,50,50	0
56	MG	CA	1657	1/1	0.92	0.12	42,42,42,42	0
56	MG	AA	1750	1/1	0.92	0.12	50,50,50,50	0
56	MG	BA	3195	1/1	0.92	0.22	46,46,46,46	0
56	MG	DA	3425	1/1	0.92	0.18	43,43,43,43	0
56	MG	BA	3437	1/1	0.92	0.12	26,26,26,26	0
56	MG	DA	3430	1/1	0.92	0.16	56,56,56,56	0
56	MG	CA	1681	1/1	0.92	0.28	43,43,43,43	0
56	MG	BA	3025	1/1	0.92	0.14	13,13,13,13	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	BA	3036	1/1	0.92	0.19	32,32,32,32	0
56	MG	AV	101	1/1	0.92	0.11	49,49,49,49	0
56	MG	DA	3456	1/1	0.92	0.16	37,37,37,37	0
56	MG	AA	1686	1/1	0.92	0.15	37,37,37,37	0
56	MG	BA	3692	1/1	0.92	0.21	41,41,41,41	0
56	MG	CA	1711	1/1	0.92	0.10	23,23,23,23	0
56	MG	BA	3045	1/1	0.92	0.12	40,40,40,40	0
56	MG	AA	1674	1/1	0.92	0.38	74,74,74,74	0
56	MG	BA	3262	1/1	0.92	0.14	31,31,31,31	0
56	MG	DA	3527	1/1	0.92	0.12	49,49,49,49	0
56	MG	CA	2007	1/1	0.92	0.30	60,60,60,60	0
56	MG	BA	3264	1/1	0.92	0.17	11,11,11,11	0
56	MG	BA	3078	1/1	0.92	0.07	22,22,22,22	0
56	MG	BA	3086	1/1	0.92	0.07	23,23,23,23	0
56	MG	CZ	102	1/1	0.92	0.12	67,67,67,67	0
56	MG	BA	3293	1/1	0.92	0.14	34,34,34,34	0
56	MG	CZ	119	1/1	0.92	0.15	55,55,55,55	0
56	MG	DA	3556	1/1	0.92	0.17	20,20,20,20	0
56	MG	BA	3498	1/1	0.92	0.13	19,19,19,19	0
56	MG	BA	3304	1/1	0.92	0.14	42,42,42,42	0
56	MG	AA	1726	1/1	0.92	0.12	44,44,44,44	0
56	MG	AA	1774	1/1	0.92	0.11	27,27,27,27	0
56	MG	CA	1769	1/1	0.92	0.11	56,56,56,56	0
56	MG	CA	1773	1/1	0.92	0.17	35,35,35,35	0
56	MG	CA	1774	1/1	0.92	0.10	31,31,31,31	0
56	MG	CC	306	1/1	0.92	0.40	52,52,52,52	0
56	MG	DA	3610	1/1	0.92	0.14	29,29,29,29	0
56	MG	CA	1777	1/1	0.92	0.14	34,34,34,34	0
56	MG	DA	3616	1/1	0.92	0.12	10,10,10,10	0
56	MG	BA	3519	1/1	0.92	0.14	38,38,38,38	0
56	MG	BA	3326	1/1	0.92	0.24	46,46,46,46	0
56	MG	CL	201	1/1	0.92	0.18	61,61,61,61	0
56	MG	CA	1794	1/1	0.92	0.07	42,42,42,42	0
56	MG	DA	3652	1/1	0.92	0.08	45,45,45,45	0
56	MG	DA	3653	1/1	0.92	0.11	55,55,55,55	0
56	MG	CA	1796	1/1	0.92	0.07	27,27,27,27	0
56	MG	CA	1797	1/1	0.92	0.17	60,60,60,60	0
56	MG	CA	1810	1/1	0.92	0.12	28,28,28,28	0
56	MG	DA	3660	1/1	0.92	0.19	44,44,44,44	0
56	MG	BA	3533	1/1	0.92	0.13	37,37,37,37	0
56	MG	BA	3743	1/1	0.92	0.09	34,34,34,34	0
56	MG	AA	1809	1/1	0.92	0.13	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	BA	3539	1/1	0.92	0.11	77,77,77,77	0
56	MG	DP	203	1/1	0.92	0.20	43,43,43,43	0
56	MG	AA	1775	1/1	0.92	0.13	74,74,74,74	0
56	MG	BA	3336	1/1	0.92	0.15	38,38,38,38	0
56	MG	AA	1824	1/1	0.92	0.14	78,78,78,78	0
56	MG	BA	3764	1/1	0.92	0.24	36,36,36,36	0
56	MG	DA	3006	1/1	0.92	0.23	27,27,27,27	0
56	MG	DA	3714	1/1	0.92	0.23	28,28,28,28	0
56	MG	BA	3566	1/1	0.92	0.18	45,45,45,45	0
56	MG	DA	3722	1/1	0.92	0.20	54,54,54,54	0
56	MG	DA	3057	1/1	0.92	0.14	31,31,31,31	0
56	MG	AA	1829	1/1	0.92	0.24	68,68,68,68	0
56	MG	DA	3736	1/1	0.92	0.14	64,64,64,64	0
56	MG	DA	3092	1/1	0.92	0.18	32,32,32,32	0
56	MG	DA	3741	1/1	0.92	0.18	25,25,25,25	0
56	MG	CA	1834	1/1	0.92	0.18	61,61,61,61	0
56	MG	DA	3748	1/1	0.92	0.70	50,50,50,50	0
56	MG	DA	3750	1/1	0.92	0.34	47,47,47,47	0
56	MG	BA	3575	1/1	0.92	0.16	52,52,52,52	0
56	MG	BA	3128	1/1	0.92	0.22	38,38,38,38	0
56	MG	CA	1849	1/1	0.92	0.15	32,32,32,32	0
56	MG	DA	3127	1/1	0.92	0.13	71,71,71,71	0
56	MG	DA	3129	1/1	0.92	0.08	32,32,32,32	0
56	MG	CA	1851	1/1	0.92	0.08	34,34,34,34	0
56	MG	BA	3364	1/1	0.92	0.15	60,60,60,60	0
56	MG	DB	216	1/1	0.92	0.17	35,35,35,35	0
56	MG	DA	3145	1/1	0.92	0.11	30,30,30,30	0
56	MG	DB	221	1/1	0.92	0.14	49,49,49,49	0
56	MG	BA	3369	1/1	0.92	0.43	48,48,48,48	0
56	MG	DB	225	1/1	0.92	0.17	34,34,34,34	0
56	MG	DA	3162	1/1	0.92	0.18	33,33,33,33	0
56	MG	AX	401	1/1	0.93	0.15	55,55,55,55	0
56	MG	BA	3149	1/1	0.93	0.13	38,38,38,38	0
56	MG	DA	3247	1/1	0.93	0.09	21,21,21,21	0
56	MG	CA	1674	1/1	0.93	0.08	63,63,63,63	0
56	MG	DA	3257	1/1	0.93	0.21	32,32,32,32	0
56	MG	AX	403	1/1	0.93	0.06	73,73,73,73	0
56	MG	DA	3268	1/1	0.93	0.23	48,48,48,48	0
56	MG	BA	3696	1/1	0.93	0.27	37,37,37,37	0
56	MG	AA	1828	1/1	0.93	0.16	47,47,47,47	0
56	MG	BA	3541	1/1	0.93	0.10	1,1,1,1	0
56	MG	DA	3308	1/1	0.93	0.18	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	AA	1714	1/1	0.93	0.19	28,28,28,28	0
56	MG	CA	1695	1/1	0.93	0.10	59,59,59,59	0
56	MG	CA	1699	1/1	0.93	0.12	45,45,45,45	0
56	MG	BA	3551	1/1	0.93	0.28	47,47,47,47	0
56	MG	BA	3172	1/1	0.93	0.08	63,63,63,63	0
56	MG	DA	3360	1/1	0.93	0.14	29,29,29,29	0
56	MG	CA	1705	1/1	0.93	0.16	31,31,31,31	0
56	MG	BA	3558	1/1	0.93	0.23	54,54,54,54	0
56	MG	AA	1719	1/1	0.93	0.12	28,28,28,28	0
56	MG	BA	3714	1/1	0.93	0.13	61,61,61,61	0
56	MG	BA	3378	1/1	0.93	0.07	28,28,28,28	0
56	MG	DA	3405	1/1	0.93	0.05	57,57,57,57	0
56	MG	DA	3411	1/1	0.93	0.10	26,26,26,26	0
56	MG	BA	3723	1/1	0.93	0.16	18,18,18,18	0
56	MG	DA	3414	1/1	0.93	0.26	43,43,43,43	0
56	MG	DA	3417	1/1	0.93	0.33	53,53,53,53	0
56	MG	DA	3418	1/1	0.93	0.16	54,54,54,54	0
56	MG	DA	3423	1/1	0.93	0.18	39,39,39,39	0
56	MG	CA	1727	1/1	0.93	0.09	55,55,55,55	0
56	MG	AA	1720	1/1	0.93	0.14	33,33,33,33	0
56	MG	CA	1732	1/1	0.93	0.20	38,38,38,38	0
56	MG	CA	1996	1/1	0.93	0.18	41,41,41,41	0
56	MG	BA	3726	1/1	0.93	0.42	66,66,66,66	0
56	MG	CA	2006	1/1	0.93	0.15	41,41,41,41	0
56	MG	CA	1741	1/1	0.93	0.14	28,28,28,28	0
56	MG	DA	3445	1/1	0.93	0.10	31,31,31,31	0
56	MG	BA	3574	1/1	0.93	0.15	35,35,35,35	0
56	MG	AA	1834	1/1	0.93	0.61	36,36,36,36	0
56	MG	BA	3733	1/1	0.93	0.29	43,43,43,43	0
56	MG	CA	1750	1/1	0.93	0.10	35,35,35,35	0
56	MG	DA	3472	1/1	0.93	0.26	39,39,39,39	0
56	MG	DA	3474	1/1	0.93	0.30	34,34,34,34	0
56	MG	DA	3477	1/1	0.93	0.15	32,32,32,32	0
56	MG	CZ	103	1/1	0.93	0.06	51,51,51,51	0
56	MG	BA	3741	1/1	0.93	0.13	28,28,28,28	0
56	MG	DA	3495	1/1	0.93	0.17	13,13,13,13	0
56	MG	DA	3504	1/1	0.93	0.12	39,39,39,39	0
56	MG	DA	3510	1/1	0.93	0.15	38,38,38,38	0
56	MG	CZ	113	1/1	0.93	0.13	64,64,64,64	0
56	MG	DA	3524	1/1	0.93	0.09	27,27,27,27	0
56	MG	CZ	116	1/1	0.93	0.14	81,81,81,81	0
56	MG	CA	1757	1/1	0.93	0.23	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	CA	1758	1/1	0.93	0.07	37,37,37,37	0
56	MG	AA	1786	1/1	0.93	0.27	76,76,76,76	0
56	MG	BA	3745	1/1	0.93	0.15	39,39,39,39	0
56	MG	CA	1772	1/1	0.93	0.28	40,40,40,40	0
56	MG	BA	3587	1/1	0.93	0.23	41,41,41,41	0
56	MG	DA	3550	1/1	0.93	0.55	35,35,35,35	0
56	MG	BA	3589	1/1	0.93	0.13	62,62,62,62	0
56	MG	AA	1683	1/1	0.93	0.13	39,39,39,39	0
56	MG	CC	305	1/1	0.93	0.11	46,46,46,46	0
56	MG	AA	1626	1/1	0.93	0.07	47,47,47,47	0
56	MG	BA	3755	1/1	0.93	0.12	64,64,64,64	0
56	MG	BA	3756	1/1	0.93	0.18	52,52,52,52	0
56	MG	DA	3581	1/1	0.93	0.12	16,16,16,16	0
56	MG	BA	3601	1/1	0.93	0.19	33,33,33,33	0
56	MG	BA	3203	1/1	0.93	0.14	27,27,27,27	0
56	MG	DA	3597	1/1	0.93	0.18	40,40,40,40	0
56	MG	BA	3420	1/1	0.93	0.12	7,7,7,7	0
56	MG	DA	3607	1/1	0.93	0.22	44,44,44,44	0
56	MG	CA	1812	1/1	0.93	0.12	51,51,51,51	0
56	MG	AA	1661	1/1	0.93	0.10	28,28,28,28	0
56	MG	AA	1629	1/1	0.93	0.34	59,59,59,59	0
56	MG	BA	3070	1/1	0.93	0.14	32,32,32,32	0
56	MG	DF	301	1/1	0.93	0.30	45,45,45,45	0
56	MG	DA	3621	1/1	0.93	0.24	51,51,51,51	0
56	MG	BA	3782	1/1	0.93	0.18	19,19,19,19	0
56	MG	AC	303	1/1	0.93	0.07	51,51,51,51	0
56	MG	DA	3640	1/1	0.93	0.28	40,40,40,40	0
56	MG	BA	3251	1/1	0.93	0.11	43,43,43,43	0
56	MG	DA	3647	1/1	0.93	0.17	19,19,19,19	0
56	MG	DA	3648	1/1	0.93	0.12	42,42,42,42	0
56	MG	DA	3651	1/1	0.93	0.15	21,21,21,21	0
56	MG	DP	202	1/1	0.93	0.19	44,44,44,44	0
56	MG	BA	3450	1/1	0.93	0.21	43,43,43,43	0
56	MG	CA	1829	1/1	0.93	0.20	35,35,35,35	0
56	MG	BA	3642	1/1	0.93	0.17	68,68,68,68	0
56	MG	DW	202	1/1	0.93	0.17	36,36,36,36	0
56	MG	AC	304	1/1	0.93	0.24	55,55,55,55	0
56	MG	BA	3455	1/1	0.93	0.23	46,46,46,46	0
56	MG	BB	218	1/1	0.93	0.17	51,51,51,51	0
56	MG	DA	3668	1/1	0.93	0.26	42,42,42,42	0
56	MG	DA	3029	1/1	0.93	0.12	25,25,25,25	0
56	MG	CA	1835	1/1	0.93	0.27	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DA	3056	1/1	0.93	0.11	25,25,25,25	0
56	MG	DA	3684	1/1	0.93	0.16	50,50,50,50	0
56	MG	BA	3652	1/1	0.93	0.23	33,33,33,33	0
56	MG	BA	3654	1/1	0.93	0.17	40,40,40,40	0
56	MG	DA	3076	1/1	0.93	0.15	51,51,51,51	0
56	MG	AA	1802	1/1	0.93	0.23	56,56,56,56	0
56	MG	DA	3703	1/1	0.93	0.39	38,38,38,38	0
56	MG	AA	1878	1/1	0.93	0.29	37,37,37,37	0
56	MG	DA	3710	1/1	0.93	0.15	21,21,21,21	0
56	MG	DA	3712	1/1	0.93	0.21	61,61,61,61	0
56	MG	AA	1624	1/1	0.93	0.13	26,26,26,26	0
56	MG	CA	1858	1/1	0.93	0.10	66,66,66,66	0
56	MG	AA	1618	1/1	0.93	0.25	49,49,49,49	0
56	MG	BA	3106	1/1	0.93	0.11	26,26,26,26	0
56	MG	DA	3728	1/1	0.93	0.18	33,33,33,33	0
56	MG	BA	3113	1/1	0.93	0.18	10,10,10,10	0
56	MG	CA	1874	1/1	0.93	0.17	52,52,52,52	0
56	MG	CA	1877	1/1	0.93	0.59	60,60,60,60	0
56	MG	CA	1880	1/1	0.93	0.06	51,51,51,51	0
56	MG	BW	202	1/1	0.93	0.25	33,33,33,33	0
56	MG	AA	1811	1/1	0.93	0.16	16,16,16,16	0
56	MG	DA	3167	1/1	0.93	0.18	23,23,23,23	0
56	MG	CA	1610	1/1	0.93	0.10	24,24,24,24	0
56	MG	DA	3173	1/1	0.93	0.13	31,31,31,31	0
56	MG	AM	201	1/1	0.93	0.28	54,54,54,54	0
56	MG	BA	3322	1/1	0.93	0.13	33,33,33,33	0
56	MG	BA	3125	1/1	0.93	0.10	23,23,23,23	0
56	MG	CA	1619	1/1	0.93	0.17	66,66,66,66	0
56	MG	AA	1767	1/1	0.93	0.39	28,28,28,28	0
56	MG	CA	1635	1/1	0.93	0.28	39,39,39,39	0
56	MG	CA	1638	1/1	0.93	0.12	26,26,26,26	0
56	MG	BA	3329	1/1	0.93	0.10	49,49,49,49	0
56	MG	BA	3689	1/1	0.93	0.13	44,44,44,44	0
56	MG	BA	3129	1/1	0.93	0.16	34,34,34,34	0
56	MG	AA	1768	1/1	0.93	0.10	32,32,32,32	0
56	MG	AA	1725	1/1	0.94	0.15	23,23,23,23	0
56	MG	CA	1918	1/1	0.94	0.13	44,44,44,44	0
56	MG	DA	3256	1/1	0.94	0.25	37,37,37,37	0
56	MG	BA	3417	1/1	0.94	0.09	25,25,25,25	0
56	MG	DA	3259	1/1	0.94	0.13	24,24,24,24	0
56	MG	AA	1653	1/1	0.94	0.14	44,44,44,44	0
56	MG	DA	3267	1/1	0.94	0.09	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	BA	3202	1/1	0.94	0.09	46,46,46,46	0
56	MG	AA	1805	1/1	0.94	0.11	53,53,53,53	0
56	MG	DA	3283	1/1	0.94	0.29	36,36,36,36	0
56	MG	CA	1636	1/1	0.94	0.09	40,40,40,40	0
56	MG	BA	3426	1/1	0.94	0.45	56,56,56,56	0
56	MG	CA	1640	1/1	0.94	0.37	56,56,56,56	0
56	MG	DA	3312	1/1	0.94	0.13	24,24,24,24	0
56	MG	BA	3209	1/1	0.94	0.16	31,31,31,31	0
56	MG	BA	3667	1/1	0.94	0.22	63,63,63,63	0
56	MG	DA	3349	1/1	0.94	0.23	44,44,44,44	0
56	MG	AB	301	1/1	0.94	0.09	44,44,44,44	0
56	MG	BA	3085	1/1	0.94	0.13	37,37,37,37	0
56	MG	AA	1856	1/1	0.94	0.12	49,49,49,49	0
56	MG	BA	3227	1/1	0.94	0.23	36,36,36,36	0
56	MG	CA	1963	1/1	0.94	0.55	35,35,35,35	0
56	MG	DA	3377	1/1	0.94	0.13	21,21,21,21	0
56	MG	AA	1861	1/1	0.94	0.73	60,60,60,60	0
56	MG	CA	1965	1/1	0.94	0.09	54,54,54,54	0
56	MG	DA	3386	1/1	0.94	0.12	27,27,27,27	0
56	MG	DA	3389	1/1	0.94	0.16	55,55,55,55	0
56	MG	AA	1602	1/1	0.94	0.08	23,23,23,23	0
56	MG	DA	3395	1/1	0.94	0.14	34,34,34,34	0
56	MG	AA	1871	1/1	0.94	0.09	35,35,35,35	0
56	MG	BA	3681	1/1	0.94	0.16	62,62,62,62	0
56	MG	CA	1684	1/1	0.94	0.10	44,44,44,44	0
56	MG	AA	1741	1/1	0.94	0.14	32,32,32,32	0
56	MG	AA	1812	1/1	0.94	0.24	33,33,33,33	0
56	MG	AA	1814	1/1	0.94	0.14	17,17,17,17	0
56	MG	BA	3272	1/1	0.94	0.10	15,15,15,15	0
56	MG	BA	3279	1/1	0.94	0.09	39,39,39,39	0
56	MG	CA	1991	1/1	0.94	0.33	57,57,57,57	0
56	MG	DA	3426	1/1	0.94	0.10	34,34,34,34	0
56	MG	BA	3480	1/1	0.94	0.19	23,23,23,23	0
56	MG	CA	1703	1/1	0.94	0.09	34,34,34,34	0
56	MG	BA	3285	1/1	0.94	0.11	40,40,40,40	0
56	MG	DA	3434	1/1	0.94	0.13	29,29,29,29	0
56	MG	CA	2004	1/1	0.94	0.10	45,45,45,45	0
56	MG	BA	3114	1/1	0.94	0.40	47,47,47,47	0
56	MG	CA	1712	1/1	0.94	0.49	18,18,18,18	0
56	MG	DA	3444	1/1	0.94	0.16	11,11,11,11	0
56	MG	AA	1820	1/1	0.94	0.06	23,23,23,23	0
56	MG	BA	3295	1/1	0.94	0.10	1,1,1,1	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	BA	3506	1/1	0.94	0.13	10,10,10,10	0
56	MG	DA	3464	1/1	0.94	0.14	26,26,26,26	0
56	MG	BA	3297	1/1	0.94	0.19	50,50,50,50	0
56	MG	BA	3709	1/1	0.94	0.19	31,31,31,31	0
56	MG	BA	3516	1/1	0.94	0.09	25,25,25,25	0
56	MG	DA	3473	1/1	0.94	0.18	55,55,55,55	0
56	MG	BA	3299	1/1	0.94	0.17	44,44,44,44	0
56	MG	BA	3120	1/1	0.94	0.07	1,1,1,1	0
56	MG	DA	3480	1/1	0.94	0.18	46,46,46,46	0
56	MG	BA	3715	1/1	0.94	0.10	42,42,42,42	0
56	MG	DA	3489	1/1	0.94	0.11	24,24,24,24	0
56	MG	BA	3527	1/1	0.94	0.21	37,37,37,37	0
56	MG	BA	3308	1/1	0.94	0.17	9,9,9,9	0
56	MG	DA	3499	1/1	0.94	0.15	25,25,25,25	0
56	MG	DA	3501	1/1	0.94	0.24	47,47,47,47	0
56	MG	AA	1748	1/1	0.94	0.17	54,54,54,54	0
56	MG	BA	3535	1/1	0.94	0.12	43,43,43,43	0
56	MG	DA	3511	1/1	0.94	0.17	7,7,7,7	0
56	MG	DA	3513	1/1	0.94	0.09	41,41,41,41	0
56	MG	CY	113	1/1	0.94	0.67	39,39,39,39	0
56	MG	DA	3523	1/1	0.94	0.10	44,44,44,44	0
56	MG	AA	1781	1/1	0.94	0.11	55,55,55,55	0
56	MG	CC	301	1/1	0.94	0.10	48,48,48,48	0
56	MG	DA	3530	1/1	0.94	0.27	51,51,51,51	0
56	MG	AA	1676	1/1	0.94	0.14	49,49,49,49	0
56	MG	DA	3535	1/1	0.94	0.09	42,42,42,42	0
56	MG	AP	101	1/1	0.94	0.25	32,32,32,32	0
56	MG	CA	1761	1/1	0.94	0.41	45,45,45,45	0
56	MG	CA	1762	1/1	0.94	0.15	30,30,30,30	0
56	MG	CC	307	1/1	0.94	0.28	27,27,27,27	0
56	MG	CD	303	1/1	0.94	0.14	21,21,21,21	0
56	MG	AA	1715	1/1	0.94	0.19	51,51,51,51	0
56	MG	CG	201	1/1	0.94	0.20	52,52,52,52	0
56	MG	BA	3548	1/1	0.94	0.20	39,39,39,39	0
56	MG	AA	1758	1/1	0.94	0.11	47,47,47,47	0
56	MG	BA	3145	1/1	0.94	0.10	36,36,36,36	0
56	MG	AA	1894	1/1	0.94	0.27	38,38,38,38	0
56	MG	DA	3572	1/1	0.94	0.08	36,36,36,36	0
56	MG	AA	1643	1/1	0.94	0.09	24,24,24,24	0
56	MG	BA	3752	1/1	0.94	0.19	30,30,30,30	0
56	MG	BA	3342	1/1	0.94	0.10	36,36,36,36	0
56	MG	DA	3590	1/1	0.94	0.18	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DA	3591	1/1	0.94	0.12	26,26,26,26	0
56	MG	CA	1790	1/1	0.94	0.09	38,38,38,38	0
56	MG	AA	1896	1/1	0.94	0.29	57,57,57,57	0
56	MG	BA	3164	1/1	0.94	0.16	51,51,51,51	0
56	MG	DA	3605	1/1	0.94	0.28	36,36,36,36	0
56	MG	BA	3346	1/1	0.94	0.15	18,18,18,18	0
56	MG	DO	201	1/1	0.94	0.28	23,23,23,23	0
56	MG	BA	3581	1/1	0.94	0.23	39,39,39,39	0
56	MG	BA	3347	1/1	0.94	0.20	19,19,19,19	0
56	MG	BA	3768	1/1	0.94	0.18	46,46,46,46	0
56	MG	BA	3769	1/1	0.94	0.07	65,65,65,65	0
56	MG	BA	3771	1/1	0.94	0.13	45,45,45,45	0
56	MG	DV	201	1/1	0.94	0.08	61,61,61,61	0
56	MG	BA	3349	1/1	0.94	0.09	42,42,42,42	0
56	MG	DA	3635	1/1	0.94	0.14	47,47,47,47	0
56	MG	DA	3637	1/1	0.94	0.46	66,66,66,66	0
56	MG	DA	3639	1/1	0.94	0.16	13,13,13,13	0
56	MG	BA	3778	1/1	0.94	0.12	33,33,33,33	0
56	MG	DA	3001	1/1	0.94	0.20	37,37,37,37	0
56	MG	DA	3003	1/1	0.94	0.18	33,33,33,33	0
56	MG	BA	3779	1/1	0.94	0.13	47,47,47,47	0
56	MG	BA	3351	1/1	0.94	0.08	39,39,39,39	0
56	MG	DA	3013	1/1	0.94	0.15	23,23,23,23	0
56	MG	DA	3019	1/1	0.94	0.09	5,5,5,5	0
56	MG	DA	3023	1/1	0.94	0.11	7,7,7,7	0
56	MG	BA	3591	1/1	0.94	0.11	50,50,50,50	0
56	MG	DA	3030	1/1	0.94	0.11	17,17,17,17	0
56	MG	BA	3358	1/1	0.94	0.34	44,44,44,44	0
56	MG	BA	3789	1/1	0.94	0.24	35,35,35,35	0
56	MG	BA	3167	1/1	0.94	0.17	34,34,34,34	0
56	MG	DA	3665	1/1	0.94	0.12	35,35,35,35	0
56	MG	BA	3598	1/1	0.94	0.19	33,33,33,33	0
56	MG	BA	3169	1/1	0.94	0.20	26,26,26,26	0
56	MG	DA	3675	1/1	0.94	0.40	55,55,55,55	0
56	MG	DA	3676	1/1	0.94	0.46	25,25,25,25	0
56	MG	BA	3602	1/1	0.94	0.08	42,42,42,42	0
56	MG	AA	1692	1/1	0.94	0.15	45,45,45,45	0
56	MG	BB	214	1/1	0.94	0.06	29,29,29,29	0
56	MG	DA	3688	1/1	0.94	0.27	63,63,63,63	0
56	MG	DA	3103	1/1	0.94	0.10	16,16,16,16	0
56	MG	AA	1902	1/1	0.94	0.08	42,42,42,42	0
56	MG	DA	3114	1/1	0.94	0.14	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	CA	1854	1/1	0.94	0.14	43,43,43,43	0
56	MG	DA	3702	1/1	0.94	0.28	42,42,42,42	0
56	MG	DA	3122	1/1	0.94	0.10	46,46,46,46	0
56	MG	BA	3624	1/1	0.94	0.25	82,82,82,82	0
56	MG	CA	1857	1/1	0.94	0.19	33,33,33,33	0
56	MG	BA	3626	1/1	0.94	0.11	29,29,29,29	0
56	MG	BA	3026	1/1	0.94	0.08	0,0,0,0	0
56	MG	AZ	106	1/1	0.94	0.07	37,37,37,37	0
56	MG	BA	3381	1/1	0.94	0.16	2,2,2,2	0
56	MG	DA	3159	1/1	0.94	0.11	52,52,52,52	0
56	MG	BA	3382	1/1	0.94	0.14	33,33,33,33	0
56	MG	AA	1837	1/1	0.94	0.10	54,54,54,54	0
56	MG	DA	3735	1/1	0.94	0.47	51,51,51,51	0
56	MG	BN	202	1/1	0.94	0.21	49,49,49,49	0
56	MG	DA	3171	1/1	0.94	0.11	52,52,52,52	0
56	MG	BA	3638	1/1	0.94	0.14	38,38,38,38	0
56	MG	DA	3744	1/1	0.94	0.19	62,62,62,62	0
56	MG	AA	1800	1/1	0.94	0.09	49,49,49,49	0
56	MG	BU	201	1/1	0.94	0.51	35,35,35,35	0
56	MG	BA	3640	1/1	0.94	0.11	34,34,34,34	0
56	MG	DA	3752	1/1	0.94	0.23	55,55,55,55	0
56	MG	CA	1888	1/1	0.94	0.20	51,51,51,51	0
56	MG	DA	3755	1/1	0.94	0.36	39,39,39,39	0
56	MG	CA	1890	1/1	0.94	0.17	37,37,37,37	0
56	MG	B7	101	1/1	0.94	0.28	24,24,24,24	0
56	MG	DA	3194	1/1	0.94	0.17	42,42,42,42	0
56	MG	BA	3402	1/1	0.94	0.09	39,39,39,39	0
56	MG	DB	208	1/1	0.94	0.20	39,39,39,39	0
56	MG	DA	3205	1/1	0.94	0.20	24,24,24,24	0
56	MG	BA	3189	1/1	0.94	0.20	48,48,48,48	0
56	MG	CA	1611	1/1	0.94	0.08	40,40,40,40	0
56	MG	DA	3215	1/1	0.94	0.14	41,41,41,41	0
56	MG	CA	1612	1/1	0.94	0.12	30,30,30,30	0
56	MG	CA	1913	1/1	0.94	0.10	41,41,41,41	0
56	MG	BA	3191	1/1	0.94	0.20	41,41,41,41	0
56	MG	DB	226	1/1	0.94	0.37	51,51,51,51	0
56	MG	CA	1916	1/1	0.94	0.17	62,62,62,62	0
56	MG	BA	3233	1/1	0.95	0.29	35,35,35,35	0
56	MG	BA	3244	1/1	0.95	0.10	34,34,34,34	0
56	MG	DA	3209	1/1	0.95	0.10	55,55,55,55	0
56	MG	DA	3213	1/1	0.95	0.09	18,18,18,18	0
56	MG	CA	1878	1/1	0.95	0.07	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	BA	3419	1/1	0.95	0.23	29,29,29,29	0
56	MG	BA	3250	1/1	0.95	0.14	39,39,39,39	0
56	MG	BF	304	1/1	0.95	0.25	40,40,40,40	0
56	MG	DA	3231	1/1	0.95	0.08	3,3,3,3	0
56	MG	DA	3237	1/1	0.95	0.12	31,31,31,31	0
56	MG	CA	1884	1/1	0.95	0.09	39,39,39,39	0
56	MG	BA	3422	1/1	0.95	0.14	24,24,24,24	0
56	MG	AA	1872	1/1	0.95	0.16	19,19,19,19	0
56	MG	BA	3424	1/1	0.95	0.07	17,17,17,17	0
56	MG	BO	202	1/1	0.95	0.08	29,29,29,29	0
56	MG	BA	3253	1/1	0.95	0.12	44,44,44,44	0
56	MG	BA	3641	1/1	0.95	0.11	47,47,47,47	0
56	MG	BA	3093	1/1	0.95	0.11	34,34,34,34	0
56	MG	DA	3265	1/1	0.95	0.09	25,25,25,25	0
56	MG	AC	306	1/1	0.95	0.09	21,21,21,21	0
56	MG	BA	3434	1/1	0.95	0.10	45,45,45,45	0
56	MG	CA	1603	1/1	0.95	0.17	41,41,41,41	0
56	MG	DA	3282	1/1	0.95	0.07	20,20,20,20	0
56	MG	CA	1606	1/1	0.95	0.11	27,27,27,27	0
56	MG	DA	3284	1/1	0.95	0.14	7,7,7,7	0
56	MG	BA	3102	1/1	0.95	0.12	22,22,22,22	0
56	MG	DA	3289	1/1	0.95	0.15	31,31,31,31	0
56	MG	BA	3269	1/1	0.95	0.10	37,37,37,37	0
56	MG	AA	1777	1/1	0.95	0.26	36,36,36,36	0
56	MG	CA	1919	1/1	0.95	0.15	64,64,64,64	0
56	MG	BA	3110	1/1	0.95	0.10	35,35,35,35	0
56	MG	BA	3658	1/1	0.95	0.14	56,56,56,56	0
56	MG	BA	3273	1/1	0.95	0.15	17,17,17,17	0
56	MG	BA	3461	1/1	0.95	0.11	23,23,23,23	0
56	MG	CA	1618	1/1	0.95	0.25	27,27,27,27	0
56	MG	AD	307	1/1	0.95	0.42	32,32,32,32	0
56	MG	DA	3359	1/1	0.95	0.27	19,19,19,19	0
56	MG	CA	1622	1/1	0.95	0.07	24,24,24,24	0
56	MG	DA	3365	1/1	0.95	0.11	8,8,8,8	0
56	MG	DA	3367	1/1	0.95	0.10	60,60,60,60	0
56	MG	DA	3371	1/1	0.95	0.16	33,33,33,33	0
56	MG	DA	3372	1/1	0.95	0.16	30,30,30,30	0
56	MG	BA	3666	1/1	0.95	0.25	51,51,51,51	0
56	MG	BA	3283	1/1	0.95	0.10	4,4,4,4	0
56	MG	CA	1939	1/1	0.95	0.24	55,55,55,55	0
56	MG	CA	1942	1/1	0.95	0.38	41,41,41,41	0
56	MG	CA	1943	1/1	0.95	0.39	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	AA	1740	1/1	0.95	0.08	53,53,53,53	0
56	MG	AA	1881	1/1	0.95	0.15	76,76,76,76	0
56	MG	AG	201	1/1	0.95	0.10	23,23,23,23	0
56	MG	DA	3399	1/1	0.95	0.34	36,36,36,36	0
56	MG	CA	1951	1/1	0.95	0.12	42,42,42,42	0
56	MG	CA	1643	1/1	0.95	0.07	35,35,35,35	0
56	MG	CA	1645	1/1	0.95	0.12	45,45,45,45	0
56	MG	AI	201	1/1	0.95	0.26	57,57,57,57	0
56	MG	BA	3474	1/1	0.95	0.33	48,48,48,48	0
56	MG	AA	1619	1/1	0.95	0.11	37,37,37,37	0
56	MG	AA	1784	1/1	0.95	0.14	22,22,22,22	0
56	MG	DA	3420	1/1	0.95	0.37	45,45,45,45	0
56	MG	CA	1665	1/1	0.95	0.15	26,26,26,26	0
56	MG	CA	1971	1/1	0.95	0.14	49,49,49,49	0
56	MG	AA	1747	1/1	0.95	0.13	40,40,40,40	0
56	MG	CA	1669	1/1	0.95	0.14	52,52,52,52	0
56	MG	CA	1670	1/1	0.95	0.29	31,31,31,31	0
56	MG	AA	1787	1/1	0.95	0.09	36,36,36,36	0
56	MG	CA	1673	1/1	0.95	0.07	48,48,48,48	0
56	MG	AA	1695	1/1	0.95	0.10	33,33,33,33	0
56	MG	CA	1677	1/1	0.95	0.10	27,27,27,27	0
56	MG	AA	1603	1/1	0.95	0.10	30,30,30,30	0
56	MG	DA	3441	1/1	0.95	0.32	41,41,41,41	0
56	MG	DA	3443	1/1	0.95	0.16	25,25,25,25	0
56	MG	CA	1995	1/1	0.95	0.19	47,47,47,47	0
56	MG	AA	1756	1/1	0.95	0.34	38,38,38,38	0
56	MG	CA	1997	1/1	0.95	0.27	24,24,24,24	0
56	MG	CA	1999	1/1	0.95	0.14	31,31,31,31	0
56	MG	DA	3459	1/1	0.95	0.15	22,22,22,22	0
56	MG	DA	3460	1/1	0.95	0.23	41,41,41,41	0
56	MG	BA	3511	1/1	0.95	0.11	26,26,26,26	0
56	MG	DA	3465	1/1	0.95	0.15	20,20,20,20	0
56	MG	CA	2001	1/1	0.95	0.07	36,36,36,36	0
56	MG	DA	3467	1/1	0.95	0.11	58,58,58,58	0
56	MG	BA	3324	1/1	0.95	0.28	33,33,33,33	0
56	MG	DA	3470	1/1	0.95	0.13	47,47,47,47	0
56	MG	CA	1688	1/1	0.95	0.10	26,26,26,26	0
56	MG	AX	402	1/1	0.95	0.15	29,29,29,29	0
56	MG	BA	3154	1/1	0.95	0.12	26,26,26,26	0
56	MG	DA	3475	1/1	0.95	0.13	34,34,34,34	0
56	MG	CA	1694	1/1	0.95	0.10	39,39,39,39	0
56	MG	DA	3479	1/1	0.95	0.10	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	AA	1680	1/1	0.95	0.13	26,26,26,26	0
56	MG	CZ	101	1/1	0.95	0.13	61,61,61,61	0
56	MG	DA	3486	1/1	0.95	0.12	35,35,35,35	0
56	MG	BA	3701	1/1	0.95	0.09	24,24,24,24	0
56	MG	BA	3521	1/1	0.95	0.06	21,21,21,21	0
56	MG	CZ	108	1/1	0.95	0.07	49,49,49,49	0
56	MG	DA	3498	1/1	0.95	0.06	59,59,59,59	0
56	MG	AA	1682	1/1	0.95	0.07	51,51,51,51	0
56	MG	BA	3334	1/1	0.95	0.16	23,23,23,23	0
56	MG	CZ	114	1/1	0.95	0.12	46,46,46,46	0
56	MG	DA	3505	1/1	0.95	0.23	30,30,30,30	0
56	MG	CZ	115	1/1	0.95	0.23	40,40,40,40	0
56	MG	AA	1634	1/1	0.95	0.09	32,32,32,32	0
56	MG	CA	1710	1/1	0.95	0.10	29,29,29,29	0
56	MG	BA	3710	1/1	0.95	0.15	13,13,13,13	0
56	MG	DA	3518	1/1	0.95	0.12	13,13,13,13	0
56	MG	DA	3520	1/1	0.95	0.27	63,63,63,63	0
56	MG	AA	1900	1/1	0.95	0.12	44,44,44,44	0
56	MG	AA	1668	1/1	0.95	0.09	14,14,14,14	0
56	MG	AA	1845	1/1	0.95	0.66	48,48,48,48	0
56	MG	CA	1716	1/1	0.95	0.10	42,42,42,42	0
56	MG	BA	3176	1/1	0.95	0.16	3,3,3,3	0
56	MG	BA	3717	1/1	0.95	0.15	40,40,40,40	0
56	MG	CA	1723	1/1	0.95	0.09	33,33,33,33	0
56	MG	DA	3542	1/1	0.95	0.14	48,48,48,48	0
56	MG	DA	3543	1/1	0.95	0.12	20,20,20,20	0
56	MG	AA	1905	1/1	0.95	0.14	40,40,40,40	0
56	MG	BA	3179	1/1	0.95	0.15	26,26,26,26	0
56	MG	CA	1731	1/1	0.95	0.11	30,30,30,30	0
56	MG	BA	3549	1/1	0.95	0.10	40,40,40,40	0
56	MG	CA	1736	1/1	0.95	0.11	52,52,52,52	0
56	MG	BA	3348	1/1	0.95	0.18	9,9,9,9	0
56	MG	CF	201	1/1	0.95	0.09	50,50,50,50	0
56	MG	DA	3557	1/1	0.95	0.13	13,13,13,13	0
56	MG	BA	3554	1/1	0.95	0.22	19,19,19,19	0
56	MG	DA	3565	1/1	0.95	0.12	36,36,36,36	0
56	MG	CA	1742	1/1	0.95	0.11	22,22,22,22	0
56	MG	DA	3568	1/1	0.95	0.10	44,44,44,44	0
56	MG	DA	3569	1/1	0.95	0.24	39,39,39,39	0
56	MG	CA	1744	1/1	0.95	0.14	48,48,48,48	0
56	MG	CK	202	1/1	0.95	0.09	40,40,40,40	0
56	MG	CA	1746	1/1	0.95	0.11	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	BA	3029	1/1	0.95	0.10	1,1,1,1	0
56	MG	BA	3731	1/1	0.95	0.11	45,45,45,45	0
56	MG	BA	3557	1/1	0.95	0.34	59,59,59,59	0
56	MG	CX	403	1/1	0.95	0.09	48,48,48,48	0
56	MG	AZ	104	1/1	0.95	0.04	45,45,45,45	0
56	MG	BA	3356	1/1	0.95	0.09	29,29,29,29	0
56	MG	DA	3599	1/1	0.95	0.18	39,39,39,39	0
56	MG	BA	3564	1/1	0.95	0.14	47,47,47,47	0
56	MG	DA	3604	1/1	0.95	0.23	43,43,43,43	0
56	MG	AA	1846	1/1	0.95	0.12	55,55,55,55	0
56	MG	BA	3567	1/1	0.95	0.07	11,11,11,11	0
56	MG	DI	201	1/1	0.95	0.10	18,18,18,18	0
56	MG	BA	3748	1/1	0.95	0.51	45,45,45,45	0
56	MG	BA	3040	1/1	0.95	0.17	35,35,35,35	0
56	MG	BA	3750	1/1	0.95	0.13	24,24,24,24	0
56	MG	CA	1771	1/1	0.95	0.08	47,47,47,47	0
56	MG	AA	1649	1/1	0.95	0.16	41,41,41,41	0
56	MG	DA	3622	1/1	0.95	0.09	34,34,34,34	0
56	MG	AY	103	1/1	0.95	0.12	53,53,53,53	0
56	MG	DA	3628	1/1	0.95	0.15	38,38,38,38	0
56	MG	DA	3632	1/1	0.95	0.20	32,32,32,32	0
56	MG	DR	201	1/1	0.95	0.15	32,32,32,32	0
56	MG	BA	3576	1/1	0.95	0.19	33,33,33,33	0
56	MG	BA	3579	1/1	0.95	0.15	41,41,41,41	0
56	MG	DX	101	1/1	0.95	0.19	50,50,50,50	0
56	MG	DZ	304	1/1	0.95	0.18	31,31,31,31	0
56	MG	DA	3642	1/1	0.95	0.12	26,26,26,26	0
56	MG	BA	3196	1/1	0.95	0.09	44,44,44,44	0
56	MG	D4	103	1/1	0.95	0.28	40,40,40,40	0
56	MG	BA	3762	1/1	0.95	0.54	35,35,35,35	0
56	MG	BA	3763	1/1	0.95	0.20	55,55,55,55	0
56	MG	AA	1849	1/1	0.95	0.20	40,40,40,40	0
56	MG	BA	3765	1/1	0.95	0.15	36,36,36,36	0
56	MG	BA	3586	1/1	0.95	0.33	34,34,34,34	0
56	MG	DA	3657	1/1	0.95	0.27	38,38,38,38	0
56	MG	CA	1800	1/1	0.95	0.30	30,30,30,30	0
56	MG	DA	3022	1/1	0.95	0.08	19,19,19,19	0
56	MG	CA	1802	1/1	0.95	0.12	31,31,31,31	0
56	MG	DA	3026	1/1	0.95	0.05	16,16,16,16	0
56	MG	DA	3027	1/1	0.95	0.22	22,22,22,22	0
56	MG	CA	1806	1/1	0.95	0.07	36,36,36,36	0
56	MG	CA	1809	1/1	0.95	0.14	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DA	3038	1/1	0.95	0.17	14,14,14,14	0
56	MG	DA	3039	1/1	0.95	0.14	17,17,17,17	0
56	MG	BA	3049	1/1	0.95	0.15	17,17,17,17	0
56	MG	BA	3055	1/1	0.95	0.17	27,27,27,27	0
56	MG	CA	1814	1/1	0.95	0.09	31,31,31,31	0
56	MG	BA	3590	1/1	0.95	0.07	27,27,27,27	0
56	MG	DA	3687	1/1	0.95	0.12	21,21,21,21	0
56	MG	DA	3072	1/1	0.95	0.13	29,29,29,29	0
56	MG	AA	1806	1/1	0.95	0.12	34,34,34,34	0
56	MG	DA	3081	1/1	0.95	0.14	47,47,47,47	0
56	MG	DA	3693	1/1	0.95	0.12	30,30,30,30	0
56	MG	DA	3694	1/1	0.95	0.09	46,46,46,46	0
56	MG	DA	3088	1/1	0.95	0.13	19,19,19,19	0
56	MG	BA	3775	1/1	0.95	0.96	49,49,49,49	0
56	MG	CA	1820	1/1	0.95	0.18	55,55,55,55	0
56	MG	BA	3387	1/1	0.95	0.19	49,49,49,49	0
56	MG	DA	3705	1/1	0.95	0.20	39,39,39,39	0
56	MG	DA	3706	1/1	0.95	0.49	42,42,42,42	0
56	MG	BA	3389	1/1	0.95	0.16	33,33,33,33	0
56	MG	DA	3709	1/1	0.95	0.40	24,24,24,24	0
56	MG	DA	3106	1/1	0.95	0.12	34,34,34,34	0
56	MG	BA	3390	1/1	0.95	0.06	33,33,33,33	0
56	MG	BA	3394	1/1	0.95	0.15	17,17,17,17	0
56	MG	DA	3716	1/1	0.95	0.30	54,54,54,54	0
56	MG	AA	1859	1/1	0.95	0.12	29,29,29,29	0
56	MG	DA	3719	1/1	0.95	0.16	47,47,47,47	0
56	MG	DA	3720	1/1	0.95	0.11	45,45,45,45	0
56	MG	BA	3784	1/1	0.95	0.11	36,36,36,36	0
56	MG	DA	3124	1/1	0.95	0.09	27,27,27,27	0
56	MG	DA	3126	1/1	0.95	0.13	37,37,37,37	0
56	MG	DA	3730	1/1	0.95	0.19	33,33,33,33	0
56	MG	BA	3786	1/1	0.95	0.15	56,56,56,56	0
56	MG	DA	3734	1/1	0.95	0.11	60,60,60,60	0
56	MG	CA	1832	1/1	0.95	0.26	38,38,38,38	0
56	MG	BA	3606	1/1	0.95	0.36	54,54,54,54	0
56	MG	BA	3612	1/1	0.95	0.12	31,31,31,31	0
56	MG	BA	3799	1/1	0.95	0.18	34,34,34,34	0
56	MG	DA	3743	1/1	0.95	0.23	43,43,43,43	0
56	MG	CA	1840	1/1	0.95	0.12	54,54,54,54	0
56	MG	BA	3801	1/1	0.95	0.12	45,45,45,45	0
56	MG	CA	1843	1/1	0.95	0.10	21,21,21,21	0
56	MG	DA	3166	1/1	0.95	0.18	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	CA	1846	1/1	0.95	0.08	69,69,69,69	0
56	MG	BA	3802	1/1	0.95	0.23	54,54,54,54	0
56	MG	AA	1636	1/1	0.95	0.12	64,64,64,64	0
56	MG	DA	3172	1/1	0.95	0.12	31,31,31,31	0
56	MG	BA	3616	1/1	0.95	0.13	2,2,2,2	0
56	MG	DA	3174	1/1	0.95	0.16	33,33,33,33	0
56	MG	DB	202	1/1	0.95	0.14	59,59,59,59	0
56	MG	AA	1727	1/1	0.95	0.17	44,44,44,44	0
56	MG	DB	206	1/1	0.95	0.12	39,39,39,39	0
56	MG	BA	3623	1/1	0.95	0.14	43,43,43,43	0
56	MG	DB	209	1/1	0.95	0.07	43,43,43,43	0
56	MG	BB	208	1/1	0.95	0.08	18,18,18,18	0
56	MG	DA	3183	1/1	0.95	0.16	12,12,12,12	0
56	MG	BB	210	1/1	0.95	0.14	62,62,62,62	0
56	MG	DB	218	1/1	0.95	0.10	46,46,46,46	0
56	MG	AA	1870	1/1	0.95	0.44	28,28,28,28	0
56	MG	DA	3191	1/1	0.95	0.09	48,48,48,48	0
56	MG	AA	1675	1/1	0.95	0.22	47,47,47,47	0
56	MG	CA	1872	1/1	0.95	0.13	24,24,24,24	0
56	MG	DA	3197	1/1	0.95	0.14	31,31,31,31	0
56	MG	BA	3627	1/1	0.95	0.07	49,49,49,49	0
56	MG	BA	3560	1/1	0.96	0.16	27,27,27,27	0
56	MG	BA	3561	1/1	0.96	0.07	30,30,30,30	0
56	MG	DA	3210	1/1	0.96	0.12	27,27,27,27	0
56	MG	BA	3319	1/1	0.96	0.14	35,35,35,35	0
56	MG	BA	3563	1/1	0.96	0.29	55,55,55,55	0
56	MG	CA	1879	1/1	0.96	0.11	28,28,28,28	0
56	MG	AA	1793	1/1	0.96	0.06	30,30,30,30	0
56	MG	AA	1857	1/1	0.96	0.18	41,41,41,41	0
56	MG	AA	1745	1/1	0.96	0.13	62,62,62,62	0
56	MG	DA	3233	1/1	0.96	0.12	5,5,5,5	0
56	MG	AA	1696	1/1	0.96	0.14	27,27,27,27	0
56	MG	BB	212	1/1	0.96	0.16	50,50,50,50	0
56	MG	AA	1862	1/1	0.96	0.14	44,44,44,44	0
56	MG	BB	215	1/1	0.96	0.09	47,47,47,47	0
56	MG	DA	3251	1/1	0.96	0.23	16,16,16,16	0
56	MG	AD	305	1/1	0.96	0.21	52,52,52,52	0
56	MG	BA	3127	1/1	0.96	0.16	38,38,38,38	0
56	MG	AA	1863	1/1	0.96	0.14	37,37,37,37	0
56	MG	DA	3258	1/1	0.96	0.11	39,39,39,39	0
56	MG	BA	3338	1/1	0.96	0.09	27,27,27,27	0
56	MG	DA	3262	1/1	0.96	0.16	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	CA	1904	1/1	0.96	0.06	42,42,42,42	0
56	MG	AD	309	1/1	0.96	0.33	36,36,36,36	0
56	MG	BE	301	1/1	0.96	0.09	42,42,42,42	0
56	MG	BA	3584	1/1	0.96	0.10	46,46,46,46	0
56	MG	DA	3270	1/1	0.96	0.08	35,35,35,35	0
56	MG	AA	1701	1/1	0.96	0.11	17,17,17,17	0
56	MG	DA	3272	1/1	0.96	0.10	0,0,0,0	0
56	MG	DA	3274	1/1	0.96	0.14	6,6,6,6	0
56	MG	DA	3279	1/1	0.96	0.18	20,20,20,20	0
56	MG	DA	3281	1/1	0.96	0.10	4,4,4,4	0
56	MG	BG	201	1/1	0.96	0.15	47,47,47,47	0
56	MG	BA	3343	1/1	0.96	0.12	32,32,32,32	0
56	MG	AA	1702	1/1	0.96	0.15	40,40,40,40	0
56	MG	BA	3134	1/1	0.96	0.51	61,61,61,61	0
56	MG	DA	3288	1/1	0.96	0.09	12,12,12,12	0
56	MG	CA	1920	1/1	0.96	0.53	32,32,32,32	0
56	MG	DA	3294	1/1	0.96	0.07	29,29,29,29	0
56	MG	CA	1921	1/1	0.96	0.34	57,57,57,57	0
56	MG	DA	3307	1/1	0.96	0.12	47,47,47,47	0
56	MG	BA	3136	1/1	0.96	0.06	32,32,32,32	0
56	MG	BQ	201	1/1	0.96	0.33	38,38,38,38	0
56	MG	BA	3592	1/1	0.96	0.22	58,58,58,58	0
56	MG	DA	3326	1/1	0.96	0.09	27,27,27,27	0
56	MG	DA	3340	1/1	0.96	0.13	33,33,33,33	0
56	MG	CA	1927	1/1	0.96	0.10	37,37,37,37	0
56	MG	DA	3344	1/1	0.96	0.10	32,32,32,32	0
56	MG	BA	3137	1/1	0.96	0.10	47,47,47,47	0
56	MG	BA	3594	1/1	0.96	0.14	46,46,46,46	0
56	MG	BA	3140	1/1	0.96	0.09	22,22,22,22	0
56	MG	B1	101	1/1	0.96	0.12	28,28,28,28	0
56	MG	DA	3356	1/1	0.96	0.10	38,38,38,38	0
56	MG	DA	3357	1/1	0.96	0.17	14,14,14,14	0
56	MG	DA	3358	1/1	0.96	0.08	17,17,17,17	0
56	MG	CA	1935	1/1	0.96	0.07	49,49,49,49	0
56	MG	BA	3597	1/1	0.96	0.47	40,40,40,40	0
56	MG	DA	3362	1/1	0.96	0.16	43,43,43,43	0
56	MG	BA	3141	1/1	0.96	0.12	39,39,39,39	0
56	MG	DA	3366	1/1	0.96	0.20	21,21,21,21	0
56	MG	CA	1938	1/1	0.96	0.41	48,48,48,48	0
56	MG	DA	3368	1/1	0.96	0.10	29,29,29,29	0
56	MG	CA	1605	1/1	0.96	0.13	27,27,27,27	0
56	MG	CA	1941	1/1	0.96	0.41	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	BA	3350	1/1	0.96	0.14	32,32,32,32	0
56	MG	BA	3142	1/1	0.96	0.11	40,40,40,40	0
56	MG	CA	1944	1/1	0.96	0.24	42,42,42,42	0
56	MG	DA	3380	1/1	0.96	0.12	26,26,26,26	0
56	MG	CA	1609	1/1	0.96	0.12	60,60,60,60	0
56	MG	DA	3385	1/1	0.96	0.18	56,56,56,56	0
56	MG	BA	3603	1/1	0.96	0.08	26,26,26,26	0
56	MG	DA	3387	1/1	0.96	0.08	13,13,13,13	0
56	MG	BA	3352	1/1	0.96	0.11	36,36,36,36	0
56	MG	BA	3608	1/1	0.96	0.08	25,25,25,25	0
56	MG	DA	3394	1/1	0.96	0.12	38,38,38,38	0
56	MG	CA	1954	1/1	0.96	0.24	22,22,22,22	0
56	MG	BA	3610	1/1	0.96	0.10	34,34,34,34	0
56	MG	DA	3400	1/1	0.96	0.13	19,19,19,19	0
56	MG	DA	3402	1/1	0.96	0.13	19,19,19,19	0
56	MG	CA	1958	1/1	0.96	0.14	51,51,51,51	0
56	MG	DA	3404	1/1	0.96	0.13	32,32,32,32	0
56	MG	BA	3355	1/1	0.96	0.16	35,35,35,35	0
56	MG	DA	3406	1/1	0.96	0.23	33,33,33,33	0
56	MG	AA	1753	1/1	0.96	0.20	31,31,31,31	0
56	MG	AA	1755	1/1	0.96	0.04	29,29,29,29	0
56	MG	DA	3413	1/1	0.96	0.14	28,28,28,28	0
56	MG	CA	1966	1/1	0.96	0.09	41,41,41,41	0
56	MG	BA	3359	1/1	0.96	0.11	21,21,21,21	0
56	MG	CA	1620	1/1	0.96	0.10	38,38,38,38	0
56	MG	CA	1621	1/1	0.96	0.20	34,34,34,34	0
56	MG	DA	3422	1/1	0.96	0.15	22,22,22,22	0
56	MG	BA	3362	1/1	0.96	0.08	60,60,60,60	0
56	MG	CA	1972	1/1	0.96	0.53	33,33,33,33	0
56	MG	BA	3150	1/1	0.96	0.15	35,35,35,35	0
56	MG	CA	1978	1/1	0.96	0.07	35,35,35,35	0
56	MG	CA	1626	1/1	0.96	0.09	52,52,52,52	0
56	MG	CA	1630	1/1	0.96	0.07	36,36,36,36	0
56	MG	BA	3368	1/1	0.96	0.16	22,22,22,22	0
56	MG	CA	1983	1/1	0.96	0.42	50,50,50,50	0
56	MG	CA	1984	1/1	0.96	0.17	54,54,54,54	0
56	MG	AA	1705	1/1	0.96	0.14	29,29,29,29	0
56	MG	CA	1987	1/1	0.96	0.72	58,58,58,58	0
56	MG	BA	3371	1/1	0.96	0.22	29,29,29,29	0
56	MG	CA	1990	1/1	0.96	0.17	56,56,56,56	0
56	MG	BA	3153	1/1	0.96	0.22	60,60,60,60	0
56	MG	DA	3448	1/1	0.96	0.11	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DA	3452	1/1	0.96	0.35	25,25,25,25	0
56	MG	AK	201	1/1	0.96	0.08	66,66,66,66	0
56	MG	DA	3457	1/1	0.96	0.21	23,23,23,23	0
56	MG	AA	1678	1/1	0.96	0.13	43,43,43,43	0
56	MG	CA	1647	1/1	0.96	0.06	25,25,25,25	0
56	MG	AA	1879	1/1	0.96	0.08	58,58,58,58	0
56	MG	DA	3462	1/1	0.96	0.09	24,24,24,24	0
56	MG	AA	1713	1/1	0.96	0.08	43,43,43,43	0
56	MG	AA	1663	1/1	0.96	0.13	35,35,35,35	0
56	MG	BA	3386	1/1	0.96	0.18	38,38,38,38	0
56	MG	CA	1661	1/1	0.96	0.07	47,47,47,47	0
56	MG	CA	2005	1/1	0.96	0.42	58,58,58,58	0
56	MG	AA	1642	1/1	0.96	0.14	46,46,46,46	0
56	MG	AA	1765	1/1	0.96	0.08	35,35,35,35	0
56	MG	BA	3644	1/1	0.96	0.14	32,32,32,32	0
56	MG	CA	2010	1/1	0.96	0.10	35,35,35,35	0
56	MG	BA	3175	1/1	0.96	0.08	12,12,12,12	0
56	MG	BA	3391	1/1	0.96	0.30	46,46,46,46	0
56	MG	CA	1672	1/1	0.96	0.13	33,33,33,33	0
56	MG	BA	3393	1/1	0.96	0.14	32,32,32,32	0
56	MG	AA	1717	1/1	0.96	0.09	28,28,28,28	0
56	MG	BA	3395	1/1	0.96	0.21	34,34,34,34	0
56	MG	AA	1823	1/1	0.96	0.24	32,32,32,32	0
56	MG	CZ	112	1/1	0.96	0.13	36,36,36,36	0
56	MG	DA	3493	1/1	0.96	0.11	30,30,30,30	0
56	MG	BA	3657	1/1	0.96	0.12	27,27,27,27	0
56	MG	DA	3497	1/1	0.96	0.08	47,47,47,47	0
56	MG	AA	1612	1/1	0.96	0.13	14,14,14,14	0
56	MG	BA	3659	1/1	0.96	0.09	37,37,37,37	0
56	MG	BA	3180	1/1	0.96	0.10	8,8,8,8	0
56	MG	CZ	117	1/1	0.96	0.11	34,34,34,34	0
56	MG	BA	3403	1/1	0.96	0.15	41,41,41,41	0
56	MG	CV	101	1/1	0.96	0.09	37,37,37,37	0
56	MG	BA	3404	1/1	0.96	0.10	43,43,43,43	0
56	MG	AA	1827	1/1	0.96	0.06	38,38,38,38	0
56	MG	DA	3514	1/1	0.96	0.09	44,44,44,44	0
56	MG	CY	106	1/1	0.96	0.17	35,35,35,35	0
56	MG	BA	3409	1/1	0.96	0.11	22,22,22,22	0
56	MG	CY	111	1/1	0.96	0.26	39,39,39,39	0
56	MG	CA	1696	1/1	0.96	0.26	54,54,54,54	0
56	MG	BA	3410	1/1	0.96	0.18	37,37,37,37	0
56	MG	CY	116	1/1	0.96	0.08	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	BA	3002	1/1	0.96	0.08	20,20,20,20	0
56	MG	BA	3186	1/1	0.96	0.23	28,28,28,28	0
56	MG	AA	1770	1/1	0.96	0.11	42,42,42,42	0
56	MG	BA	3009	1/1	0.96	0.12	0,0,0,0	0
56	MG	BA	3190	1/1	0.96	0.26	36,36,36,36	0
56	MG	AA	1771	1/1	0.96	0.11	62,62,62,62	0
56	MG	BA	3680	1/1	0.96	0.21	44,44,44,44	0
56	MG	AA	1684	1/1	0.96	0.29	27,27,27,27	0
56	MG	BA	3685	1/1	0.96	0.34	37,37,37,37	0
56	MG	BA	3686	1/1	0.96	0.10	30,30,30,30	0
56	MG	DA	3549	1/1	0.96	0.07	13,13,13,13	0
56	MG	AA	1671	1/1	0.96	0.08	20,20,20,20	0
56	MG	AA	1673	1/1	0.96	0.11	21,21,21,21	0
56	MG	CI	201	1/1	0.96	0.15	45,45,45,45	0
56	MG	BA	3199	1/1	0.96	0.18	31,31,31,31	0
56	MG	CA	1724	1/1	0.96	0.23	56,56,56,56	0
56	MG	BA	3035	1/1	0.96	0.09	38,38,38,38	0
56	MG	AA	1836	1/1	0.96	0.28	45,45,45,45	0
56	MG	BA	3205	1/1	0.96	0.14	21,21,21,21	0
56	MG	BA	3208	1/1	0.96	0.10	27,27,27,27	0
56	MG	BA	3448	1/1	0.96	0.21	45,45,45,45	0
56	MG	DA	3571	1/1	0.96	0.10	26,26,26,26	0
56	MG	CX	405	1/1	0.96	0.22	49,49,49,49	0
56	MG	DA	3574	1/1	0.96	0.07	45,45,45,45	0
56	MG	BA	3698	1/1	0.96	0.26	57,57,57,57	0
56	MG	DA	3577	1/1	0.96	0.24	42,42,42,42	0
56	MG	AA	1904	1/1	0.96	0.17	47,47,47,47	0
56	MG	CX	408	1/1	0.96	0.21	44,44,44,44	0
56	MG	DA	3588	1/1	0.96	0.12	14,14,14,14	0
56	MG	AA	1628	1/1	0.96	0.11	34,34,34,34	0
56	MG	DG	201	1/1	0.96	0.39	34,34,34,34	0
56	MG	CA	1743	1/1	0.96	0.19	30,30,30,30	0
56	MG	BA	3216	1/1	0.96	0.11	33,33,33,33	0
56	MG	CA	1745	1/1	0.96	0.22	42,42,42,42	0
56	MG	BA	3704	1/1	0.96	0.12	42,42,42,42	0
56	MG	BA	3705	1/1	0.96	0.16	47,47,47,47	0
56	MG	BA	3459	1/1	0.96	0.29	40,40,40,40	0
56	MG	AZ	102	1/1	0.96	0.05	60,60,60,60	0
56	MG	AZ	103	1/1	0.96	0.09	34,34,34,34	0
56	MG	CA	1751	1/1	0.96	0.38	19,19,19,19	0
56	MG	AA	1728	1/1	0.96	0.10	14,14,14,14	0
56	MG	AZ	105	1/1	0.96	0.10	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	BA	3231	1/1	0.96	0.07	32,32,32,32	0
56	MG	DW	203	1/1	0.96	0.12	7,7,7,7	0
56	MG	CA	1760	1/1	0.96	0.07	59,59,59,59	0
56	MG	BA	3053	1/1	0.96	0.13	50,50,50,50	0
56	MG	BA	3470	1/1	0.96	0.23	51,51,51,51	0
56	MG	DA	3631	1/1	0.96	0.13	26,26,26,26	0
56	MG	D3	101	1/1	0.96	0.10	43,43,43,43	0
56	MG	DA	3633	1/1	0.96	0.18	19,19,19,19	0
56	MG	D4	101	1/1	0.96	0.05	23,23,23,23	0
56	MG	CA	1765	1/1	0.96	0.11	38,38,38,38	0
56	MG	BA	3716	1/1	0.96	0.12	28,28,28,28	0
56	MG	BA	3234	1/1	0.96	0.18	25,25,25,25	0
56	MG	CA	1770	1/1	0.96	0.11	30,30,30,30	0
56	MG	BA	3235	1/1	0.96	0.07	21,21,21,21	0
56	MG	DA	3012	1/1	0.96	0.10	16,16,16,16	0
56	MG	BA	3721	1/1	0.96	0.18	34,34,34,34	0
56	MG	DA	3015	1/1	0.96	0.11	11,11,11,11	0
56	MG	DA	3016	1/1	0.96	0.17	3,3,3,3	0
56	MG	BA	3475	1/1	0.96	0.15	15,15,15,15	0
56	MG	BA	3241	1/1	0.96	0.13	19,19,19,19	0
56	MG	BA	3477	1/1	0.96	0.21	31,31,31,31	0
56	MG	DA	3655	1/1	0.96	0.17	41,41,41,41	0
56	MG	CA	1780	1/1	0.96	0.09	15,15,15,15	0
56	MG	AA	1657	1/1	0.96	0.11	37,37,37,37	0
56	MG	CA	1783	1/1	0.96	0.13	32,32,32,32	0
56	MG	CA	1786	1/1	0.96	0.38	19,19,19,19	0
56	MG	DA	3034	1/1	0.96	0.12	9,9,9,9	0
56	MG	DA	3663	1/1	0.96	0.16	19,19,19,19	0
56	MG	DA	3036	1/1	0.96	0.06	13,13,13,13	0
56	MG	CA	1788	1/1	0.96	0.15	40,40,40,40	0
56	MG	BA	3481	1/1	0.96	0.34	45,45,45,45	0
56	MG	DA	3041	1/1	0.96	0.05	12,12,12,12	0
56	MG	DA	3048	1/1	0.96	0.23	20,20,20,20	0
56	MG	DA	3054	1/1	0.96	0.20	2,2,2,2	0
56	MG	AA	1733	1/1	0.96	0.07	24,24,24,24	0
56	MG	DA	3681	1/1	0.96	0.24	28,28,28,28	0
56	MG	BA	3488	1/1	0.96	0.22	26,26,26,26	0
56	MG	CA	1795	1/1	0.96	0.15	42,42,42,42	0
56	MG	DA	3685	1/1	0.96	0.09	20,20,20,20	0
56	MG	DA	3059	1/1	0.96	0.16	27,27,27,27	0
56	MG	DA	3062	1/1	0.96	0.12	31,31,31,31	0
56	MG	BA	3735	1/1	0.96	0.18	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DA	3691	1/1	0.96	0.14	50,50,50,50	0
56	MG	BA	3072	1/1	0.96	0.18	26,26,26,26	0
56	MG	DA	3074	1/1	0.96	0.12	19,19,19,19	0
56	MG	BA	3742	1/1	0.96	0.15	46,46,46,46	0
56	MG	DA	3078	1/1	0.96	0.09	15,15,15,15	0
56	MG	DA	3696	1/1	0.96	0.23	76,76,76,76	0
56	MG	DA	3697	1/1	0.96	0.10	36,36,36,36	0
56	MG	DA	3079	1/1	0.96	0.14	12,12,12,12	0
56	MG	CA	1801	1/1	0.96	0.05	30,30,30,30	0
56	MG	DA	3082	1/1	0.96	0.10	19,19,19,19	0
56	MG	BA	3073	1/1	0.96	0.16	23,23,23,23	0
56	MG	CA	1804	1/1	0.96	0.16	32,32,32,32	0
56	MG	DA	3707	1/1	0.96	0.14	45,45,45,45	0
56	MG	BA	3074	1/1	0.96	0.06	24,24,24,24	0
56	MG	BA	3500	1/1	0.96	0.16	16,16,16,16	0
56	MG	BA	3502	1/1	0.96	0.06	38,38,38,38	0
56	MG	BA	3258	1/1	0.96	0.08	30,30,30,30	0
56	MG	BA	3509	1/1	0.96	0.07	33,33,33,33	0
56	MG	DA	3113	1/1	0.96	0.26	13,13,13,13	0
56	MG	AA	1622	1/1	0.96	0.11	24,24,24,24	0
56	MG	BA	3751	1/1	0.96	0.15	53,53,53,53	0
56	MG	DA	3118	1/1	0.96	0.09	26,26,26,26	0
56	MG	BA	3263	1/1	0.96	0.18	0,0,0,0	0
56	MG	BA	3515	1/1	0.96	0.11	9,9,9,9	0
56	MG	BA	3079	1/1	0.96	0.11	29,29,29,29	0
56	MG	DA	3729	1/1	0.96	0.54	50,50,50,50	0
56	MG	BA	3080	1/1	0.96	0.12	19,19,19,19	0
56	MG	AY	104	1/1	0.96	0.14	38,38,38,38	0
56	MG	AY	105	1/1	0.96	0.28	64,64,64,64	0
56	MG	BA	3522	1/1	0.96	0.15	0,0,0,0	0
56	MG	DA	3142	1/1	0.96	0.15	24,24,24,24	0
56	MG	AY	108	1/1	0.96	0.12	33,33,33,33	0
56	MG	BA	3275	1/1	0.96	0.18	12,12,12,12	0
56	MG	BA	3532	1/1	0.96	0.23	56,56,56,56	0
56	MG	BA	3088	1/1	0.96	0.10	10,10,10,10	0
56	MG	DA	3164	1/1	0.96	0.10	13,13,13,13	0
56	MG	AA	1662	1/1	0.96	0.18	48,48,48,48	0
56	MG	AA	1790	1/1	0.96	0.18	32,32,32,32	0
56	MG	BA	3537	1/1	0.96	0.09	17,17,17,17	0
56	MG	DA	3753	1/1	0.96	0.33	32,32,32,32	0
56	MG	BA	3288	1/1	0.96	0.15	8,8,8,8	0
56	MG	CA	1842	1/1	0.96	0.12	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	AA	1742	1/1	0.96	0.08	17,17,17,17	0
56	MG	BA	3094	1/1	0.96	0.10	23,23,23,23	0
56	MG	BA	3547	1/1	0.96	0.09	26,26,26,26	0
56	MG	BA	3098	1/1	0.96	0.09	28,28,28,28	0
56	MG	AY	117	1/1	0.96	0.21	32,32,32,32	0
56	MG	CA	1853	1/1	0.96	0.15	50,50,50,50	0
56	MG	AY	123	1/1	0.96	0.34	42,42,42,42	0
56	MG	BA	3104	1/1	0.96	0.10	15,15,15,15	0
56	MG	DA	3190	1/1	0.96	0.16	32,32,32,32	0
56	MG	BA	3788	1/1	0.96	0.17	49,49,49,49	0
56	MG	DB	214	1/1	0.96	0.28	34,34,34,34	0
56	MG	AA	1852	1/1	0.96	0.12	45,45,45,45	0
56	MG	DB	217	1/1	0.96	0.17	24,24,24,24	0
56	MG	BA	3108	1/1	0.96	0.12	24,24,24,24	0
56	MG	DA	3195	1/1	0.96	0.12	28,28,28,28	0
56	MG	CA	1866	1/1	0.96	0.18	22,22,22,22	0
56	MG	AA	1854	1/1	0.96	0.09	44,44,44,44	0
56	MG	DB	224	1/1	0.96	0.54	41,41,41,41	0
56	MG	DA	3200	1/1	0.96	0.18	43,43,43,43	0
56	MG	DA	3201	1/1	0.96	0.06	45,45,45,45	0
56	MG	DB	227	1/1	0.96	0.17	53,53,53,53	0
56	MG	BA	3800	1/1	0.96	0.70	32,32,32,32	0
56	MG	BA	3492	1/1	0.97	0.09	47,47,47,47	0
56	MG	DA	3155	1/1	0.97	0.10	35,35,35,35	0
56	MG	DA	3157	1/1	0.97	0.12	30,30,30,30	0
56	MG	BA	3494	1/1	0.97	0.17	25,25,25,25	0
56	MG	DA	3160	1/1	0.97	0.04	35,35,35,35	0
56	MG	CA	1817	1/1	0.97	0.06	19,19,19,19	0
56	MG	BA	3496	1/1	0.97	0.11	39,39,39,39	0
56	MG	DA	3165	1/1	0.97	0.11	8,8,8,8	0
56	MG	BA	3267	1/1	0.97	0.06	21,21,21,21	0
56	MG	BA	3268	1/1	0.97	0.14	6,6,6,6	0
56	MG	CA	1821	1/1	0.97	0.09	22,22,22,22	0
56	MG	DA	3170	1/1	0.97	0.12	8,8,8,8	0
56	MG	CA	1823	1/1	0.97	0.09	40,40,40,40	0
56	MG	AA	1658	1/1	0.97	0.11	19,19,19,19	0
56	MG	AA	1864	1/1	0.97	0.21	36,36,36,36	0
56	MG	AA	1867	1/1	0.97	0.48	49,49,49,49	0
56	MG	DA	3175	1/1	0.97	0.10	32,32,32,32	0
56	MG	BA	3095	1/1	0.97	0.06	27,27,27,27	0
56	MG	AA	1754	1/1	0.97	0.06	21,21,21,21	0
56	MG	BA	3277	1/1	0.97	0.14	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DA	3180	1/1	0.97	0.10	22,22,22,22	0
56	MG	AC	305	1/1	0.97	0.27	45,45,45,45	0
56	MG	BA	3280	1/1	0.97	0.20	26,26,26,26	0
56	MG	DA	3185	1/1	0.97	0.24	44,44,44,44	0
56	MG	DA	3187	1/1	0.97	0.14	14,14,14,14	0
56	MG	BA	3281	1/1	0.97	0.09	7,7,7,7	0
56	MG	BA	3518	1/1	0.97	0.10	9,9,9,9	0
56	MG	BA	3101	1/1	0.97	0.08	0,0,0,0	0
56	MG	CA	1836	1/1	0.97	0.20	14,14,14,14	0
56	MG	CA	1837	1/1	0.97	0.28	45,45,45,45	0
56	MG	CA	1839	1/1	0.97	0.09	31,31,31,31	0
56	MG	BA	3520	1/1	0.97	0.10	7,7,7,7	0
56	MG	BA	3770	1/1	0.97	0.14	30,30,30,30	0
56	MG	AA	1646	1/1	0.97	0.18	21,21,21,21	0
56	MG	BA	3287	1/1	0.97	0.11	27,27,27,27	0
56	MG	DA	3203	1/1	0.97	0.11	38,38,38,38	0
56	MG	CA	1844	1/1	0.97	0.08	26,26,26,26	0
56	MG	DA	3206	1/1	0.97	0.16	20,20,20,20	0
56	MG	DA	3207	1/1	0.97	0.07	20,20,20,20	0
56	MG	BA	3774	1/1	0.97	0.12	44,44,44,44	0
56	MG	AD	303	1/1	0.97	0.12	17,17,17,17	0
56	MG	BA	3777	1/1	0.97	0.06	40,40,40,40	0
56	MG	DA	3211	1/1	0.97	0.09	23,23,23,23	0
56	MG	DA	3212	1/1	0.97	0.16	34,34,34,34	0
56	MG	BA	3528	1/1	0.97	0.09	9,9,9,9	0
56	MG	CA	1852	1/1	0.97	0.09	43,43,43,43	0
56	MG	BA	3105	1/1	0.97	0.10	36,36,36,36	0
56	MG	BA	3530	1/1	0.97	0.17	35,35,35,35	0
56	MG	DA	3226	1/1	0.97	0.06	21,21,21,21	0
56	MG	AA	1807	1/1	0.97	0.11	22,22,22,22	0
56	MG	DA	3228	1/1	0.97	0.15	12,12,12,12	0
56	MG	BA	3294	1/1	0.97	0.15	43,43,43,43	0
56	MG	AA	1712	1/1	0.97	0.20	26,26,26,26	0
56	MG	DA	3234	1/1	0.97	0.27	8,8,8,8	0
56	MG	CA	1860	1/1	0.97	0.11	31,31,31,31	0
56	MG	DA	3238	1/1	0.97	0.20	2,2,2,2	0
56	MG	CA	1861	1/1	0.97	0.20	64,64,64,64	0
56	MG	BA	3785	1/1	0.97	0.23	47,47,47,47	0
56	MG	CA	1863	1/1	0.97	0.16	33,33,33,33	0
56	MG	DA	3250	1/1	0.97	0.18	32,32,32,32	0
56	MG	CA	1864	1/1	0.97	0.23	40,40,40,40	0
56	MG	BA	3109	1/1	0.97	0.17	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DA	3255	1/1	0.97	0.09	19,19,19,19	0
56	MG	AD	306	1/1	0.97	0.16	38,38,38,38	0
56	MG	CA	1870	1/1	0.97	0.19	25,25,25,25	0
56	MG	CA	1871	1/1	0.97	0.15	34,34,34,34	0
56	MG	AA	1873	1/1	0.97	0.10	36,36,36,36	0
56	MG	BA	3306	1/1	0.97	0.06	36,36,36,36	0
56	MG	BA	3792	1/1	0.97	0.06	42,42,42,42	0
56	MG	BA	3795	1/1	0.97	0.32	35,35,35,35	0
56	MG	DA	3266	1/1	0.97	0.08	31,31,31,31	0
56	MG	BA	3796	1/1	0.97	0.25	27,27,27,27	0
56	MG	BA	3307	1/1	0.97	0.07	26,26,26,26	0
56	MG	DA	3269	1/1	0.97	0.07	31,31,31,31	0
56	MG	BA	3546	1/1	0.97	0.11	17,17,17,17	0
56	MG	AD	308	1/1	0.97	0.09	42,42,42,42	0
56	MG	CA	1882	1/1	0.97	0.36	35,35,35,35	0
56	MG	BA	3115	1/1	0.97	0.20	33,33,33,33	0
56	MG	BA	3116	1/1	0.97	0.15	68,68,68,68	0
56	MG	BA	3316	1/1	0.97	0.09	12,12,12,12	0
56	MG	BA	3552	1/1	0.97	0.16	12,12,12,12	0
56	MG	CA	1887	1/1	0.97	0.24	40,40,40,40	0
56	MG	BA	3317	1/1	0.97	0.13	25,25,25,25	0
56	MG	CA	1889	1/1	0.97	0.23	31,31,31,31	0
56	MG	BB	207	1/1	0.97	0.06	28,28,28,28	0
56	MG	AA	1647	1/1	0.97	0.11	44,44,44,44	0
56	MG	CA	1897	1/1	0.97	0.27	23,23,23,23	0
56	MG	DA	3295	1/1	0.97	0.19	37,37,37,37	0
56	MG	DA	3296	1/1	0.97	0.10	4,4,4,4	0
56	MG	DA	3299	1/1	0.97	0.07	1,1,1,1	0
56	MG	AA	1877	1/1	0.97	0.23	32,32,32,32	0
56	MG	CA	1900	1/1	0.97	0.10	56,56,56,56	0
56	MG	CA	1901	1/1	0.97	0.12	7,7,7,7	0
56	MG	BB	211	1/1	0.97	0.08	16,16,16,16	0
56	MG	DA	3313	1/1	0.97	0.12	42,42,42,42	0
56	MG	DA	3314	1/1	0.97	0.06	25,25,25,25	0
56	MG	DA	3320	1/1	0.97	0.10	19,19,19,19	0
56	MG	DA	3321	1/1	0.97	0.10	28,28,28,28	0
56	MG	BA	3323	1/1	0.97	0.14	40,40,40,40	0
56	MG	DA	3324	1/1	0.97	0.14	11,11,11,11	0
56	MG	DA	3325	1/1	0.97	0.14	34,34,34,34	0
56	MG	AA	1681	1/1	0.97	0.07	49,49,49,49	0
56	MG	DA	3330	1/1	0.97	0.21	36,36,36,36	0
56	MG	DA	3332	1/1	0.97	0.10	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DA	3334	1/1	0.97	0.11	8,8,8,8	0
56	MG	DA	3336	1/1	0.97	0.08	38,38,38,38	0
56	MG	CA	1907	1/1	0.97	0.08	31,31,31,31	0
56	MG	AA	1813	1/1	0.97	0.06	23,23,23,23	0
56	MG	CA	1912	1/1	0.97	0.13	45,45,45,45	0
56	MG	AA	1761	1/1	0.97	0.08	26,26,26,26	0
56	MG	DA	3350	1/1	0.97	0.10	24,24,24,24	0
56	MG	CA	1914	1/1	0.97	0.17	29,29,29,29	0
56	MG	AA	1648	1/1	0.97	0.10	26,26,26,26	0
56	MG	BB	219	1/1	0.97	0.43	52,52,52,52	0
56	MG	BB	220	1/1	0.97	0.13	60,60,60,60	0
56	MG	AA	1666	1/1	0.97	0.30	34,34,34,34	0
56	MG	BA	3333	1/1	0.97	0.23	19,19,19,19	0
56	MG	AA	1667	1/1	0.97	0.15	38,38,38,38	0
56	MG	BB	226	1/1	0.97	0.14	59,59,59,59	0
56	MG	CA	1922	1/1	0.97	0.09	33,33,33,33	0
56	MG	BD	301	1/1	0.97	0.08	2,2,2,2	0
56	MG	BA	3131	1/1	0.97	0.13	30,30,30,30	0
56	MG	BA	3337	1/1	0.97	0.18	28,28,28,28	0
56	MG	BF	302	1/1	0.97	0.12	13,13,13,13	0
56	MG	DA	3369	1/1	0.97	0.07	7,7,7,7	0
56	MG	DA	3370	1/1	0.97	0.15	23,23,23,23	0
56	MG	AL	202	1/1	0.97	0.20	46,46,46,46	0
56	MG	AA	1637	1/1	0.97	0.20	32,32,32,32	0
56	MG	DA	3373	1/1	0.97	0.08	41,41,41,41	0
56	MG	DA	3374	1/1	0.97	0.12	24,24,24,24	0
56	MG	BA	3577	1/1	0.97	0.21	17,17,17,17	0
56	MG	BH	202	1/1	0.97	0.08	34,34,34,34	0
56	MG	BA	3578	1/1	0.97	0.12	19,19,19,19	0
56	MG	BA	3341	1/1	0.97	0.12	26,26,26,26	0
56	MG	AA	1722	1/1	0.97	0.07	35,35,35,35	0
56	MG	DA	3384	1/1	0.97	0.20	20,20,20,20	0
56	MG	AA	1723	1/1	0.97	0.09	29,29,29,29	0
56	MG	BQ	202	1/1	0.97	0.26	45,45,45,45	0
56	MG	AA	1687	1/1	0.97	0.07	11,11,11,11	0
56	MG	AQ	201	1/1	0.97	0.51	47,47,47,47	0
56	MG	BT	202	1/1	0.97	0.10	42,42,42,42	0
56	MG	AA	1620	1/1	0.97	0.08	35,35,35,35	0
56	MG	CA	1945	1/1	0.97	0.23	18,18,18,18	0
56	MG	BW	201	1/1	0.97	0.23	23,23,23,23	0
56	MG	BA	3143	1/1	0.97	0.15	40,40,40,40	0
56	MG	DA	3401	1/1	0.97	0.11	1,1,1,1	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	CA	1948	1/1	0.97	0.36	43,43,43,43	0
56	MG	CA	1949	1/1	0.97	0.10	37,37,37,37	0
56	MG	BY	201	1/1	0.97	0.39	36,36,36,36	0
56	MG	BA	3144	1/1	0.97	0.14	34,34,34,34	0
56	MG	CA	1952	1/1	0.97	0.18	37,37,37,37	0
56	MG	B1	102	1/1	0.97	0.24	24,24,24,24	0
56	MG	B2	101	1/1	0.97	0.20	32,32,32,32	0
56	MG	B2	103	1/1	0.97	0.44	38,38,38,38	0
56	MG	CA	1962	1/1	0.97	0.26	41,41,41,41	0
56	MG	DA	3415	1/1	0.97	0.09	27,27,27,27	0
56	MG	AA	1689	1/1	0.97	0.08	39,39,39,39	0
56	MG	CA	1601	1/1	0.97	0.10	54,54,54,54	0
56	MG	CA	1602	1/1	0.97	0.13	15,15,15,15	0
56	MG	AA	1833	1/1	0.97	0.30	52,52,52,52	0
56	MG	CA	1604	1/1	0.97	0.24	37,37,37,37	0
56	MG	AA	1899	1/1	0.97	0.17	42,42,42,42	0
56	MG	AA	1776	1/1	0.97	0.08	11,11,11,11	0
56	MG	BA	3353	1/1	0.97	0.07	40,40,40,40	0
56	MG	DA	3429	1/1	0.97	0.37	48,48,48,48	0
56	MG	CA	1608	1/1	0.97	0.11	27,27,27,27	0
56	MG	CA	1973	1/1	0.97	0.11	37,37,37,37	0
56	MG	BA	3354	1/1	0.97	0.12	19,19,19,19	0
56	MG	BA	3001	1/1	0.97	0.11	26,26,26,26	0
56	MG	BA	3599	1/1	0.97	0.15	34,34,34,34	0
56	MG	AA	1690	1/1	0.97	0.09	47,47,47,47	0
56	MG	AA	1778	1/1	0.97	0.10	50,50,50,50	0
56	MG	BA	3157	1/1	0.97	0.10	8,8,8,8	0
56	MG	BA	3160	1/1	0.97	0.11	23,23,23,23	0
56	MG	BA	3161	1/1	0.97	0.09	25,25,25,25	0
56	MG	DA	3446	1/1	0.97	0.15	20,20,20,20	0
56	MG	BA	3365	1/1	0.97	0.24	40,40,40,40	0
56	MG	DA	3449	1/1	0.97	0.09	16,16,16,16	0
56	MG	DA	3451	1/1	0.97	0.17	5,5,5,5	0
56	MG	BA	3006	1/1	0.97	0.10	9,9,9,9	0
56	MG	DA	3455	1/1	0.97	0.26	35,35,35,35	0
56	MG	CA	1989	1/1	0.97	0.10	33,33,33,33	0
56	MG	BA	3008	1/1	0.97	0.23	5,5,5,5	0
56	MG	BA	3370	1/1	0.97	0.28	24,24,24,24	0
56	MG	CA	1993	1/1	0.97	0.30	48,48,48,48	0
56	MG	CA	1624	1/1	0.97	0.36	54,54,54,54	0
56	MG	BA	3619	1/1	0.97	0.10	32,32,32,32	0
56	MG	AA	1903	1/1	0.97	0.13	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	CA	1629	1/1	0.97	0.09	8,8,8,8	0
56	MG	BA	3622	1/1	0.97	0.12	32,32,32,32	0
56	MG	CA	1631	1/1	0.97	0.13	27,27,27,27	0
56	MG	CA	1634	1/1	0.97	0.17	41,41,41,41	0
56	MG	BA	3010	1/1	0.97	0.12	2,2,2,2	0
56	MG	BA	3373	1/1	0.97	0.10	24,24,24,24	0
56	MG	BA	3011	1/1	0.97	0.41	33,33,33,33	0
56	MG	BA	3376	1/1	0.97	0.09	35,35,35,35	0
56	MG	CA	2008	1/1	0.97	0.45	53,53,53,53	0
56	MG	DA	3476	1/1	0.97	0.10	37,37,37,37	0
56	MG	CA	1641	1/1	0.97	0.08	14,14,14,14	0
56	MG	CA	1642	1/1	0.97	0.10	29,29,29,29	0
56	MG	CA	2011	1/1	0.97	0.18	28,28,28,28	0
56	MG	DA	3481	1/1	0.97	0.08	31,31,31,31	0
56	MG	BA	3628	1/1	0.97	0.16	24,24,24,24	0
56	MG	DA	3484	1/1	0.97	0.31	6,6,6,6	0
56	MG	DA	3485	1/1	0.97	0.22	10,10,10,10	0
56	MG	AA	1838	1/1	0.97	0.13	39,39,39,39	0
56	MG	DA	3487	1/1	0.97	0.06	48,48,48,48	0
56	MG	CA	1646	1/1	0.97	0.12	45,45,45,45	0
56	MG	BA	3630	1/1	0.97	0.30	41,41,41,41	0
56	MG	CA	1649	1/1	0.97	0.15	16,16,16,16	0
56	MG	CZ	106	1/1	0.97	0.06	19,19,19,19	0
56	MG	DA	3496	1/1	0.97	0.17	18,18,18,18	0
56	MG	BA	3020	1/1	0.97	0.07	2,2,2,2	0
56	MG	AA	1730	1/1	0.97	0.10	12,12,12,12	0
56	MG	AA	1907	1/1	0.97	0.08	54,54,54,54	0
56	MG	CA	1654	1/1	0.97	0.10	23,23,23,23	0
56	MG	CA	1656	1/1	0.97	0.13	48,48,48,48	0
56	MG	BA	3635	1/1	0.97	0.13	32,32,32,32	0
56	MG	CA	1659	1/1	0.97	0.09	44,44,44,44	0
56	MG	BA	3636	1/1	0.97	0.09	47,47,47,47	0
56	MG	CA	1664	1/1	0.97	0.24	41,41,41,41	0
56	MG	BA	3028	1/1	0.97	0.21	10,10,10,10	0
56	MG	CV	102	1/1	0.97	0.14	25,25,25,25	0
56	MG	DA	3517	1/1	0.97	0.06	48,48,48,48	0
56	MG	AA	1910	1/1	0.97	0.23	32,32,32,32	0
56	MG	CY	101	1/1	0.97	0.13	12,12,12,12	0
56	MG	DA	3522	1/1	0.97	0.11	33,33,33,33	0
56	MG	CY	104	1/1	0.97	0.07	20,20,20,20	0
56	MG	CA	1667	1/1	0.97	0.11	21,21,21,21	0
56	MG	DA	3525	1/1	0.97	0.10	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	CA	1668	1/1	0.97	0.11	55,55,55,55	0
56	MG	CY	107	1/1	0.97	0.27	38,38,38,38	0
56	MG	BA	3388	1/1	0.97	0.23	46,46,46,46	0
56	MG	CY	110	1/1	0.97	0.08	17,17,17,17	0
56	MG	BA	3030	1/1	0.97	0.08	26,26,26,26	0
56	MG	BA	3032	1/1	0.97	0.10	11,11,11,11	0
56	MG	BA	3033	1/1	0.97	0.12	24,24,24,24	0
56	MG	CY	114	1/1	0.97	0.13	16,16,16,16	0
56	MG	BA	3188	1/1	0.97	0.13	3,3,3,3	0
56	MG	CY	117	1/1	0.97	0.11	23,23,23,23	0
56	MG	BA	3646	1/1	0.97	0.12	12,12,12,12	0
56	MG	CY	119	1/1	0.97	0.38	35,35,35,35	0
56	MG	CY	120	1/1	0.97	0.17	29,29,29,29	0
56	MG	CB	302	1/1	0.97	0.58	48,48,48,48	0
56	MG	BA	3034	1/1	0.97	0.07	17,17,17,17	0
56	MG	AA	1780	1/1	0.97	0.14	34,34,34,34	0
56	MG	AA	1670	1/1	0.97	0.05	22,22,22,22	0
56	MG	DA	3562	1/1	0.97	0.07	17,17,17,17	0
56	MG	BA	3653	1/1	0.97	0.13	38,38,38,38	0
56	MG	BA	3397	1/1	0.97	0.10	45,45,45,45	0
56	MG	CA	1686	1/1	0.97	0.29	29,29,29,29	0
56	MG	CA	1687	1/1	0.97	0.06	19,19,19,19	0
56	MG	BA	3192	1/1	0.97	0.22	20,20,20,20	0
56	MG	BA	3038	1/1	0.97	0.09	37,37,37,37	0
56	MG	AA	1652	1/1	0.97	0.07	17,17,17,17	0
56	MG	DA	3573	1/1	0.97	0.11	25,25,25,25	0
56	MG	CA	1692	1/1	0.97	0.11	6,6,6,6	0
56	MG	AA	1736	1/1	0.97	0.10	50,50,50,50	0
56	MG	CI	202	1/1	0.97	0.47	52,52,52,52	0
56	MG	DA	3579	1/1	0.97	0.14	24,24,24,24	0
56	MG	BA	3405	1/1	0.97	0.11	20,20,20,20	0
56	MG	DA	3582	1/1	0.97	0.17	27,27,27,27	0
56	MG	BA	3406	1/1	0.97	0.14	42,42,42,42	0
56	MG	DA	3584	1/1	0.97	0.08	35,35,35,35	0
56	MG	DA	3585	1/1	0.97	0.14	31,31,31,31	0
56	MG	DA	3586	1/1	0.97	0.18	55,55,55,55	0
56	MG	CA	1697	1/1	0.97	0.09	10,10,10,10	0
56	MG	CA	1698	1/1	0.97	0.14	28,28,28,28	0
56	MG	BA	3198	1/1	0.97	0.08	21,21,21,21	0
56	MG	DA	3592	1/1	0.97	0.28	47,47,47,47	0
56	MG	DA	3593	1/1	0.97	0.27	28,28,28,28	0
56	MG	AA	1847	1/1	0.97	0.12	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	BA	3200	1/1	0.97	0.09	20,20,20,20	0
56	MG	CX	404	1/1	0.97	0.11	34,34,34,34	0
56	MG	BA	3412	1/1	0.97	0.20	22,22,22,22	0
56	MG	DA	3602	1/1	0.97	0.09	32,32,32,32	0
56	MG	DA	3603	1/1	0.97	0.22	32,32,32,32	0
56	MG	AA	1737	1/1	0.97	0.08	40,40,40,40	0
56	MG	CA	1706	1/1	0.97	0.07	16,16,16,16	0
56	MG	DA	3606	1/1	0.97	0.30	54,54,54,54	0
56	MG	CA	1707	1/1	0.97	0.07	48,48,48,48	0
56	MG	CX	409	1/1	0.97	0.30	33,33,33,33	0
56	MG	BA	3047	1/1	0.97	0.14	17,17,17,17	0
56	MG	DA	3612	1/1	0.97	0.19	41,41,41,41	0
56	MG	DA	3614	1/1	0.97	0.19	55,55,55,55	0
56	MG	BA	3204	1/1	0.97	0.11	41,41,41,41	0
56	MG	AA	1672	1/1	0.97	0.12	46,46,46,46	0
56	MG	DA	3617	1/1	0.97	0.05	47,47,47,47	0
56	MG	AA	1850	1/1	0.97	0.30	23,23,23,23	0
56	MG	BA	3421	1/1	0.97	0.20	45,45,45,45	0
56	MG	AA	1851	1/1	0.97	0.16	50,50,50,50	0
56	MG	DA	3623	1/1	0.97	0.11	39,39,39,39	0
56	MG	CA	1717	1/1	0.97	0.12	32,32,32,32	0
56	MG	DA	3627	1/1	0.97	0.19	24,24,24,24	0
56	MG	CA	1718	1/1	0.97	0.11	38,38,38,38	0
56	MG	DA	3630	1/1	0.97	0.10	21,21,21,21	0
56	MG	BA	3678	1/1	0.97	0.13	42,42,42,42	0
56	MG	BA	3210	1/1	0.97	0.14	31,31,31,31	0
56	MG	CA	1722	1/1	0.97	0.23	36,36,36,36	0
56	MG	BA	3054	1/1	0.97	0.12	6,6,6,6	0
56	MG	DT	201	1/1	0.97	0.10	25,25,25,25	0
56	MG	DA	3636	1/1	0.97	0.14	46,46,46,46	0
56	MG	AA	1606	1/1	0.97	0.08	0,0,0,0	0
56	MG	DW	201	1/1	0.97	0.16	54,54,54,54	0
56	MG	CA	1725	1/1	0.97	0.07	26,26,26,26	0
56	MG	CA	1726	1/1	0.97	0.14	32,32,32,32	0
56	MG	DA	3644	1/1	0.97	0.14	5,5,5,5	0
56	MG	BA	3219	1/1	0.97	0.13	14,14,14,14	0
56	MG	BA	3687	1/1	0.97	0.08	19,19,19,19	0
56	MG	CA	1730	1/1	0.97	0.34	45,45,45,45	0
56	MG	BA	3688	1/1	0.97	0.21	38,38,38,38	0
56	MG	BA	3427	1/1	0.97	0.14	10,10,10,10	0
56	MG	D4	102	1/1	0.97	0.21	40,40,40,40	0
56	MG	BA	3428	1/1	0.97	0.07	17,17,17,17	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	D7	102	1/1	0.97	0.11	28,28,28,28	0
56	MG	DA	3656	1/1	0.97	0.48	35,35,35,35	0
56	MG	D8	101	1/1	0.97	0.18	20,20,20,20	0
56	MG	BA	3058	1/1	0.97	0.15	39,39,39,39	0
56	MG	DA	3002	1/1	0.97	0.25	45,45,45,45	0
56	MG	CA	1738	1/1	0.97	0.19	20,20,20,20	0
56	MG	CA	1739	1/1	0.97	0.25	39,39,39,39	0
56	MG	BA	3221	1/1	0.97	0.14	21,21,21,21	0
56	MG	DA	3007	1/1	0.97	0.23	24,24,24,24	0
56	MG	BA	3436	1/1	0.97	0.10	1,1,1,1	0
56	MG	DA	3667	1/1	0.97	0.17	38,38,38,38	0
56	MG	BA	3068	1/1	0.97	0.16	14,14,14,14	0
56	MG	DA	3669	1/1	0.97	0.09	7,7,7,7	0
56	MG	DA	3672	1/1	0.97	0.07	29,29,29,29	0
56	MG	BA	3069	1/1	0.97	0.14	11,11,11,11	0
56	MG	BA	3443	1/1	0.97	0.28	29,29,29,29	0
56	MG	DA	3017	1/1	0.97	0.11	4,4,4,4	0
56	MG	DA	3677	1/1	0.97	0.23	27,27,27,27	0
56	MG	DA	3678	1/1	0.97	0.10	20,20,20,20	0
56	MG	DA	3018	1/1	0.97	0.09	3,3,3,3	0
56	MG	DA	3680	1/1	0.97	0.18	6,6,6,6	0
56	MG	BA	3445	1/1	0.97	0.14	45,45,45,45	0
56	MG	DA	3020	1/1	0.97	0.24	9,9,9,9	0
56	MG	DA	3021	1/1	0.97	0.26	2,2,2,2	0
56	MG	AA	1635	1/1	0.97	0.09	30,30,30,30	0
56	MG	DA	3686	1/1	0.97	0.19	30,30,30,30	0
56	MG	BA	3449	1/1	0.97	0.10	31,31,31,31	0
56	MG	DA	3024	1/1	0.97	0.07	12,12,12,12	0
56	MG	DA	3025	1/1	0.97	0.21	24,24,24,24	0
56	MG	BA	3702	1/1	0.97	0.14	47,47,47,47	0
56	MG	BA	3230	1/1	0.97	0.16	0,0,0,0	0
56	MG	BA	3451	1/1	0.97	0.18	51,51,51,51	0
56	MG	CA	1752	1/1	0.97	0.11	24,24,24,24	0
56	MG	DA	3033	1/1	0.97	0.09	10,10,10,10	0
56	MG	CA	1753	1/1	0.97	0.14	23,23,23,23	0
56	MG	BA	3452	1/1	0.97	0.12	18,18,18,18	0
56	MG	AA	1699	1/1	0.97	0.10	35,35,35,35	0
56	MG	DA	3699	1/1	0.97	0.47	38,38,38,38	0
56	MG	AY	111	1/1	0.97	0.09	34,34,34,34	0
56	MG	BA	3458	1/1	0.97	0.09	6,6,6,6	0
56	MG	DA	3704	1/1	0.97	0.12	34,34,34,34	0
56	MG	DA	3043	1/1	0.97	0.06	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	AA	1656	1/1	0.97	0.07	41,41,41,41	0
56	MG	DA	3050	1/1	0.97	0.16	11,11,11,11	0
56	MG	AY	116	1/1	0.97	0.31	51,51,51,51	0
56	MG	CA	1763	1/1	0.97	0.10	19,19,19,19	0
56	MG	CA	1764	1/1	0.97	0.14	30,30,30,30	0
56	MG	DA	3711	1/1	0.97	0.08	49,49,49,49	0
56	MG	BA	3236	1/1	0.97	0.15	6,6,6,6	0
56	MG	DA	3713	1/1	0.97	0.10	27,27,27,27	0
56	MG	BA	3713	1/1	0.97	0.23	28,28,28,28	0
56	MG	DA	3060	1/1	0.97	0.07	19,19,19,19	0
56	MG	DA	3717	1/1	0.97	0.15	24,24,24,24	0
56	MG	AA	1601	1/1	0.97	0.15	18,18,18,18	0
56	MG	BA	3464	1/1	0.97	0.14	30,30,30,30	0
56	MG	DA	3067	1/1	0.97	0.07	17,17,17,17	0
56	MG	DA	3721	1/1	0.97	0.27	11,11,11,11	0
56	MG	DA	3069	1/1	0.97	0.12	15,15,15,15	0
56	MG	DA	3723	1/1	0.97	0.11	28,28,28,28	0
56	MG	DA	3070	1/1	0.97	0.07	20,20,20,20	0
56	MG	DA	3725	1/1	0.97	0.13	44,44,44,44	0
56	MG	DA	3727	1/1	0.97	0.08	27,27,27,27	0
56	MG	BA	3243	1/1	0.97	0.12	14,14,14,14	0
56	MG	AY	119	1/1	0.97	0.10	22,22,22,22	0
56	MG	BA	3718	1/1	0.97	0.10	33,33,33,33	0
56	MG	DA	3077	1/1	0.97	0.09	7,7,7,7	0
56	MG	DA	3732	1/1	0.97	0.15	29,29,29,29	0
56	MG	BA	3247	1/1	0.97	0.13	39,39,39,39	0
56	MG	CA	1775	1/1	0.97	0.19	30,30,30,30	0
56	MG	BA	3720	1/1	0.97	0.07	30,30,30,30	0
56	MG	CA	1779	1/1	0.97	0.12	14,14,14,14	0
56	MG	DA	3083	1/1	0.97	0.15	24,24,24,24	0
56	MG	DA	3085	1/1	0.97	0.09	35,35,35,35	0
56	MG	BA	3248	1/1	0.97	0.11	42,42,42,42	0
56	MG	BA	3722	1/1	0.97	0.28	16,16,16,16	0
56	MG	CA	1782	1/1	0.97	0.09	19,19,19,19	0
56	MG	DA	3095	1/1	0.97	0.15	24,24,24,24	0
56	MG	BA	3081	1/1	0.97	0.07	0,0,0,0	0
56	MG	BA	3082	1/1	0.97	0.08	48,48,48,48	0
56	MG	DA	3104	1/1	0.97	0.15	21,21,21,21	0
56	MG	AY	120	1/1	0.97	0.12	47,47,47,47	0
56	MG	DA	3109	1/1	0.97	0.13	19,19,19,19	0
56	MG	AY	122	1/1	0.97	0.07	17,17,17,17	0
56	MG	BA	3729	1/1	0.97	0.14	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	AA	1749	1/1	0.97	0.14	32,32,32,32	0
56	MG	DB	203	1/1	0.97	0.07	21,21,21,21	0
56	MG	BA	3259	1/1	0.97	0.16	27,27,27,27	0
56	MG	DB	205	1/1	0.97	0.07	60,60,60,60	0
56	MG	DA	3117	1/1	0.97	0.08	24,24,24,24	0
56	MG	AY	124	1/1	0.97	0.08	21,21,21,21	0
56	MG	DA	3119	1/1	0.97	0.06	10,10,10,10	0
56	MG	BA	3734	1/1	0.97	0.17	32,32,32,32	0
56	MG	BA	3483	1/1	0.97	0.11	29,29,29,29	0
56	MG	DB	213	1/1	0.97	0.07	20,20,20,20	0
56	MG	BA	3736	1/1	0.97	0.23	39,39,39,39	0
56	MG	BA	3090	1/1	0.97	0.06	56,56,56,56	0
56	MG	AA	1703	1/1	0.97	0.22	36,36,36,36	0
56	MG	BA	3265	1/1	0.97	0.19	0,0,0,0	0
56	MG	DA	3136	1/1	0.97	0.15	11,11,11,11	0
56	MG	DA	3137	1/1	0.97	0.11	20,20,20,20	0
56	MG	BA	3744	1/1	0.97	0.36	21,21,21,21	0
56	MG	DB	223	1/1	0.97	0.11	53,53,53,53	0
56	MG	DA	3141	1/1	0.97	0.09	9,9,9,9	0
56	MG	BA	3490	1/1	0.97	0.10	22,22,22,22	0
56	MG	DA	3144	1/1	0.97	0.24	11,11,11,11	0
56	MG	BA	3491	1/1	0.97	0.13	31,31,31,31	0
56	MG	DA	3149	1/1	0.97	0.29	37,37,37,37	0
56	MG	AA	1700	1/1	0.98	0.19	46,46,46,46	0
56	MG	BR	201	1/1	0.98	0.07	24,24,24,24	0
56	MG	CA	1906	1/1	0.98	0.27	24,24,24,24	0
56	MG	AA	1826	1/1	0.98	0.09	35,35,35,35	0
56	MG	CA	1908	1/1	0.98	0.06	5,5,5,5	0
56	MG	CA	1909	1/1	0.98	0.24	33,33,33,33	0
56	MG	AA	1887	1/1	0.98	0.13	18,18,18,18	0
56	MG	BT	201	1/1	0.98	0.13	23,23,23,23	0
56	MG	BA	3201	1/1	0.98	0.06	22,22,22,22	0
56	MG	DA	3217	1/1	0.98	0.05	20,20,20,20	0
56	MG	BA	3600	1/1	0.98	0.11	13,13,13,13	0
56	MG	DA	3219	1/1	0.98	0.08	12,12,12,12	0
56	MG	DA	3221	1/1	0.98	0.14	11,11,11,11	0
56	MG	DA	3223	1/1	0.98	0.05	26,26,26,26	0
56	MG	DA	3224	1/1	0.98	0.07	9,9,9,9	0
56	MG	BV	201	1/1	0.98	0.17	21,21,21,21	0
56	MG	BA	3375	1/1	0.98	0.06	14,14,14,14	0
56	MG	AA	1640	1/1	0.98	0.09	35,35,35,35	0
56	MG	BA	3075	1/1	0.98	0.15	11,11,11,11	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	BZ	301	1/1	0.98	0.19	21,21,21,21	0
56	MG	BA	3604	1/1	0.98	0.16	36,36,36,36	0
56	MG	DA	3235	1/1	0.98	0.10	0,0,0,0	0
56	MG	DA	3236	1/1	0.98	0.31	14,14,14,14	0
56	MG	BA	3605	1/1	0.98	0.18	41,41,41,41	0
56	MG	BA	3379	1/1	0.98	0.09	25,25,25,25	0
56	MG	DA	3242	1/1	0.98	0.08	24,24,24,24	0
56	MG	B2	102	1/1	0.98	0.24	31,31,31,31	0
56	MG	BA	3607	1/1	0.98	0.24	23,23,23,23	0
56	MG	DA	3245	1/1	0.98	0.09	5,5,5,5	0
56	MG	DA	3246	1/1	0.98	0.10	15,15,15,15	0
56	MG	B5	101	1/1	0.98	0.09	18,18,18,18	0
56	MG	BA	3076	1/1	0.98	0.04	26,26,26,26	0
56	MG	CA	1929	1/1	0.98	0.09	48,48,48,48	0
56	MG	DA	3252	1/1	0.98	0.06	16,16,16,16	0
56	MG	B7	102	1/1	0.98	0.09	13,13,13,13	0
56	MG	DA	3254	1/1	0.98	0.27	35,35,35,35	0
56	MG	B7	103	1/1	0.98	0.10	47,47,47,47	0
56	MG	AA	1889	1/1	0.98	0.22	20,20,20,20	0
56	MG	CA	1933	1/1	0.98	0.08	36,36,36,36	0
56	MG	BA	3206	1/1	0.98	0.09	37,37,37,37	0
56	MG	BA	3383	1/1	0.98	0.08	29,29,29,29	0
56	MG	DA	3260	1/1	0.98	0.07	15,15,15,15	0
56	MG	BA	3614	1/1	0.98	0.22	32,32,32,32	0
56	MG	BA	3207	1/1	0.98	0.17	31,31,31,31	0
56	MG	DA	3264	1/1	0.98	0.08	29,29,29,29	0
56	MG	AA	1735	1/1	0.98	0.04	24,24,24,24	0
56	MG	BA	3620	1/1	0.98	0.28	49,49,49,49	0
56	MG	CA	1940	1/1	0.98	0.08	35,35,35,35	0
56	MG	AA	1651	1/1	0.98	0.07	53,53,53,53	0
56	MG	AA	1641	1/1	0.98	0.06	8,8,8,8	0
56	MG	BA	3211	1/1	0.98	0.10	27,27,27,27	0
56	MG	BA	3213	1/1	0.98	0.15	33,33,33,33	0
56	MG	BA	3625	1/1	0.98	0.07	25,25,25,25	0
56	MG	DA	3273	1/1	0.98	0.19	0,0,0,0	0
56	MG	CA	1613	1/1	0.98	0.09	17,17,17,17	0
56	MG	DA	3276	1/1	0.98	0.17	29,29,29,29	0
56	MG	AF	201	1/1	0.98	0.09	30,30,30,30	0
56	MG	BA	3215	1/1	0.98	0.08	28,28,28,28	0
56	MG	AA	1704	1/1	0.98	0.04	18,18,18,18	0
56	MG	CA	1617	1/1	0.98	0.04	11,11,11,11	0
56	MG	BA	3217	1/1	0.98	0.12	0,0,0,0	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	BA	3218	1/1	0.98	0.09	20,20,20,20	0
56	MG	CA	1953	1/1	0.98	0.12	18,18,18,18	0
56	MG	BA	3398	1/1	0.98	0.28	16,16,16,16	0
56	MG	DA	3290	1/1	0.98	0.13	25,25,25,25	0
56	MG	DA	3292	1/1	0.98	0.09	8,8,8,8	0
56	MG	DA	3293	1/1	0.98	0.10	10,10,10,10	0
56	MG	BA	3399	1/1	0.98	0.19	17,17,17,17	0
56	MG	CA	1956	1/1	0.98	0.16	57,57,57,57	0
56	MG	CA	1957	1/1	0.98	0.23	28,28,28,28	0
56	MG	DA	3297	1/1	0.98	0.09	34,34,34,34	0
56	MG	DA	3298	1/1	0.98	0.04	0,0,0,0	0
56	MG	AA	1607	1/1	0.98	0.10	8,8,8,8	0
56	MG	DA	3301	1/1	0.98	0.07	31,31,31,31	0
56	MG	CA	1959	1/1	0.98	0.09	3,3,3,3	0
56	MG	DA	3306	1/1	0.98	0.07	15,15,15,15	0
56	MG	CA	1961	1/1	0.98	0.15	27,27,27,27	0
56	MG	CA	1623	1/1	0.98	0.08	22,22,22,22	0
56	MG	DA	3309	1/1	0.98	0.11	30,30,30,30	0
56	MG	DA	3310	1/1	0.98	0.12	34,34,34,34	0
56	MG	AH	201	1/1	0.98	0.05	24,24,24,24	0
56	MG	AA	1707	1/1	0.98	0.08	26,26,26,26	0
56	MG	BA	3222	1/1	0.98	0.08	13,13,13,13	0
56	MG	DA	3316	1/1	0.98	0.25	31,31,31,31	0
56	MG	DA	3318	1/1	0.98	0.11	21,21,21,21	0
56	MG	DA	3319	1/1	0.98	0.14	18,18,18,18	0
56	MG	CA	1628	1/1	0.98	0.12	23,23,23,23	0
56	MG	BA	3089	1/1	0.98	0.07	17,17,17,17	0
56	MG	CA	1968	1/1	0.98	0.22	25,25,25,25	0
56	MG	BA	3225	1/1	0.98	0.09	21,21,21,21	0
56	MG	AI	202	1/1	0.98	0.11	17,17,17,17	0
56	MG	CA	1632	1/1	0.98	0.05	24,24,24,24	0
56	MG	DA	3329	1/1	0.98	0.07	42,42,42,42	0
56	MG	CA	1633	1/1	0.98	0.08	12,12,12,12	0
56	MG	BA	3408	1/1	0.98	0.11	12,12,12,12	0
56	MG	DA	3333	1/1	0.98	0.07	4,4,4,4	0
56	MG	AA	1835	1/1	0.98	0.15	17,17,17,17	0
56	MG	DA	3335	1/1	0.98	0.08	7,7,7,7	0
56	MG	CA	1976	1/1	0.98	0.09	32,32,32,32	0
56	MG	DA	3339	1/1	0.98	0.08	47,47,47,47	0
56	MG	CA	1977	1/1	0.98	0.52	31,31,31,31	0
56	MG	DA	3341	1/1	0.98	0.10	31,31,31,31	0
56	MG	BA	3643	1/1	0.98	0.09	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	AA	1897	1/1	0.98	0.11	13,13,13,13	0
56	MG	DA	3347	1/1	0.98	0.28	10,10,10,10	0
56	MG	CA	1980	1/1	0.98	0.10	40,40,40,40	0
56	MG	BA	3645	1/1	0.98	0.06	25,25,25,25	0
56	MG	BA	3411	1/1	0.98	0.15	20,20,20,20	0
56	MG	DA	3353	1/1	0.98	0.11	0,0,0,0	0
56	MG	BA	3647	1/1	0.98	0.30	20,20,20,20	0
56	MG	BA	3648	1/1	0.98	0.15	4,4,4,4	0
56	MG	AA	1898	1/1	0.98	0.14	27,27,27,27	0
56	MG	CA	1986	1/1	0.98	0.18	23,23,23,23	0
56	MG	BA	3650	1/1	0.98	0.42	33,33,33,33	0
56	MG	BA	3232	1/1	0.98	0.08	25,25,25,25	0
56	MG	AA	1783	1/1	0.98	0.18	50,50,50,50	0
56	MG	BA	3416	1/1	0.98	0.09	15,15,15,15	0
56	MG	DA	3363	1/1	0.98	0.11	36,36,36,36	0
56	MG	DA	3364	1/1	0.98	0.13	43,43,43,43	0
56	MG	AA	1743	1/1	0.98	0.07	33,33,33,33	0
56	MG	CA	1992	1/1	0.98	0.24	47,47,47,47	0
56	MG	CA	1652	1/1	0.98	0.07	40,40,40,40	0
56	MG	BA	3418	1/1	0.98	0.07	34,34,34,34	0
56	MG	BA	3097	1/1	0.98	0.09	16,16,16,16	0
56	MG	CA	1655	1/1	0.98	0.14	24,24,24,24	0
56	MG	AA	1744	1/1	0.98	0.05	30,30,30,30	0
56	MG	CA	1998	1/1	0.98	0.09	48,48,48,48	0
56	MG	BA	3237	1/1	0.98	0.16	28,28,28,28	0
56	MG	CA	1658	1/1	0.98	0.12	37,37,37,37	0
56	MG	BA	3239	1/1	0.98	0.26	22,22,22,22	0
56	MG	DA	3376	1/1	0.98	0.08	35,35,35,35	0
56	MG	CA	2002	1/1	0.98	0.08	39,39,39,39	0
56	MG	CA	2003	1/1	0.98	0.15	18,18,18,18	0
56	MG	BA	3660	1/1	0.98	0.12	38,38,38,38	0
56	MG	CA	1663	1/1	0.98	0.05	8,8,8,8	0
56	MG	DA	3382	1/1	0.98	0.07	39,39,39,39	0
56	MG	BA	3240	1/1	0.98	0.10	10,10,10,10	0
56	MG	BA	3662	1/1	0.98	0.47	40,40,40,40	0
56	MG	BA	3663	1/1	0.98	0.46	32,32,32,32	0
56	MG	AA	1685	1/1	0.98	0.15	30,30,30,30	0
56	MG	BA	3242	1/1	0.98	0.10	22,22,22,22	0
56	MG	AA	1746	1/1	0.98	0.10	14,14,14,14	0
56	MG	DA	3391	1/1	0.98	0.09	17,17,17,17	0
56	MG	DA	3393	1/1	0.98	0.28	37,37,37,37	0
56	MG	AA	1608	1/1	0.98	0.08	16,16,16,16	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	BA	3245	1/1	0.98	0.10	29,29,29,29	0
56	MG	DA	3396	1/1	0.98	0.05	21,21,21,21	0
56	MG	DA	3397	1/1	0.98	0.07	19,19,19,19	0
56	MG	BA	3430	1/1	0.98	0.17	32,32,32,32	0
56	MG	BA	3246	1/1	0.98	0.06	41,41,41,41	0
56	MG	BA	3103	1/1	0.98	0.18	35,35,35,35	0
56	MG	CZ	104	1/1	0.98	0.07	42,42,42,42	0
56	MG	CA	1676	1/1	0.98	0.13	25,25,25,25	0
56	MG	CZ	107	1/1	0.98	0.07	36,36,36,36	0
56	MG	AA	1791	1/1	0.98	0.09	30,30,30,30	0
56	MG	BA	3249	1/1	0.98	0.09	41,41,41,41	0
56	MG	DA	3407	1/1	0.98	0.06	32,32,32,32	0
56	MG	DA	3408	1/1	0.98	0.14	31,31,31,31	0
56	MG	DA	3409	1/1	0.98	0.09	24,24,24,24	0
56	MG	CZ	110	1/1	0.98	0.09	33,33,33,33	0
56	MG	CA	1679	1/1	0.98	0.11	40,40,40,40	0
56	MG	CA	1680	1/1	0.98	0.10	37,37,37,37	0
56	MG	BA	3675	1/1	0.98	0.07	40,40,40,40	0
56	MG	BA	3676	1/1	0.98	0.09	20,20,20,20	0
56	MG	AA	1906	1/1	0.98	0.18	26,26,26,26	0
56	MG	CA	1685	1/1	0.98	0.05	6,6,6,6	0
56	MG	CZ	118	1/1	0.98	0.43	69,69,69,69	0
56	MG	DA	3421	1/1	0.98	0.16	26,26,26,26	0
56	MG	BA	3441	1/1	0.98	0.14	28,28,28,28	0
56	MG	BA	3679	1/1	0.98	0.14	26,26,26,26	0
56	MG	AA	1655	1/1	0.98	0.06	26,26,26,26	0
56	MG	BA	3444	1/1	0.98	0.05	33,33,33,33	0
56	MG	BA	3682	1/1	0.98	0.23	25,25,25,25	0
56	MG	CY	103	1/1	0.98	0.07	49,49,49,49	0
56	MG	CA	1691	1/1	0.98	0.09	15,15,15,15	0
56	MG	DA	3431	1/1	0.98	0.21	29,29,29,29	0
56	MG	BA	3683	1/1	0.98	0.16	18,18,18,18	0
56	MG	DA	3433	1/1	0.98	0.09	21,21,21,21	0
56	MG	BA	3684	1/1	0.98	0.20	46,46,46,46	0
56	MG	BA	3107	1/1	0.98	0.08	21,21,21,21	0
56	MG	CY	108	1/1	0.98	0.11	22,22,22,22	0
56	MG	BA	3446	1/1	0.98	0.11	39,39,39,39	0
56	MG	BA	3254	1/1	0.98	0.11	31,31,31,31	0
56	MG	DA	3442	1/1	0.98	0.10	32,32,32,32	0
56	MG	AA	1609	1/1	0.98	0.07	28,28,28,28	0
56	MG	BA	3256	1/1	0.98	0.05	13,13,13,13	0
56	MG	BA	3690	1/1	0.98	0.14	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	BA	3257	1/1	0.98	0.05	18,18,18,18	0
56	MG	DA	3447	1/1	0.98	0.17	36,36,36,36	0
56	MG	CY	115	1/1	0.98	0.06	38,38,38,38	0
56	MG	AA	1645	1/1	0.98	0.23	31,31,31,31	0
56	MG	DA	3450	1/1	0.98	0.48	29,29,29,29	0
56	MG	CA	1704	1/1	0.98	0.42	31,31,31,31	0
56	MG	AX	406	1/1	0.98	0.28	36,36,36,36	0
56	MG	BA	3260	1/1	0.98	0.07	35,35,35,35	0
56	MG	BA	3456	1/1	0.98	0.12	35,35,35,35	0
56	MG	CY	121	1/1	0.98	0.09	0,0,0,0	0
56	MG	CB	301	1/1	0.98	0.19	11,11,11,11	0
56	MG	CA	1708	1/1	0.98	0.11	17,17,17,17	0
56	MG	BA	3457	1/1	0.98	0.06	24,24,24,24	0
56	MG	DA	3461	1/1	0.98	0.14	8,8,8,8	0
56	MG	BA	3112	1/1	0.98	0.08	26,26,26,26	0
56	MG	DA	3463	1/1	0.98	0.09	37,37,37,37	0
56	MG	CC	303	1/1	0.98	0.19	22,22,22,22	0
56	MG	AA	1796	1/1	0.98	0.11	15,15,15,15	0
56	MG	BA	3699	1/1	0.98	0.55	35,35,35,35	0
56	MG	AA	1798	1/1	0.98	0.06	32,32,32,32	0
56	MG	BA	3003	1/1	0.98	0.11	44,44,44,44	0
56	MG	DA	3469	1/1	0.98	0.18	19,19,19,19	0
56	MG	CD	302	1/1	0.98	0.07	41,41,41,41	0
56	MG	DA	3471	1/1	0.98	0.08	18,18,18,18	0
56	MG	AA	1752	1/1	0.98	0.06	13,13,13,13	0
56	MG	BA	3117	1/1	0.98	0.11	33,33,33,33	0
56	MG	BA	3005	1/1	0.98	0.07	2,2,2,2	0
56	MG	BA	3466	1/1	0.98	0.09	22,22,22,22	0
56	MG	CA	1721	1/1	0.98	0.10	45,45,45,45	0
56	MG	AA	1716	1/1	0.98	0.08	35,35,35,35	0
56	MG	BA	3707	1/1	0.98	0.31	31,31,31,31	0
56	MG	CJ	201	1/1	0.98	0.46	33,33,33,33	0
56	MG	BA	3468	1/1	0.98	0.06	1,1,1,1	0
56	MG	BA	3121	1/1	0.98	0.08	40,40,40,40	0
56	MG	BA	3007	1/1	0.98	0.06	34,34,34,34	0
56	MG	BA	3123	1/1	0.98	0.11	34,34,34,34	0
56	MG	BA	3473	1/1	0.98	0.12	35,35,35,35	0
56	MG	CA	1729	1/1	0.98	0.23	15,15,15,15	0
56	MG	BA	3124	1/1	0.98	0.16	33,33,33,33	0
56	MG	DA	3490	1/1	0.98	0.07	5,5,5,5	0
56	MG	DA	3491	1/1	0.98	0.07	44,44,44,44	0
56	MG	BA	3278	1/1	0.98	0.07	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	AA	1627	1/1	0.98	0.06	29,29,29,29	0
56	MG	CA	1734	1/1	0.98	0.12	42,42,42,42	0
56	MG	BA	3126	1/1	0.98	0.07	37,37,37,37	0
56	MG	BA	3479	1/1	0.98	0.08	45,45,45,45	0
56	MG	AA	1718	1/1	0.98	0.09	27,27,27,27	0
56	MG	DD	301	1/1	0.98	0.05	0,0,0,0	0
56	MG	DA	3500	1/1	0.98	0.07	13,13,13,13	0
56	MG	AA	1804	1/1	0.98	0.22	18,18,18,18	0
56	MG	DA	3502	1/1	0.98	0.08	13,13,13,13	0
56	MG	CA	1740	1/1	0.98	0.07	8,8,8,8	0
56	MG	AA	1660	1/1	0.98	0.07	19,19,19,19	0
56	MG	DA	3506	1/1	0.98	0.11	6,6,6,6	0
56	MG	BA	3286	1/1	0.98	0.09	1,1,1,1	0
56	MG	DH	204	1/1	0.98	0.20	11,11,11,11	0
56	MG	DA	3512	1/1	0.98	0.15	15,15,15,15	0
56	MG	BA	3486	1/1	0.98	0.06	41,41,41,41	0
56	MG	DI	202	1/1	0.98	0.08	18,18,18,18	0
56	MG	BA	3487	1/1	0.98	0.07	16,16,16,16	0
56	MG	AY	106	1/1	0.98	0.05	32,32,32,32	0
56	MG	BA	3015	1/1	0.98	0.08	16,16,16,16	0
56	MG	BA	3727	1/1	0.98	0.33	36,36,36,36	0
56	MG	DA	3521	1/1	0.98	0.14	7,7,7,7	0
56	MG	BA	3016	1/1	0.98	0.14	0,0,0,0	0
56	MG	DP	206	1/1	0.98	0.15	33,33,33,33	0
56	MG	BA	3290	1/1	0.98	0.07	12,12,12,12	0
56	MG	BA	3291	1/1	0.98	0.17	19,19,19,19	0
56	MG	BA	3292	1/1	0.98	0.08	10,10,10,10	0
56	MG	DA	3528	1/1	0.98	0.23	14,14,14,14	0
56	MG	DA	3529	1/1	0.98	0.17	7,7,7,7	0
56	MG	BA	3732	1/1	0.98	0.25	41,41,41,41	0
56	MG	DA	3531	1/1	0.98	0.14	39,39,39,39	0
56	MG	BA	3495	1/1	0.98	0.11	10,10,10,10	0
56	MG	DA	3533	1/1	0.98	0.13	12,12,12,12	0
56	MG	DA	3534	1/1	0.98	0.16	26,26,26,26	0
56	MG	BA	3017	1/1	0.98	0.12	18,18,18,18	0
56	MG	DA	3536	1/1	0.98	0.18	35,35,35,35	0
56	MG	DA	3537	1/1	0.98	0.21	19,19,19,19	0
56	MG	DA	3538	1/1	0.98	0.12	34,34,34,34	0
56	MG	CA	1756	1/1	0.98	0.18	32,32,32,32	0
56	MG	AY	107	1/1	0.98	0.09	18,18,18,18	0
56	MG	DZ	301	1/1	0.98	0.08	27,27,27,27	0
56	MG	DA	3544	1/1	0.98	0.08	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DZ	303	1/1	0.98	0.22	32,32,32,32	0
56	MG	BA	3022	1/1	0.98	0.17	2,2,2,2	0
56	MG	D2	101	1/1	0.98	0.12	58,58,58,58	0
56	MG	CA	1759	1/1	0.98	0.07	25,25,25,25	0
56	MG	BA	3737	1/1	0.98	0.26	22,22,22,22	0
56	MG	BA	3738	1/1	0.98	0.36	44,44,44,44	0
56	MG	DA	3552	1/1	0.98	0.09	16,16,16,16	0
56	MG	BA	3739	1/1	0.98	0.07	37,37,37,37	0
56	MG	DA	3555	1/1	0.98	0.10	24,24,24,24	0
56	MG	BA	3138	1/1	0.98	0.07	34,34,34,34	0
56	MG	D7	101	1/1	0.98	0.07	22,22,22,22	0
56	MG	DA	3558	1/1	0.98	0.08	30,30,30,30	0
56	MG	BA	3139	1/1	0.98	0.05	33,33,33,33	0
56	MG	DA	3560	1/1	0.98	0.15	8,8,8,8	0
56	MG	BA	3504	1/1	0.98	0.07	12,12,12,12	0
56	MG	DA	3563	1/1	0.98	0.09	8,8,8,8	0
56	MG	CA	1766	1/1	0.98	0.04	26,26,26,26	0
56	MG	DA	3566	1/1	0.98	0.07	15,15,15,15	0
56	MG	CA	1767	1/1	0.98	0.08	22,22,22,22	0
56	MG	BA	3301	1/1	0.98	0.10	15,15,15,15	0
56	MG	BA	3508	1/1	0.98	0.14	5,5,5,5	0
56	MG	BA	3302	1/1	0.98	0.12	21,21,21,21	0
56	MG	BA	3510	1/1	0.98	0.15	39,39,39,39	0
56	MG	DA	3009	1/1	0.98	0.10	8,8,8,8	0
56	MG	DA	3010	1/1	0.98	0.17	2,2,2,2	0
56	MG	BA	3303	1/1	0.98	0.05	22,22,22,22	0
56	MG	AA	1621	1/1	0.98	0.12	15,15,15,15	0
56	MG	DA	3576	1/1	0.98	0.25	18,18,18,18	0
56	MG	BA	3513	1/1	0.98	0.07	24,24,24,24	0
56	MG	BA	3514	1/1	0.98	0.17	29,29,29,29	0
56	MG	DA	3580	1/1	0.98	0.38	21,21,21,21	0
56	MG	AA	1604	1/1	0.98	0.15	26,26,26,26	0
56	MG	CA	1778	1/1	0.98	0.13	34,34,34,34	0
56	MG	BA	3027	1/1	0.98	0.07	20,20,20,20	0
56	MG	AA	1694	1/1	0.98	0.25	45,45,45,45	0
56	MG	AA	1724	1/1	0.98	0.07	26,26,26,26	0
56	MG	BA	3312	1/1	0.98	0.11	7,7,7,7	0
56	MG	DA	3587	1/1	0.98	0.11	42,42,42,42	0
56	MG	BA	3758	1/1	0.98	0.19	24,24,24,24	0
56	MG	BA	3759	1/1	0.98	0.09	41,41,41,41	0
56	MG	CA	1787	1/1	0.98	0.04	19,19,19,19	0
56	MG	BA	3760	1/1	0.98	0.20	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	BA	3761	1/1	0.98	0.18	15,15,15,15	0
56	MG	DA	3028	1/1	0.98	0.07	34,34,34,34	0
56	MG	DA	3595	1/1	0.98	0.09	17,17,17,17	0
56	MG	DA	3596	1/1	0.98	0.06	41,41,41,41	0
56	MG	BA	3313	1/1	0.98	0.06	25,25,25,25	0
56	MG	DA	3598	1/1	0.98	0.08	9,9,9,9	0
56	MG	CA	1793	1/1	0.98	0.08	9,9,9,9	0
56	MG	DA	3031	1/1	0.98	0.10	21,21,21,21	0
56	MG	BA	3314	1/1	0.98	0.09	10,10,10,10	0
56	MG	AY	112	1/1	0.98	0.11	39,39,39,39	0
56	MG	BA	3524	1/1	0.98	0.07	36,36,36,36	0
56	MG	DA	3037	1/1	0.98	0.07	57,57,57,57	0
56	MG	BA	3526	1/1	0.98	0.12	4,4,4,4	0
56	MG	CA	1799	1/1	0.98	0.08	14,14,14,14	0
56	MG	DA	3608	1/1	0.98	0.05	36,36,36,36	0
56	MG	BA	3767	1/1	0.98	0.15	20,20,20,20	0
56	MG	DA	3042	1/1	0.98	0.08	7,7,7,7	0
56	MG	BA	3147	1/1	0.98	0.14	53,53,53,53	0
56	MG	DA	3613	1/1	0.98	0.18	26,26,26,26	0
56	MG	DA	3047	1/1	0.98	0.06	10,10,10,10	0
56	MG	BA	3031	1/1	0.98	0.13	11,11,11,11	0
56	MG	DA	3049	1/1	0.98	0.08	11,11,11,11	0
56	MG	BA	3318	1/1	0.98	0.07	39,39,39,39	0
56	MG	DA	3618	1/1	0.98	0.13	47,47,47,47	0
56	MG	DA	3052	1/1	0.98	0.14	38,38,38,38	0
56	MG	DA	3053	1/1	0.98	0.12	46,46,46,46	0
56	MG	CA	1805	1/1	0.98	0.11	9,9,9,9	0
56	MG	AA	1865	1/1	0.98	0.25	32,32,32,32	0
56	MG	CA	1808	1/1	0.98	0.10	13,13,13,13	0
56	MG	DA	3625	1/1	0.98	0.08	28,28,28,28	0
56	MG	DA	3626	1/1	0.98	0.15	46,46,46,46	0
56	MG	BA	3531	1/1	0.98	0.06	16,16,16,16	0
56	MG	BA	3320	1/1	0.98	0.14	2,2,2,2	0
56	MG	DA	3629	1/1	0.98	0.27	22,22,22,22	0
56	MG	CA	1811	1/1	0.98	0.10	43,43,43,43	0
56	MG	DA	3061	1/1	0.98	0.07	4,4,4,4	0
56	MG	BA	3321	1/1	0.98	0.13	51,51,51,51	0
56	MG	DA	3063	1/1	0.98	0.07	0,0,0,0	0
56	MG	DA	3064	1/1	0.98	0.12	11,11,11,11	0
56	MG	DA	3065	1/1	0.98	0.09	0,0,0,0	0
56	MG	BA	3776	1/1	0.98	0.09	6,6,6,6	0
56	MG	BA	3534	1/1	0.98	0.15	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DA	3638	1/1	0.98	0.19	37,37,37,37	0
56	MG	DA	3068	1/1	0.98	0.08	0,0,0,0	0
56	MG	AY	115	1/1	0.98	0.09	18,18,18,18	0
56	MG	AA	1623	1/1	0.98	0.07	7,7,7,7	0
56	MG	AA	1679	1/1	0.98	0.07	32,32,32,32	0
56	MG	DA	3645	1/1	0.98	0.10	20,20,20,20	0
56	MG	DA	3073	1/1	0.98	0.05	34,34,34,34	0
56	MG	BA	3538	1/1	0.98	0.05	10,10,10,10	0
56	MG	AY	118	1/1	0.98	0.08	45,45,45,45	0
56	MG	DA	3649	1/1	0.98	0.08	19,19,19,19	0
56	MG	DA	3650	1/1	0.98	0.16	63,63,63,63	0
56	MG	CA	1822	1/1	0.98	0.14	26,26,26,26	0
56	MG	BA	3783	1/1	0.98	0.28	29,29,29,29	0
56	MG	BA	3037	1/1	0.98	0.11	8,8,8,8	0
56	MG	BA	3159	1/1	0.98	0.07	18,18,18,18	0
56	MG	AA	1697	1/1	0.98	0.09	1,1,1,1	0
56	MG	BA	3331	1/1	0.98	0.06	10,10,10,10	0
56	MG	DA	3084	1/1	0.98	0.18	26,26,26,26	0
56	MG	CA	1828	1/1	0.98	0.10	2,2,2,2	0
56	MG	DA	3086	1/1	0.98	0.12	42,42,42,42	0
56	MG	AA	1815	1/1	0.98	0.20	24,24,24,24	0
56	MG	DA	3090	1/1	0.98	0.05	12,12,12,12	0
56	MG	DA	3091	1/1	0.98	0.06	8,8,8,8	0
56	MG	BA	3162	1/1	0.98	0.17	41,41,41,41	0
56	MG	BA	3791	1/1	0.98	0.07	54,54,54,54	0
56	MG	DA	3666	1/1	0.98	0.06	23,23,23,23	0
56	MG	AA	1816	1/1	0.98	0.13	23,23,23,23	0
56	MG	DA	3096	1/1	0.98	0.09	22,22,22,22	0
56	MG	DA	3099	1/1	0.98	0.15	23,23,23,23	0
56	MG	DA	3671	1/1	0.98	0.11	6,6,6,6	0
56	MG	DA	3100	1/1	0.98	0.07	3,3,3,3	0
56	MG	BA	3793	1/1	0.98	0.07	31,31,31,31	0
56	MG	DA	3102	1/1	0.98	0.07	5,5,5,5	0
56	MG	BA	3166	1/1	0.98	0.10	28,28,28,28	0
56	MG	BA	3553	1/1	0.98	0.08	24,24,24,24	0
56	MG	DA	3105	1/1	0.98	0.08	12,12,12,12	0
56	MG	BA	3797	1/1	0.98	0.21	18,18,18,18	0
56	MG	DA	3108	1/1	0.98	0.11	1,1,1,1	0
56	MG	BA	3041	1/1	0.98	0.09	25,25,25,25	0
56	MG	DA	3682	1/1	0.98	0.15	10,10,10,10	0
56	MG	CA	1838	1/1	0.98	0.14	28,28,28,28	0
56	MG	DA	3112	1/1	0.98	0.09	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	BA	3339	1/1	0.98	0.08	34,34,34,34	0
56	MG	BA	3168	1/1	0.98	0.06	4,4,4,4	0
56	MG	DA	3115	1/1	0.98	0.17	5,5,5,5	0
56	MG	BA	3042	1/1	0.98	0.07	12,12,12,12	0
56	MG	DA	3689	1/1	0.98	0.21	45,45,45,45	0
56	MG	BA	3559	1/1	0.98	0.09	15,15,15,15	0
56	MG	BA	3804	1/1	0.98	0.11	29,29,29,29	0
56	MG	AA	1817	1/1	0.98	0.12	39,39,39,39	0
56	MG	DA	3121	1/1	0.98	0.14	24,24,24,24	0
56	MG	CA	1845	1/1	0.98	0.07	21,21,21,21	0
56	MG	DA	3123	1/1	0.98	0.06	1,1,1,1	0
56	MG	BA	3171	1/1	0.98	0.16	30,30,30,30	0
56	MG	DA	3125	1/1	0.98	0.21	15,15,15,15	0
56	MG	BB	201	1/1	0.98	0.09	35,35,35,35	0
56	MG	CA	1848	1/1	0.98	0.06	41,41,41,41	0
56	MG	DA	3701	1/1	0.98	0.06	27,27,27,27	0
56	MG	DA	3128	1/1	0.98	0.18	46,46,46,46	0
56	MG	BB	202	1/1	0.98	0.07	34,34,34,34	0
56	MG	DA	3130	1/1	0.98	0.05	20,20,20,20	0
56	MG	DA	3133	1/1	0.98	0.12	21,21,21,21	0
56	MG	CA	1850	1/1	0.98	0.10	20,20,20,20	0
56	MG	DA	3135	1/1	0.98	0.22	25,25,25,25	0
56	MG	BB	204	1/1	0.98	0.08	46,46,46,46	0
56	MG	BB	205	1/1	0.98	0.28	36,36,36,36	0
56	MG	AA	1874	1/1	0.98	0.26	10,10,10,10	0
56	MG	DA	3139	1/1	0.98	0.12	47,47,47,47	0
56	MG	DA	3140	1/1	0.98	0.19	18,18,18,18	0
56	MG	BA	3174	1/1	0.98	0.10	28,28,28,28	0
56	MG	AA	1818	1/1	0.98	0.18	33,33,33,33	0
56	MG	DA	3715	1/1	0.98	0.21	50,50,50,50	0
56	MG	DA	3143	1/1	0.98	0.09	31,31,31,31	0
56	MG	AA	1698	1/1	0.98	0.10	27,27,27,27	0
56	MG	BA	3177	1/1	0.98	0.10	0,0,0,0	0
56	MG	DA	3147	1/1	0.98	0.10	18,18,18,18	0
56	MG	CA	1859	1/1	0.98	0.05	22,22,22,22	0
56	MG	DA	3150	1/1	0.98	0.08	1,1,1,1	0
56	MG	AB	302	1/1	0.98	0.10	33,33,33,33	0
56	MG	DA	3152	1/1	0.98	0.11	28,28,28,28	0
56	MG	DA	3153	1/1	0.98	0.07	10,10,10,10	0
56	MG	DA	3154	1/1	0.98	0.26	38,38,38,38	0
56	MG	BB	213	1/1	0.98	0.08	35,35,35,35	0
56	MG	BA	3573	1/1	0.98	0.08	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DA	3158	1/1	0.98	0.15	15,15,15,15	0
56	MG	BA	3050	1/1	0.98	0.07	4,4,4,4	0
56	MG	AC	301	1/1	0.98	0.15	41,41,41,41	0
56	MG	AA	1821	1/1	0.98	0.09	27,27,27,27	0
56	MG	CA	1867	1/1	0.98	0.09	33,33,33,33	0
56	MG	BA	3183	1/1	0.98	0.10	15,15,15,15	0
56	MG	CA	1869	1/1	0.98	0.09	32,32,32,32	0
56	MG	AA	1729	1/1	0.98	0.07	12,12,12,12	0
56	MG	DA	3740	1/1	0.98	0.27	27,27,27,27	0
56	MG	DA	3168	1/1	0.98	0.07	49,49,49,49	0
56	MG	BA	3056	1/1	0.98	0.09	1,1,1,1	0
56	MG	BB	222	1/1	0.98	0.20	39,39,39,39	0
56	MG	BA	3580	1/1	0.98	0.18	19,19,19,19	0
56	MG	DA	3746	1/1	0.98	0.32	43,43,43,43	0
56	MG	DA	3747	1/1	0.98	0.12	23,23,23,23	0
56	MG	AA	1665	1/1	0.98	0.07	6,6,6,6	0
56	MG	DA	3749	1/1	0.98	0.27	34,34,34,34	0
56	MG	CA	1875	1/1	0.98	0.16	19,19,19,19	0
56	MG	DA	3751	1/1	0.98	0.25	48,48,48,48	0
56	MG	BA	3357	1/1	0.98	0.06	4,4,4,4	0
56	MG	BA	3583	1/1	0.98	0.08	24,24,24,24	0
56	MG	BA	3059	1/1	0.98	0.08	11,11,11,11	0
56	MG	BA	3585	1/1	0.98	0.09	20,20,20,20	0
56	MG	BA	3062	1/1	0.98	0.09	24,24,24,24	0
56	MG	BA	3063	1/1	0.98	0.05	0,0,0,0	0
56	MG	DA	3181	1/1	0.98	0.13	26,26,26,26	0
56	MG	BF	305	1/1	0.98	0.11	27,27,27,27	0
56	MG	BA	3588	1/1	0.98	0.05	22,22,22,22	0
56	MG	BG	202	1/1	0.98	0.07	26,26,26,26	0
56	MG	DA	3186	1/1	0.98	0.06	47,47,47,47	0
56	MG	BA	3363	1/1	0.98	0.14	24,24,24,24	0
56	MG	DB	207	1/1	0.98	0.11	37,37,37,37	0
56	MG	DA	3188	1/1	0.98	0.11	9,9,9,9	0
56	MG	BH	201	1/1	0.98	0.12	15,15,15,15	0
56	MG	BA	3064	1/1	0.98	0.14	21,21,21,21	0
56	MG	BI	201	1/1	0.98	0.24	29,29,29,29	0
56	MG	BI	203	1/1	0.98	0.30	40,40,40,40	0
56	MG	DA	3193	1/1	0.98	0.19	17,17,17,17	0
56	MG	DB	215	1/1	0.98	0.08	47,47,47,47	0
56	MG	BA	3065	1/1	0.98	0.10	18,18,18,18	0
56	MG	CA	1894	1/1	0.98	0.06	19,19,19,19	0
56	MG	DA	3196	1/1	0.98	0.10	12,12,12,12	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	CA	1896	1/1	0.98	0.07	31,31,31,31	0
56	MG	DB	220	1/1	0.98	0.09	23,23,23,23	0
56	MG	BA	3066	1/1	0.98	0.13	37,37,37,37	0
56	MG	DA	3199	1/1	0.98	0.14	12,12,12,12	0
56	MG	CA	1898	1/1	0.98	0.22	14,14,14,14	0
56	MG	BO	201	1/1	0.98	0.06	17,17,17,17	0
56	MG	AA	1882	1/1	0.98	0.36	30,30,30,30	0
56	MG	DA	3204	1/1	0.98	0.07	28,28,28,28	0
56	MG	BP	201	1/1	0.98	0.18	34,34,34,34	0
56	MG	AA	1883	1/1	0.98	0.23	21,21,21,21	0
57	ZN	AN	101	1/1	0.98	0.04	68,68,68,68	0
57	ZN	CD	301	1/1	0.98	0.24	70,70,70,70	0
57	ZN	CN	101	1/1	0.98	0.04	82,82,82,82	0
56	MG	DA	3436	1/1	0.99	0.16	7,7,7,7	0
56	MG	BN	201	1/1	0.99	0.04	20,20,20,20	0
56	MG	DA	3438	1/1	0.99	0.15	24,24,24,24	0
56	MG	DA	3439	1/1	0.99	0.27	17,17,17,17	0
56	MG	BA	3503	1/1	0.99	0.08	29,29,29,29	0
56	MG	BA	3670	1/1	0.99	0.08	29,29,29,29	0
56	MG	AA	1855	1/1	0.99	0.11	23,23,23,23	0
56	MG	CA	1776	1/1	0.99	0.15	17,17,17,17	0
56	MG	BO	203	1/1	0.99	0.04	19,19,19,19	0
56	MG	BA	3505	1/1	0.99	0.05	1,1,1,1	0
56	MG	BA	3360	1/1	0.99	0.07	17,17,17,17	0
56	MG	BA	3507	1/1	0.99	0.11	29,29,29,29	0
56	MG	BQ	203	1/1	0.99	0.12	43,43,43,43	0
56	MG	DA	3131	1/1	0.99	0.10	16,16,16,16	0
56	MG	DA	3132	1/1	0.99	0.14	11,11,11,11	0
56	MG	BA	3361	1/1	0.99	0.07	33,33,33,33	0
56	MG	BA	3057	1/1	0.99	0.06	3,3,3,3	0
56	MG	DA	3453	1/1	0.99	0.06	23,23,23,23	0
56	MG	DA	3454	1/1	0.99	0.08	12,12,12,12	0
56	MG	CA	1784	1/1	0.99	0.18	45,45,45,45	0
56	MG	CA	1785	1/1	0.99	0.08	9,9,9,9	0
56	MG	AA	1664	1/1	0.99	0.10	6,6,6,6	0
56	MG	AA	1908	1/1	0.99	0.10	13,13,13,13	0
56	MG	BA	3060	1/1	0.99	0.08	7,7,7,7	0
56	MG	BA	3366	1/1	0.99	0.06	10,10,10,10	0
56	MG	BA	3367	1/1	0.99	0.11	24,24,24,24	0
56	MG	CA	2013	1/1	0.99	0.04	7,7,7,7	0
56	MG	CA	1791	1/1	0.99	0.06	43,43,43,43	0
56	MG	CA	1792	1/1	0.99	0.09	16,16,16,16	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	BA	3146	1/1	0.99	0.04	22,22,22,22	0
56	MG	DA	3146	1/1	0.99	0.09	20,20,20,20	0
56	MG	BA	3061	1/1	0.99	0.09	26,26,26,26	0
56	MG	DA	3148	1/1	0.99	0.22	50,50,50,50	0
56	MG	BA	3148	1/1	0.99	0.05	17,17,17,17	0
56	MG	CZ	105	1/1	0.99	0.03	16,16,16,16	0
56	MG	AA	1909	1/1	0.99	0.05	40,40,40,40	0
56	MG	AA	1611	1/1	0.99	0.07	6,6,6,6	0
56	MG	CA	1798	1/1	0.99	0.24	51,51,51,51	0
56	MG	AZ	101	1/1	0.99	0.21	42,42,42,42	0
56	MG	BA	3252	1/1	0.99	0.21	7,7,7,7	0
56	MG	DA	3156	1/1	0.99	0.10	14,14,14,14	0
56	MG	CZ	111	1/1	0.99	0.10	49,49,49,49	0
56	MG	DA	3478	1/1	0.99	0.10	18,18,18,18	0
56	MG	BA	3152	1/1	0.99	0.05	7,7,7,7	0
56	MG	BA	3523	1/1	0.99	0.08	0,0,0,0	0
56	MG	CA	1803	1/1	0.99	0.17	6,6,6,6	0
56	MG	AO	101	1/1	0.99	0.09	30,30,30,30	0
56	MG	DA	3483	1/1	0.99	0.17	19,19,19,19	0
56	MG	DA	3163	1/1	0.99	0.04	21,21,21,21	0
56	MG	BA	3525	1/1	0.99	0.06	8,8,8,8	0
56	MG	BA	3377	1/1	0.99	0.06	4,4,4,4	0
56	MG	CA	1807	1/1	0.99	0.27	14,14,14,14	0
56	MG	DA	3488	1/1	0.99	0.20	10,10,10,10	0
56	MG	AA	1858	1/1	0.99	0.05	15,15,15,15	0
56	MG	BA	3155	1/1	0.99	0.13	15,15,15,15	0
56	MG	BA	3067	1/1	0.99	0.06	27,27,27,27	0
56	MG	CV	103	1/1	0.99	0.12	29,29,29,29	0
56	MG	AA	1605	1/1	0.99	0.07	15,15,15,15	0
56	MG	DA	3494	1/1	0.99	0.08	5,5,5,5	0
56	MG	BA	3158	1/1	0.99	0.25	44,44,44,44	0
56	MG	CY	102	1/1	0.99	0.07	11,11,11,11	0
56	MG	CA	1813	1/1	0.99	0.10	41,41,41,41	0
56	MG	AA	1860	1/1	0.99	0.05	11,11,11,11	0
56	MG	BA	3384	1/1	0.99	0.07	1,1,1,1	0
56	MG	DA	3177	1/1	0.99	0.33	3,3,3,3	0
56	MG	CA	1816	1/1	0.99	0.28	48,48,48,48	0
56	MG	BA	3385	1/1	0.99	0.06	18,18,18,18	0
56	MG	DA	3503	1/1	0.99	0.07	24,24,24,24	0
56	MG	BA	3261	1/1	0.99	0.34	36,36,36,36	0
56	MG	AA	1751	1/1	0.99	0.12	20,20,20,20	0
56	MG	DA	3182	1/1	0.99	0.08	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DA	3507	1/1	0.99	0.10	0,0,0,0	0
56	MG	DA	3508	1/1	0.99	0.07	16,16,16,16	0
56	MG	DA	3509	1/1	0.99	0.10	33,33,33,33	0
56	MG	BA	3071	1/1	0.99	0.03	34,34,34,34	0
56	MG	AA	1613	1/1	0.99	0.18	20,20,20,20	0
56	MG	BA	3163	1/1	0.99	0.10	25,25,25,25	0
56	MG	BA	3540	1/1	0.99	0.08	23,23,23,23	0
56	MG	BA	3266	1/1	0.99	0.09	10,10,10,10	0
56	MG	DA	3515	1/1	0.99	0.06	5,5,5,5	0
56	MG	BA	3542	1/1	0.99	0.15	13,13,13,13	0
56	MG	BA	3543	1/1	0.99	0.11	19,19,19,19	0
56	MG	BA	3392	1/1	0.99	0.15	27,27,27,27	0
56	MG	DA	3519	1/1	0.99	0.13	6,6,6,6	0
56	MG	BA	3545	1/1	0.99	0.12	25,25,25,25	0
56	MG	AA	1732	1/1	0.99	0.06	35,35,35,35	0
56	MG	BA	3165	1/1	0.99	0.05	8,8,8,8	0
56	MG	AY	101	1/1	0.99	0.11	26,26,26,26	0
56	MG	AY	102	1/1	0.99	0.09	32,32,32,32	0
56	MG	BA	3550	1/1	0.99	0.04	13,13,13,13	0
56	MG	DA	3526	1/1	0.99	0.14	12,12,12,12	0
56	MG	BA	3271	1/1	0.99	0.11	0,0,0,0	0
56	MG	AA	1782	1/1	0.99	0.07	21,21,21,21	0
56	MG	BA	3077	1/1	0.99	0.13	8,8,8,8	0
56	MG	CA	1627	1/1	0.99	0.10	29,29,29,29	0
56	MG	BA	3274	1/1	0.99	0.09	6,6,6,6	0
56	MG	DA	3202	1/1	0.99	0.08	32,32,32,32	0
56	MG	BA	3401	1/1	0.99	0.10	44,44,44,44	0
56	MG	BA	3556	1/1	0.99	0.16	7,7,7,7	0
56	MG	BA	3724	1/1	0.99	0.12	32,32,32,32	0
56	MG	AA	1819	1/1	0.99	0.07	1,1,1,1	0
56	MG	BA	3276	1/1	0.99	0.05	0,0,0,0	0
56	MG	AA	1866	1/1	0.99	0.05	13,13,13,13	0
56	MG	DA	3539	1/1	0.99	0.06	3,3,3,3	0
56	MG	DA	3540	1/1	0.99	0.16	0,0,0,0	0
56	MG	AA	1639	1/1	0.99	0.05	25,25,25,25	0
56	MG	BA	3173	1/1	0.99	0.07	12,12,12,12	0
56	MG	CA	1637	1/1	0.99	0.09	21,21,21,21	0
56	MG	AA	1734	1/1	0.99	0.06	21,21,21,21	0
56	MG	CA	1639	1/1	0.99	0.07	28,28,28,28	0
56	MG	AA	1869	1/1	0.99	0.16	33,33,33,33	0
56	MG	BA	3282	1/1	0.99	0.07	6,6,6,6	0
56	MG	DA	3216	1/1	0.99	0.05	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	BA	3565	1/1	0.99	0.08	24,24,24,24	0
56	MG	CO	101	1/1	0.99	0.05	25,25,25,25	0
56	MG	DA	3551	1/1	0.99	0.17	17,17,17,17	0
56	MG	BA	3083	1/1	0.99	0.06	9,9,9,9	0
56	MG	DA	3553	1/1	0.99	0.07	6,6,6,6	0
56	MG	DA	3220	1/1	0.99	0.08	22,22,22,22	0
56	MG	CA	1644	1/1	0.99	0.07	6,6,6,6	0
56	MG	DA	3222	1/1	0.99	0.15	2,2,2,2	0
56	MG	CX	401	1/1	0.99	0.07	13,13,13,13	0
56	MG	CA	1855	1/1	0.99	0.10	37,37,37,37	0
56	MG	DA	3225	1/1	0.99	0.10	27,27,27,27	0
56	MG	BA	3284	1/1	0.99	0.07	12,12,12,12	0
56	MG	DA	3561	1/1	0.99	0.21	19,19,19,19	0
56	MG	BA	3568	1/1	0.99	0.07	13,13,13,13	0
56	MG	BA	3569	1/1	0.99	0.06	0,0,0,0	0
56	MG	DA	3564	1/1	0.99	0.06	7,7,7,7	0
56	MG	DA	3229	1/1	0.99	0.06	1,1,1,1	0
56	MG	DA	3230	1/1	0.99	0.07	19,19,19,19	0
56	MG	CA	1648	1/1	0.99	0.10	28,28,28,28	0
56	MG	DA	3232	1/1	0.99	0.09	6,6,6,6	0
56	MG	BA	3570	1/1	0.99	0.14	21,21,21,21	0
56	MG	BA	3571	1/1	0.99	0.04	40,40,40,40	0
56	MG	BA	3740	1/1	0.99	0.14	22,22,22,22	0
56	MG	BA	3084	1/1	0.99	0.05	1,1,1,1	0
56	MG	AA	1785	1/1	0.99	0.14	27,27,27,27	0
56	MG	CA	1865	1/1	0.99	0.07	12,12,12,12	0
56	MG	DA	3239	1/1	0.99	0.09	12,12,12,12	0
56	MG	DA	3240	1/1	0.99	0.07	21,21,21,21	0
56	MG	DA	3241	1/1	0.99	0.20	12,12,12,12	0
56	MG	DA	3578	1/1	0.99	0.08	11,11,11,11	0
56	MG	BA	3414	1/1	0.99	0.09	24,24,24,24	0
56	MG	AA	1614	1/1	0.99	0.08	4,4,4,4	0
56	MG	DH	203	1/1	0.99	0.14	19,19,19,19	0
56	MG	AA	1659	1/1	0.99	0.10	33,33,33,33	0
56	MG	AA	1825	1/1	0.99	0.10	28,28,28,28	0
56	MG	BA	3182	1/1	0.99	0.11	22,22,22,22	0
56	MG	DA	3248	1/1	0.99	0.15	19,19,19,19	0
56	MG	DA	3249	1/1	0.99	0.31	32,32,32,32	0
56	MG	DN	201	1/1	0.99	0.06	29,29,29,29	0
56	MG	AA	1788	1/1	0.99	0.14	12,12,12,12	0
56	MG	DA	3589	1/1	0.99	0.11	19,19,19,19	0
56	MG	DO	202	1/1	0.99	0.07	14,14,14,14	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	CA	1660	1/1	0.99	0.06	10,10,10,10	0
56	MG	AY	114	1/1	0.99	0.08	20,20,20,20	0
56	MG	CA	1662	1/1	0.99	0.04	12,12,12,12	0
56	MG	BA	3185	1/1	0.99	0.07	5,5,5,5	0
56	MG	CA	1876	1/1	0.99	0.14	22,22,22,22	0
56	MG	AA	1875	1/1	0.99	0.05	16,16,16,16	0
56	MG	AA	1615	1/1	0.99	0.06	8,8,8,8	0
56	MG	BA	3753	1/1	0.99	0.37	28,28,28,28	0
56	MG	DA	3261	1/1	0.99	0.06	33,33,33,33	0
56	MG	DA	3600	1/1	0.99	0.07	17,17,17,17	0
56	MG	BA	3296	1/1	0.99	0.06	20,20,20,20	0
56	MG	BA	3013	1/1	0.99	0.06	0,0,0,0	0
56	MG	BA	3298	1/1	0.99	0.11	5,5,5,5	0
56	MG	BA	3014	1/1	0.99	0.08	11,11,11,11	0
56	MG	BA	3300	1/1	0.99	0.05	20,20,20,20	0
56	MG	BA	3429	1/1	0.99	0.06	5,5,5,5	0
56	MG	DZ	302	1/1	0.99	0.06	24,24,24,24	0
56	MG	AA	1759	1/1	0.99	0.08	6,6,6,6	0
56	MG	BA	3431	1/1	0.99	0.11	11,11,11,11	0
56	MG	CA	1675	1/1	0.99	0.05	26,26,26,26	0
56	MG	DA	3611	1/1	0.99	0.06	21,21,21,21	0
56	MG	BA	3096	1/1	0.99	0.14	16,16,16,16	0
56	MG	BA	3433	1/1	0.99	0.15	40,40,40,40	0
56	MG	AA	1760	1/1	0.99	0.13	24,24,24,24	0
56	MG	DA	3275	1/1	0.99	0.31	2,2,2,2	0
56	MG	CA	1892	1/1	0.99	0.15	5,5,5,5	0
56	MG	DA	3277	1/1	0.99	0.18	0,0,0,0	0
56	MG	DA	3278	1/1	0.99	0.11	11,11,11,11	0
56	MG	DA	3619	1/1	0.99	0.12	23,23,23,23	0
56	MG	CA	1893	1/1	0.99	0.27	23,23,23,23	0
56	MG	DA	3280	1/1	0.99	0.04	3,3,3,3	0
56	MG	D5	101	1/1	0.99	0.06	2,2,2,2	0
56	MG	BA	3435	1/1	0.99	0.32	43,43,43,43	0
56	MG	CA	1895	1/1	0.99	0.23	30,30,30,30	0
56	MG	BA	3596	1/1	0.99	0.14	8,8,8,8	0
56	MG	DA	3285	1/1	0.99	0.05	15,15,15,15	0
56	MG	DA	3286	1/1	0.99	0.09	6,6,6,6	0
56	MG	BA	3193	1/1	0.99	0.08	2,2,2,2	0
56	MG	BA	3194	1/1	0.99	0.07	21,21,21,21	0
56	MG	CA	1683	1/1	0.99	0.14	16,16,16,16	0
56	MG	AA	1830	1/1	0.99	0.18	35,35,35,35	0
56	MG	DA	3291	1/1	0.99	0.19	6,6,6,6	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DA	3005	1/1	0.99	0.17	1,1,1,1	0
56	MG	BA	3439	1/1	0.99	0.04	7,7,7,7	0
56	MG	BA	3440	1/1	0.99	0.16	15,15,15,15	0
56	MG	DA	3008	1/1	0.99	0.15	9,9,9,9	0
56	MG	CA	1903	1/1	0.99	0.14	31,31,31,31	0
56	MG	BA	3099	1/1	0.99	0.06	1,1,1,1	0
56	MG	DA	3011	1/1	0.99	0.20	17,17,17,17	0
56	MG	BA	3773	1/1	0.99	0.16	44,44,44,44	0
56	MG	DA	3641	1/1	0.99	0.18	13,13,13,13	0
56	MG	DA	3300	1/1	0.99	0.04	16,16,16,16	0
56	MG	DA	3643	1/1	0.99	0.07	28,28,28,28	0
56	MG	BA	3442	1/1	0.99	0.36	26,26,26,26	0
56	MG	DA	3014	1/1	0.99	0.05	9,9,9,9	0
56	MG	DA	3303	1/1	0.99	0.08	12,12,12,12	0
56	MG	DA	3304	1/1	0.99	0.04	10,10,10,10	0
56	MG	DA	3305	1/1	0.99	0.06	29,29,29,29	0
56	MG	BA	3309	1/1	0.99	0.13	25,25,25,25	0
56	MG	BA	3310	1/1	0.99	0.09	23,23,23,23	0
56	MG	BA	3018	1/1	0.99	0.07	2,2,2,2	0
56	MG	CA	1910	1/1	0.99	0.08	15,15,15,15	0
56	MG	CA	1693	1/1	0.99	0.22	10,10,10,10	0
56	MG	DA	3311	1/1	0.99	0.07	15,15,15,15	0
56	MG	BA	3019	1/1	0.99	0.14	5,5,5,5	0
56	MG	BA	3447	1/1	0.99	0.04	16,16,16,16	0
56	MG	BA	3609	1/1	0.99	0.15	10,10,10,10	0
56	MG	DA	3315	1/1	0.99	0.14	39,39,39,39	0
56	MG	AA	1880	1/1	0.99	0.22	8,8,8,8	0
56	MG	DA	3317	1/1	0.99	0.08	1,1,1,1	0
56	MG	BA	3611	1/1	0.99	0.06	11,11,11,11	0
56	MG	DA	3662	1/1	0.99	0.09	24,24,24,24	0
56	MG	BA	3021	1/1	0.99	0.05	11,11,11,11	0
56	MG	CA	1700	1/1	0.99	0.06	14,14,14,14	0
56	MG	AY	121	1/1	0.99	0.15	30,30,30,30	0
56	MG	BA	3024	1/1	0.99	0.26	37,37,37,37	0
56	MG	DA	3323	1/1	0.99	0.05	8,8,8,8	0
56	MG	BA	3615	1/1	0.99	0.10	3,3,3,3	0
56	MG	BA	3787	1/1	0.99	0.08	11,11,11,11	0
56	MG	DA	3670	1/1	0.99	0.18	59,59,59,59	0
56	MG	CA	1923	1/1	0.99	0.11	28,28,28,28	0
56	MG	DA	3327	1/1	0.99	0.12	13,13,13,13	0
56	MG	DA	3328	1/1	0.99	0.06	10,10,10,10	0
56	MG	DA	3674	1/1	0.99	0.10	4,4,4,4	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DA	3032	1/1	0.99	0.14	0,0,0,0	0
56	MG	AA	1738	1/1	0.99	0.05	6,6,6,6	0
56	MG	DA	3331	1/1	0.99	0.11	0,0,0,0	0
56	MG	BA	3617	1/1	0.99	0.06	32,32,32,32	0
56	MG	DA	3035	1/1	0.99	0.09	6,6,6,6	0
56	MG	BA	3618	1/1	0.99	0.10	10,10,10,10	0
56	MG	AA	1739	1/1	0.99	0.05	3,3,3,3	0
56	MG	CA	1928	1/1	0.99	0.06	17,17,17,17	0
56	MG	DA	3337	1/1	0.99	0.07	23,23,23,23	0
56	MG	DA	3338	1/1	0.99	0.05	25,25,25,25	0
56	MG	CA	1709	1/1	0.99	0.27	39,39,39,39	0
56	MG	DA	3040	1/1	0.99	0.13	10,10,10,10	0
56	MG	BA	3454	1/1	0.99	0.17	26,26,26,26	0
56	MG	DA	3342	1/1	0.99	0.09	12,12,12,12	0
56	MG	AA	1794	1/1	0.99	0.16	13,13,13,13	0
56	MG	BA	3794	1/1	0.99	0.23	12,12,12,12	0
56	MG	DA	3345	1/1	0.99	0.10	24,24,24,24	0
56	MG	DA	3346	1/1	0.99	0.08	3,3,3,3	0
56	MG	DA	3044	1/1	0.99	0.16	5,5,5,5	0
56	MG	DA	3348	1/1	0.99	0.15	40,40,40,40	0
56	MG	DA	3045	1/1	0.99	0.03	7,7,7,7	0
56	MG	DA	3046	1/1	0.99	0.06	10,10,10,10	0
56	MG	AA	1763	1/1	0.99	0.12	30,30,30,30	0
56	MG	DA	3352	1/1	0.99	0.14	15,15,15,15	0
56	MG	CA	1714	1/1	0.99	0.15	13,13,13,13	0
56	MG	DA	3700	1/1	0.99	0.13	10,10,10,10	0
56	MG	AA	1616	1/1	0.99	0.15	7,7,7,7	0
56	MG	BA	3111	1/1	0.99	0.06	10,10,10,10	0
56	MG	DA	3051	1/1	0.99	0.04	11,11,11,11	0
56	MG	BA	3798	1/1	0.99	0.06	38,38,38,38	0
56	MG	AA	1886	1/1	0.99	0.12	39,39,39,39	0
56	MG	BA	3460	1/1	0.99	0.09	10,10,10,10	0
56	MG	AA	1797	1/1	0.99	0.05	30,30,30,30	0
56	MG	DA	3361	1/1	0.99	0.30	19,19,19,19	0
56	MG	BA	3325	1/1	0.99	0.05	5,5,5,5	0
56	MG	AA	1721	1/1	0.99	0.05	0,0,0,0	0
56	MG	DA	3058	1/1	0.99	0.06	15,15,15,15	0
56	MG	BA	3212	1/1	0.99	0.03	17,17,17,17	0
56	MG	BA	3328	1/1	0.99	0.07	2,2,2,2	0
56	MG	AA	1766	1/1	0.99	0.09	18,18,18,18	0
56	MG	AA	1839	1/1	0.99	0.12	39,39,39,39	0
56	MG	BA	3634	1/1	0.99	0.17	18,18,18,18	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	BB	203	1/1	0.99	0.07	22,22,22,22	0
56	MG	AA	1706	1/1	0.99	0.07	26,26,26,26	0
56	MG	BA	3332	1/1	0.99	0.12	9,9,9,9	0
56	MG	AA	1841	1/1	0.99	0.05	24,24,24,24	0
56	MG	BA	3471	1/1	0.99	0.08	17,17,17,17	0
56	MG	CA	1733	1/1	0.99	0.22	52,52,52,52	0
56	MG	AD	302	1/1	0.99	0.04	13,13,13,13	0
56	MG	DA	3071	1/1	0.99	0.19	31,31,31,31	0
56	MG	DA	3378	1/1	0.99	0.06	17,17,17,17	0
56	MG	DA	3726	1/1	0.99	0.33	34,34,34,34	0
56	MG	CA	1735	1/1	0.99	0.19	20,20,20,20	0
56	MG	BB	209	1/1	0.99	0.06	26,26,26,26	0
56	MG	BA	3335	1/1	0.99	0.06	4,4,4,4	0
56	MG	DA	3075	1/1	0.99	0.17	8,8,8,8	0
56	MG	DA	3383	1/1	0.99	0.06	10,10,10,10	0
56	MG	AA	1801	1/1	0.99	0.04	21,21,21,21	0
56	MG	DA	3733	1/1	0.99	0.08	19,19,19,19	0
56	MG	AA	1843	1/1	0.99	0.07	28,28,28,28	0
56	MG	CA	1960	1/1	0.99	0.12	26,26,26,26	0
56	MG	AA	1617	1/1	0.99	0.06	0,0,0,0	0
56	MG	DA	3737	1/1	0.99	0.23	56,56,56,56	0
56	MG	DA	3388	1/1	0.99	0.06	3,3,3,3	0
56	MG	DA	3739	1/1	0.99	0.12	20,20,20,20	0
56	MG	DA	3080	1/1	0.99	0.16	23,23,23,23	0
56	MG	AA	1769	1/1	0.99	0.04	47,47,47,47	0
56	MG	DA	3742	1/1	0.99	0.35	2,2,2,2	0
56	MG	BA	3478	1/1	0.99	0.08	10,10,10,10	0
56	MG	DA	3392	1/1	0.99	0.06	4,4,4,4	0
56	MG	BB	216	1/1	0.99	0.07	51,51,51,51	0
56	MG	AA	1610	1/1	0.99	0.22	23,23,23,23	0
56	MG	BA	3223	1/1	0.99	0.20	9,9,9,9	0
56	MG	AA	1709	1/1	0.99	0.15	15,15,15,15	0
56	MG	DA	3087	1/1	0.99	0.18	27,27,27,27	0
56	MG	DA	3398	1/1	0.99	0.13	26,26,26,26	0
56	MG	BA	3044	1/1	0.99	0.15	18,18,18,18	0
56	MG	DA	3089	1/1	0.99	0.19	30,30,30,30	0
56	MG	BA	3226	1/1	0.99	0.12	24,24,24,24	0
56	MG	BA	3485	1/1	0.99	0.13	12,12,12,12	0
56	MG	AA	1772	1/1	0.99	0.06	17,17,17,17	0
56	MG	BB	224	1/1	0.99	0.24	25,25,25,25	0
56	MG	DA	3094	1/1	0.99	0.14	13,13,13,13	0
56	MG	BA	3228	1/1	0.99	0.05	0,0,0,0	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DB	201	1/1	0.99	0.08	14,14,14,14	0
56	MG	BA	3046	1/1	0.99	0.07	20,20,20,20	0
56	MG	DA	3097	1/1	0.99	0.08	5,5,5,5	0
56	MG	DA	3098	1/1	0.99	0.07	1,1,1,1	0
56	MG	DA	3410	1/1	0.99	0.14	17,17,17,17	0
56	MG	CA	1975	1/1	0.99	0.21	32,32,32,32	0
56	MG	AA	1773	1/1	0.99	0.04	26,26,26,26	0
56	MG	CA	1755	1/1	0.99	0.09	31,31,31,31	0
56	MG	BD	302	1/1	0.99	0.14	2,2,2,2	0
56	MG	AA	1808	1/1	0.99	0.07	23,23,23,23	0
56	MG	DB	211	1/1	0.99	0.04	15,15,15,15	0
56	MG	DA	3416	1/1	0.99	0.08	26,26,26,26	0
56	MG	BA	3132	1/1	0.99	0.15	21,21,21,21	0
56	MG	AA	1710	1/1	0.99	0.05	1,1,1,1	0
56	MG	DA	3419	1/1	0.99	0.08	33,33,33,33	0
56	MG	BF	303	1/1	0.99	0.24	37,37,37,37	0
56	MG	BA	3493	1/1	0.99	0.05	17,17,17,17	0
56	MG	AA	1810	1/1	0.99	0.09	24,24,24,24	0
56	MG	BA	3051	1/1	0.99	0.22	16,16,16,16	0
56	MG	DA	3424	1/1	0.99	0.08	22,22,22,22	0
56	MG	DA	3111	1/1	0.99	0.09	6,6,6,6	0
56	MG	BA	3052	1/1	0.99	0.06	0,0,0,0	0
56	MG	DA	3427	1/1	0.99	0.10	7,7,7,7	0
56	MG	BA	3497	1/1	0.99	0.07	2,2,2,2	0
56	MG	AA	1853	1/1	0.99	0.06	12,12,12,12	0
56	MG	BA	3238	1/1	0.99	0.17	14,14,14,14	0
56	MG	AH	202	1/1	0.99	0.17	41,41,41,41	0
56	MG	BI	202	1/1	0.99	0.06	29,29,29,29	0
57	ZN	AD	301	1/1	0.99	0.21	46,46,46,46	0
56	MG	BA	3501	1/1	0.99	0.07	60,60,60,60	0
56	MG	AA	1711	1/1	0.99	0.05	17,17,17,17	0
56	MG	DA	3120	1/1	0.99	0.27	23,23,23,23	0
56	MG	DA	3161	1/1	1.00	0.25	1,1,1,1	0
56	MG	BA	3118	1/1	1.00	0.17	20,20,20,20	0
56	MG	BA	3482	1/1	1.00	0.05	11,11,11,11	0
56	MG	DA	3107	1/1	1.00	0.06	16,16,16,16	0
56	MG	AA	1632	1/1	1.00	0.08	5,5,5,5	0
56	MG	BA	3135	1/1	1.00	0.05	13,13,13,13	0
56	MG	DP	204	1/1	1.00	0.07	3,3,3,3	0
56	MG	BA	3023	1/1	1.00	0.10	2,2,2,2	0
56	MG	BA	3305	1/1	1.00	0.09	5,5,5,5	0

6.5 Other polymers (i)

There are no such residues in this entry.