wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 18, 2023 – 02:13 PM EST

PDB ID	:	1VY6
Title	:	Crystal structure of the Thermus thermophilus 70S ribosome in the pre-attack state of peptide bond formation containing short substrate-mimic Cytidine-Puromycin in the A site and acylated tRNA in the P site.
Authors	:	Polikanov, Y.S.; Steitz, T.A.; Innis, C.A.
Deposited on	:	2014-05-13
Resolution	:	2.90 Å(reported)

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

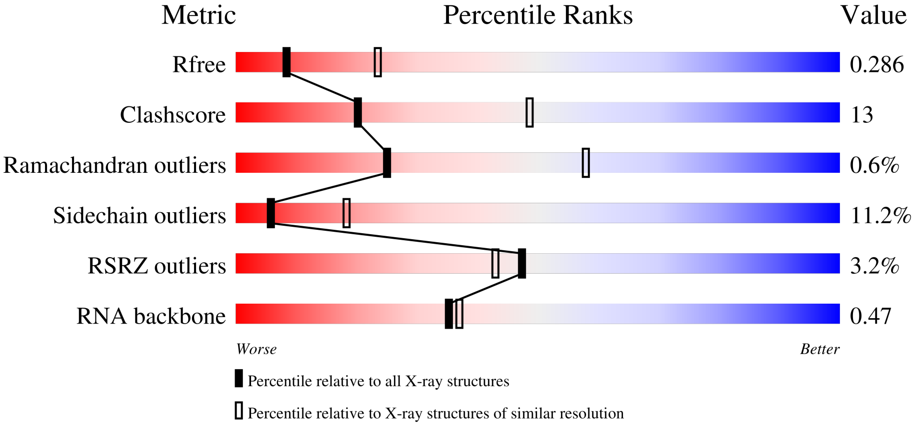
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

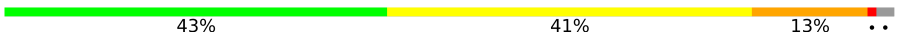
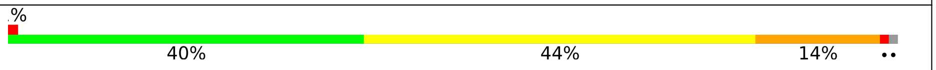
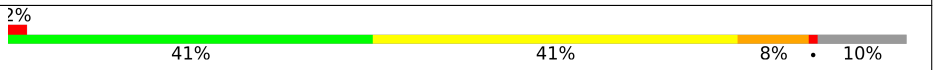
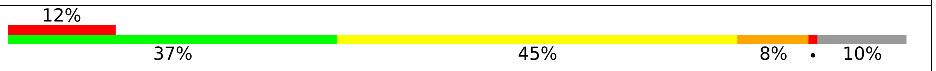
The reported resolution of this entry is 2.90 Å.

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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)
RNA backbone	3102	1007 (3.16-2.64)

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	1521	
1	CA	1521	
2	AB	256	
2	CB	256	

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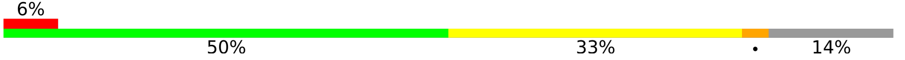
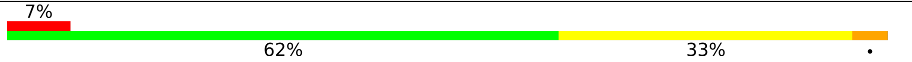
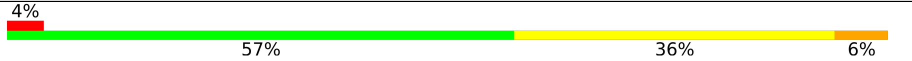
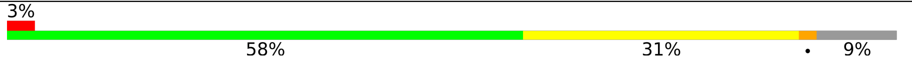
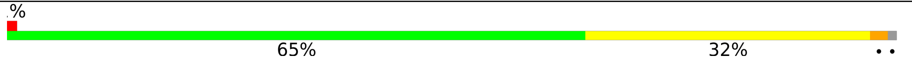
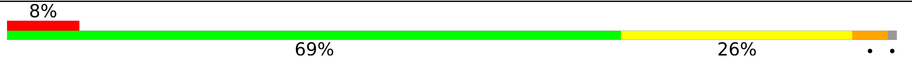
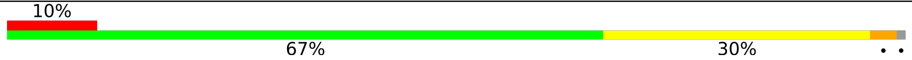
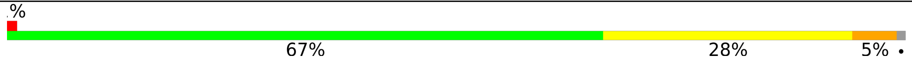
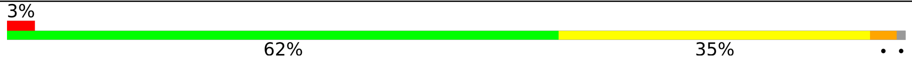
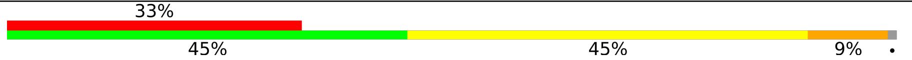
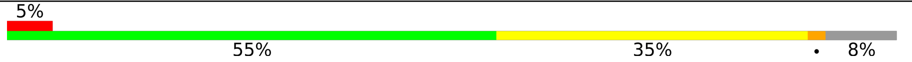
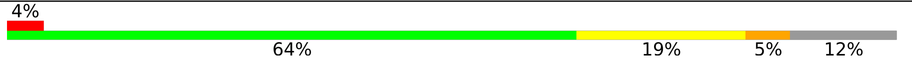
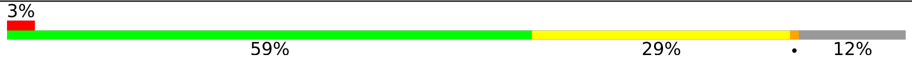
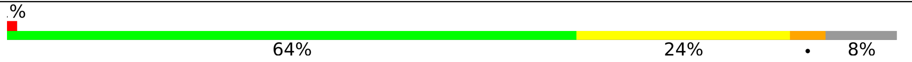
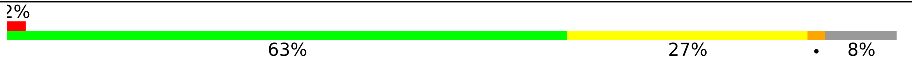
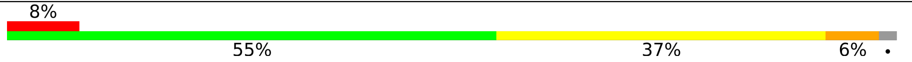
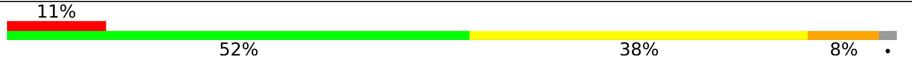
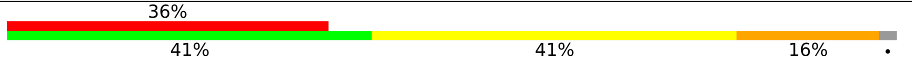
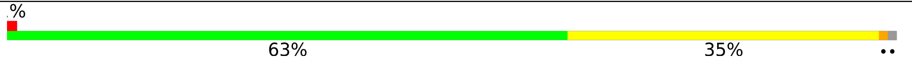
Mol	Chain	Length	Quality of chain
3	AC	239	
3	CC	239	
4	AD	209	
4	CD	209	
5	AE	162	
5	CE	162	
6	AF	101	
6	CF	101	
7	AG	156	
7	CG	156	
8	AH	138	
8	CH	138	
9	AI	128	
9	CI	128	
10	AJ	105	
10	CJ	105	
11	AK	129	
11	CK	129	
12	AL	132	
12	CL	132	
13	AM	126	
13	CM	126	
14	AN	61	
14	CN	61	
15	AO	89	

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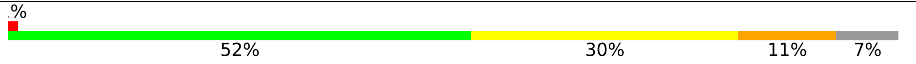
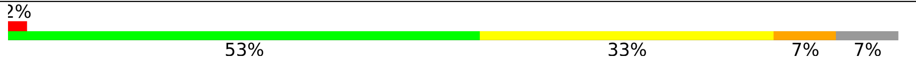
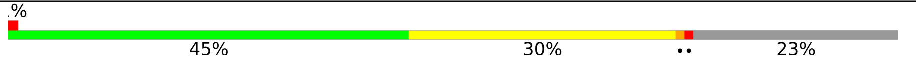
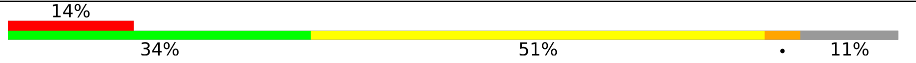
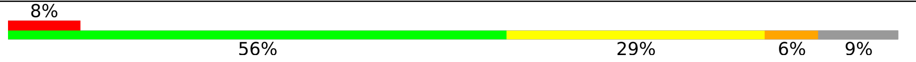
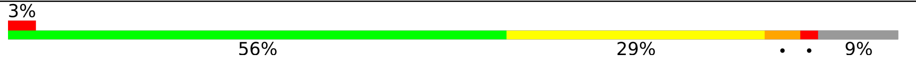
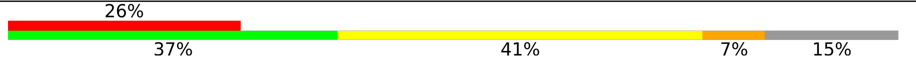
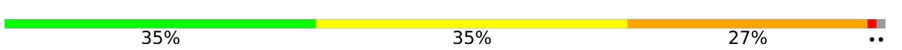
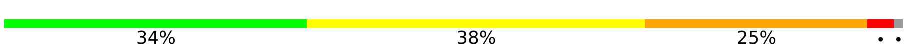
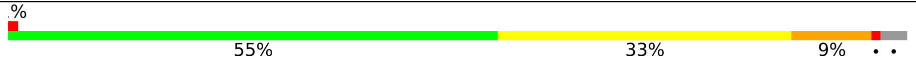
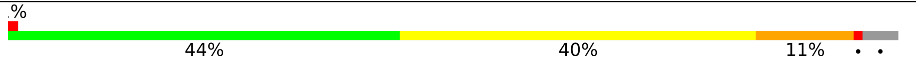
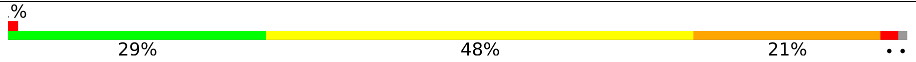
Mol	Chain	Length	Quality of chain
15	CO	89	
16	AP	88	
16	CP	88	
17	AQ	105	
17	CQ	105	
18	AR	88	
18	CR	88	
19	AS	93	
19	CS	93	
20	AT	106	
20	CT	106	
21	AU	27	
21	CU	27	
22	AV	24	
22	CV	24	
23	AW	2	
23	CW	2	
24	AX	77	
24	CX	77	
25	BA	2915	
25	DA	2915	
26	BB	121	
26	DB	121	
27	BD	276	
27	DD	276	

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Mol	Chain	Length	Quality of chain
28	BE	206	% 66% 29% • •
28	DE	206	2% 65% 27% 6% ••
29	BF	210	71% 22% • •
29	DF	210	% 55% 37% 5% •
30	BG	182	3% 66% 25% 8% •
30	DG	182	19% 50% 39% 10% •
31	BH	180	2% 69% 26% • •
31	DH	180	14% 61% 31% 5% •
32	BI	148	64% 26% 9% •
32	DI	148	7% 63% 28% 7% ••
33	BN	140	% 71% 25% •
33	DN	140	5% 65% 29% 6%
34	BO	122	66% 32% •
34	DO	122	% 62% 35% •
35	BP	150	3% 69% 26% • ••
35	DP	150	3% 61% 33% • ••
36	BQ	141	2% 65% 32% •
36	DQ	141	% 60% 35% •
37	BR	118	2% 63% 30% 8%
37	DR	118	3% 69% 25% 6%
38	BS	112	69% 24% 5% •
38	DS	112	2% 48% 44% 6% •
39	BT	146	58% 28% • 10%
39	DT	146	3% 56% 27% 6% 10%
40	BU	118	3% 78% 18% • •

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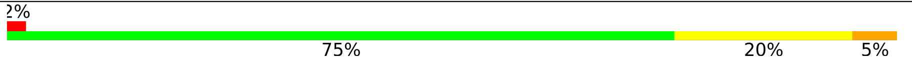
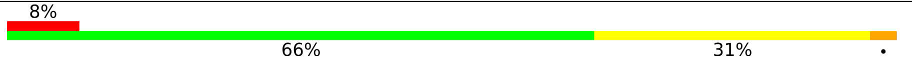
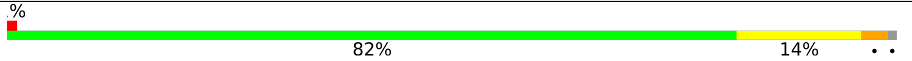
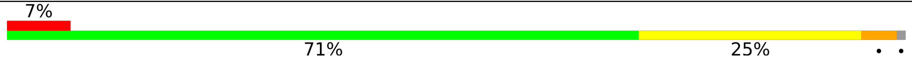
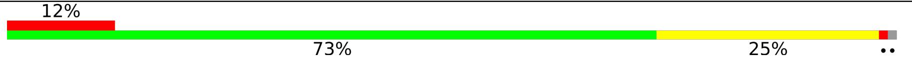
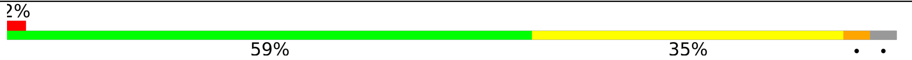
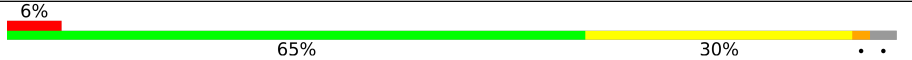
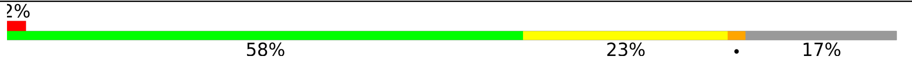
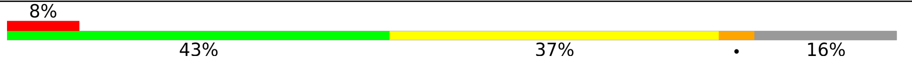
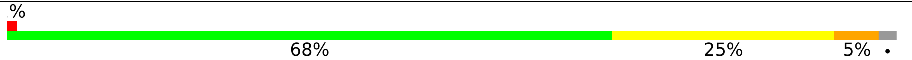
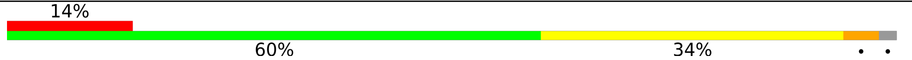
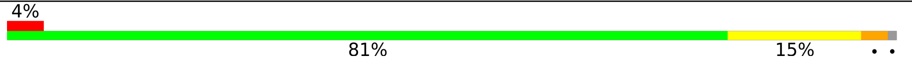
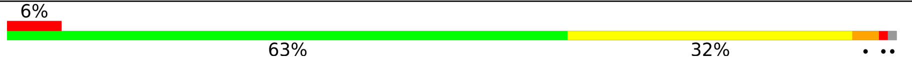
Mol	Chain	Length	Quality of chain
40	DU	118	
41	BV	101	
41	DV	101	
42	BW	113	
42	DW	113	
43	BX	96	
43	DX	96	
44	BY	110	
44	DY	110	
45	BZ	206	
45	DZ	206	
46	B0	85	
46	D0	85	
47	B1	98	
47	D1	98	
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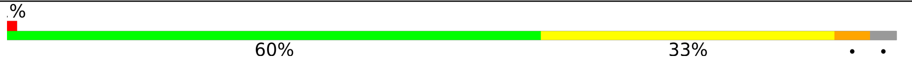
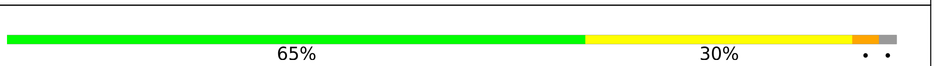
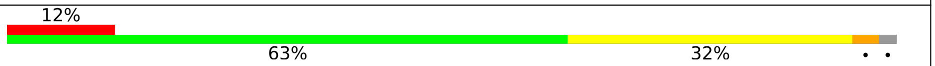
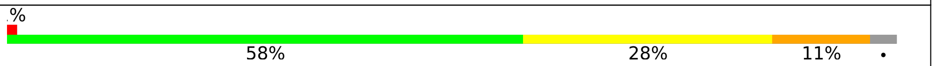
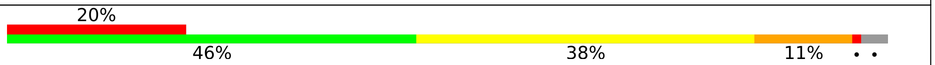
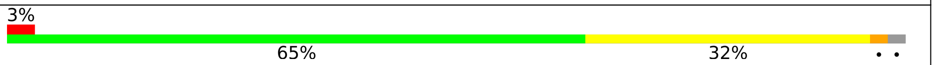
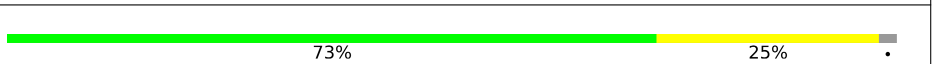
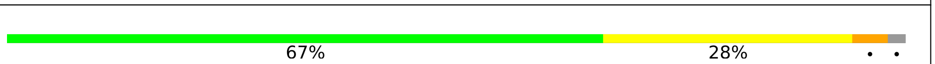
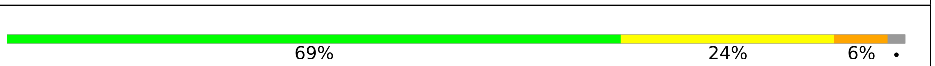
48	D2	72	
49	B3	60	
49	D3	60	
50	B4	71	
50	D4	71	
51	B5	60	
51	D5	60	
52	B6	54	
52	D6	54	

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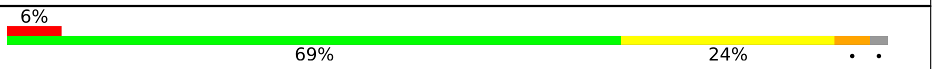
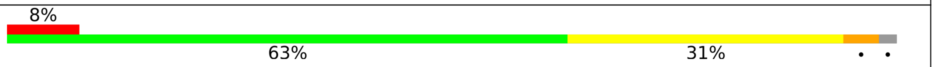
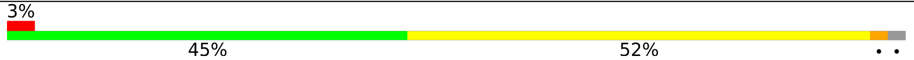
Mol	Chain	Length	Quality of chain
53	B7	49	
53	D7	49	
54	B8	65	
54	D8	65	
55	B9	37	
55	D9	37	

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	DA	3121	-	-	-	X

2 Entry composition

There are 60 unique types of molecules in this entry. The entry contains 289646 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	AA	1498	32205	14333	5970	10404	1498	0	0	0
1	CA	1503	32312	14381	5990	10438	1503	0	0	0

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	AB	231	1846	1179	331	331	5	0	0	0
2	CB	231	1825	1167	326	327	5	0	0	0

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	AC	206	1552	976	302	273	1	0	0	0
3	CC	206	1542	968	300	273	1	0	0	0

- Molecule 4 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	AD	208	1659	1040	326	286	7	0	0	0
4	CD	208	1670	1047	332	284	7	0	0	0

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
5	AE	148	Total C N O S 1129 714 213 198 4	0	0	0
5	CE	148	Total C N O S 1133 716 214 199 4	0	0	0

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
6	AF	100	Total C N O S 806 511 143 149 3	0	0	0
6	CF	100	Total C N O S 816 516 146 151 3	0	0	0

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
7	AG	155	Total C N O S 1231 766 243 216 6	0	0	0
7	CG	155	Total C N O S 1235 769 244 216 6	0	0	0

- Molecule 8 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
8	AH	137	Total C N O S 1088 689 206 191 2	0	0	0
8	CH	137	Total C N O S 1088 689 206 191 2	0	0	0

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
9	AI	127	Total C N O 983 623 193 167	0	0	0
9	CI	127	Total C N O 978 619 190 169	0	0	0

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
10	AJ	97	Total C N O 709 440 138 131	0	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
10	CJ	96	Total C N O 714 445 138 131	0	0	0

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
11	AK	114	Total C N O S 829 516 155 155 3	0	0	0
11	CK	114	Total C N O S 833 519 156 155 3	0	0	0

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
12	AL	122	Total C N O S 930 585 185 159 1	0	0	0
12	CL	122	Total C N O S 930 585 185 159 1	0	0	0

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
13	AM	123	Total C N O S 958 592 198 166 2	0	0	0
13	CM	122	Total C N O S 950 586 197 165 2	0	0	0

- Molecule 14 is a protein called 30S ribosomal protein S14 type Z.

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

- Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
15	AO	88	Total C N O S 728 456 144 126 2	0	0	0
15	CO	88	Total C N O S 728 456 144 126 2	0	0	0

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AP	82	Total	C	N	O	S	0	0	0
			681	433	134	113	1			
16	CP	82	Total	C	N	O	S	0	0	0
			677	430	133	113	1			

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AQ	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			
17	CQ	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	AR	68	Total	C	N	O	0	0	0
			555	355	108	92			
18	CR	68	Total	C	N	O	0	0	0
			555	355	108	92			

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AS	83	Total	C	N	O	S	0	0	0
			652	417	120	113	2			
19	CS	83	Total	C	N	O	S	0	0	0
			646	412	119	113	2			

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AT	96	Total	C	N	O	S	0	0	0
			728	446	156	124	2			
20	CT	96	Total	C	N	O	S	0	0	0
			727	446	155	124	2			

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
21	AU	23	Total C N O 199 122 48 29	0	0	0
21	CU	23	Total C N O 199 122 48 29	0	0	0

- Molecule 22 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
22	AV	13	Total C N O P 277 125 51 88 13	0	0	0
22	CV	12	Total C N O P 252 115 46 80 11	0	0	0

- Molecule 23 is a RNA chain called Cytidine-Puromycin.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
23	AW	2	Total C N O P 54 31 10 12 1	0	0	0
23	CW	2	Total C N O P 54 31 10 12 1	0	0	0

- Molecule 24 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
24	AX	76	Total C N O P S 1635 731 296 530 76 2	0	0	0
24	CX	76	Total C N O P S 1635 731 296 530 76 2	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
25	BA	2819	Total C N O P 60729 27026 11370 19515 2818	0	0	0
25	DA	2800	Total C N O P 60311 26840 11284 19388 2799	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
26	BB	120	Total C N O P 2573 1146 476 832 119	0	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
26	DB	120	Total C N O P 2573 1146 476 832 119	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
27	BD	275	Total C N O S 2136 1349 423 361 3	0	0	0
27	DD	275	Total C N O S 2136 1349 423 361 3	0	0	0

- 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 1559 985 298 270 6	0	0	0
28	DE	204	Total C N O S 1559 985 298 270 6	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
29	BF	203	Total C N O S 1584 1009 298 275 2	0	0	1
29	DF	203	Total C N O S 1580 1007 297 274 2	0	0	1

- 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 1425 914 256 251 4	0	0	0
30	DG	181	Total C N O S 1424 911 258 251 4	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
31	BH	174	Total C N O S 1330 845 248 236 1	0	0	0
31	DH	174	Total C N O S 1330 845 248 236 1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	BI	146	Total 1085	C 693	N 189	O 202	S 1	0	0	0
32	DI	146	Total 1061	C 680	N 186	O 194	S 1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	BN	140	Total 1117	C 719	N 207	O 187	S 4	0	0	0
33	DN	140	Total 1117	C 719	N 207	O 187	S 4	0	0	0

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BP	149	Total 1135	C 706	N 230	O 196	S 3	0	0	0
35	DP	149	Total 1135	C 706	N 230	O 196	S 3	0	0	0

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	BR	118	Total 968	C 604	N 203	O 160	S 1	0	0	0
37	DR	118	Total 968	C 604	N 203	O 160	S 1	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
38	BS	110	Total 877	C 553	N 175	O 149	0	0	0
38	DS	110	Total 870	C 549	N 173	O 148	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BT	131	Total 1091	C 680	N 225	O 185	S 1	0	0	0
39	DT	131	Total 1083	C 675	N 224	O 183	S 1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	BU	116	Total 959	C 608	N 201	O 149	S 1	0	0	0
40	DU	116	Total 959	C 608	N 201	O 149	S 1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BV	101	Total 771	C 495	N 140	O 135	S 1	0	0	0
41	DV	101	Total 771	C 495	N 140	O 135	S 1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BW	112	Total 886	C 557	N 174	O 153	S 2	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	DW	112	Total	C	N	O	S	0	0	0
			886	557	174	153	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BX	95	Total	C	N	O	S	0	0	0
			750	488	135	126	1			
43	DX	95	Total	C	N	O	S	0	0	0
			750	488	135	126	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	BY	107	Total	C	N	O	S	0	0	0
			806	517	152	131	6			
44	DY	107	Total	C	N	O	S	0	0	0
			806	517	152	131	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	BZ	171	Total	C	N	O	S	0	0	0
			1349	862	243	242	2			
45	DZ	174	Total	C	N	O	S	0	0	0
			1360	870	243	245	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	B0	83	Total	C	N	O	S	0	0	0
			653	404	139	109	1			
46	D0	83	Total	C	N	O	S	0	0	0
			653	404	139	109	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	B1	97	Total	C	N	O	S	0	0	0
			755	475	148	131	1			
47	D1	97	Total	C	N	O	S	0	0	0
			755	475	148	131	1			

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
48	B2	70	Total C N O S 588 365 118 103 2	0	0	0
48	D2	70	Total C N O S 588 365 118 103 2	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
49	B3	59	Total C N O 469 298 90 81	0	0	0
49	D3	59	Total C N O 464 296 90 78	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
50	B4	69	Total C N O S 552 349 99 99 5	0	0	0
50	D4	69	Total C N O S 532 339 97 91 5	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
51	B5	59	Total C N O S 455 285 89 76 5	0	0	0
51	D5	59	Total C N O S 455 285 89 76 5	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
52	B6	53	Total C N O S 453 281 91 77 4	0	0	0
52	D6	53	Total C N O S 449 279 91 75 4	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	B7	48	Total 418	C 257	N 104	O 55	S 2	0	0	0
53	D7	48	Total 418	C 257	N 104	O 55	S 2	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	B8	64	Total 511	C 328	N 99	O 82	S 2	0	0	0
54	D8	64	Total 517	C 331	N 102	O 82	S 2	0	0	0

- Molecule 55 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	B9	37	Total 307	C 188	N 68	O 47	S 4	0	0	0
55	D9	37	Total 307	C 188	N 68	O 47	S 4	0	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	AA	187	Total 187	Mg 187	0	0
56	AD	1	Total 1	Mg 1	0	0
56	AE	2	Total 2	Mg 2	0	0
56	AF	1	Total 1	Mg 1	0	0
56	AK	1	Total 1	Mg 1	0	0
56	AL	1	Total 1	Mg 1	0	0
56	AM	1	Total 1	Mg 1	0	0
56	AN	1	Total 1	Mg 1	0	0
56	AX	7	Total 7	Mg 7	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	BA	675	Total Mg 675 675	0	0
56	BB	18	Total Mg 18 18	0	0
56	BD	8	Total Mg 8 8	0	0
56	BE	6	Total Mg 6 6	0	0
56	BF	5	Total Mg 5 5	0	0
56	BG	3	Total Mg 3 3	0	0
56	BH	1	Total Mg 1 1	0	0
56	BN	2	Total Mg 2 2	0	0
56	BO	1	Total Mg 1 1	0	0
56	BP	4	Total Mg 4 4	0	0
56	BQ	3	Total Mg 3 3	0	0
56	BR	3	Total Mg 3 3	0	0
56	BU	5	Total Mg 5 5	0	0
56	BV	3	Total Mg 3 3	0	0
56	BW	4	Total Mg 4 4	0	0
56	BX	3	Total Mg 3 3	0	0
56	BY	2	Total Mg 2 2	0	0
56	BZ	1	Total Mg 1 1	0	0
56	B0	5	Total Mg 5 5	0	0
56	B3	2	Total Mg 2 2	0	0
56	B4	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	B5	2	Total Mg 2 2	0	0
56	B7	4	Total Mg 4 4	0	0
56	B8	1	Total Mg 1 1	0	0
56	B9	1	Total Mg 1 1	0	0
56	CA	154	Total Mg 154 154	0	0
56	CE	2	Total Mg 2 2	0	0
56	CF	1	Total Mg 1 1	0	0
56	CJ	1	Total Mg 1 1	0	0
56	CK	1	Total Mg 1 1	0	0
56	CT	1	Total Mg 1 1	0	0
56	CX	1	Total Mg 1 1	0	0
56	DA	595	Total Mg 595 595	0	0
56	DB	12	Total Mg 12 12	0	0
56	DD	2	Total Mg 2 2	0	0
56	DE	5	Total Mg 5 5	0	0
56	DF	3	Total Mg 3 3	0	0
56	DG	1	Total Mg 1 1	0	0
56	DN	1	Total Mg 1 1	0	0
56	DP	1	Total Mg 1 1	0	0
56	DQ	3	Total Mg 3 3	0	0
56	DR	2	Total Mg 2 2	0	0

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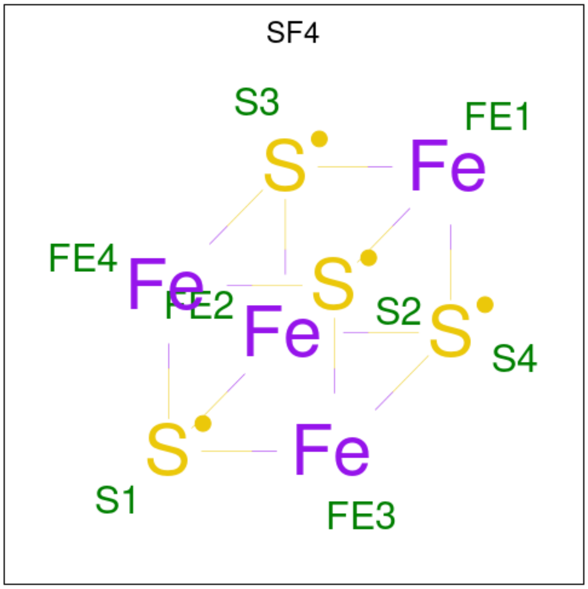
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	DT	1	Total Mg 1 1	0	0
56	DU	1	Total Mg 1 1	0	0
56	DV	2	Total Mg 2 2	0	0
56	DW	2	Total Mg 2 2	0	0
56	DY	1	Total Mg 1 1	0	0
56	D0	1	Total Mg 1 1	0	0
56	D3	1	Total Mg 1 1	0	0
56	D5	1	Total Mg 1 1	0	0
56	D7	1	Total Mg 1 1	0	0
56	D8	2	Total Mg 2 2	0	0

- Molecule 57 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	AD	1	Total Fe S 8 4 4	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	CD	1	Total Fe S 8 4 4	0	0

- Molecule 58 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	AN	1	Total Zn 1 1	0	0
58	BY	1	Total Zn 1 1	0	0
58	B4	1	Total Zn 1 1	0	0
58	B5	1	Total Zn 1 1	0	0
58	B6	1	Total Zn 1 1	0	0
58	B9	1	Total Zn 1 1	0	0
58	CN	1	Total Zn 1 1	0	0
58	DY	1	Total Zn 1 1	0	0
58	D4	1	Total Zn 1 1	0	0
58	D5	1	Total Zn 1 1	0	0
58	D6	1	Total Zn 1 1	0	0
58	D9	1	Total Zn 1 1	0	0

- Molecule 59 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	AX	1	Total K 1 1	0	0
59	DA	1	Total K 1 1	0	0

- Molecule 60 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	AA	165	Total O 165 165	0	0
60	AJ	1	Total O 1 1	0	0
60	AL	3	Total O 3 3	0	0
60	AP	1	Total O 1 1	0	0
60	AU	1	Total O 1 1	0	0
60	AV	2	Total O 2 2	0	0
60	AW	3	Total O 3 3	0	0
60	BA	924	Total O 924 924	0	0
60	BB	27	Total O 27 27	0	0
60	BD	6	Total O 6 6	0	0
60	BE	8	Total O 8 8	0	0
60	BF	6	Total O 6 6	0	0
60	BG	1	Total O 1 1	0	0
60	BH	1	Total O 1 1	0	0
60	BN	3	Total O 3 3	0	0
60	BO	1	Total O 1 1	0	0
60	BP	14	Total O 14 14	0	0
60	BQ	2	Total O 2 2	0	0
60	BS	1	Total O 1 1	0	0
60	BT	4	Total O 4 4	0	0
60	BU	2	Total O 2 2	0	0
60	BV	5	Total O 5 5	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	BW	1	Total O 1 1	0	0
60	BX	2	Total O 2 2	0	0
60	BZ	1	Total O 1 1	0	0
60	B0	4	Total O 4 4	0	0
60	B1	2	Total O 2 2	0	0
60	B2	1	Total O 1 1	0	0
60	B3	1	Total O 1 1	0	0
60	B5	2	Total O 2 2	0	0
60	B7	2	Total O 2 2	0	0
60	B8	8	Total O 8 8	0	0
60	CA	113	Total O 113 113	0	0
60	CE	2	Total O 2 2	0	0
60	CJ	2	Total O 2 2	0	0
60	CL	1	Total O 1 1	0	0
60	CO	1	Total O 1 1	0	0
60	CW	1	Total O 1 1	0	0
60	CX	1	Total O 1 1	0	0
60	DA	689	Total O 689 689	0	0
60	DB	9	Total O 9 9	0	0
60	DD	11	Total O 11 11	0	0
60	DE	5	Total O 5 5	0	0

Continued on next page...

Continued from previous page...

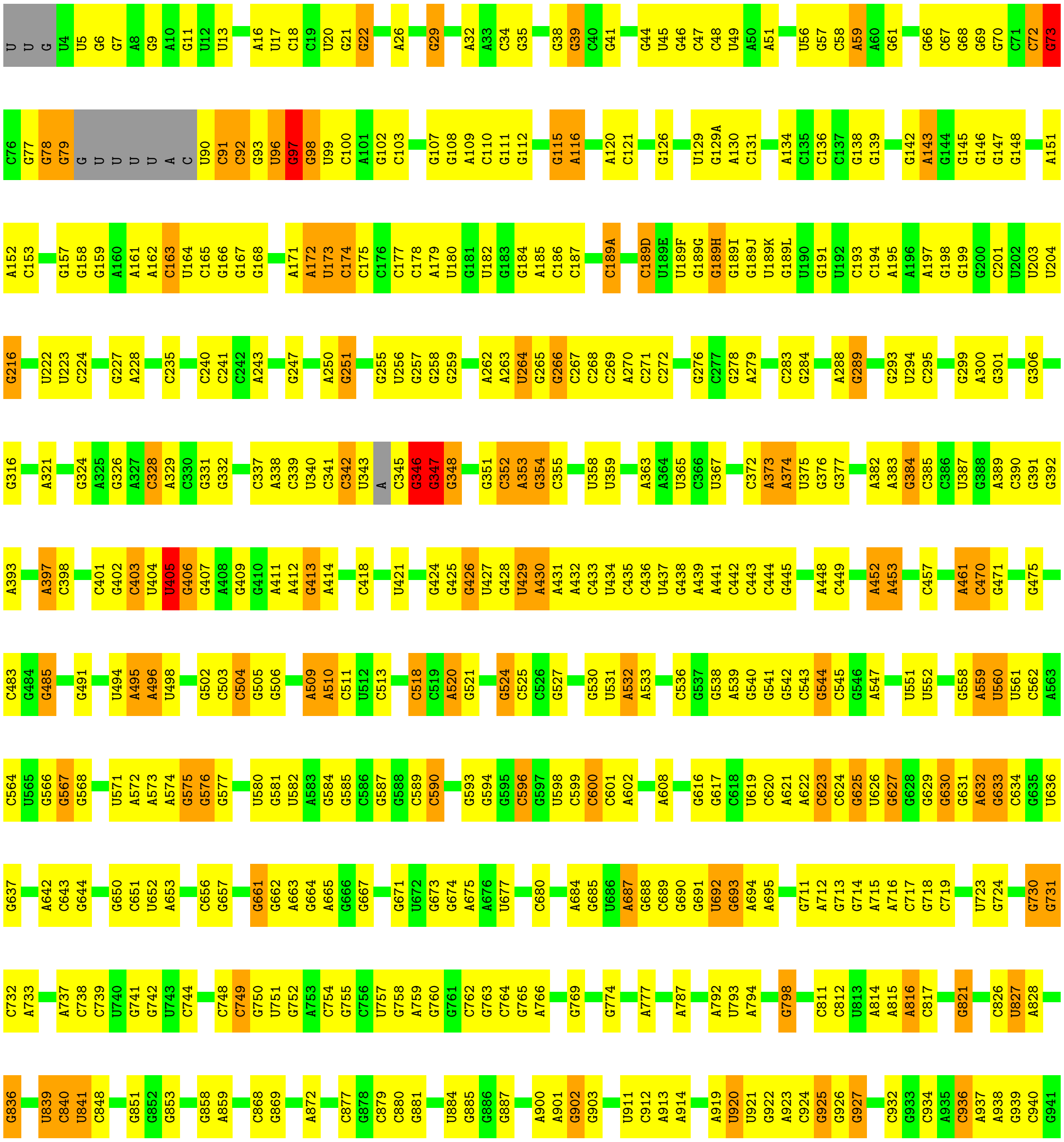
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	DF	6	Total O 6 6	0	0
60	DO	1	Total O 1 1	0	0
60	DP	6	Total O 6 6	0	0
60	DU	3	Total O 3 3	0	0
60	DV	1	Total O 1 1	0	0
60	DW	1	Total O 1 1	0	0
60	DX	3	Total O 3 3	0	0
60	D0	5	Total O 5 5	0	0
60	D1	1	Total O 1 1	0	0
60	D3	1	Total O 1 1	0	0
60	D8	3	Total O 3 3	0	0

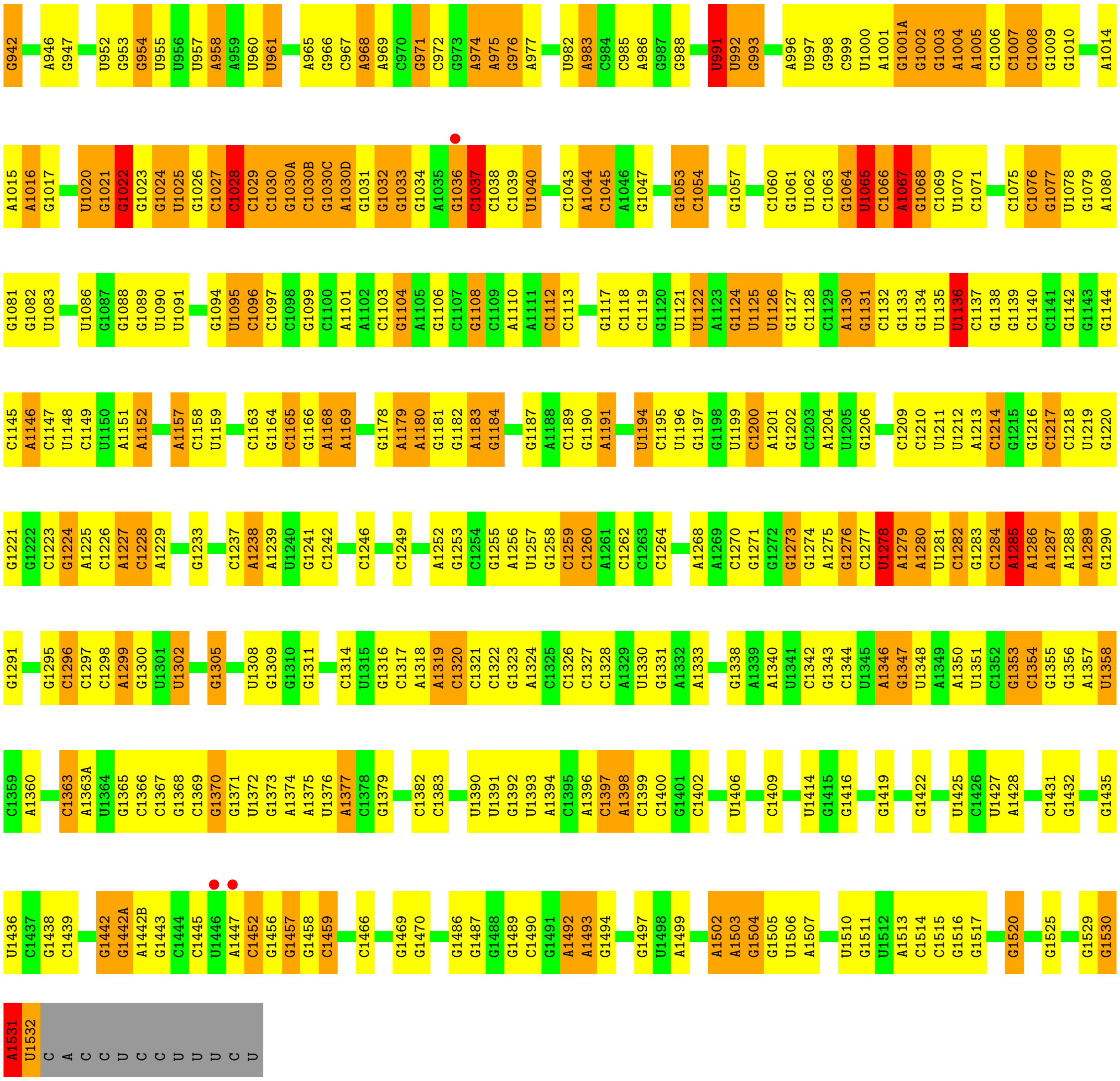
3 Residue-property plots ⓘ

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

- Molecule 1: 16S Ribosomal RNA

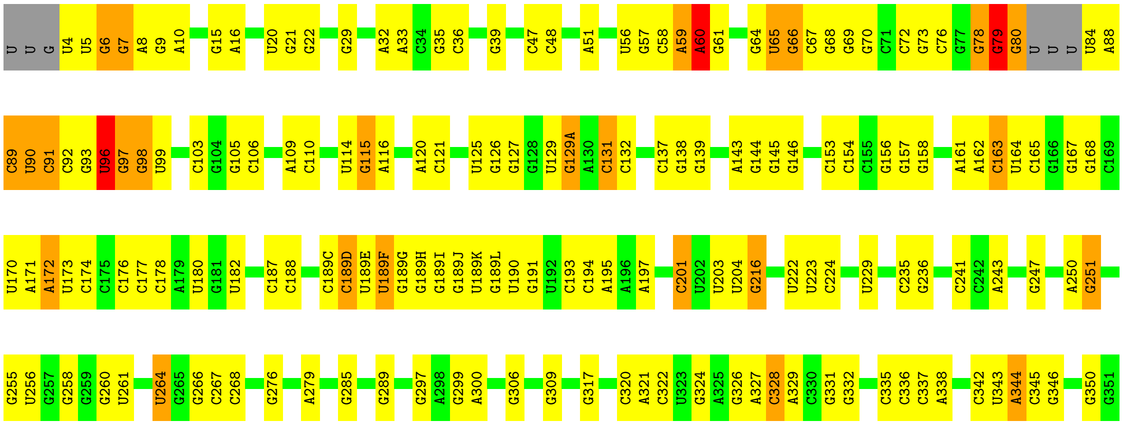
Chain AA:

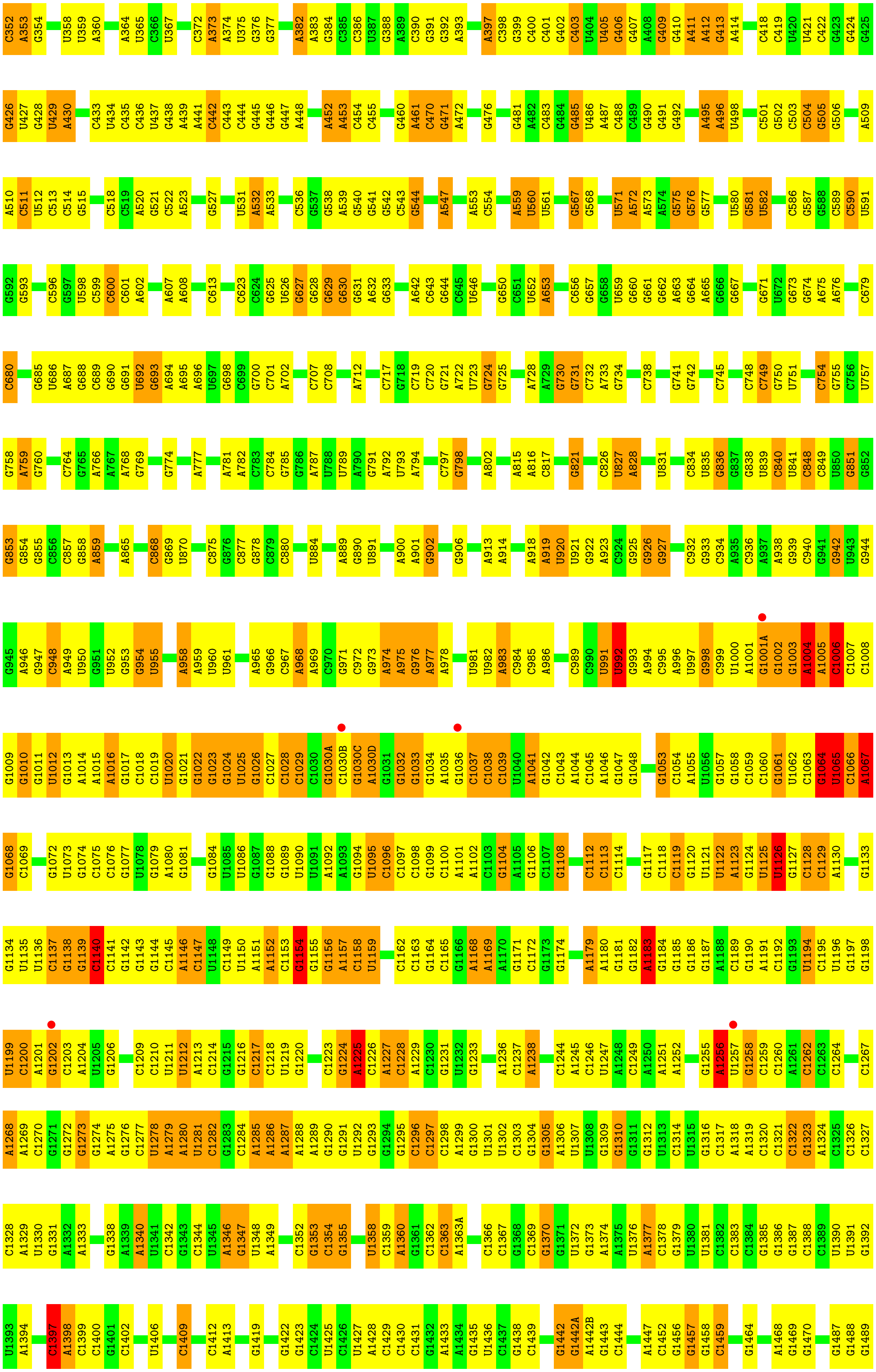




- Molecule 1: 16S Ribosomal RNA

Chain CA:

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G426 U427 G428 U429 A430 C433 U434 C435 C436 U437 G438 A439 A441 C442 C443 C444 G445 G446 G447 A448 A452 A453 C454 C455 G460 A461 C470 G471 A472 G476 G481 A482 C483 G484 G485 U486 A487 C488 C489 G490 G491 G492 A495 A496 U498 C501 G502 C503 C504 G505 G506 A509
A510 C511 U512 C513 C514 G515 C518 C519 A520 G521 C522 A523 G527 U531 A532 A533 C536 G537 C538 A539 G540 G541 G542 C543 G544 A547 A553 C554 A559 U560 U561 G567 G568 U571 A572 A573 A574 G575 G576 G577 U580 G581 U582 C586 G587 G588 C589 C590 U591
G592 G593 C596 G597 U598 C599 C600 C601 A602 A607 A608 C613 C623 C624 G625 U626 G627 G628 G629 G630 G631 A632 G633 A642 C643 G644 C645 U646 G650 C651 U652 A653 C656 G657 G658 U659 G660 G661 G662 A663 G664 A665 G666 G667 G671 U672 G673 G674 A675 A676 C679
C680 G685 U686 A687 G688 C689 G690 G691 U692 G693 A694 A695 A696 U697 G698 C699 G700 C701 A702 C707 C708 A712 C717 G718 C719 C720 G721 A722 U723 G724 G725 A728 A729 G730 G731 C732 A733 G734 C738 G741 G742 C745 C748 C749 G750 U751 C754 G755 C756 U757
G758 A759 G760 C764 G765 A766 A767 A768 G769 G774 A777 A781 A782 C783 C784 G785 G786 A787 U788 U789 A790 G791 A792 U793 A794 C797 G798 A802 A815 A816 C817 G821 C826 U827 A828 U831 C834 U835 G836 G837 G838 U839 C840 U841 C848 C849 U850 G851 G852
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G945 A946 G947 C948 A949 U950 G951 U952 G953 G954 U955 A958 A959 U960 U961 A965 G966 C967 A968 A969 C970 G971 C972 G973 A974 A975 G976 A977 A978 U981 U982 A983 C984 C985 A986 C989 C990 U991 U992 G993 A994 C995 A996 U997 G998 C999 U1000 A1001 G1001A G1002 G1003 A1004 A1005 C1006 C1007 C1008
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G1068 C1069 G1072 U1073 G1074 C1075 C1076 G1077 U1078 G1079 A1080 G1081 G1084 U1085 U1086 G1087 G1088 G1089 U1090 U1091 A1092 A1093 G1094 U1095 C1096 C1097 C1098 G1099 C1100 A1101 A1102 C1103 G1104 A1105 G1106 C1107 G1108 C1112 C1113 C1114 G1117 C1118 C1119 G1120 U1121 U1122 A1123 G1124 U1125 U1126 G1127 C1128 C1129 A1130 G1133
G1134 U1135 U1136 C1137 G1138 G1139 C1140 C1141 G1142 G1143 G1144 C1145 A1146 C1147 U1148 C1149 U1150 A1151 A1152 C1153 G1154 G1155 G1156 A1157 C1158 U1159 C1162 C1163 G1164 C1165 G1166 A1168 A1169 A1170 G1171 C1172 G1173 G1174 A1179 A1180 G1181 G1182 A1183 G1184 G1185 G1186 G1187 A1188 C1189 G1190 A1191 C1192 G1193 U1194 C1195 U1196 G1197 G1198
U1199 C1200 A1201 G1202 C1203 A1204 U1205 G1206 C1209 C1210 U1211 U1212 A1213 C1214 G1215 G1216 C1217 C1218 U1219 G1220 C1223 G1224 A1225 C1226 A1227 C1228 A1229 C1230 G1231 U1232 G1233 A1236 C1237 A1238 C1244 A1245 C1246 U1247 A1248 C1249 A1250 A1251 A1252 G1255 A1256 U1257 G1258 C1259 C1260 A1261 C1262 C1263 C1264 C1267
A1268 A1269 C1270 G1271 G1272 G1273 G1274 A1275 G1276 C1277 U1278 A1279 A1280 U1281 C1282 G1283 C1284 A1285 A1286 A1287 A1288 A1289 G1290 G1291 U1292 G1293 G1294 G1295 C1296 C1297 C1298 A1299 G1300 U1301 U1302 C1303 G1304 G1305 A1306 U1307 U1308 G1309 G1310 G1311 G1312 U1313 C1314 U1315 G1316 C1317 A1318 A1319 C1320 C1321 C1322 G1323 A1324 C1325 C1326 C1327
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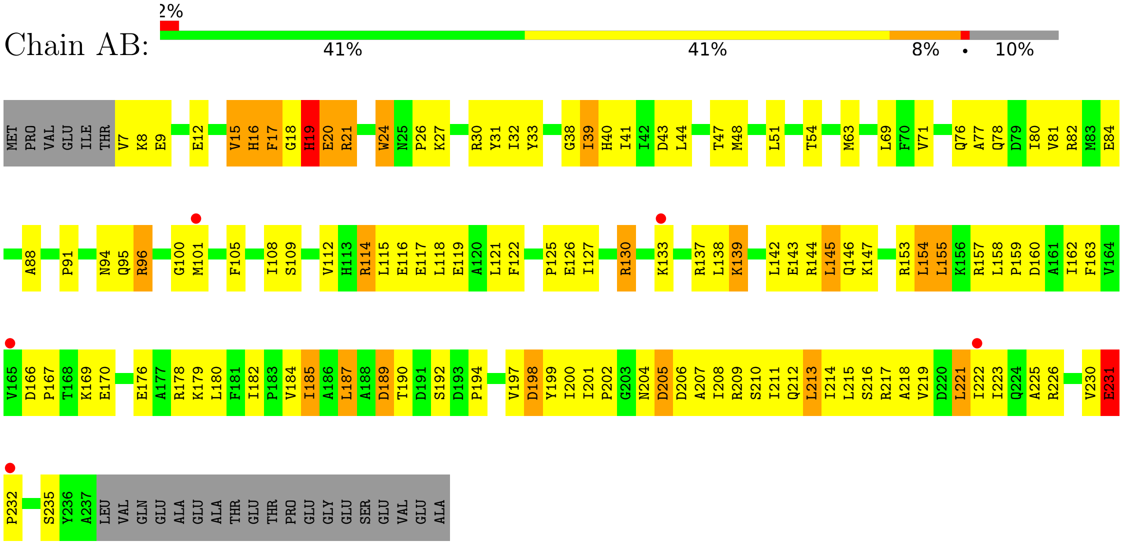
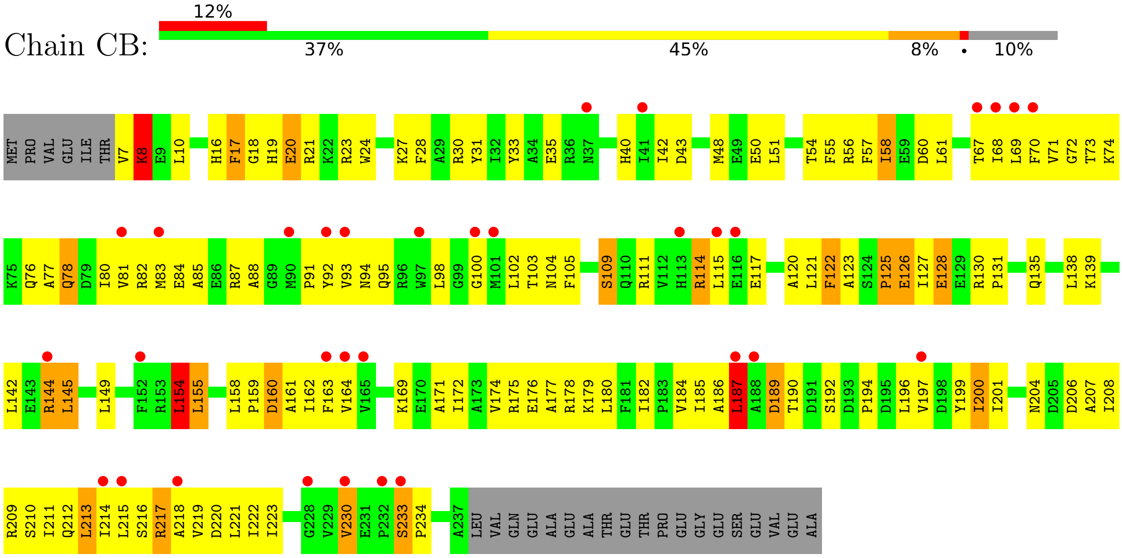
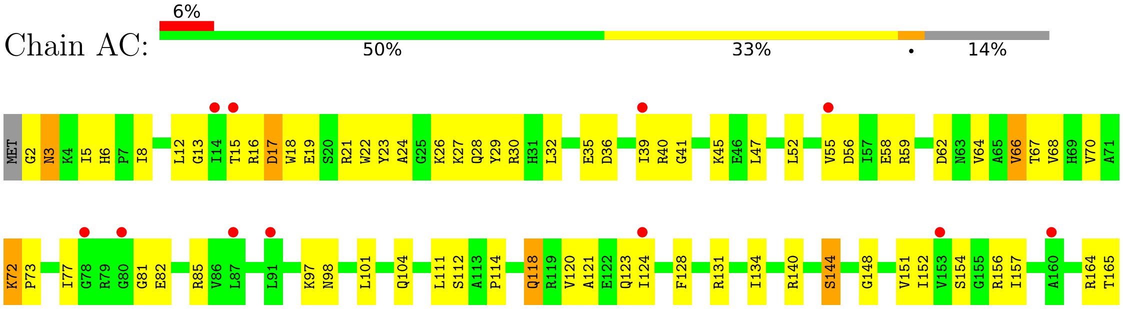
- Molecule 2: 30S ribosomal protein S2

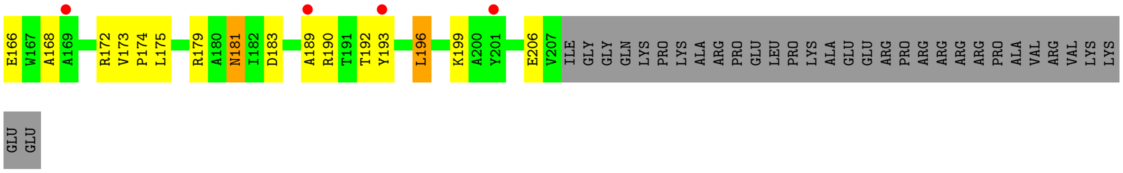


- Molecule 2: 30S ribosomal protein S2

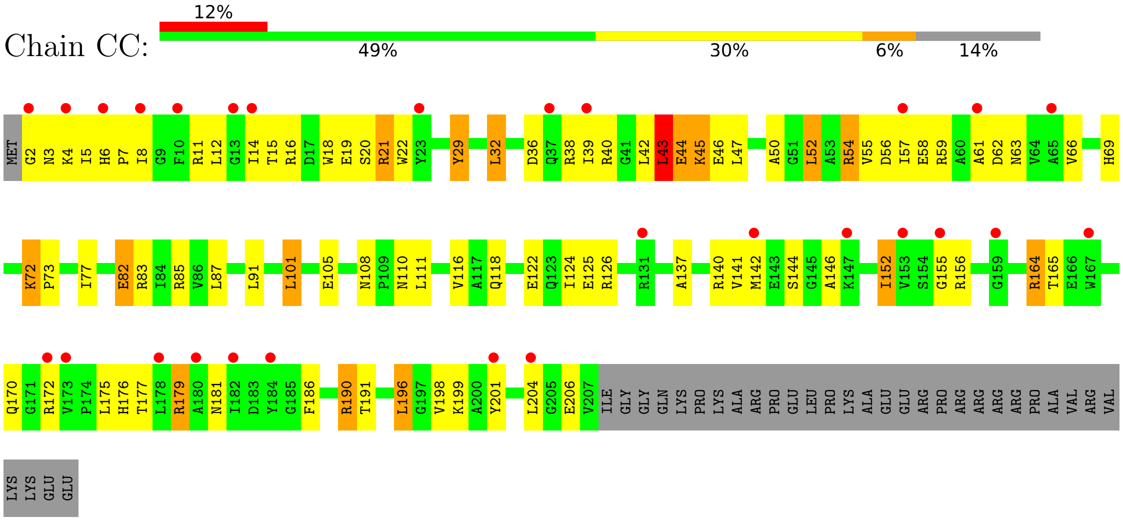


- Molecule 3: 30S ribosomal protein S3

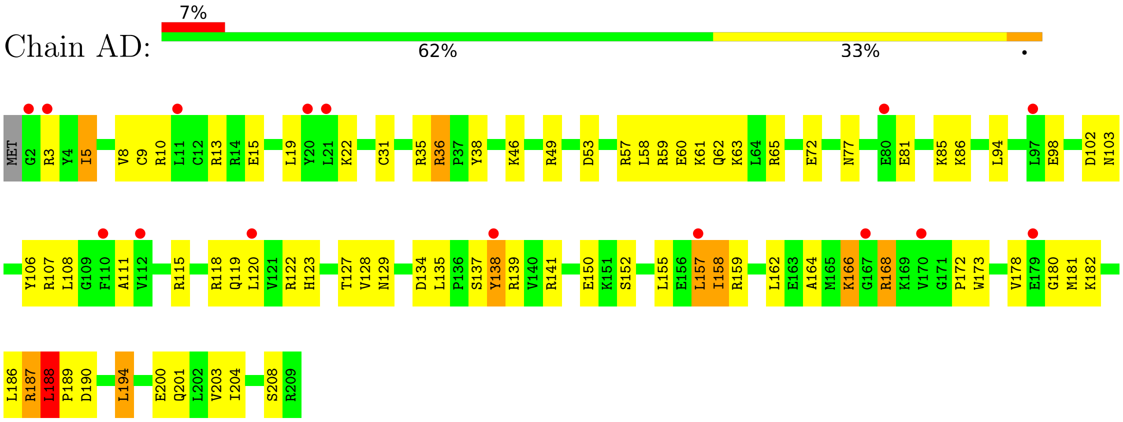




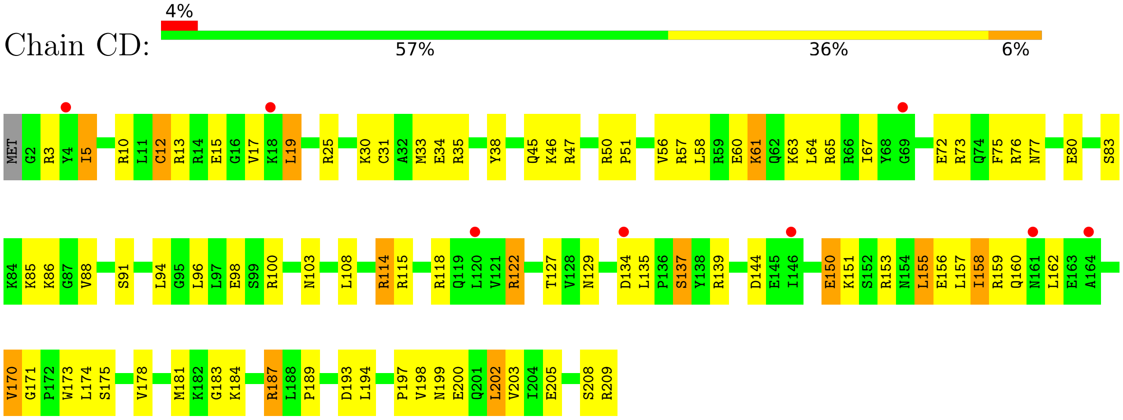
- Molecule 3: 30S ribosomal protein S3



- Molecule 4: 30S ribosomal protein S4

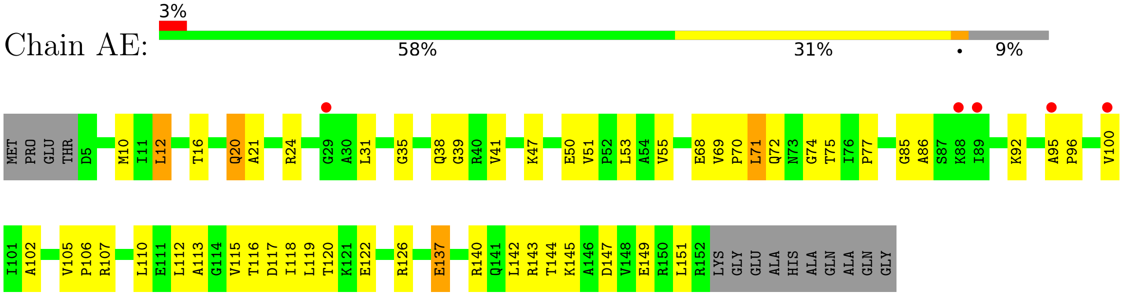


- Molecule 4: 30S ribosomal protein S4



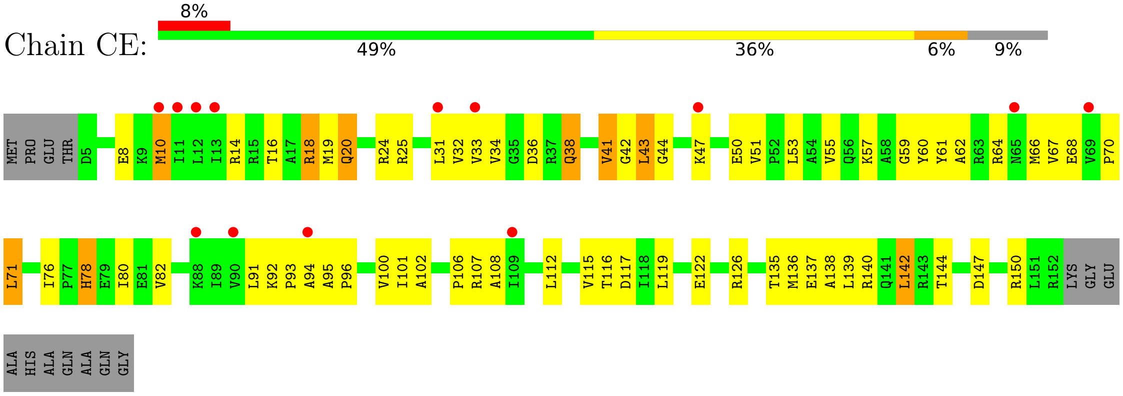
- Molecule 5: 30S ribosomal protein S5

Chain AE:



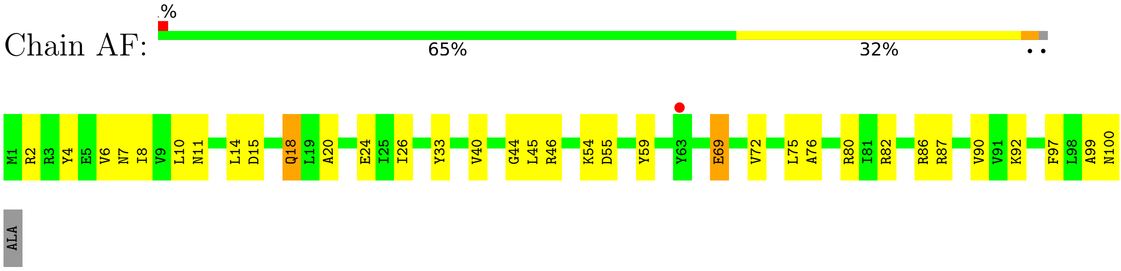
- Molecule 5: 30S ribosomal protein S5

Chain CE:



- Molecule 6: 30S ribosomal protein S6

Chain AF:



- Molecule 6: 30S ribosomal protein S6

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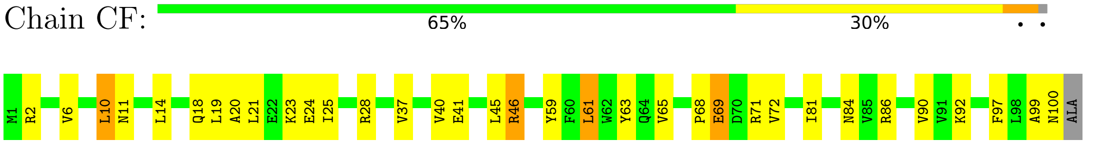
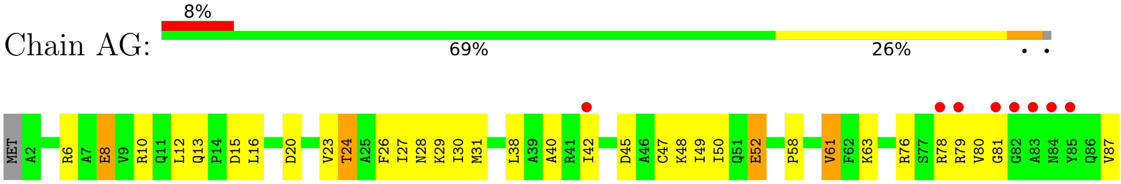
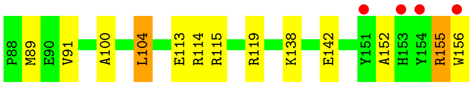


- Molecule 7: 30S ribosomal protein S7

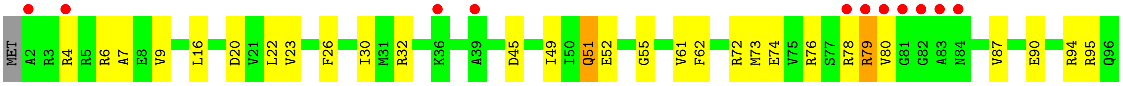
Chain AG:

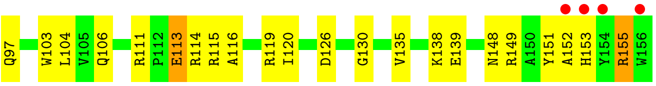




- Molecule 7: 30S ribosomal protein S7

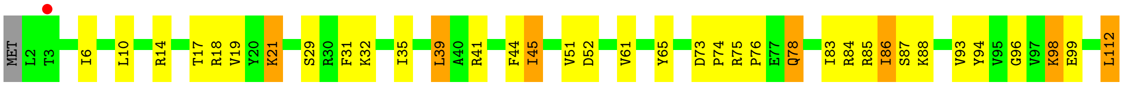
Chain CG:

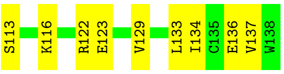




- Molecule 8: 30S ribosomal protein S8

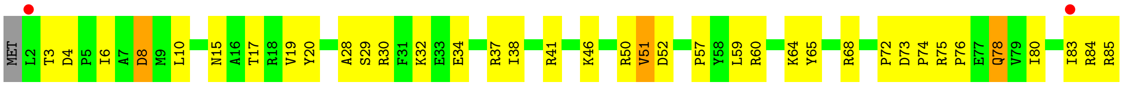
Chain AH:





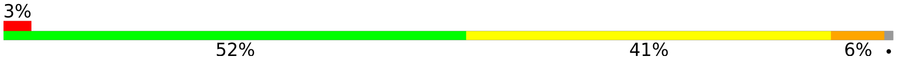
- Molecule 8: 30S ribosomal protein S8

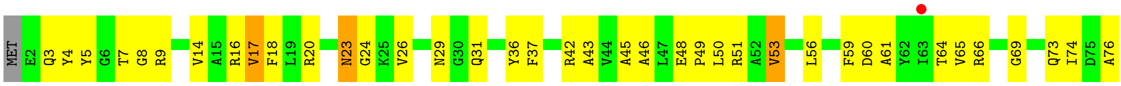
Chain CH:

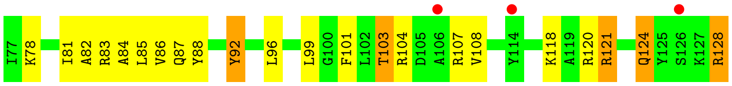


- Molecule 9: 30S ribosomal protein S9

Chain AI:







- Molecule 9: 30S ribosomal protein S9

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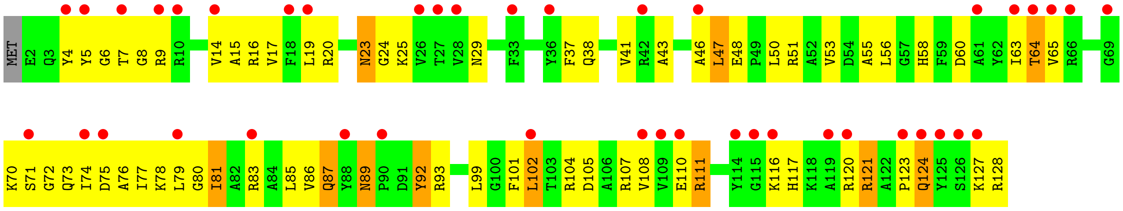
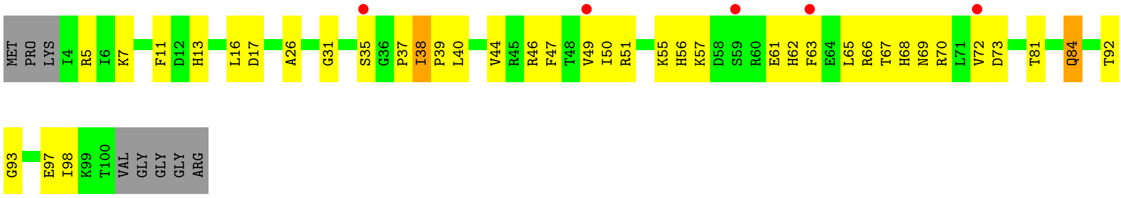


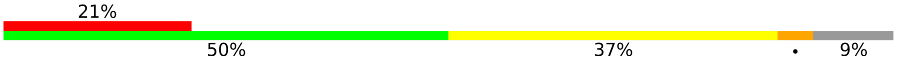
- Molecule 10: 30S ribosomal protein S10

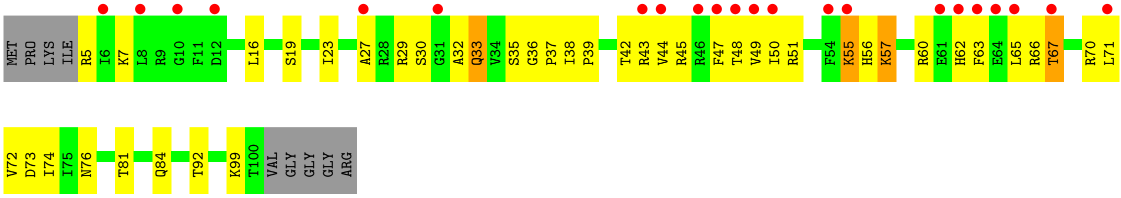
Chain AJ:



- Molecule 10: 30S ribosomal protein S10

Chain CJ:



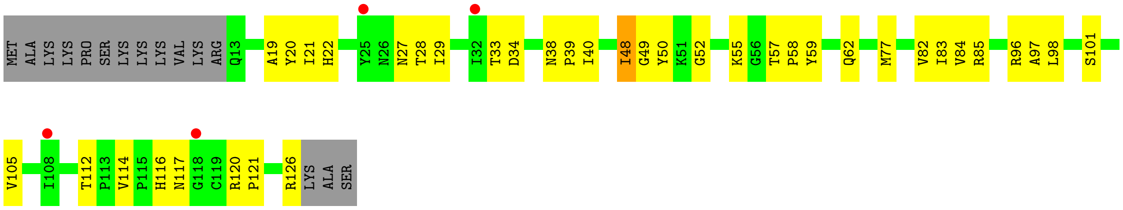


- Molecule 11: 30S ribosomal protein S11

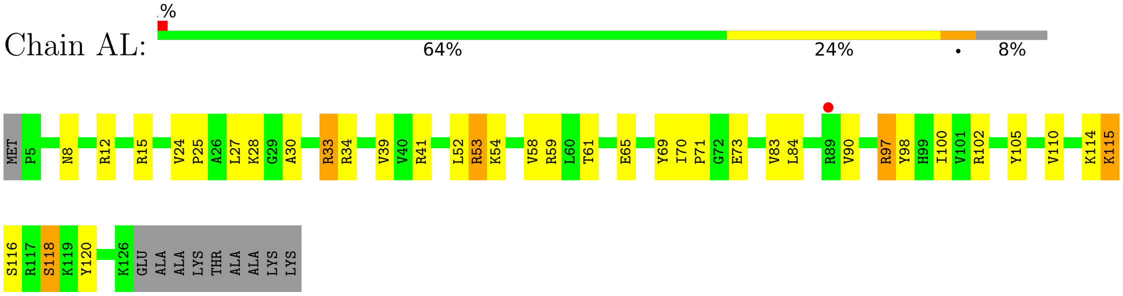
Chain AK:

- Molecule 11: 30S ribosomal protein S11

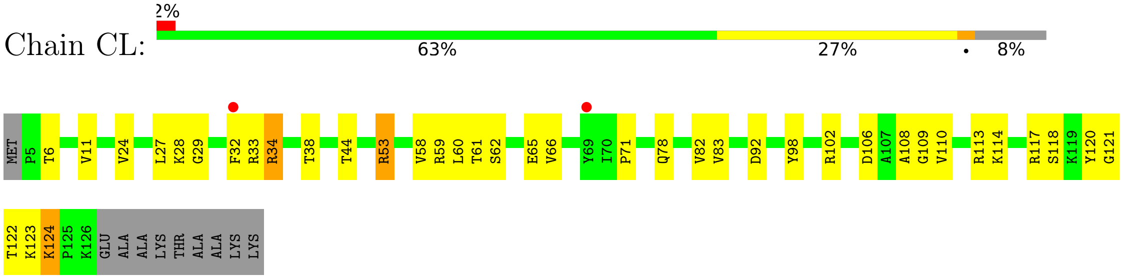
Chain CK:



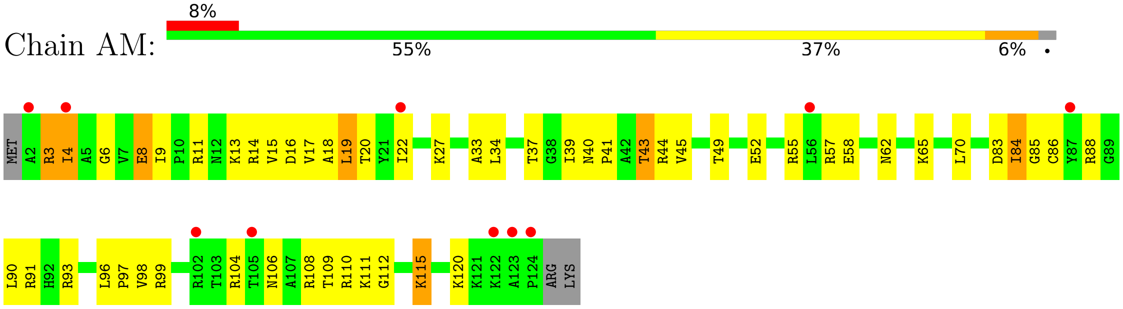
- Molecule 12: 30S ribosomal protein S12



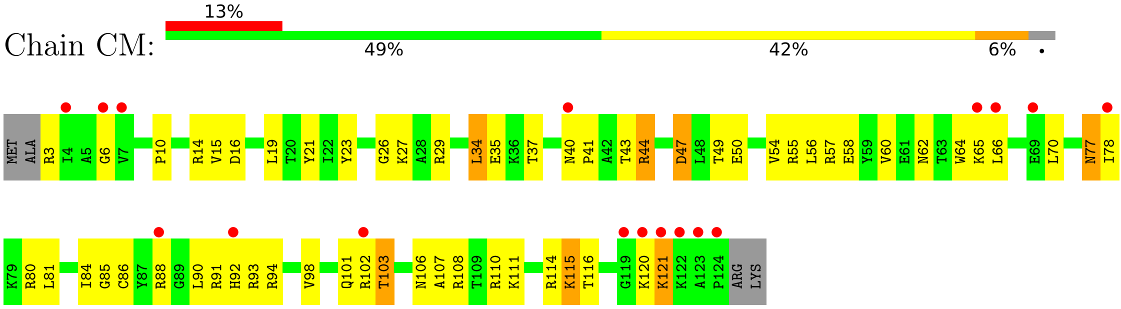
- Molecule 12: 30S ribosomal protein S12



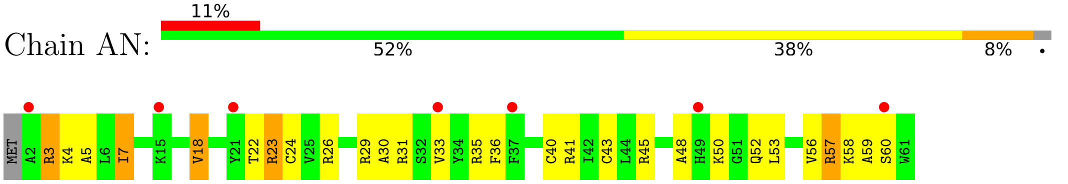
- Molecule 13: 30S ribosomal protein S13



- Molecule 13: 30S ribosomal protein S13



- Molecule 14: 30S ribosomal protein S14 type Z



- Molecule 14: 30S ribosomal protein S14 type Z

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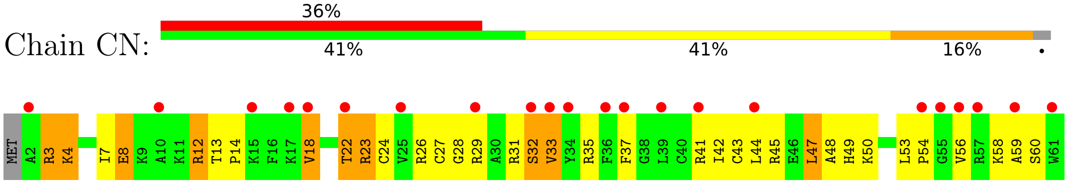
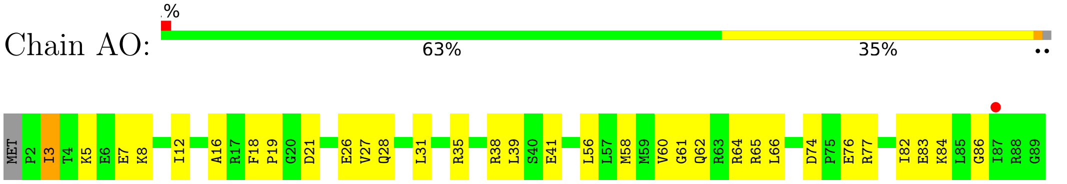


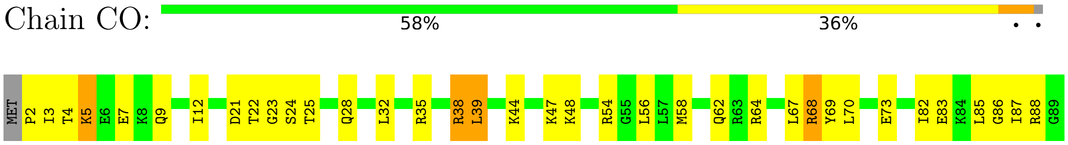
- Molecule 15: 30S ribosomal protein S15

Chain AO:



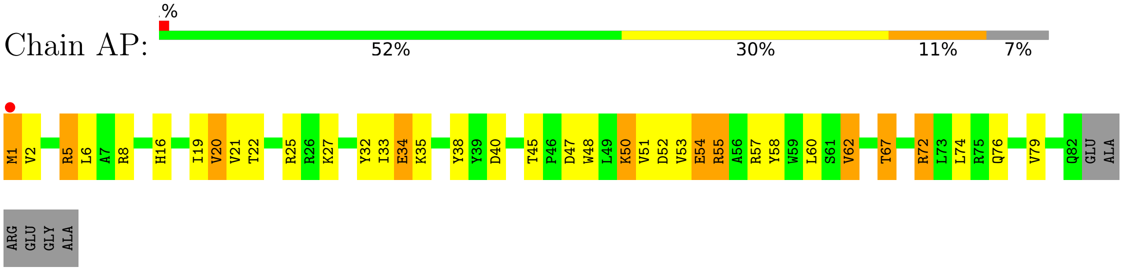
- Molecule 15: 30S ribosomal protein S15

Chain CO:



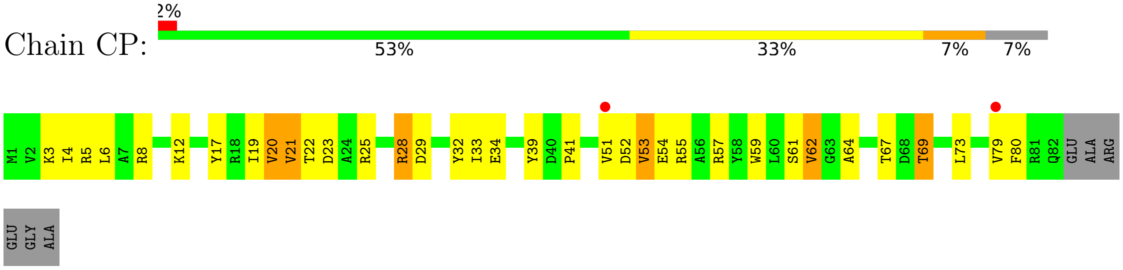
- Molecule 16: 30S ribosomal protein S16

Chain AP:



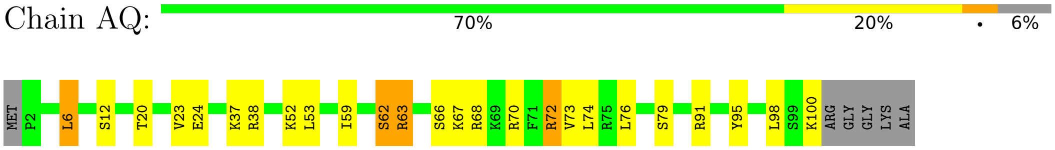
- Molecule 16: 30S ribosomal protein S16

Chain CP:



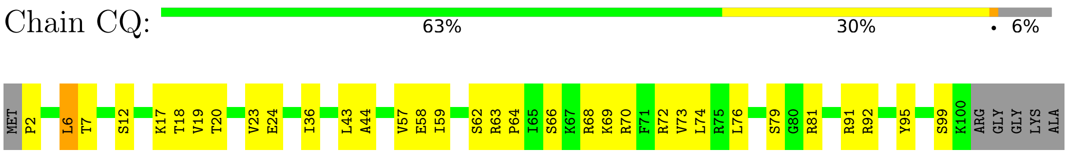
- Molecule 17: 30S ribosomal protein S17

Chain AQ:



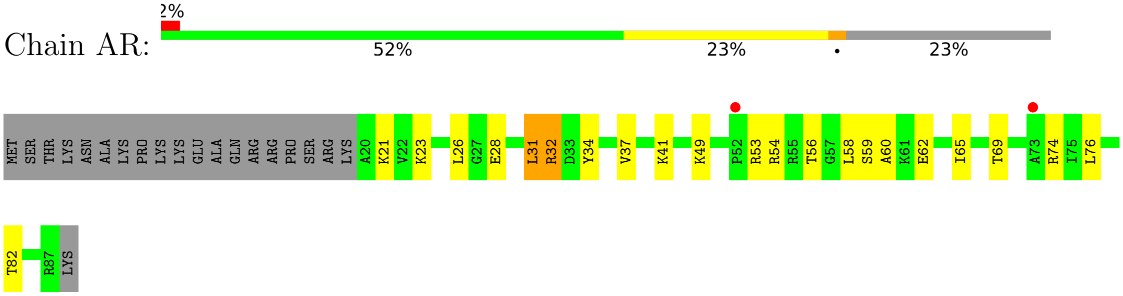
- Molecule 17: 30S ribosomal protein S17

Chain CQ:



- Molecule 18: 30S ribosomal protein S18

Chain AR:



- Molecule 18: 30S ribosomal protein S18

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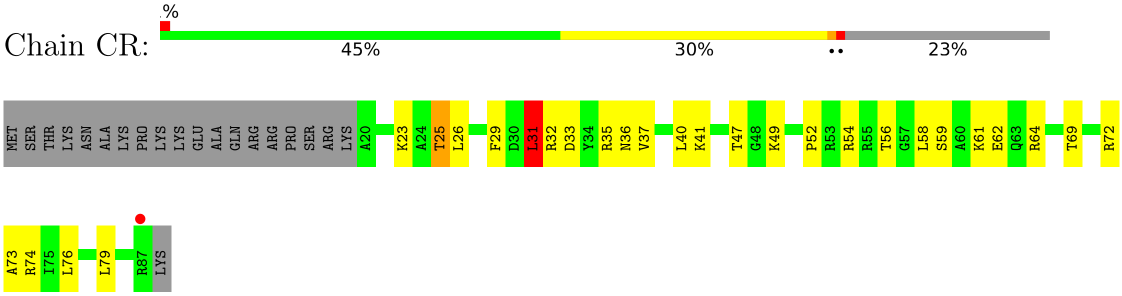
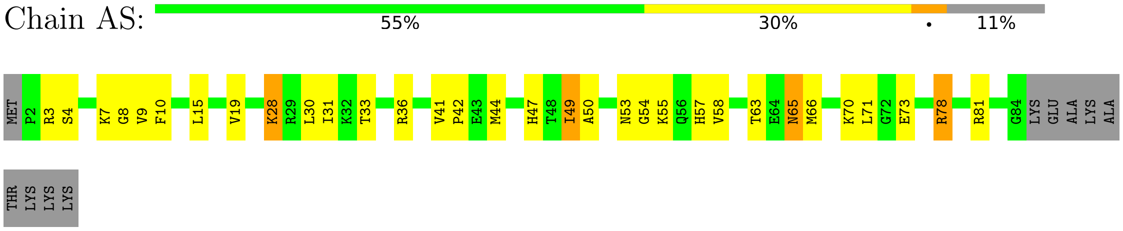


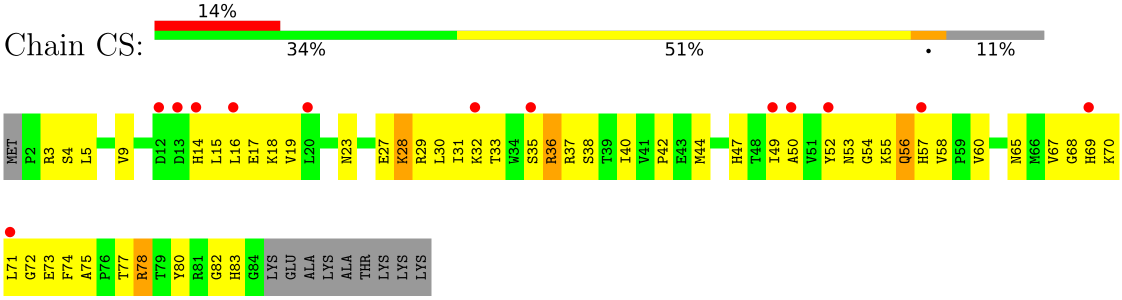
- Molecule 19: 30S ribosomal protein S19

Chain AS:



- Molecule 19: 30S ribosomal protein S19

Chain CS:



- Molecule 20: 30S ribosomal protein S20

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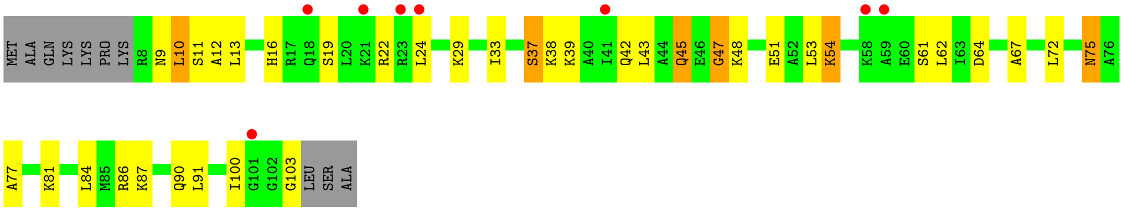

- Molecule 20: 30S ribosomal protein S20

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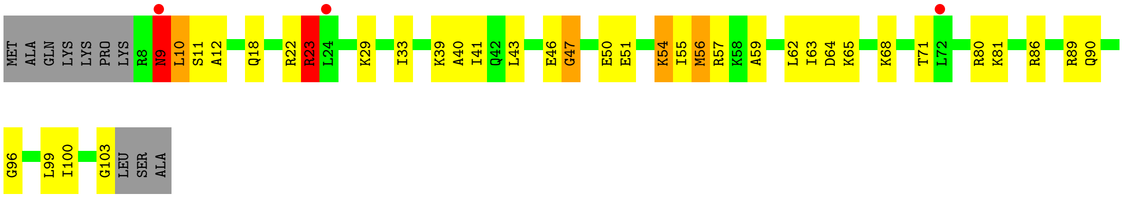

- Molecule 21: 30S ribosomal protein Thx

Chain AU:

- Molecule 21: 30S ribosomal protein Thx

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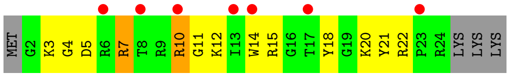

- Molecule 22: mRNA

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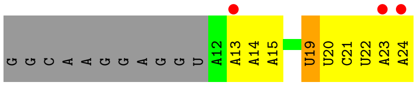

- Molecule 22: mRNA

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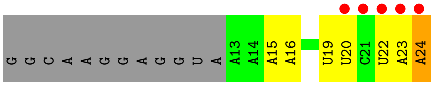


- Molecule 23: Cytidine-Puromycin

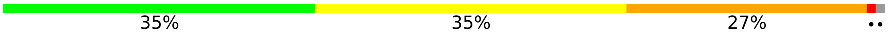
Chain AW:

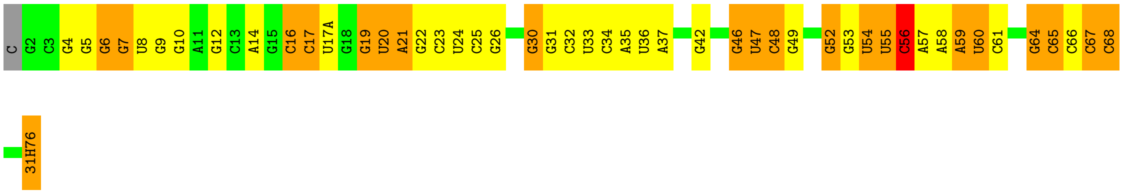
- Molecule 23: Cytidine-Puromycin

Chain CW:

- Molecule 24: P-site tRNA

Chain AX:





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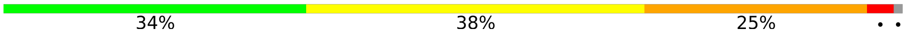

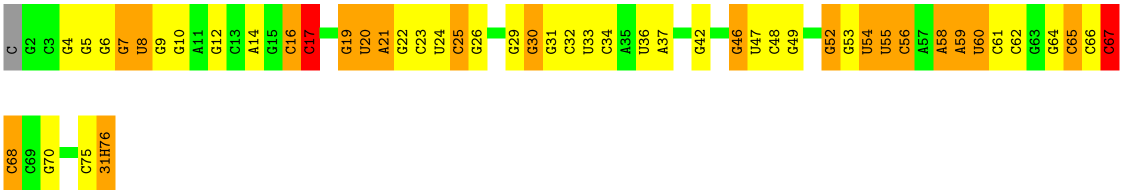

- Molecule 25: 23S Ribosomal RNA

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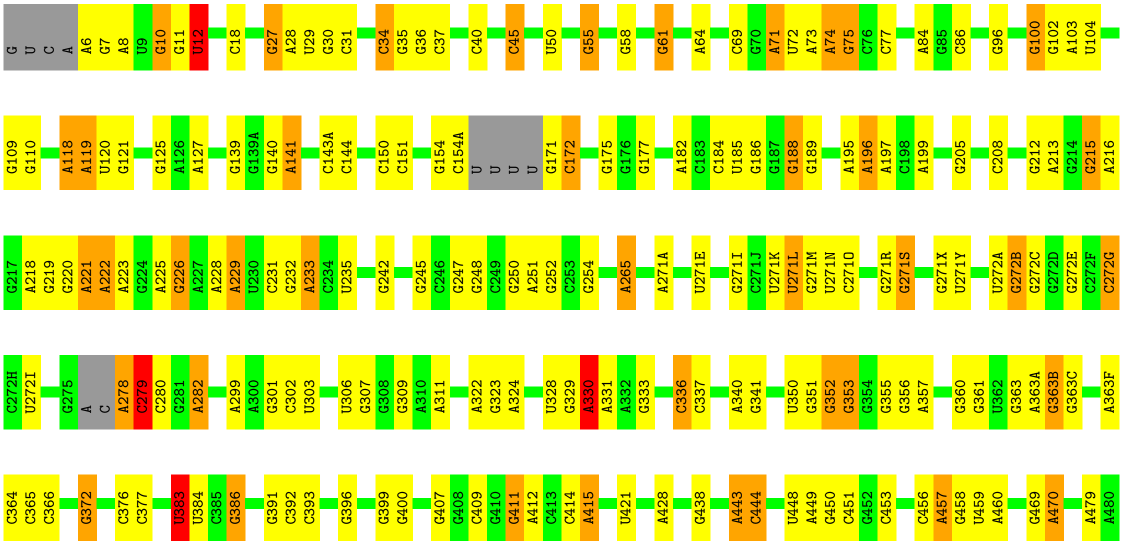

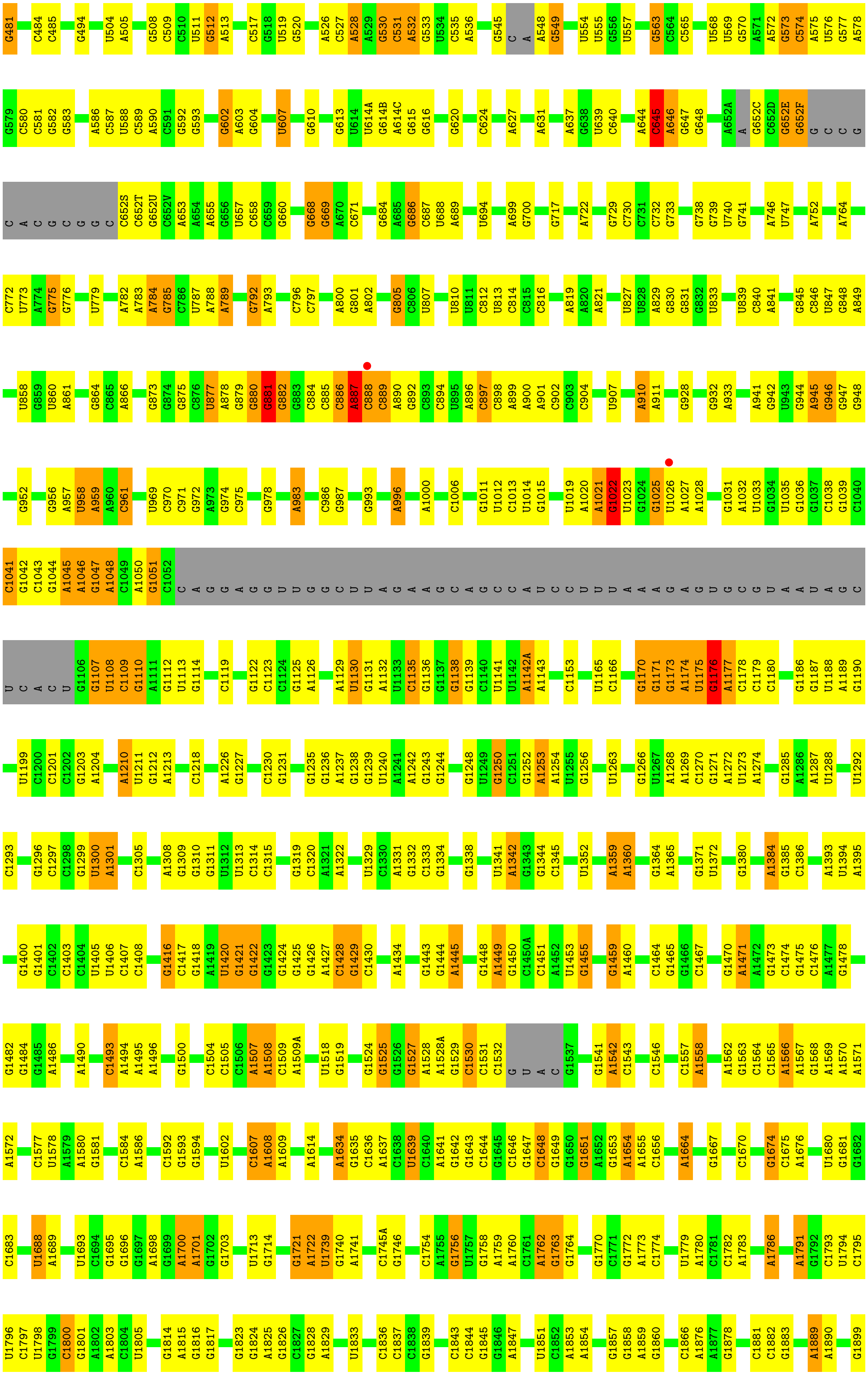
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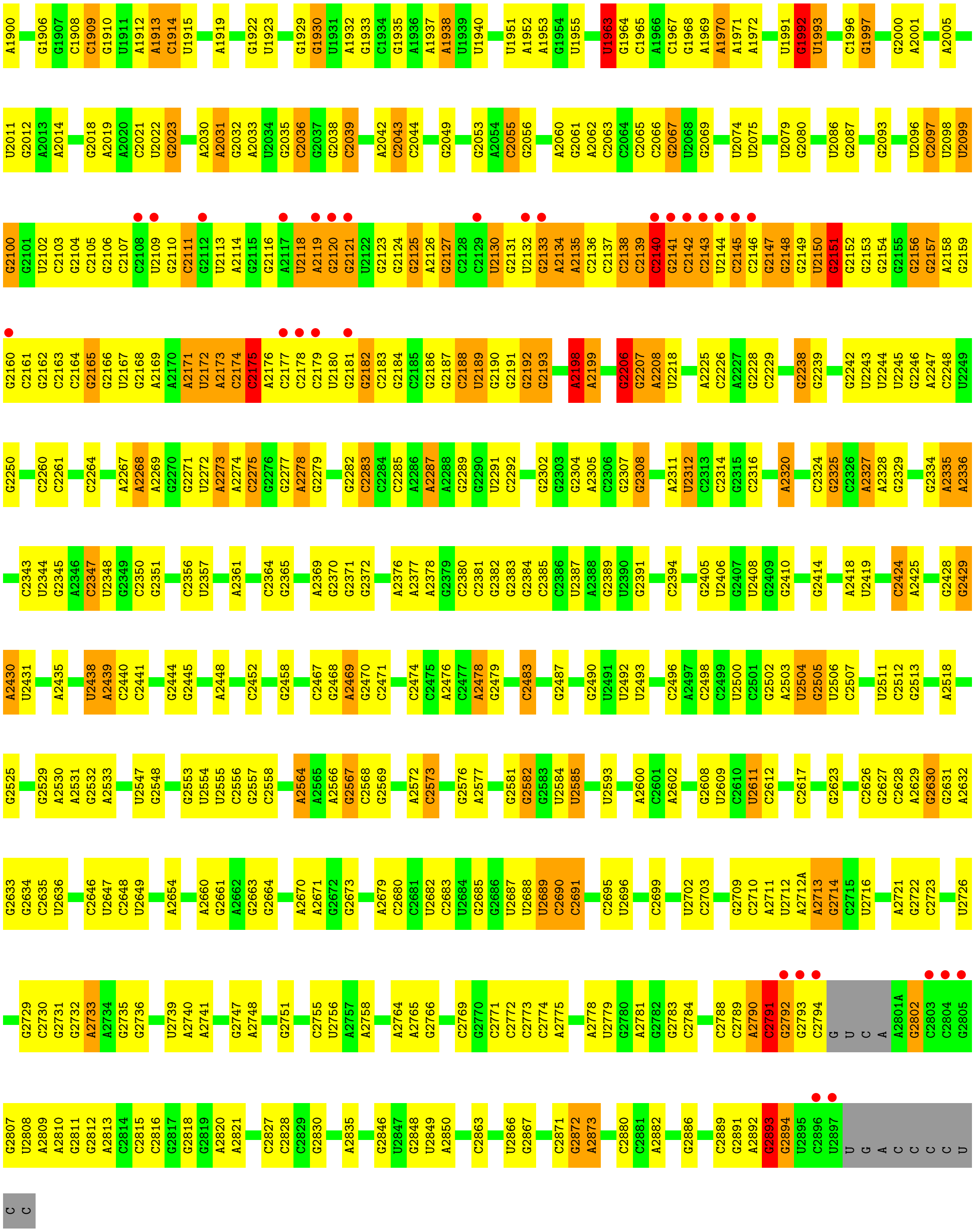
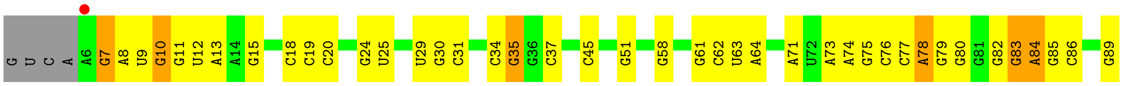
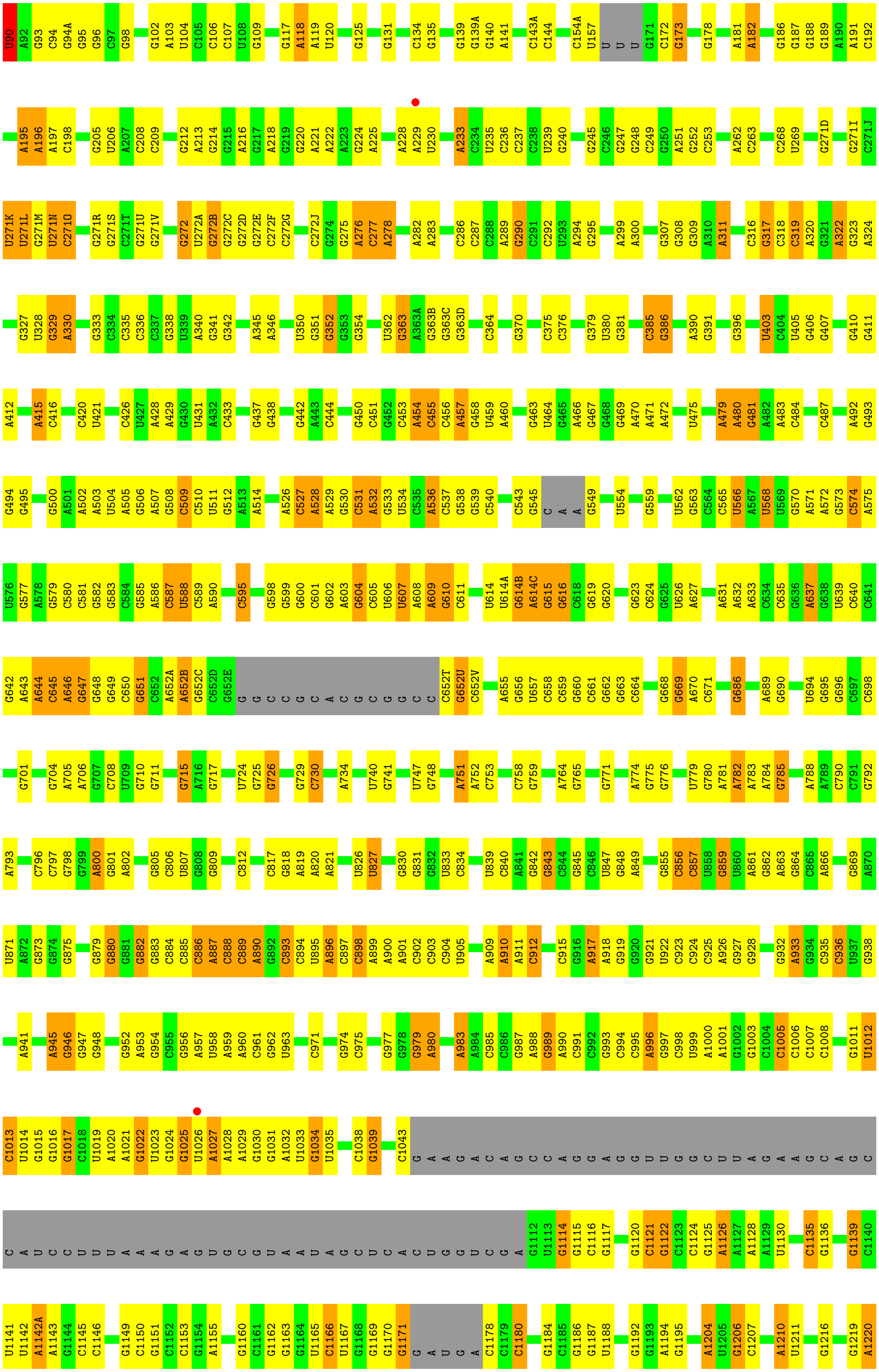


• Molecule 25: 23S Ribosomal RNA

Chain DA:

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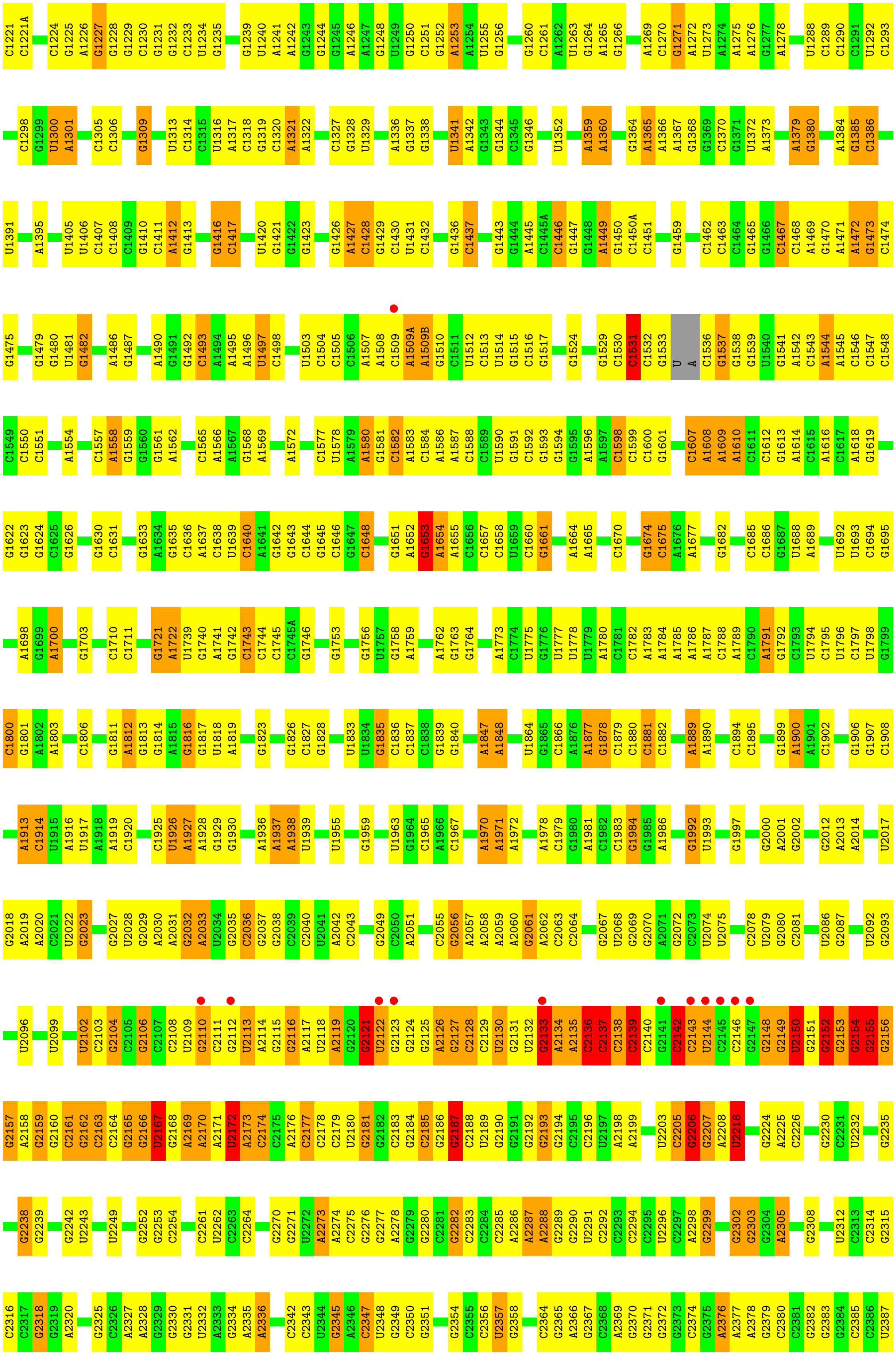
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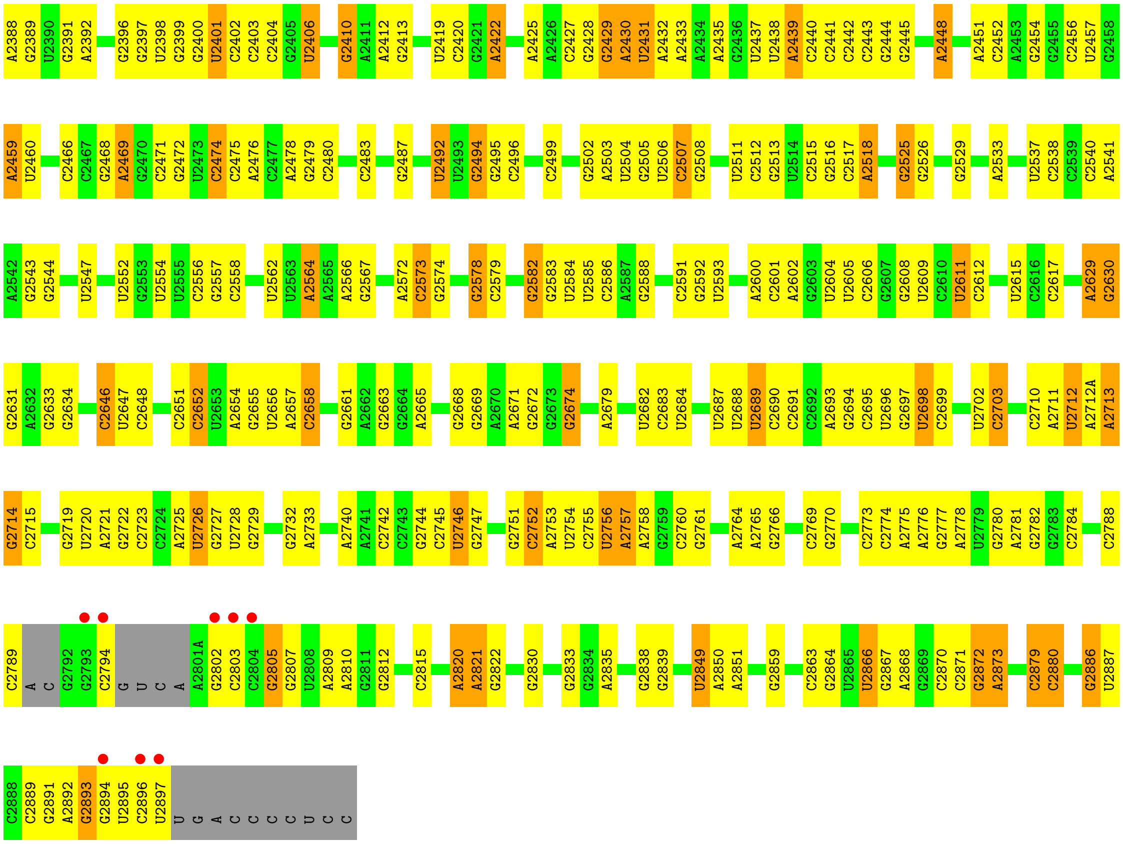
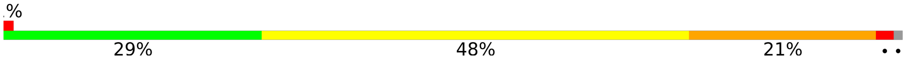


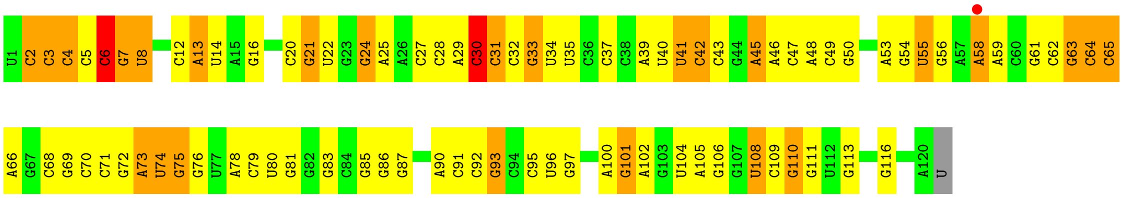
- Molecule 26: 5S Ribosomal RNA

Chain BB:

- Molecule 26: 5S Ribosomal RNA

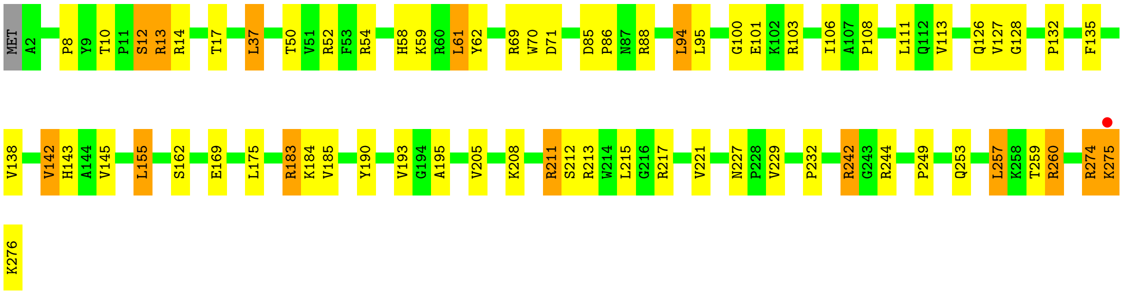
Chain DB:





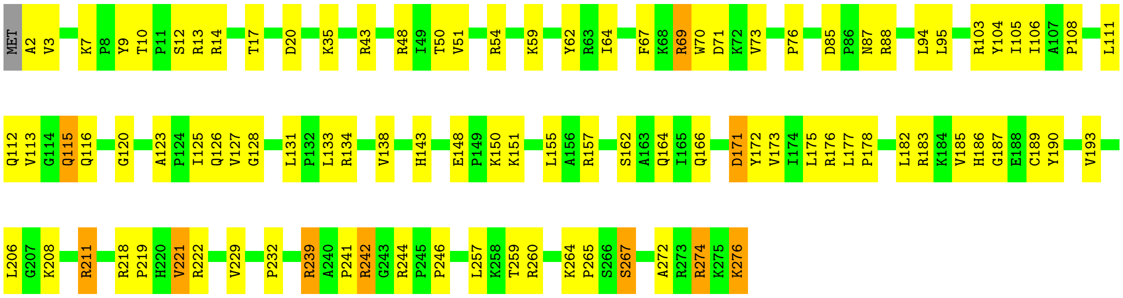
- Molecule 27: 50S ribosomal protein L2

Chain BD:



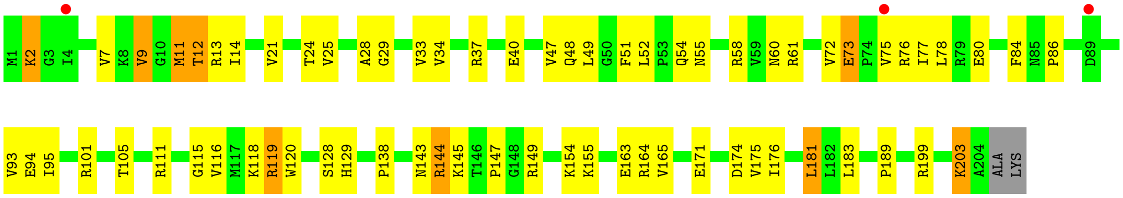
- Molecule 27: 50S ribosomal protein L2

Chain DD:



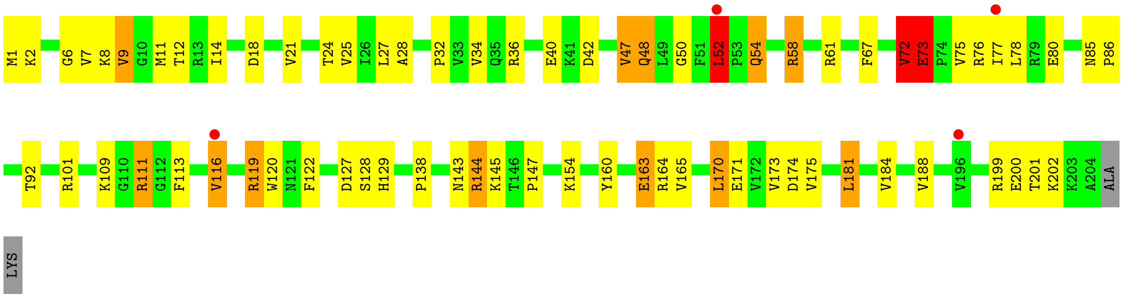
- Molecule 28: 50S ribosomal protein L3

Chain BE:



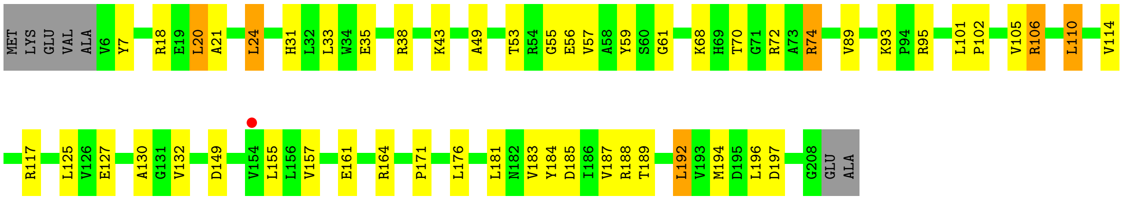
- Molecule 28: 50S ribosomal protein L3

Chain DE:



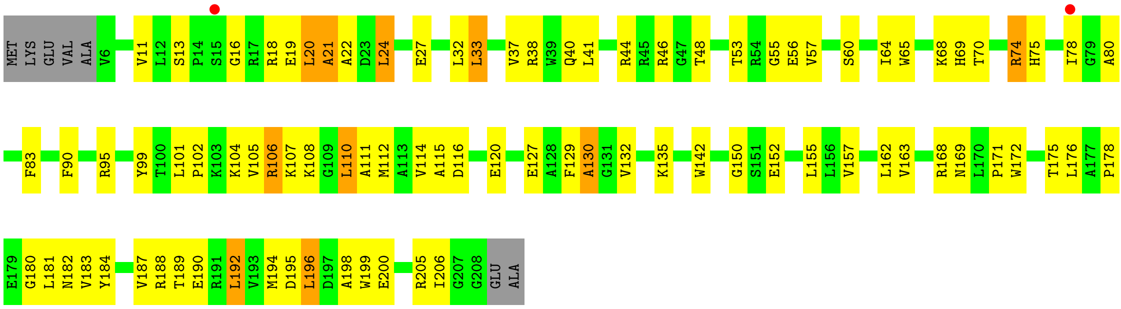
- Molecule 29: 50S ribosomal protein L4

Chain BF:



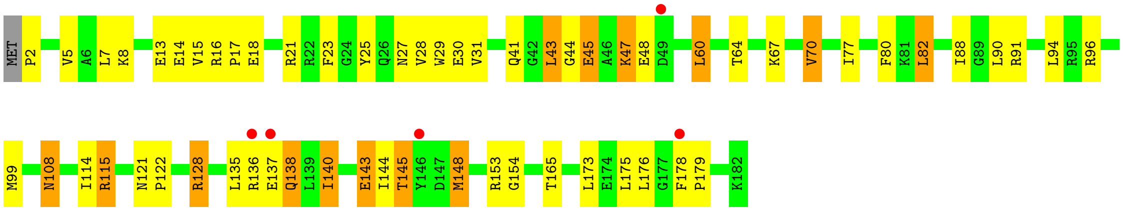
- Molecule 29: 50S ribosomal protein L4

Chain DF:



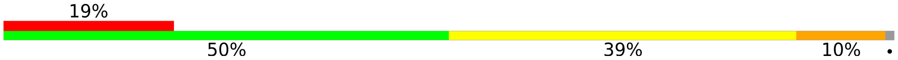
- Molecule 30: 50S ribosomal protein L5

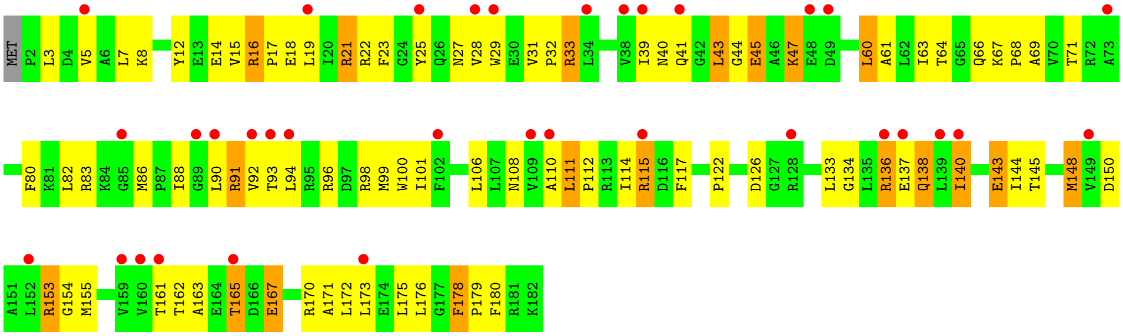
Chain BG:



- Molecule 30: 50S ribosomal protein L5

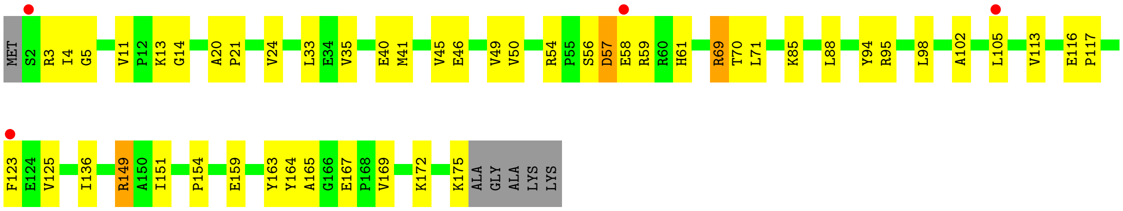
Chain DG:



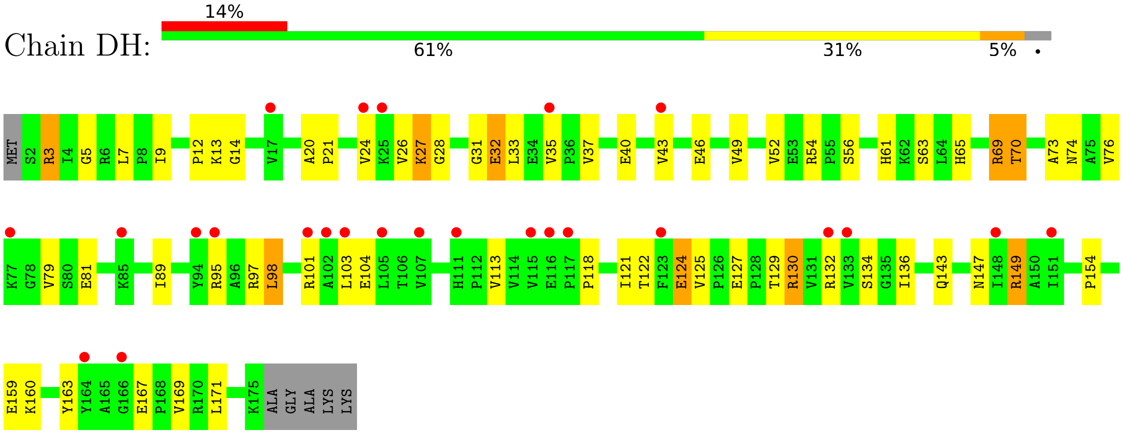


- Molecule 31: 50S ribosomal protein L6

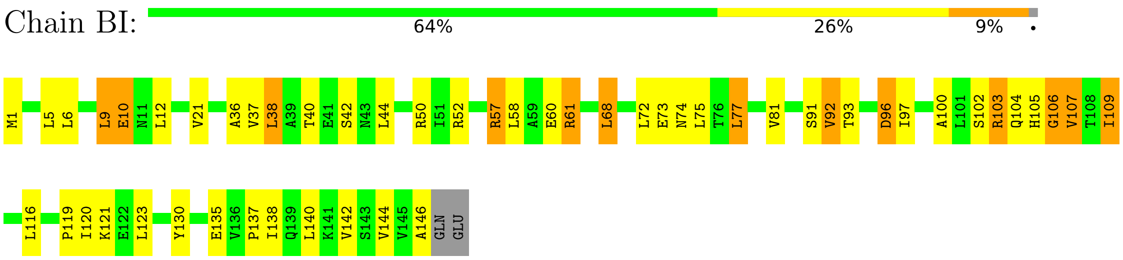
Chain BH:



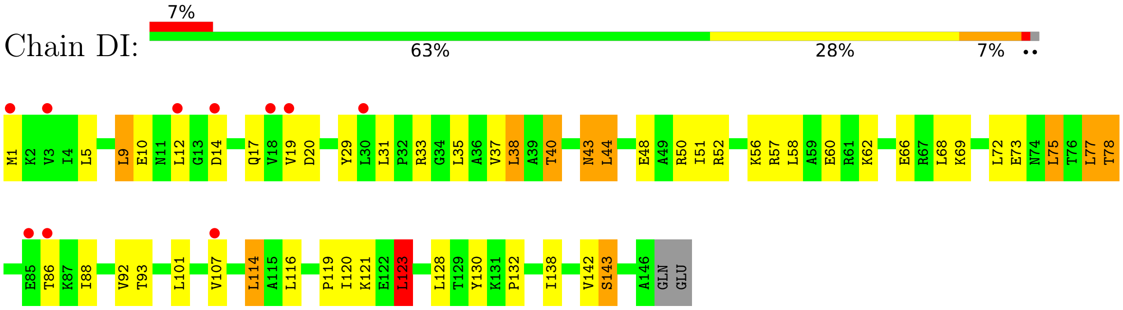
- Molecule 31: 50S ribosomal protein L6



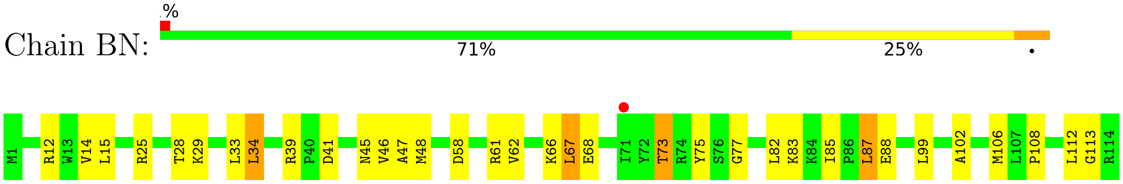
- Molecule 32: 50S ribosomal protein L9

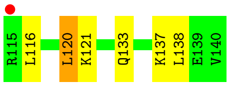


- Molecule 32: 50S ribosomal protein L9



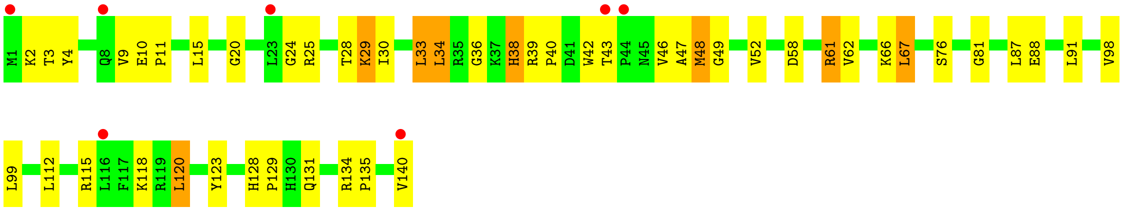
- Molecule 33: 50S ribosomal protein L13





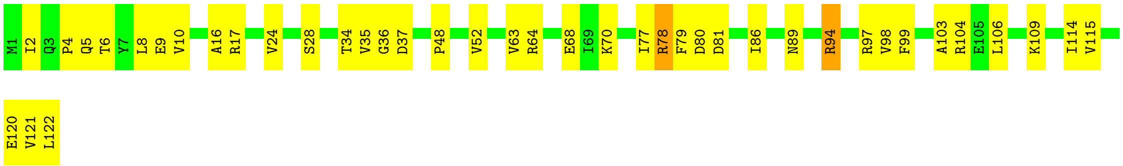
- Molecule 33: 50S ribosomal protein L13

Chain DN:



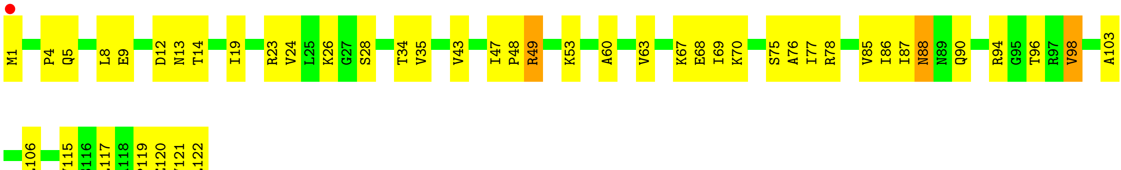
- Molecule 34: 50S ribosomal protein L14

Chain BO:



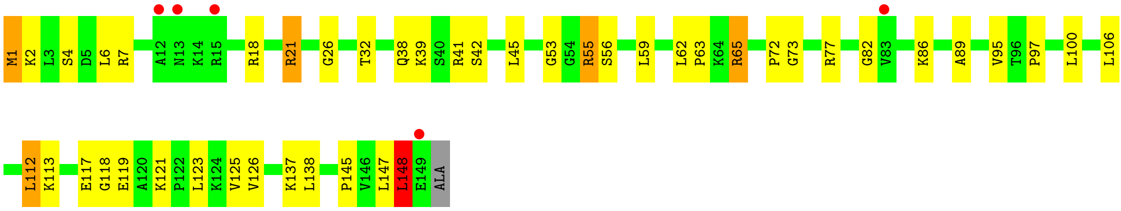
- Molecule 34: 50S ribosomal protein L14

Chain DO:



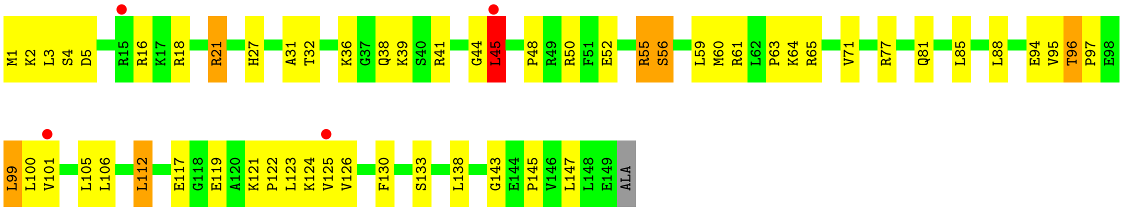
- Molecule 35: 50S ribosomal protein L15

Chain BP:



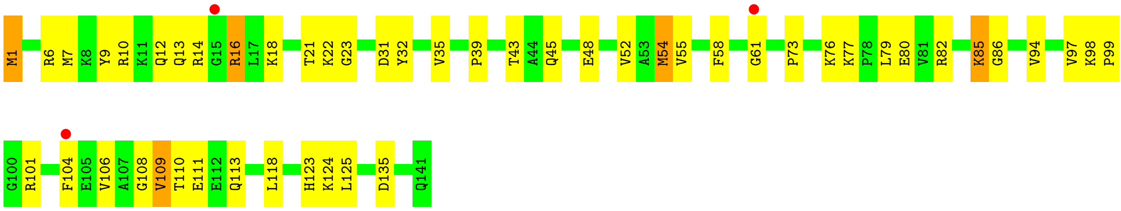
- Molecule 35: 50S ribosomal protein L15

Chain DP:



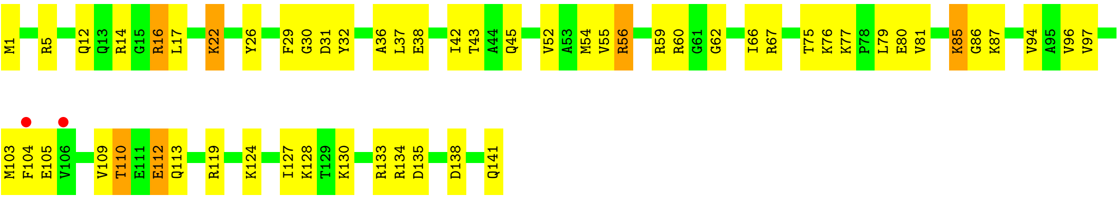
- Molecule 36: 50S ribosomal protein L16

Chain BQ:



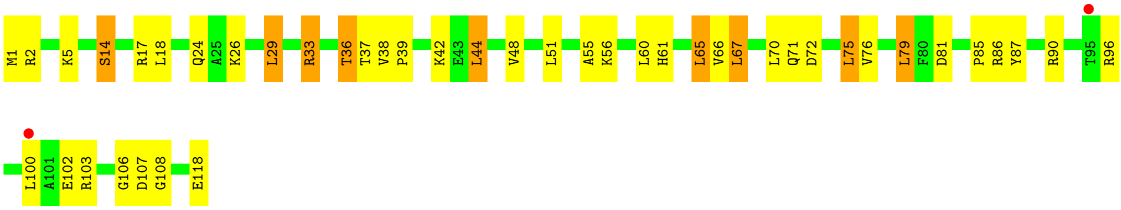
- Molecule 36: 50S ribosomal protein L16

Chain DQ:



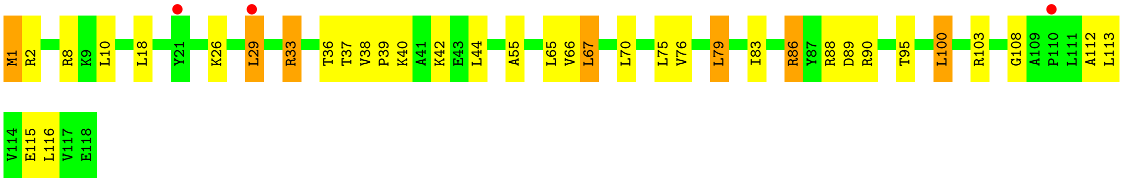
- Molecule 37: 50S ribosomal protein L17

Chain BR:



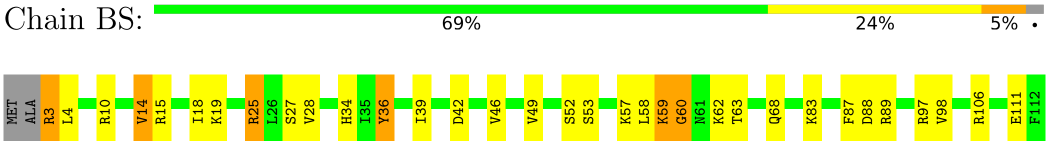
- Molecule 37: 50S ribosomal protein L17

Chain DR:



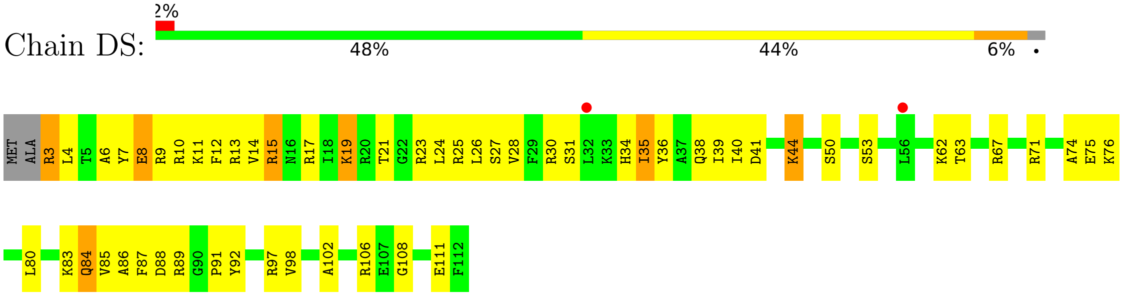
- Molecule 38: 50S ribosomal protein L18

Chain BS:



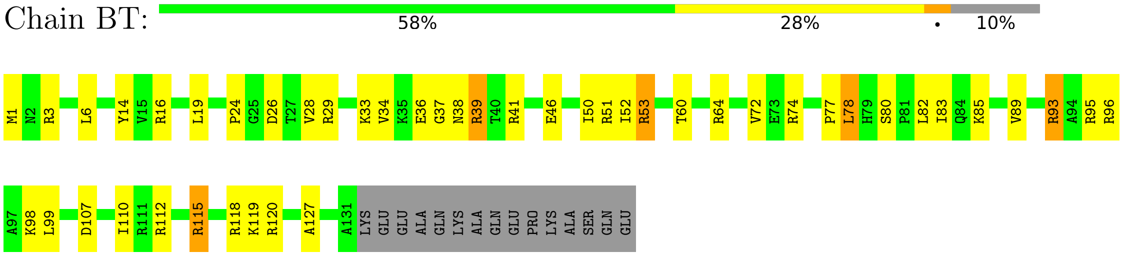
- Molecule 38: 50S ribosomal protein L18

Chain DS:



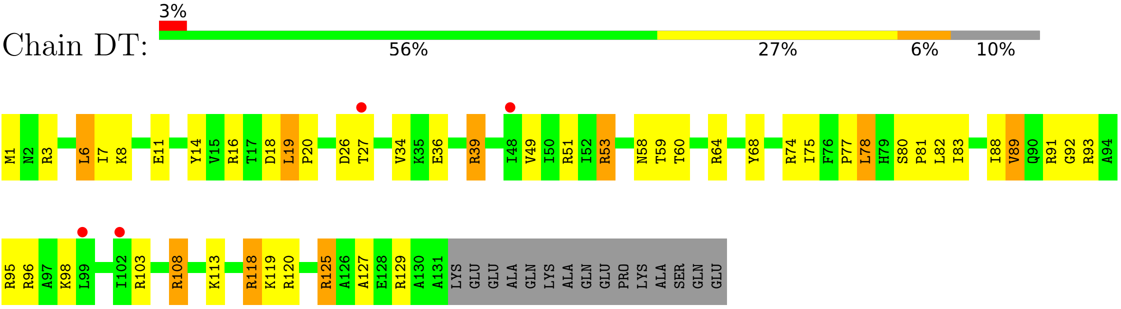
- Molecule 39: 50S ribosomal protein L19

Chain BT:



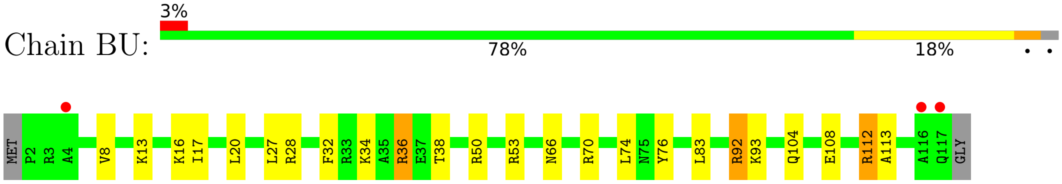
- Molecule 39: 50S ribosomal protein L19

Chain DT:



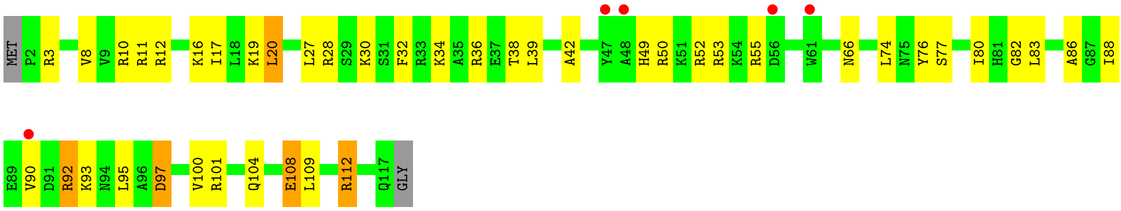
- Molecule 40: 50S ribosomal protein L20

Chain BU:



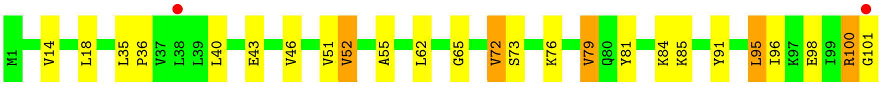
- Molecule 40: 50S ribosomal protein L20

Chain DU:



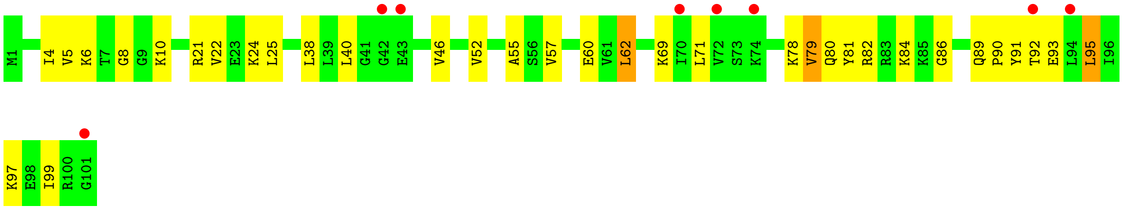
- Molecule 41: 50S ribosomal protein L21

Chain BV:



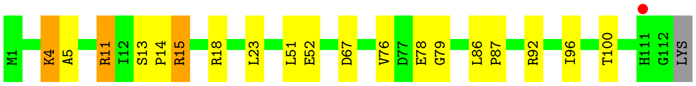
- Molecule 41: 50S ribosomal protein L21

Chain DV:



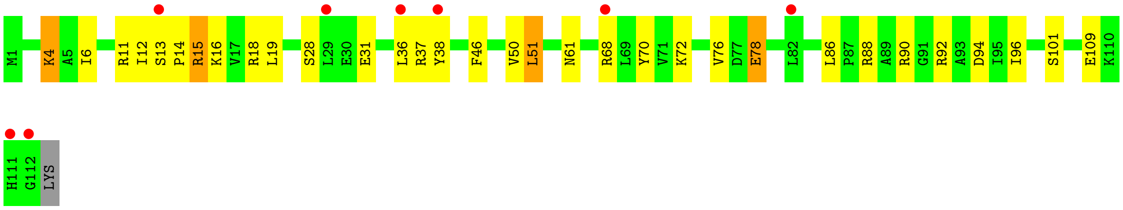
- Molecule 42: 50S ribosomal protein L22

Chain BW:



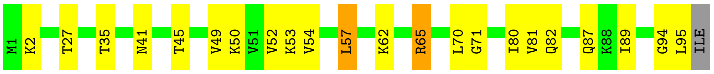
- Molecule 42: 50S ribosomal protein L22

Chain DW:

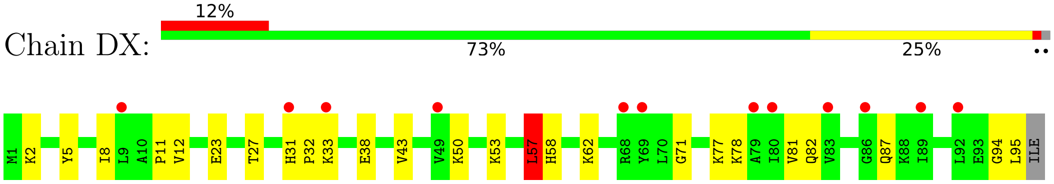


- Molecule 43: 50S ribosomal protein L23

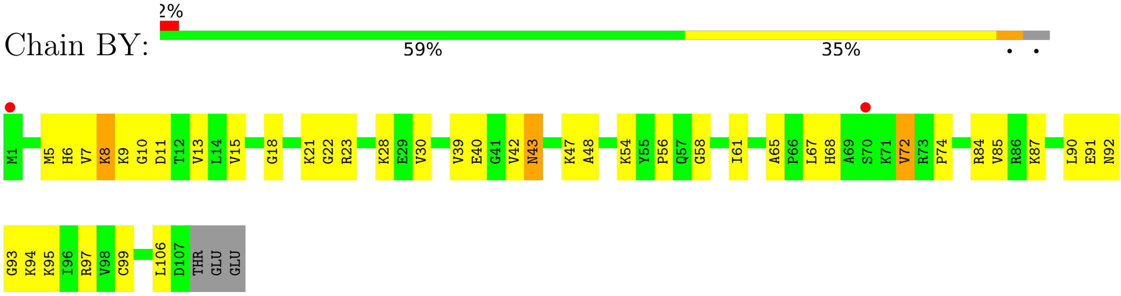
Chain BX:



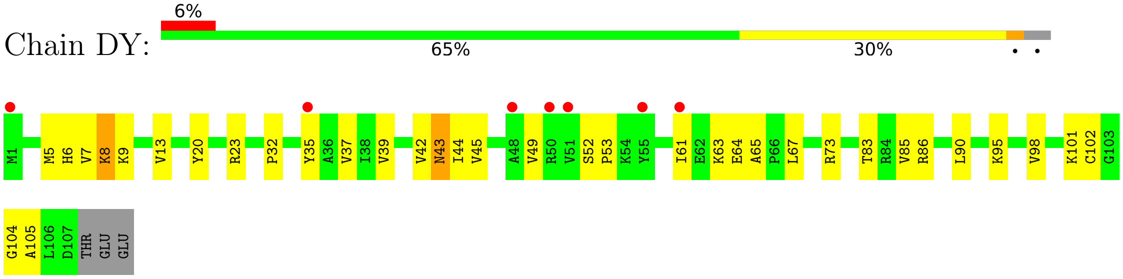
- Molecule 43: 50S ribosomal protein L23



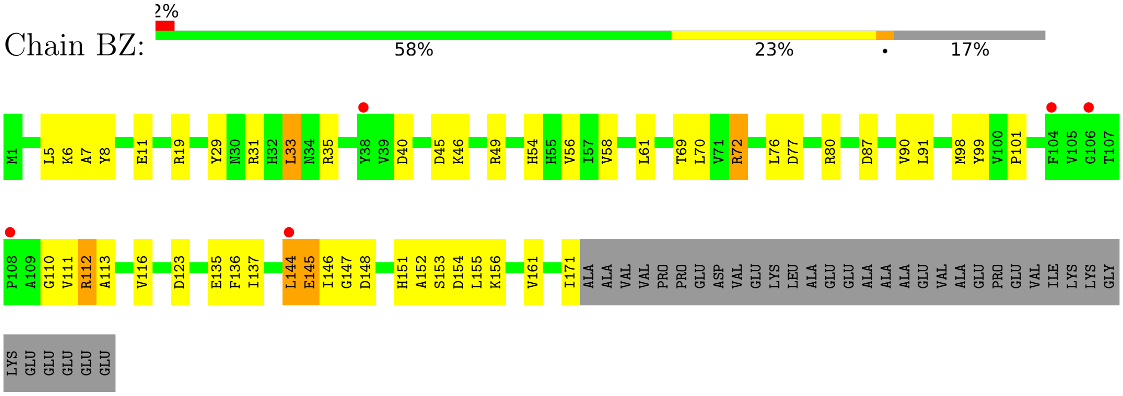
- Molecule 44: 50S ribosomal protein L24



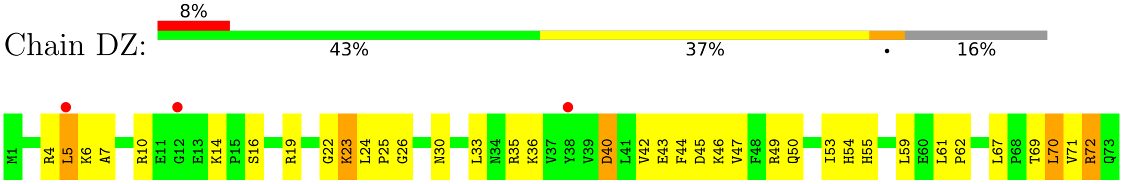
- Molecule 44: 50S ribosomal protein L24

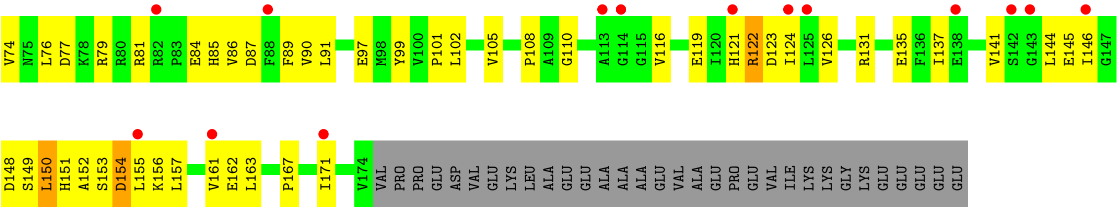


- Molecule 45: 50S ribosomal protein L25



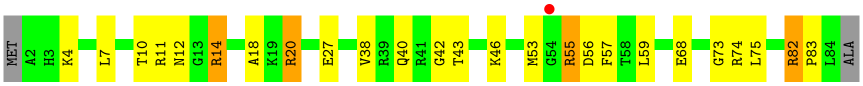
- Molecule 45: 50S ribosomal protein L25





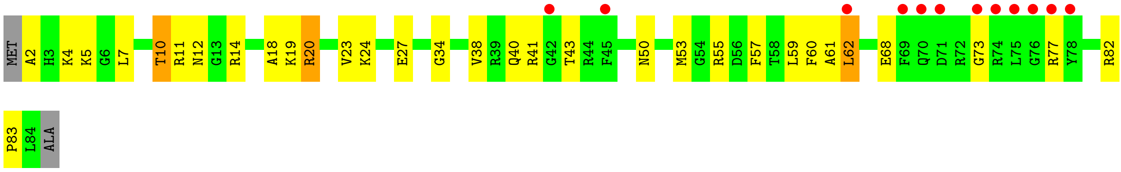
- Molecule 46: 50S ribosomal protein L27

Chain B0:



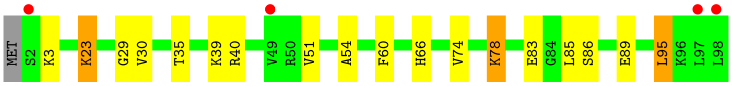
- Molecule 46: 50S ribosomal protein L27

Chain D0:



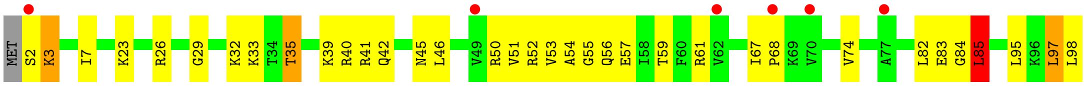
- Molecule 47: 50S ribosomal protein L28

Chain B1:



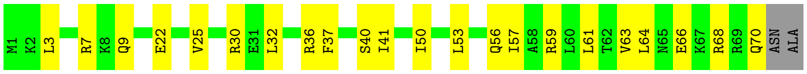
- Molecule 47: 50S ribosomal protein L28

Chain D1:



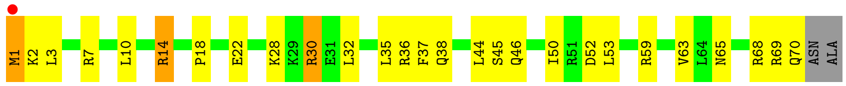
- Molecule 48: 50S ribosomal protein L29

Chain B2:



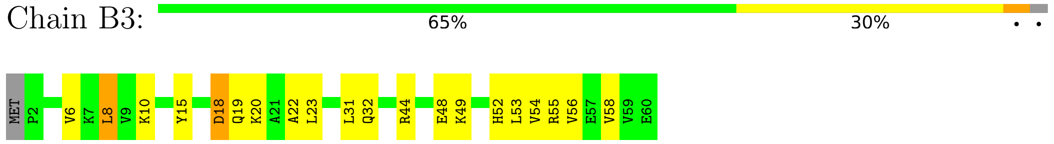
- Molecule 48: 50S ribosomal protein L29

Chain D2:



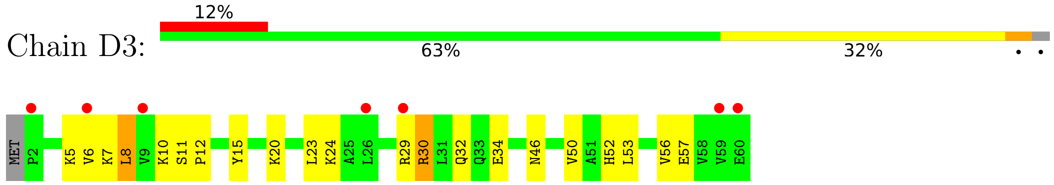
- Molecule 49: 50S ribosomal protein L30

Chain B3:



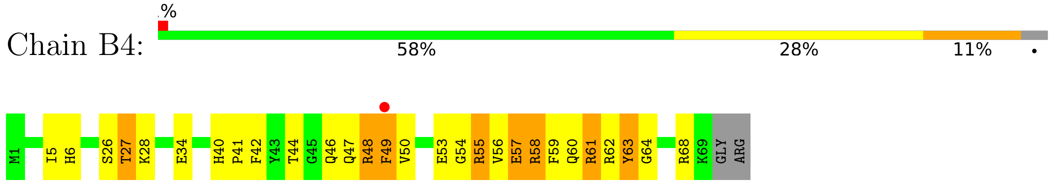
- Molecule 49: 50S ribosomal protein L30

Chain D3:



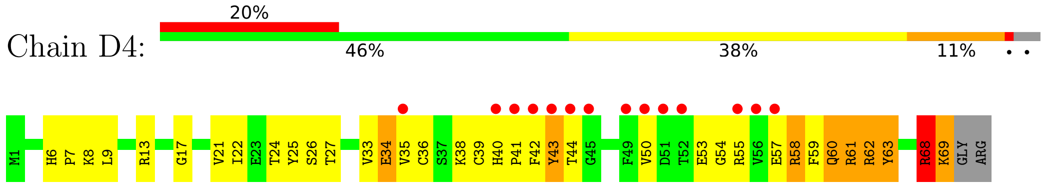
- Molecule 50: 50S ribosomal protein L31

Chain B4:



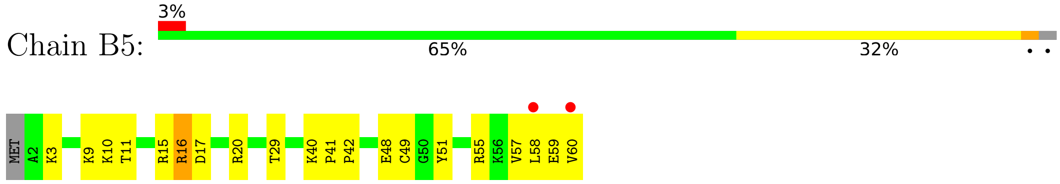
- Molecule 50: 50S ribosomal protein L31

Chain D4:



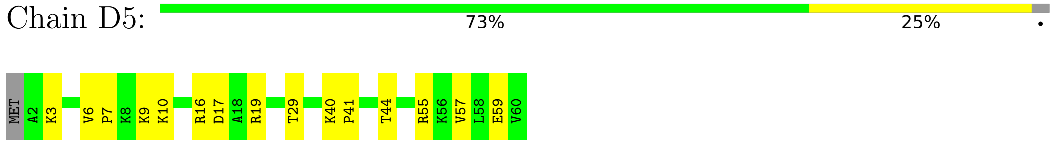
- Molecule 51: 50S ribosomal protein L32

Chain B5:



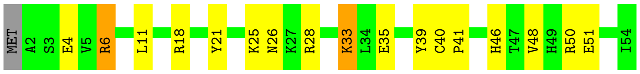
- Molecule 51: 50S ribosomal protein L32

Chain D5:



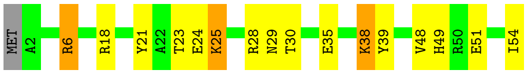
- Molecule 52: 50S ribosomal protein L33

Chain B6:



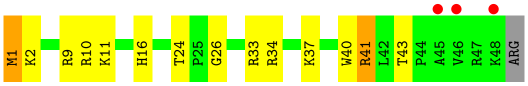
- Molecule 52: 50S ribosomal protein L33

Chain D6:



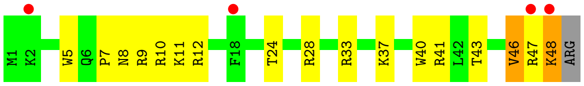
- Molecule 53: 50S ribosomal protein L34

Chain B7:



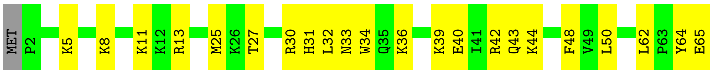
- Molecule 53: 50S ribosomal protein L34

Chain D7:



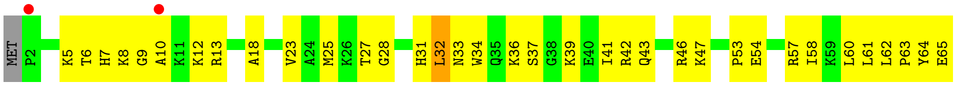
- Molecule 54: 50S ribosomal protein L35

Chain B8:



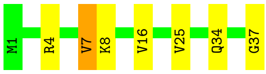
- Molecule 54: 50S ribosomal protein L35

Chain D8:



- Molecule 55: 50S ribosomal protein L36

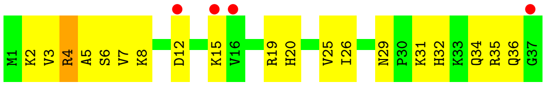
Chain B9:



- Molecule 55: 50S ribosomal protein L36

Chain D9:


11%
49%
49%
•


M1
K2
V3
R4
A5
S6
V7
K8
D12
K15
V16
R19
H20
V25
I26
N29
P30
K31
H32
K33
Q34
R35
Q36
G37

4 Data and refinement statistics ⓘ

Property	**Value**	**Source**
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	209.25Å 448.46Å 618.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	362.98 – 2.90 362.98 – 2.90	Depositor EDS
% Data completeness (in resolution range)	96.9 (362.98-2.90) 96.9 (362.98-2.90)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.31 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.231 , 0.286 0.231 , 0.286	Depositor DCC
R_{free} test set	61606 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	54.8	Xtriage
Anisotropy	0.140	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 72.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.37$, $< L^2 > = 0.19$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	289646	wwPDB-VP
Average B, all atoms (Å^2)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.87% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, 31H, PPU, ZN, MG, K, 4SU, 5MC, PSU, SF4

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	0.39	0/36049	0.94	50/56261 (0.1%)
1	CA	0.41	6/36170 (0.0%)	1.02	84/56452 (0.1%)
2	AB	0.31	0/1881	0.63	0/2542
2	CB	0.32	0/1860	0.65	3/2518 (0.1%)
3	AC	0.30	0/1576	0.51	0/2130
3	CC	0.31	0/1566	0.61	2/2119 (0.1%)
4	AD	0.31	0/1689	0.59	1/2267 (0.0%)
4	CD	0.30	0/1700	0.54	0/2280
5	AE	0.29	0/1145	0.56	0/1543
5	CE	0.32	0/1149	0.59	0/1548
6	AF	0.30	0/819	0.51	0/1111
6	CF	0.30	0/829	0.50	0/1123
7	AG	0.28	0/1250	0.51	0/1679
7	CG	0.30	0/1254	0.54	0/1683
8	AH	0.29	0/1108	0.51	0/1494
8	CH	0.28	0/1108	0.55	0/1494
9	AI	0.31	0/1002	0.59	0/1346
9	CI	0.32	0/997	0.56	0/1343
10	AJ	0.28	0/722	0.57	0/982
10	CJ	0.30	0/727	0.56	0/988
11	AK	0.28	0/844	0.51	0/1145
11	CK	0.29	0/848	0.51	0/1149
12	AL	0.31	0/946	0.51	0/1274
12	CL	0.31	0/946	0.57	0/1274
13	AM	0.28	0/969	0.63	0/1302
13	CM	0.32	0/961	0.61	0/1291
14	AN	0.32	0/501	0.54	0/664
14	CN	0.31	0/501	0.60	0/664
15	AO	0.29	0/739	0.50	0/985
15	CO	0.28	0/739	0.52	0/985
16	AP	0.30	0/697	0.54	0/939
16	CP	0.29	0/693	0.52	0/935

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\lvert Z\rvert >5$	RMSZ	$\#\lvert Z\rvert >5$
17	AQ	0.30	0/836	0.54	0/1117
17	CQ	0.29	0/836	0.52	0/1117
18	AR	0.29	0/560	0.54	0/746
18	CR	0.29	0/560	0.57	1/746 (0.1%)
19	AS	0.28	0/667	0.53	0/900
19	CS	0.32	0/661	0.67	0/893
20	AT	0.31	0/730	0.60	0/965
20	CT	0.29	0/729	0.63	1/965 (0.1%)
21	AU	0.28	0/203	0.49	0/266
21	CU	0.33	0/203	0.47	0/266
22	AV	0.42	0/310	0.95	0/480
22	CV	0.45	0/282	0.97	0/437
23	AW	0.35	0/18	0.66	0/26
23	CW	0.27	0/18	0.91	0/26
24	AX	0.52	0/1700	1.21	18/2650 (0.7%)
24	CX	0.55	3/1700 (0.2%)	1.24	16/2650 (0.6%)
25	BA	0.48	1/68013 (0.0%)	0.94	53/106165 (0.0%)
25	DA	0.42	0/67542	0.95	80/105428 (0.1%)
26	BB	0.42	0/2878	0.93	0/4490
26	DB	0.45	0/2878	1.00	3/4490 (0.1%)
27	BD	0.37	0/2186	0.57	0/2944
27	DD	0.33	0/2186	0.56	0/2944
28	BE	0.35	0/1592	0.55	0/2149
28	DE	0.33	0/1592	0.58	1/2149 (0.0%)
29	BF	0.34	0/1619	0.54	0/2193
29	DF	0.32	0/1615	0.57	0/2188
30	BG	0.30	0/1450	0.57	0/1959
30	DG	0.35	0/1449	0.61	0/1958
31	BH	0.32	0/1356	0.53	0/1834
31	DH	0.29	0/1356	0.55	0/1834
32	BI	0.29	0/1100	0.58	0/1501
32	DI	0.30	0/1076	0.60	1/1471 (0.1%)
33	BN	0.32	0/1144	0.52	0/1543
33	DN	0.31	0/1144	0.54	0/1543
34	BO	0.37	0/943	0.59	0/1269
34	DO	0.33	0/943	0.55	0/1269
35	BP	0.34	0/1152	0.58	1/1533 (0.1%)
35	DP	0.32	0/1152	0.60	0/1533
36	BQ	0.35	0/1143	0.53	0/1527
36	DQ	0.33	0/1143	0.55	0/1527
37	BR	0.34	0/982	0.55	0/1312
37	DR	0.30	0/982	0.53	0/1312
38	BS	0.33	0/887	0.56	0/1180

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\| >5$	RMSZ	#$\|Z\| >5$
38	DS	0.30	0/880	0.59	0/1172
39	BT	0.33	0/1105	0.56	0/1477
39	DT	0.30	0/1097	0.54	0/1468
40	BU	0.36	0/977	0.53	0/1301
40	DU	0.31	0/977	0.55	0/1301
41	BV	0.36	0/782	0.54	0/1049
41	DV	0.32	0/782	0.57	0/1049
42	BW	0.35	0/897	0.54	0/1205
42	DW	0.31	0/897	0.52	0/1205
43	BX	0.38	0/764	0.58	1/1025 (0.1%)
43	DX	0.32	0/764	0.56	1/1025 (0.1%)
44	BY	0.35	0/819	0.56	0/1095
44	DY	0.31	0/819	0.56	0/1095
45	BZ	0.33	0/1379	0.61	0/1873
45	DZ	0.30	0/1390	0.55	0/1890
46	B0	0.35	0/662	0.59	0/881
46	D0	0.31	0/662	0.50	0/881
47	B1	0.34	0/762	0.56	0/1014
47	D1	0.33	0/762	0.57	1/1014 (0.1%)
48	B2	0.32	0/590	0.57	0/781
48	D2	0.30	0/590	0.49	0/781
49	B3	0.35	0/474	0.55	0/635
49	D3	0.30	0/469	0.53	0/630
50	B4	0.36	0/565	0.71	0/761
50	D4	0.35	0/545	0.69	0/737
51	B5	0.33	0/469	0.55	0/635
51	D5	0.32	0/469	0.54	0/635
52	B6	0.39	0/460	0.53	0/613
52	D6	0.33	0/456	0.53	0/608
53	B7	0.37	0/426	0.56	0/561
53	D7	0.34	0/426	0.48	0/561
54	B8	0.37	0/519	0.55	0/684
54	D8	0.31	0/525	0.52	0/691
55	B9	0.35	0/310	0.50	0/407
55	D9	0.34	0/310	0.54	0/407
All	All	0.40	10/310281 (0.0%)	0.87	318/464152 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	AB	0	2
7	AG	0	1
20	CT	0	1
27	BD	0	1
38	BS	0	1
All	All	0	6

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	CA	1154	G	C6-N1	-12.01	1.31	1.39
1	CA	1154	G	N1-C2	-11.43	1.28	1.37
1	CA	1119	C	N3-C4	-10.12	1.26	1.33
1	CA	1154	G	N7-C5	-6.67	1.35	1.39
24	CX	14	A	N7-C5	-5.86	1.35	1.39

The worst 5 of 318 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	CA	1119	C	N1-C2-O2	29.84	136.81	118.90
1	CA	1154	G	C5-C6-O6	27.03	144.82	128.60
1	CA	1154	G	N3-C2-N2	25.60	137.82	119.90
1	CA	1154	G	N1-C2-N2	-23.27	95.25	116.20
1	CA	1119	C	C2-N3-C4	19.75	129.77	119.90

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	AB	231	GLU	Peptide
2	AB	9	GLU	Peptide
7	AG	79	ARG	Peptide
27	BD	274	ARG	Peptide
38	BS	58	LEU	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32205	0	16254	640	0
1	CA	32312	0	16307	729	0
2	AB	1846	0	1867	85	0
2	CB	1825	0	1828	97	0
3	AC	1552	0	1546	67	0
3	CC	1542	0	1517	73	0
4	AD	1659	0	1676	65	0
4	CD	1670	0	1703	68	0
5	AE	1129	0	1185	30	0
5	CE	1133	0	1191	53	0
6	AF	806	0	793	28	0
6	CF	816	0	808	22	0
7	AG	1231	0	1238	28	0
7	CG	1235	0	1249	30	0
8	AH	1088	0	1126	25	0
8	CH	1088	0	1126	38	0
9	AI	983	0	986	53	0
9	CI	978	0	966	55	0
10	AJ	709	0	650	34	0
10	CJ	714	0	672	35	0
11	AK	829	0	825	18	0
11	CK	833	0	836	23	0
12	AL	930	0	979	31	0
12	CL	930	0	980	33	0
13	AM	958	0	1002	39	0
13	CM	950	0	988	56	0
14	AN	492	0	529	25	0
14	CN	492	0	529	36	0
15	AO	728	0	760	22	0
15	CO	728	0	760	30	0
16	AP	681	0	697	31	0
16	CP	677	0	686	26	0
17	AQ	823	0	891	24	0
17	CQ	823	0	891	21	0
18	AR	555	0	618	13	0
18	CR	555	0	618	21	0
19	AS	652	0	662	28	0
19	CS	646	0	644	52	0
20	AT	728	0	798	26	0
20	CT	727	0	796	28	0
21	AU	199	0	208	8	0
21	CU	199	0	208	12	0
22	AV	277	0	140	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	CV	252	0	130	8	0
23	AW	54	0	40	5	0
23	CW	54	0	40	7	0
24	AX	1635	0	838	34	0
24	CX	1635	0	838	40	0
25	BA	60729	0	30621	812	0
25	DA	60311	0	30408	1066	0
26	BB	2573	0	1306	29	0
26	DB	2573	0	1306	91	0
27	BD	2136	0	2218	58	0
27	DD	2136	0	2217	68	0
28	BE	1559	0	1618	52	0
28	DE	1559	0	1618	56	0
29	BF	1584	0	1625	36	0
29	DF	1580	0	1619	68	0
30	BG	1425	0	1443	45	0
30	DG	1424	0	1434	77	0
31	BH	1330	0	1407	29	0
31	DH	1330	0	1407	42	0
32	BI	1085	0	1114	39	0
32	DI	1061	0	1080	34	0
33	BN	1117	0	1184	24	0
33	DN	1117	0	1184	33	0
34	BO	933	0	996	26	0
34	DO	933	0	996	34	0
35	BP	1135	0	1212	34	0
35	DP	1135	0	1211	50	0
36	BQ	1122	0	1179	35	0
36	DQ	1122	0	1179	43	0
37	BR	968	0	1033	28	0
37	DR	968	0	1033	27	0
38	BS	877	0	938	22	0
38	DS	870	0	923	53	0
39	BT	1091	0	1151	30	0
39	DT	1083	0	1136	37	0
40	BU	959	0	1019	18	0
40	DU	959	0	1019	33	0
41	BV	771	0	830	14	0
41	DV	771	0	830	26	0
42	BW	886	0	940	9	0
42	DW	886	0	940	18	0
43	BX	750	0	814	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	DX	750	0	814	17	0
44	BY	806	0	881	31	0
44	DY	806	0	881	26	0
45	BZ	1349	0	1355	30	0
45	DZ	1360	0	1363	64	0
46	B0	653	0	674	26	0
46	D0	653	0	674	25	0
47	B1	755	0	826	12	0
47	D1	755	0	826	26	0
48	B2	588	0	643	12	0
48	D2	588	0	643	17	0
49	B3	469	0	518	9	0
49	D3	464	0	514	17	0
50	B4	552	0	533	25	0
50	D4	532	0	503	30	0
51	B5	455	0	465	12	0
51	D5	455	0	465	13	0
52	B6	453	0	473	9	0
52	D6	449	0	469	13	0
53	B7	418	0	467	13	0
53	D7	418	0	467	14	0
54	B8	511	0	571	18	0
54	D8	517	0	582	33	0
55	B9	307	0	335	4	0
55	D9	307	0	335	13	0
56	AA	187	0	0	0	0
56	AD	1	0	0	0	0
56	AE	2	0	0	0	0
56	AF	1	0	0	0	0
56	AK	1	0	0	0	0
56	AL	1	0	0	0	0
56	AM	1	0	0	0	0
56	AN	1	0	0	0	0
56	AX	7	0	0	0	0
56	B0	5	0	0	0	0
56	B3	2	0	0	0	0
56	B4	1	0	0	0	0
56	B5	2	0	0	0	0
56	B7	4	0	0	0	0
56	B8	1	0	0	0	0
56	B9	1	0	0	0	0
56	BA	675	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	BB	18	0	0	0	0
56	BD	8	0	0	0	0
56	BE	6	0	0	0	0
56	BF	5	0	0	0	0
56	BG	3	0	0	0	0
56	BH	1	0	0	0	0
56	BN	2	0	0	0	0
56	BO	1	0	0	0	0
56	BP	4	0	0	0	0
56	BQ	3	0	0	0	0
56	BR	3	0	0	0	0
56	BU	5	0	0	0	0
56	BV	3	0	0	0	0
56	BW	4	0	0	0	0
56	BX	3	0	0	0	0
56	BY	2	0	0	0	0
56	BZ	1	0	0	0	0
56	CA	154	0	0	0	0
56	CE	2	0	0	0	0
56	CF	1	0	0	0	0
56	CJ	1	0	0	0	0
56	CK	1	0	0	0	0
56	CT	1	0	0	0	0
56	CX	1	0	0	0	0
56	D0	1	0	0	0	0
56	D3	1	0	0	0	0
56	D5	1	0	0	0	0
56	D7	1	0	0	0	0
56	D8	2	0	0	0	0
56	DA	595	0	0	0	0
56	DB	12	0	0	0	0
56	DD	2	0	0	0	0
56	DE	5	0	0	0	0
56	DF	3	0	0	0	0
56	DG	1	0	0	0	0
56	DN	1	0	0	0	0
56	DP	1	0	0	0	0
56	DQ	3	0	0	0	0
56	DR	2	0	0	0	0
56	DT	1	0	0	0	0
56	DU	1	0	0	0	0
56	DV	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	DW	2	0	0	0	0
56	DY	1	0	0	0	0
57	AD	8	0	0	0	0
57	CD	8	0	0	0	0
58	AN	1	0	0	0	0
58	B4	1	0	0	0	0
58	B5	1	0	0	0	0
58	B6	1	0	0	0	0
58	B9	1	0	0	0	0
58	BY	1	0	0	0	0
58	CN	1	0	0	0	0
58	D4	1	0	0	0	0
58	D5	1	0	0	0	0
58	D6	1	0	0	0	0
58	D9	1	0	0	0	0
58	DY	1	0	0	0	0
59	AX	1	0	0	0	0
59	DA	1	0	0	0	0
60	AA	165	0	0	12	0
60	AJ	1	0	0	0	0
60	AL	3	0	0	2	0
60	AP	1	0	0	0	0
60	AU	1	0	0	0	0
60	AV	2	0	0	0	0
60	AW	3	0	0	0	0
60	B0	4	0	0	0	0
60	B1	2	0	0	0	0
60	B2	1	0	0	0	0
60	B3	1	0	0	0	0
60	B5	2	0	0	0	0
60	B7	2	0	0	1	0
60	B8	8	0	0	2	0
60	BA	924	0	0	62	0
60	BB	27	0	0	0	0
60	BD	6	0	0	2	0
60	BE	8	0	0	0	0
60	BF	6	0	0	1	0
60	BG	1	0	0	0	0
60	BH	1	0	0	1	0
60	BN	3	0	0	0	0
60	BO	1	0	0	0	0
60	BP	14	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	BQ	2	0	0	0	0
60	BS	1	0	0	0	0
60	BT	4	0	0	1	0
60	BU	2	0	0	0	0
60	BV	5	0	0	0	0
60	BW	1	0	0	0	0
60	BX	2	0	0	0	0
60	BZ	1	0	0	0	0
60	CA	113	0	0	5	0
60	CE	2	0	0	0	0
60	CJ	2	0	0	1	0
60	CL	1	0	0	1	0
60	CO	1	0	0	0	0
60	CW	1	0	0	1	0
60	CX	1	0	0	1	0
60	D0	5	0	0	0	0
60	D1	1	0	0	0	0
60	D3	1	0	0	3	0
60	D8	3	0	0	0	0
60	DA	689	0	0	58	0
60	DB	9	0	0	0	0
60	DD	11	0	0	2	0
60	DE	5	0	0	1	0
60	DF	6	0	0	0	0
60	DO	1	0	0	0	0
60	DP	6	0	0	0	0
60	DU	3	0	0	0	0
60	DV	1	0	0	0	0
60	DW	1	0	0	0	0
60	DX	3	0	0	0	0
All	All	289646	0	193084	5717	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 13.

The worst 5 of 5717 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)
25:DA:2121:G:H1	25:DA:2177:C:N4	1.35	1.23
19:CS:42:PRO:HG3	50:D4:61:ARG:HG2	1.39	1.04
1:AA:1028:C:N4	1:AA:1033:G:H1	1.56	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:DA:2128:C:H42	25:DA:2160:G:H1	1.08	1.00
25:DA:2137:C:H42	25:DA:2154:G:H1	1.05	0.99

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	229/256 (90%)	208 (91%)	18 (8%)	3 (1%)	12	37
2	CB	229/256 (90%)	206 (90%)	17 (7%)	6 (3%)	5	20
3	AC	204/239 (85%)	193 (95%)	10 (5%)	1 (0%)	29	61
3	CC	204/239 (85%)	187 (92%)	15 (7%)	2 (1%)	15	45
4	AD	206/209 (99%)	195 (95%)	9 (4%)	2 (1%)	15	45
4	CD	206/209 (99%)	194 (94%)	11 (5%)	1 (0%)	29	61
5	AE	146/162 (90%)	140 (96%)	4 (3%)	2 (1%)	11	36
5	CE	146/162 (90%)	142 (97%)	4 (3%)	0	100	100
6	AF	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
6	CF	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
7	AG	153/156 (98%)	148 (97%)	2 (1%)	3 (2%)	7	27
7	CG	153/156 (98%)	151 (99%)	1 (1%)	1 (1%)	22	54
8	AH	135/138 (98%)	133 (98%)	2 (2%)	0	100	100
8	CH	135/138 (98%)	132 (98%)	3 (2%)	0	100	100
9	AI	125/128 (98%)	118 (94%)	7 (6%)	0	100	100
9	CI	125/128 (98%)	120 (96%)	5 (4%)	0	100	100
10	AJ	95/105 (90%)	87 (92%)	7 (7%)	1 (1%)	14	42
10	CJ	94/105 (90%)	87 (93%)	5 (5%)	2 (2%)	7	26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	AK	112/129 (87%)	104 (93%)	5 (4%)	3 (3%)	5	19
11	CK	112/129 (87%)	103 (92%)	7 (6%)	2 (2%)	8	29
12	AL	120/132 (91%)	115 (96%)	5 (4%)	0	100	100
12	CL	120/132 (91%)	113 (94%)	7 (6%)	0	100	100
13	AM	121/126 (96%)	113 (93%)	8 (7%)	0	100	100
13	CM	120/126 (95%)	114 (95%)	5 (4%)	1 (1%)	19	51
14	AN	58/61 (95%)	55 (95%)	3 (5%)	0	100	100
14	CN	58/61 (95%)	55 (95%)	3 (5%)	0	100	100
15	AO	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
15	CO	86/89 (97%)	81 (94%)	5 (6%)	0	100	100
16	AP	80/88 (91%)	77 (96%)	3 (4%)	0	100	100
16	CP	80/88 (91%)	77 (96%)	2 (2%)	1 (1%)	12	37
17	AQ	97/105 (92%)	92 (95%)	4 (4%)	1 (1%)	15	45
17	CQ	97/105 (92%)	94 (97%)	3 (3%)	0	100	100
18	AR	66/88 (75%)	65 (98%)	1 (2%)	0	100	100
18	CR	66/88 (75%)	65 (98%)	1 (2%)	0	100	100
19	AS	81/93 (87%)	76 (94%)	5 (6%)	0	100	100
19	CS	81/93 (87%)	75 (93%)	6 (7%)	0	100	100
20	AT	94/106 (89%)	87 (93%)	6 (6%)	1 (1%)	14	42
20	CT	94/106 (89%)	86 (92%)	5 (5%)	3 (3%)	4	16
21	AU	21/27 (78%)	21 (100%)	0	0	100	100
21	CU	21/27 (78%)	21 (100%)	0	0	100	100
27	BD	273/276 (99%)	263 (96%)	9 (3%)	1 (0%)	34	66
27	DD	273/276 (99%)	262 (96%)	9 (3%)	2 (1%)	22	54
28	BE	202/206 (98%)	195 (96%)	6 (3%)	1 (0%)	29	61
28	DE	202/206 (98%)	193 (96%)	7 (4%)	2 (1%)	15	45
29	BF	201/210 (96%)	197 (98%)	3 (2%)	1 (0%)	29	61
29	DF	201/210 (96%)	197 (98%)	2 (1%)	2 (1%)	15	45
30	BG	179/182 (98%)	171 (96%)	7 (4%)	1 (1%)	25	58
30	DG	179/182 (98%)	167 (93%)	11 (6%)	1 (1%)	25	58
31	BH	172/180 (96%)	169 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	DH	172/180 (96%)	168 (98%)	4 (2%)	0	100	100
32	BI	144/148 (97%)	130 (90%)	10 (7%)	4 (3%)	5	19
32	DI	144/148 (97%)	137 (95%)	6 (4%)	1 (1%)	22	54
33	BN	138/140 (99%)	137 (99%)	1 (1%)	0	100	100
33	DN	138/140 (99%)	135 (98%)	2 (1%)	1 (1%)	22	54
34	BO	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
34	DO	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
35	BP	147/150 (98%)	141 (96%)	6 (4%)	0	100	100
35	DP	147/150 (98%)	140 (95%)	5 (3%)	2 (1%)	11	36
36	BQ	139/141 (99%)	134 (96%)	5 (4%)	0	100	100
36	DQ	139/141 (99%)	133 (96%)	6 (4%)	0	100	100
37	BR	116/118 (98%)	112 (97%)	4 (3%)	0	100	100
37	DR	116/118 (98%)	111 (96%)	5 (4%)	0	100	100
38	BS	108/112 (96%)	103 (95%)	4 (4%)	1 (1%)	17	48
38	DS	108/112 (96%)	105 (97%)	2 (2%)	1 (1%)	17	48
39	BT	129/146 (88%)	123 (95%)	4 (3%)	2 (2%)	9	32
39	DT	129/146 (88%)	125 (97%)	3 (2%)	1 (1%)	19	51
40	BU	114/118 (97%)	114 (100%)	0	0	100	100
40	DU	114/118 (97%)	114 (100%)	0	0	100	100
41	BV	99/101 (98%)	93 (94%)	6 (6%)	0	100	100
41	DV	99/101 (98%)	95 (96%)	4 (4%)	0	100	100
42	BW	110/113 (97%)	110 (100%)	0	0	100	100
42	DW	110/113 (97%)	110 (100%)	0	0	100	100
43	BX	93/96 (97%)	89 (96%)	4 (4%)	0	100	100
43	DX	93/96 (97%)	90 (97%)	3 (3%)	0	100	100
44	BY	105/110 (96%)	99 (94%)	6 (6%)	0	100	100
44	DY	105/110 (96%)	102 (97%)	3 (3%)	0	100	100
45	BZ	169/206 (82%)	152 (90%)	16 (10%)	1 (1%)	25	58
45	DZ	172/206 (84%)	158 (92%)	14 (8%)	0	100	100
46	B0	81/85 (95%)	81 (100%)	0	0	100	100
46	D0	81/85 (95%)	79 (98%)	1 (1%)	1 (1%)	13	40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	B1	95/98 (97%)	94 (99%)	1 (1%)	0	100	100
47	D1	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	14	42
48	B2	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
48	D2	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
49	B3	57/60 (95%)	57 (100%)	0	0	100	100
49	D3	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
50	B4	67/71 (94%)	56 (84%)	9 (13%)	2 (3%)	4	17
50	D4	67/71 (94%)	54 (81%)	8 (12%)	5 (8%)	1	2
51	B5	57/60 (95%)	57 (100%)	0	0	100	100
51	D5	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
52	B6	51/54 (94%)	50 (98%)	1 (2%)	0	100	100
52	D6	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
53	B7	46/49 (94%)	46 (100%)	0	0	100	100
53	D7	46/49 (94%)	45 (98%)	0	1 (2%)	6	24
54	B8	62/65 (95%)	62 (100%)	0	0	100	100
54	D8	62/65 (95%)	62 (100%)	0	0	100	100
55	B9	35/37 (95%)	35 (100%)	0	0	100	100
55	D9	35/37 (95%)	35 (100%)	0	0	100	100
All	All	11409/12128 (94%)	10906 (96%)	432 (4%)	71 (1%)	25	58

5 of 71 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	19	HIS
2	AB	231	GLU
4	AD	166	LYS
7	AG	80	VAL
27	BD	275	LYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AB	192/220 (87%)	151 (79%)	41 (21%)	1	3
2	CB	187/220 (85%)	154 (82%)	33 (18%)	2	5
3	AC	143/188 (76%)	125 (87%)	18 (13%)	4	13
3	CC	140/188 (74%)	121 (86%)	19 (14%)	3	11
4	AD	170/181 (94%)	146 (86%)	24 (14%)	3	10
4	CD	172/181 (95%)	145 (84%)	27 (16%)	2	8
5	AE	113/123 (92%)	103 (91%)	10 (9%)	10	30
5	CE	114/123 (93%)	98 (86%)	16 (14%)	3	10
6	AF	83/90 (92%)	78 (94%)	5 (6%)	19	49
6	CF	85/90 (94%)	77 (91%)	8 (9%)	8	26
7	AG	119/127 (94%)	108 (91%)	11 (9%)	9	27
7	CG	120/127 (94%)	109 (91%)	11 (9%)	9	27
8	AH	114/119 (96%)	103 (90%)	11 (10%)	8	25
8	CH	114/119 (96%)	104 (91%)	10 (9%)	10	30
9	AI	90/99 (91%)	76 (84%)	14 (16%)	2	8
9	CI	89/99 (90%)	70 (79%)	19 (21%)	1	3
10	AJ	66/92 (72%)	63 (96%)	3 (4%)	27	61
10	CJ	69/92 (75%)	64 (93%)	5 (7%)	14	39
11	AK	82/99 (83%)	75 (92%)	7 (8%)	10	31
11	CK	83/99 (84%)	79 (95%)	4 (5%)	25	58
12	AL	97/109 (89%)	89 (92%)	8 (8%)	11	32
12	CL	97/109 (89%)	88 (91%)	9 (9%)	9	27
13	AM	93/101 (92%)	79 (85%)	14 (15%)	3	9
13	CM	92/101 (91%)	77 (84%)	15 (16%)	2	7
14	AN	49/50 (98%)	42 (86%)	7 (14%)	3	10
14	CN	49/50 (98%)	39 (80%)	10 (20%)	1	3
15	AO	78/80 (98%)	70 (90%)	8 (10%)	7	22
15	CO	78/80 (98%)	71 (91%)	7 (9%)	9	29
16	AP	69/74 (93%)	54 (78%)	15 (22%)	1	3
16	CP	68/74 (92%)	59 (87%)	9 (13%)	4	12
17	AQ	94/97 (97%)	87 (93%)	7 (7%)	13	38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	CQ	94/97 (97%)	88 (94%)	6 (6%)	17	45
18	AR	59/77 (77%)	52 (88%)	7 (12%)	5	15
18	CR	59/77 (77%)	52 (88%)	7 (12%)	5	15
19	AS	69/80 (86%)	63 (91%)	6 (9%)	10	30
19	CS	67/80 (84%)	59 (88%)	8 (12%)	5	15
20	AT	70/82 (85%)	61 (87%)	9 (13%)	4	13
20	CT	70/82 (85%)	59 (84%)	11 (16%)	2	8
21	AU	18/22 (82%)	15 (83%)	3 (17%)	2	6
21	CU	18/22 (82%)	15 (83%)	3 (17%)	2	6
27	BD	215/218 (99%)	196 (91%)	19 (9%)	10	30
27	DD	215/218 (99%)	194 (90%)	21 (10%)	8	24
28	BE	164/166 (99%)	144 (88%)	20 (12%)	5	15
28	DE	164/166 (99%)	143 (87%)	21 (13%)	4	13
29	BF	160/166 (96%)	146 (91%)	14 (9%)	10	30
29	DF	159/166 (96%)	144 (91%)	15 (9%)	8	26
30	BG	143/156 (92%)	123 (86%)	20 (14%)	3	10
30	DG	142/156 (91%)	118 (83%)	24 (17%)	2	6
31	BH	144/148 (97%)	136 (94%)	8 (6%)	21	52
31	DH	144/148 (97%)	131 (91%)	13 (9%)	9	29
32	BI	110/124 (89%)	93 (84%)	17 (16%)	2	8
32	DI	104/124 (84%)	87 (84%)	17 (16%)	2	7
33	BN	118/119 (99%)	104 (88%)	14 (12%)	5	15
33	DN	118/119 (99%)	104 (88%)	14 (12%)	5	15
34	BO	100/100 (100%)	92 (92%)	8 (8%)	12	33
34	DO	100/100 (100%)	90 (90%)	10 (10%)	7	23
35	BP	115/116 (99%)	102 (89%)	13 (11%)	6	18
35	DP	115/116 (99%)	103 (90%)	12 (10%)	7	21
36	BQ	111/111 (100%)	100 (90%)	11 (10%)	8	24
36	DQ	111/111 (100%)	98 (88%)	13 (12%)	5	16
37	BR	101/101 (100%)	86 (85%)	15 (15%)	3	9
37	DR	101/101 (100%)	90 (89%)	11 (11%)	6	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	BS	87/88 (99%)	80 (92%)	7 (8%)	12	33
38	DS	85/88 (97%)	76 (89%)	9 (11%)	6	20
39	BT	115/127 (91%)	104 (90%)	11 (10%)	8	25
39	DT	113/127 (89%)	98 (87%)	15 (13%)	4	11
40	BU	93/94 (99%)	85 (91%)	8 (9%)	10	30
40	DU	93/94 (99%)	85 (91%)	8 (9%)	10	30
41	BV	80/82 (98%)	72 (90%)	8 (10%)	7	23
41	DV	80/82 (98%)	75 (94%)	5 (6%)	18	46
42	BW	90/92 (98%)	82 (91%)	8 (9%)	9	29
42	DW	90/92 (98%)	84 (93%)	6 (7%)	16	43
43	BX	77/78 (99%)	73 (95%)	4 (5%)	23	55
43	DX	77/78 (99%)	75 (97%)	2 (3%)	46	77
44	BY	85/91 (93%)	77 (91%)	8 (9%)	8	26
44	DY	85/91 (93%)	81 (95%)	4 (5%)	26	59
45	BZ	145/179 (81%)	126 (87%)	19 (13%)	4	12
45	DZ	145/179 (81%)	128 (88%)	17 (12%)	5	16
46	B0	65/67 (97%)	61 (94%)	4 (6%)	18	47
46	D0	65/67 (97%)	61 (94%)	4 (6%)	18	47
47	B1	80/83 (96%)	75 (94%)	5 (6%)	18	46
47	D1	80/83 (96%)	73 (91%)	7 (9%)	10	30
48	B2	65/67 (97%)	61 (94%)	4 (6%)	18	47
48	D2	65/67 (97%)	57 (88%)	8 (12%)	4	14
49	B3	51/52 (98%)	45 (88%)	6 (12%)	5	16
49	D3	50/52 (96%)	46 (92%)	4 (8%)	12	33
50	B4	59/63 (94%)	50 (85%)	9 (15%)	2	8
50	D4	53/63 (84%)	40 (76%)	13 (24%)	0	2
51	B5	50/52 (96%)	44 (88%)	6 (12%)	5	15
51	D5	50/52 (96%)	46 (92%)	4 (8%)	12	33
52	B6	51/52 (98%)	45 (88%)	6 (12%)	5	16
52	D6	50/52 (96%)	45 (90%)	5 (10%)	7	23
53	B7	41/42 (98%)	37 (90%)	4 (10%)	8	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
53	D7	41/42 (98%)	37 (90%)	4 (10%)	8	24
54	B8	53/55 (96%)	49 (92%)	4 (8%)	13	37
54	D8	54/55 (98%)	50 (93%)	4 (7%)	13	38
55	B9	34/34 (100%)	32 (94%)	2 (6%)	19	49
55	D9	34/34 (100%)	30 (88%)	4 (12%)	5	16
All	All	9318/10066 (93%)	8277 (89%)	1041 (11%)	6	18

5 of 1041 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
38	DS	83	LYS
41	DV	79	VAL
38	DS	80	LEU
55	D9	26	ILE
38	BS	14	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 128 such sidechains are listed below:

Mol	Chain	Res	Type
35	DP	38	GLN
41	DV	64	HIS
40	BU	94	ASN
39	BT	123	GLN
44	DY	43	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1495/1521 (98%)	387 (25%)	22 (1%)
1	CA	1501/1521 (98%)	391 (26%)	24 (1%)
22	AV	12/24 (50%)	4 (33%)	0
22	CV	11/24 (45%)	4 (36%)	0
23	AW	0/2	-	-
23	CW	0/2	-	-
24	AX	74/77 (96%)	25 (33%)	1 (1%)
24	CX	74/77 (96%)	26 (35%)	1 (1%)
25	BA	2811/2915 (96%)	537 (19%)	24 (0%)
25	DA	2791/2915 (95%)	622 (22%)	29 (1%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
26	BB	120/121 (99%)	19 (15%)	3 (2%)
26	DB	119/121 (98%)	36 (30%)	0
All	All	9008/9320 (96%)	2051 (22%)	104 (1%)

5 of 2051 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	5	U
1	AA	6	G
1	AA	7	G
1	AA	9	G
1	AA	22	G

5 of 104 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	CA	532	A
1	CA	1279	A
25	DA	2406	U
1	CA	748	C
1	CA	1067	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
23	PPU	AW	76	23,25	32,40,41	1.00	2 (6%)	33,57,60	1.77	9 (27%)
24	5MU	CX	54	24	19,22,23	1.29	4 (21%)	28,32,35	2.14	6 (21%)
24	5MU	AX	54	24,56	19,22,23	1.38	5 (26%)	28,32,35	2.05	6 (21%)
24	PSU	AX	55	24	18,21,22	1.36	3 (16%)	22,30,33	1.90	3 (13%)
24	31H	CX	76	24	28,34,35	1.16	3 (10%)	23,47,50	1.62	4 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
24	4SU	AX	8	24	18,21,22	2.17	5 (27%)	26,30,33	1.64	5 (19%)
24	5MC	AX	32	24	18,22,23	0.98	2 (11%)	26,32,35	1.32	3 (11%)
24	PSU	CX	55	24	18,21,22	1.33	2 (11%)	22,30,33	1.84	4 (18%)
24	4SU	CX	8	24	18,21,22	2.02	6 (33%)	26,30,33	1.54	5 (19%)
23	PPU	CW	76	23	32,40,41	0.90	1 (3%)	33,57,60	1.67	7 (21%)
24	5MC	CX	32	24	18,22,23	0.93	2 (11%)	26,32,35	1.12	2 (7%)
24	31H	AX	76	24,56	28,34,35	1.13	3 (10%)	23,47,50	1.70	4 (17%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	PPU	AW	76	23,25	-	5/21/43/44	0/4/4/4
24	5MU	CX	54	24	-	0/7/25/26	0/2/2/2
24	5MU	AX	54	24,56	-	0/7/25/26	0/2/2/2
24	PSU	AX	55	24	-	1/7/25/26	0/2/2/2
24	31H	CX	76	24	-	10/18/40/41	0/3/3/3
24	4SU	AX	8	24	-	0/7/25/26	0/2/2/2
24	5MC	AX	32	24	-	0/7/25/26	0/2/2/2
24	PSU	CX	55	24	-	0/7/25/26	0/2/2/2
24	4SU	CX	8	24	-	0/7/25/26	0/2/2/2
23	PPU	CW	76	23	-	5/21/43/44	0/4/4/4
24	5MC	CX	32	24	-	0/7/25/26	0/2/2/2
24	31H	AX	76	24,56	-	5/18/40/41	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AX	8	4SU	C4-N3	-5.13	1.32	1.37
24	CX	8	4SU	C4-N3	-4.50	1.32	1.37
24	AX	8	4SU	C4-S4	-4.37	1.60	1.68
24	CX	8	4SU	C4-S4	-4.17	1.60	1.68
24	AX	8	4SU	C2-N3	-4.01	1.30	1.38

The worst 5 of 58 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	AX	55	PSU	N1-C2-N3	5.90	121.81	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	CX	55	PSU	N1-C2-N3	5.82	121.73	115.13
24	AX	76	31H	N3-C2-N1	-5.81	119.59	128.68
24	CX	76	31H	N3-C2-N1	-5.51	120.06	128.68
24	AX	54	5MU	N3-C2-N1	5.44	122.12	114.89

There are no chirality outliers.

5 of 26 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	AW	76	PPU	O4'-C4'-C5'-O5'
23	AW	76	PPU	C3'-C4'-C5'-O5'
24	AX	76	31H	C3'-C4'-C5'-O5'
24	AX	76	31H	OCN-CN-N-CA
23	CW	76	PPU	C3'-C4'-C5'-O5'

There are no ring outliers.

9 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	AW	76	PPU	5	0
24	CX	54	5MU	2	0
24	AX	54	5MU	1	0
24	AX	55	PSU	1	0
24	CX	76	31H	4	0
24	CX	55	PSU	1	0
24	CX	8	4SU	1	0
23	CW	76	PPU	7	0
24	AX	76	31H	3	0

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 1780 ligands modelled in this entry, 1778 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
57	SF4	AD	501	4	0,12,12	-	-	-		
57	SF4	CD	501	4	0,12,12	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	SF4	AD	501	4	-	-	0/6/5/5
57	SF4	CD	501	4	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	AA	1498/1521 (98%)	0.06	3 (0%) 95 95	39, 74, 94, 105	0
1	CA	1503/1521 (98%)	0.01	8 (0%) 91 91	41, 75, 94, 105	0
2	AB	231/256 (90%)	0.28	5 (2%) 62 59	65, 82, 90, 96	0
2	CB	231/256 (90%)	0.84	32 (13%) 2 2	67, 83, 92, 96	0
3	AC	206/239 (86%)	0.54	15 (7%) 15 11	67, 78, 86, 94	0
3	CC	206/239 (86%)	0.76	28 (13%) 3 2	69, 80, 87, 92	0
4	AD	208/209 (99%)	0.56	15 (7%) 15 11	57, 72, 82, 86	0
4	CD	208/209 (99%)	0.45	8 (3%) 40 36	57, 73, 82, 87	0
5	AE	148/162 (91%)	0.45	5 (3%) 45 40	55, 71, 81, 86	0
5	CE	148/162 (91%)	0.68	13 (8%) 10 7	58, 73, 82, 89	0
6	AF	100/101 (99%)	0.21	1 (1%) 82 82	55, 71, 80, 82	0
6	CF	100/101 (99%)	0.05	0 100 100	58, 73, 80, 82	0
7	AG	155/156 (99%)	0.39	12 (7%) 13 10	67, 76, 85, 94	0
7	CG	155/156 (99%)	0.55	15 (9%) 7 6	68, 78, 86, 96	0
8	AH	137/138 (99%)	0.20	1 (0%) 87 87	62, 72, 78, 86	0
8	CH	137/138 (99%)	0.43	4 (2%) 51 47	62, 73, 80, 88	0
9	AI	127/128 (99%)	0.26	4 (3%) 49 44	64, 82, 87, 90	0
9	CI	127/128 (99%)	1.55	42 (33%) 0 0	67, 83, 89, 91	0
10	AJ	97/105 (92%)	0.19	5 (5%) 27 23	63, 80, 89, 95	0
10	CJ	96/105 (91%)	1.10	22 (22%) 0 0	70, 86, 93, 100	0
11	AK	114/129 (88%)	0.47	5 (4%) 34 30	54, 72, 81, 83	0
11	CK	114/129 (88%)	0.37	4 (3%) 44 38	56, 72, 80, 83	0
12	AL	122/132 (92%)	0.29	1 (0%) 86 86	55, 65, 75, 78	0
12	CL	122/132 (92%)	0.31	2 (1%) 72 71	57, 67, 75, 80	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	AM	123/126 (97%)	0.53	10 (8%) 12 9	64, 78, 86, 91	0
13	CM	122/126 (96%)	0.80	17 (13%) 2 2	68, 80, 88, 93	0
14	AN	60/61 (98%)	0.85	7 (11%) 4 3	65, 76, 83, 86	0
14	CN	60/61 (98%)	1.78	22 (36%) 0 0	69, 79, 84, 88	0
15	AO	88/89 (98%)	0.13	1 (1%) 80 80	56, 69, 80, 90	0
15	CO	88/89 (98%)	0.26	0 100 100	56, 70, 80, 90	0
16	AP	82/88 (93%)	0.35	1 (1%) 79 79	58, 73, 83, 85	0
16	CP	82/88 (93%)	0.46	2 (2%) 59 56	58, 72, 82, 85	0
17	AQ	99/105 (94%)	0.26	0 100 100	60, 70, 81, 85	0
17	CQ	99/105 (94%)	0.26	0 100 100	57, 70, 80, 84	0
18	AR	68/88 (77%)	0.38	2 (2%) 51 47	60, 70, 81, 85	0
18	CR	68/88 (77%)	0.32	1 (1%) 73 73	61, 72, 82, 86	0
19	AS	83/93 (89%)	0.27	0 100 100	67, 81, 88, 96	0
19	CS	83/93 (89%)	0.97	13 (15%) 2 1	71, 83, 91, 97	0
20	AT	96/106 (90%)	0.59	8 (8%) 11 8	58, 72, 82, 89	0
20	CT	96/106 (90%)	0.31	3 (3%) 49 44	59, 72, 82, 88	0
21	AU	23/27 (85%)	0.65	0 100 100	65, 75, 80, 86	0
21	CU	23/27 (85%)	1.43	7 (30%) 0 0	66, 76, 83, 87	0
22	AV	13/24 (54%)	1.49	3 (23%) 0 0	60, 92, 100, 100	0
22	CV	12/24 (50%)	2.00	5 (41%) 0 0	63, 93, 99, 99	0
23	AW	1/2 (50%)	0.70	0 100 100	42, 42, 42, 42	0
23	CW	1/2 (50%)	1.07	0 100 100	59, 59, 59, 59	0
24	AX	71/77 (92%)	0.09	0 100 100	37, 72, 84, 92	0
24	CX	71/77 (92%)	0.01	0 100 100	39, 73, 86, 92	0
25	BA	2819/2915 (96%)	0.32	32 (1%) 80 80	23, 46, 89, 107	0
25	DA	2800/2915 (96%)	0.02	23 (0%) 86 86	26, 50, 90, 107	0
26	BB	120/121 (99%)	0.23	0 100 100	40, 65, 76, 91	0
26	DB	120/121 (99%)	0.05	1 (0%) 86 86	44, 70, 81, 93	0
27	BD	275/276 (99%)	0.26	1 (0%) 92 93	24, 45, 61, 77	0
27	DD	275/276 (99%)	0.27	0 100 100	27, 47, 63, 78	0
28	BE	204/206 (99%)	0.39	3 (1%) 73 73	18, 44, 66, 80	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
28	DE	204/206 (99%)	0.30	4 (1%)	65	63	32, 57, 72, 86	0
29	BF	203/210 (96%)	0.41	1 (0%)	91	91	26, 55, 74, 84	0
29	DF	203/210 (96%)	0.11	2 (0%)	82	82	26, 58, 75, 85	0
30	BG	181/182 (99%)	0.38	5 (2%)	53	49	56, 70, 82, 91	0
30	DG	181/182 (99%)	0.88	34 (18%)	1	0	61, 73, 85, 91	0
31	BH	174/180 (96%)	0.38	4 (2%)	60	58	51, 66, 76, 82	0
31	DH	174/180 (96%)	0.85	25 (14%)	2	2	55, 69, 80, 85	0
32	BI	146/148 (98%)	0.16	0	100	100	46, 74, 85, 87	0
32	DI	146/148 (98%)	0.28	10 (6%)	17	13	50, 75, 84, 87	0
33	BN	140/140 (100%)	0.41	2 (1%)	75	75	33, 53, 72, 80	0
33	DN	140/140 (100%)	0.59	7 (5%)	28	25	36, 56, 72, 81	0
34	BO	122/122 (100%)	0.15	0	100	100	25, 43, 60, 76	0
34	DO	122/122 (100%)	0.18	1 (0%)	86	86	42, 59, 73, 77	0
35	BP	149/150 (99%)	0.45	5 (3%)	45	40	27, 57, 73, 87	0
35	DP	149/150 (99%)	0.41	4 (2%)	54	50	29, 59, 76, 86	0
36	BQ	141/141 (100%)	0.44	3 (2%)	63	61	35, 53, 64, 71	0
36	DQ	141/141 (100%)	0.47	2 (1%)	75	75	38, 56, 68, 76	0
37	BR	118/118 (100%)	0.32	2 (1%)	70	69	25, 37, 56, 66	0
37	DR	118/118 (100%)	0.44	3 (2%)	57	55	40, 54, 66, 76	0
38	BS	110/112 (98%)	0.16	0	100	100	40, 52, 63, 68	0
38	DS	110/112 (98%)	0.39	2 (1%)	68	67	57, 76, 86, 92	0
39	BT	131/146 (89%)	0.03	0	100	100	32, 50, 74, 86	0
39	DT	131/146 (89%)	0.33	4 (3%)	49	44	44, 60, 75, 85	0
40	BU	116/118 (98%)	0.42	3 (2%)	56	52	23, 35, 55, 76	0
40	DU	116/118 (98%)	0.75	5 (4%)	35	31	41, 61, 77, 87	0
41	BV	101/101 (100%)	0.25	2 (1%)	65	63	19, 43, 64, 76	0
41	DV	101/101 (100%)	0.57	8 (7%)	12	10	44, 71, 80, 88	0
42	BW	112/113 (99%)	0.41	1 (0%)	84	84	21, 38, 53, 75	0
42	DW	112/113 (99%)	0.72	8 (7%)	16	12	31, 51, 69, 85	0
43	BX	95/96 (98%)	0.36	0	100	100	25, 43, 64, 82	0
43	DX	95/96 (98%)	0.85	12 (12%)	3	3	43, 62, 78, 91	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB($\AA^2$)	Q<0.9
44	BY	107/110 (97%)	0.38	2 (1%) 66 65	36, 51, 69, 80	0
44	DY	107/110 (97%)	0.63	7 (6%) 18 14	55, 72, 81, 89	0
45	BZ	171/206 (83%)	0.35	5 (2%) 51 47	42, 63, 77, 92	0
45	DZ	174/206 (84%)	0.75	17 (9%) 7 5	61, 80, 90, 100	0
46	B0	83/85 (97%)	0.26	1 (1%) 79 79	16, 43, 56, 66	0
46	D0	83/85 (97%)	0.85	12 (14%) 2 1	44, 65, 74, 80	0
47	B1	97/98 (98%)	0.24	4 (4%) 37 32	27, 49, 70, 77	0
47	D1	97/98 (98%)	0.43	6 (6%) 20 16	38, 59, 75, 78	0
48	B2	70/72 (97%)	0.27	0 100 100	37, 50, 66, 72	0
48	D2	70/72 (97%)	0.38	1 (1%) 75 75	58, 70, 79, 85	0
49	B3	59/60 (98%)	0.25	0 100 100	26, 41, 61, 72	0
49	D3	59/60 (98%)	0.93	7 (11%) 4 3	44, 64, 77, 80	0
50	B4	69/71 (97%)	0.14	1 (1%) 75 75	57, 76, 91, 94	0
50	D4	69/71 (97%)	0.94	14 (20%) 1 0	77, 87, 97, 104	0
51	B5	59/60 (98%)	0.38	2 (3%) 45 40	19, 38, 57, 78	0
51	D5	59/60 (98%)	0.35	0 100 100	31, 52, 69, 76	0
52	B6	53/54 (98%)	0.04	0 100 100	29, 43, 60, 71	0
52	D6	53/54 (98%)	0.12	0 100 100	50, 63, 75, 83	0
53	B7	48/49 (97%)	0.47	3 (6%) 20 16	20, 30, 53, 72	0
53	D7	48/49 (97%)	0.54	4 (8%) 11 8	35, 46, 71, 76	0
54	B8	64/65 (98%)	0.39	0 100 100	27, 36, 47, 55	0
54	D8	64/65 (98%)	0.60	2 (3%) 49 44	44, 58, 67, 75	0
55	B9	37/37 (100%)	0.58	0 100 100	31, 52, 64, 69	0
55	D9	37/37 (100%)	0.68	4 (10%) 5 4	44, 58, 67, 73	0
All	All	20634/21448 (96%)	0.31	663 (3%) 47 43	16, 64, 87, 107	0

The worst 5 of 663 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	CM	124	PRO	11.0
14	CN	25	VAL	7.0
13	CM	123	ALA	6.4
22	AV	24	A	6.3
31	DH	115	VAL	6.1

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

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
24	4SU	CX	8	20/21	0.92	0.15	65,84,90,94	0
24	PSU	CX	55	20/21	0.92	0.14	59,68,84,85	0
24	5MU	CX	54	21/22	0.93	0.20	66,78,87,98	0
24	31H	CX	76	32/33	0.94	0.30	33,54,78,89	0
24	4SU	AX	8	20/21	0.95	0.17	50,63,78,79	0
24	PSU	AX	55	20/21	0.95	0.14	57,66,78,79	0
23	PPU	CW	76	37/38	0.96	0.27	31,50,63,70	0
24	5MU	AX	54	21/22	0.96	0.15	55,69,75,82	0
24	5MC	CX	32	21/22	0.96	0.15	52,69,78,83	0
23	PPU	AW	76	37/38	0.97	0.23	25,33,43,45	0
24	5MC	AX	32	21/22	0.97	0.17	46,61,70,75	0
24	31H	AX	76	32/33	0.97	0.27	27,44,76,98	0

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	DG	3001	1/1	0.35	0.26	81,81,81,81	0
56	MG	CA	3016	1/1	0.67	0.14	68,68,68,68	0
56	MG	DA	3251	1/1	0.69	0.18	62,62,62,62	0
56	MG	AA	3181	1/1	0.69	0.18	53,53,53,53	0
56	MG	BA	3649	1/1	0.70	0.14	50,50,50,50	0
56	MG	DA	3275	1/1	0.71	0.10	45,45,45,45	0
56	MG	DA	3506	1/1	0.73	0.14	65,65,65,65	0
56	MG	BB	3010	1/1	0.74	0.14	77,77,77,77	0
56	MG	BA	3619	1/1	0.75	0.16	30,30,30,30	0
56	MG	AA	3023	1/1	0.75	0.20	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DA	3479	1/1	0.75	0.12	63,63,63,63	0
56	MG	CA	3086	1/1	0.75	0.09	68,68,68,68	0
56	MG	DA	3121	1/1	0.75	0.43	50,50,50,50	0
56	MG	CA	3011	1/1	0.76	0.17	66,66,66,66	0
56	MG	DA	3561	1/1	0.76	0.18	63,63,63,63	0
56	MG	CA	3154	1/1	0.76	0.14	62,62,62,62	0
56	MG	AA	3184	1/1	0.77	0.17	74,74,74,74	0
56	MG	DA	3485	1/1	0.77	0.12	60,60,60,60	0
56	MG	BA	3278	1/1	0.77	0.12	50,50,50,50	0
56	MG	AA	3147	1/1	0.77	0.08	67,67,67,67	0
56	MG	DB	3005	1/1	0.77	0.21	56,56,56,56	0
56	MG	AA	3062	1/1	0.77	0.18	58,58,58,58	0
56	MG	BA	3639	1/1	0.78	0.19	64,64,64,64	0
56	MG	DA	3187	1/1	0.78	0.13	46,46,46,46	0
56	MG	BZ	3001	1/1	0.78	0.25	58,58,58,58	0
56	MG	CA	3126	1/1	0.78	0.23	73,73,73,73	0
56	MG	BA	3090	1/1	0.78	0.20	44,44,44,44	0
56	MG	CA	3083	1/1	0.79	0.20	66,66,66,66	0
56	MG	BA	3350	1/1	0.79	0.17	59,59,59,59	0
56	MG	CA	3121	1/1	0.79	0.13	61,61,61,61	0
56	MG	BA	3373	1/1	0.79	0.17	41,41,41,41	0
56	MG	BA	3127	1/1	0.79	0.25	45,45,45,45	0
56	MG	BA	3028	1/1	0.80	0.16	41,41,41,41	0
56	MG	DA	3354	1/1	0.80	0.19	51,51,51,51	0
56	MG	CA	3136	1/1	0.80	0.12	53,53,53,53	0
56	MG	CA	3036	1/1	0.80	0.11	56,56,56,56	0
56	MG	BA	3569	1/1	0.80	0.18	55,55,55,55	0
56	MG	BA	3056	1/1	0.80	0.13	46,46,46,46	0
56	MG	AA	3024	1/1	0.80	0.18	60,60,60,60	0
56	MG	DA	3264	1/1	0.80	0.17	47,47,47,47	0
56	MG	BA	3125	1/1	0.81	0.19	51,51,51,51	0
56	MG	AA	3010	1/1	0.81	0.15	60,60,60,60	0
56	MG	AA	3088	1/1	0.81	0.16	62,62,62,62	0
56	MG	BB	3003	1/1	0.81	0.09	61,61,61,61	0
56	MG	DA	3150	1/1	0.81	0.70	55,55,55,55	0
56	MG	DB	3007	1/1	0.81	0.14	38,38,38,38	0
56	MG	DA	3398	1/1	0.81	0.13	51,51,51,51	0
56	MG	CA	3071	1/1	0.82	0.18	51,51,51,51	0
56	MG	DA	3474	1/1	0.82	0.11	62,62,62,62	0
56	MG	CA	3004	1/1	0.82	0.13	51,51,51,51	0
56	MG	AA	3027	1/1	0.83	0.16	71,71,71,71	0
56	MG	BA	3576	1/1	0.83	0.17	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	CA	3131	1/1	0.83	0.08	65,65,65,65	0
56	MG	BA	3580	1/1	0.83	0.14	62,62,62,62	0
56	MG	BA	3585	1/1	0.83	0.16	50,50,50,50	0
56	MG	DA	3022	1/1	0.83	0.13	39,39,39,39	0
56	MG	BA	3601	1/1	0.83	0.14	50,50,50,50	0
56	MG	AA	3183	1/1	0.83	0.19	55,55,55,55	0
56	MG	BA	3075	1/1	0.83	0.28	58,58,58,58	0
56	MG	BA	3082	1/1	0.83	0.21	47,47,47,47	0
56	MG	AA	3180	1/1	0.83	0.11	56,56,56,56	0
56	MG	BB	3009	1/1	0.84	0.12	67,67,67,67	0
56	MG	BA	3446	1/1	0.84	0.20	61,61,61,61	0
56	MG	DA	3021	1/1	0.84	0.15	55,55,55,55	0
56	MG	BE	303	1/1	0.84	0.19	41,41,41,41	0
56	MG	BP	203	1/1	0.84	0.14	47,47,47,47	0
56	MG	BA	3550	1/1	0.84	0.17	44,44,44,44	0
56	MG	B8	5001	1/1	0.84	0.15	36,36,36,36	0
56	MG	AA	3071	1/1	0.84	0.12	36,36,36,36	0
56	MG	DA	3256	1/1	0.84	0.15	45,45,45,45	0
56	MG	AF	3001	1/1	0.84	0.15	52,52,52,52	0
56	MG	BA	3136	1/1	0.84	0.18	44,44,44,44	0
56	MG	CA	3035	1/1	0.84	0.14	66,66,66,66	0
56	MG	BA	3235	1/1	0.84	0.22	51,51,51,51	0
56	MG	CA	3050	1/1	0.84	0.13	67,67,67,67	0
56	MG	BA	3237	1/1	0.84	0.19	57,57,57,57	0
56	MG	CA	3081	1/1	0.84	0.16	56,56,56,56	0
56	MG	BA	3616	1/1	0.84	0.13	34,34,34,34	0
56	MG	BA	3012	1/1	0.84	0.14	39,39,39,39	0
56	MG	DA	3568	1/1	0.84	0.13	60,60,60,60	0
56	MG	AA	3019	1/1	0.84	0.22	62,62,62,62	0
56	MG	BA	3371	1/1	0.84	0.18	25,25,25,25	0
56	MG	BA	3093	1/1	0.84	0.21	40,40,40,40	0
56	MG	DW	3002	1/1	0.84	0.19	60,60,60,60	0
56	MG	BA	3521	1/1	0.85	0.11	54,54,54,54	0
56	MG	BA	3309	1/1	0.85	0.14	32,32,32,32	0
56	MG	BA	3347	1/1	0.85	0.11	53,53,53,53	0
56	MG	DA	3359	1/1	0.85	0.13	43,43,43,43	0
56	MG	CA	3152	1/1	0.85	0.16	75,75,75,75	0
56	MG	BA	3112	1/1	0.85	0.26	40,40,40,40	0
56	MG	AA	3160	1/1	0.85	0.09	71,71,71,71	0
56	MG	BA	3244	1/1	0.85	0.56	46,46,46,46	0
56	MG	DA	3054	1/1	0.85	0.23	45,45,45,45	0
56	MG	DA	3544	1/1	0.85	0.18	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DA	3090	1/1	0.85	0.10	54,54,54,54	0
56	MG	CA	3084	1/1	0.85	0.10	72,72,72,72	0
56	MG	BA	3169	1/1	0.85	0.13	39,39,39,39	0
56	MG	CA	3104	1/1	0.85	0.17	74,74,74,74	0
56	MG	CA	3118	1/1	0.85	0.10	78,78,78,78	0
56	MG	CA	3019	1/1	0.85	0.20	71,71,71,71	0
56	MG	CA	3049	1/1	0.86	0.17	51,51,51,51	0
56	MG	DA	3091	1/1	0.86	0.15	45,45,45,45	0
56	MG	DA	3478	1/1	0.86	0.14	53,53,53,53	0
56	MG	BA	3634	1/1	0.86	0.30	41,41,41,41	0
56	MG	BA	3579	1/1	0.86	0.18	46,46,46,46	0
56	MG	DA	3487	1/1	0.86	0.18	50,50,50,50	0
56	MG	DA	3504	1/1	0.86	0.12	49,49,49,49	0
56	MG	BA	3129	1/1	0.86	0.17	42,42,42,42	0
56	MG	BA	3546	1/1	0.86	0.10	57,57,57,57	0
56	MG	AA	3109	1/1	0.86	0.18	44,44,44,44	0
56	MG	BA	3331	1/1	0.86	0.15	59,59,59,59	0
56	MG	DA	3582	1/1	0.86	0.17	38,38,38,38	0
56	MG	BA	3081	1/1	0.86	0.19	42,42,42,42	0
56	MG	DA	3347	1/1	0.86	0.14	41,41,41,41	0
56	MG	BA	3624	1/1	0.86	0.29	49,49,49,49	0
56	MG	DA	3069	1/1	0.86	0.12	35,35,35,35	0
56	MG	AA	3061	1/1	0.87	0.13	62,62,62,62	0
56	MG	DA	3430	1/1	0.87	0.19	30,30,30,30	0
56	MG	DA	3443	1/1	0.87	0.08	49,49,49,49	0
56	MG	DA	3446	1/1	0.87	0.09	46,46,46,46	0
56	MG	BA	3253	1/1	0.87	0.38	47,47,47,47	0
56	MG	DA	3477	1/1	0.87	0.13	42,42,42,42	0
56	MG	DA	3135	1/1	0.87	0.16	47,47,47,47	0
56	MG	CA	3138	1/1	0.87	0.15	58,58,58,58	0
56	MG	DA	3151	1/1	0.87	0.14	34,34,34,34	0
56	MG	DA	3172	1/1	0.87	0.11	35,35,35,35	0
56	MG	BA	3171	1/1	0.87	0.14	44,44,44,44	0
56	MG	BA	3441	1/1	0.87	0.12	44,44,44,44	0
56	MG	DA	3516	1/1	0.87	0.08	61,61,61,61	0
56	MG	DA	3531	1/1	0.87	0.12	69,69,69,69	0
56	MG	BW	3002	1/1	0.87	0.19	57,57,57,57	0
56	MG	BA	3230	1/1	0.87	0.21	40,40,40,40	0
56	MG	AA	3081	1/1	0.87	0.11	44,44,44,44	0
56	MG	DA	3574	1/1	0.87	0.13	56,56,56,56	0
56	MG	AA	3058	1/1	0.87	0.13	62,62,62,62	0
56	MG	DA	3073	1/1	0.87	0.14	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DA	3357	1/1	0.87	0.11	33,33,33,33	0
56	MG	CA	3129	1/1	0.87	0.14	55,55,55,55	0
56	MG	DA	3373	1/1	0.87	0.13	42,42,42,42	0
56	MG	AA	3106	1/1	0.88	0.17	50,50,50,50	0
56	MG	AA	3087	1/1	0.88	0.21	62,62,62,62	0
56	MG	CA	3090	1/1	0.88	0.16	66,66,66,66	0
56	MG	BA	3395	1/1	0.88	0.23	54,54,54,54	0
56	MG	DA	3301	1/1	0.88	0.13	56,56,56,56	0
56	MG	BA	3206	1/1	0.88	0.20	41,41,41,41	0
56	MG	AA	3092	1/1	0.88	0.17	61,61,61,61	0
56	MG	BD	304	1/1	0.88	0.20	28,28,28,28	0
56	MG	AA	3148	1/1	0.88	0.06	56,56,56,56	0
56	MG	BA	3531	1/1	0.88	0.09	41,41,41,41	0
56	MG	AA	3149	1/1	0.88	0.12	68,68,68,68	0
56	MG	BW	3004	1/1	0.88	0.23	30,30,30,30	0
56	MG	BA	3094	1/1	0.88	0.20	45,45,45,45	0
56	MG	AX	3006	1/1	0.88	0.09	54,54,54,54	0
56	MG	CT	3001	1/1	0.88	0.09	50,50,50,50	0
56	MG	BA	3260	1/1	0.88	0.22	49,49,49,49	0
56	MG	BA	3267	1/1	0.88	0.17	40,40,40,40	0
56	MG	DA	3028	1/1	0.88	0.35	47,47,47,47	0
56	MG	CA	3013	1/1	0.88	0.16	53,53,53,53	0
56	MG	DA	3056	1/1	0.88	0.09	36,36,36,36	0
56	MG	AA	3153	1/1	0.88	0.16	50,50,50,50	0
56	MG	BA	3126	1/1	0.88	0.12	45,45,45,45	0
56	MG	DA	3076	1/1	0.88	0.11	43,43,43,43	0
56	MG	AA	3093	1/1	0.88	0.18	45,45,45,45	0
56	MG	DA	3538	1/1	0.88	0.10	39,39,39,39	0
56	MG	BA	3605	1/1	0.88	0.17	46,46,46,46	0
56	MG	DA	3108	1/1	0.88	0.10	46,46,46,46	0
56	MG	BA	3334	1/1	0.88	0.10	32,32,32,32	0
56	MG	BA	3340	1/1	0.88	0.13	42,42,42,42	0
56	MG	CA	3055	1/1	0.88	0.14	62,62,62,62	0
56	MG	BA	3048	1/1	0.88	0.15	47,47,47,47	0
56	MG	BA	3631	1/1	0.88	0.12	41,41,41,41	0
56	MG	AA	3164	1/1	0.88	0.14	61,61,61,61	0
56	MG	DA	3212	1/1	0.88	0.17	39,39,39,39	0
56	MG	AA	3089	1/1	0.89	0.14	36,36,36,36	0
56	MG	DA	3162	1/1	0.89	0.11	57,57,57,57	0
56	MG	AA	3167	1/1	0.89	0.14	73,73,73,73	0
56	MG	CA	3085	1/1	0.89	0.12	52,52,52,52	0
56	MG	DA	3209	1/1	0.89	0.11	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	3567	1/1	0.89	0.18	53,53,53,53	0
56	MG	DA	3220	1/1	0.89	0.13	43,43,43,43	0
56	MG	DA	3239	1/1	0.89	0.20	56,56,56,56	0
56	MG	DA	3243	1/1	0.89	0.09	50,50,50,50	0
56	MG	DA	3247	1/1	0.89	0.13	49,49,49,49	0
56	MG	BA	3177	1/1	0.89	0.13	44,44,44,44	0
56	MG	BE	305	1/1	0.89	0.26	51,51,51,51	0
56	MG	BH	3001	1/1	0.89	0.20	56,56,56,56	0
56	MG	BA	3185	1/1	0.89	0.13	43,43,43,43	0
56	MG	AX	3007	1/1	0.89	0.11	60,60,60,60	0
56	MG	DA	3307	1/1	0.89	0.21	53,53,53,53	0
56	MG	AA	3172	1/1	0.89	0.09	69,69,69,69	0
56	MG	BY	503	1/1	0.89	0.12	42,42,42,42	0
56	MG	BA	3013	1/1	0.89	0.16	35,35,35,35	0
56	MG	B0	104	1/1	0.89	0.36	48,48,48,48	0
56	MG	B4	502	1/1	0.89	0.16	61,61,61,61	0
56	MG	AA	3035	1/1	0.89	0.19	65,65,65,65	0
56	MG	DA	3412	1/1	0.89	0.20	53,53,53,53	0
56	MG	DA	3425	1/1	0.89	0.14	37,37,37,37	0
56	MG	CJ	5001	1/1	0.89	0.09	60,60,60,60	0
56	MG	AA	3049	1/1	0.89	0.22	47,47,47,47	0
56	MG	AA	3056	1/1	0.89	0.15	69,69,69,69	0
56	MG	BA	3617	1/1	0.89	0.26	66,66,66,66	0
56	MG	DA	3475	1/1	0.89	0.20	41,41,41,41	0
56	MG	BA	3058	1/1	0.89	0.15	43,43,43,43	0
56	MG	DA	3037	1/1	0.89	0.10	40,40,40,40	0
56	MG	DA	3052	1/1	0.89	0.15	49,49,49,49	0
56	MG	BA	3466	1/1	0.89	0.22	49,49,49,49	0
56	MG	DA	3486	1/1	0.89	0.17	37,37,37,37	0
56	MG	CA	3028	1/1	0.89	0.12	52,52,52,52	0
56	MG	DA	3065	1/1	0.89	0.15	49,49,49,49	0
56	MG	AA	3068	1/1	0.89	0.20	31,31,31,31	0
56	MG	BA	3633	1/1	0.89	0.14	57,57,57,57	0
56	MG	DA	3518	1/1	0.89	0.19	53,53,53,53	0
56	MG	DA	3530	1/1	0.89	0.10	60,60,60,60	0
56	MG	CA	3041	1/1	0.89	0.13	67,67,67,67	0
56	MG	BA	3523	1/1	0.89	0.10	50,50,50,50	0
56	MG	BA	3527	1/1	0.89	0.12	40,40,40,40	0
56	MG	BA	3078	1/1	0.89	0.13	53,53,53,53	0
56	MG	DA	3119	1/1	0.89	0.20	37,37,37,37	0
56	MG	CA	3068	1/1	0.89	0.09	74,74,74,74	0
56	MG	DA	3131	1/1	0.89	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	3672	1/1	0.89	0.10	46,46,46,46	0
56	MG	DA	3141	1/1	0.89	0.07	42,42,42,42	0
56	MG	DA	3145	1/1	0.89	0.14	31,31,31,31	0
56	MG	DQ	3003	1/1	0.89	0.18	50,50,50,50	0
56	MG	BA	3533	1/1	0.89	0.11	45,45,45,45	0
56	MG	BA	3401	1/1	0.90	0.14	32,32,32,32	0
56	MG	BA	3416	1/1	0.90	0.17	64,64,64,64	0
56	MG	BA	3623	1/1	0.90	0.10	48,48,48,48	0
56	MG	BA	3243	1/1	0.90	0.17	45,45,45,45	0
56	MG	BA	3002	1/1	0.90	0.14	39,39,39,39	0
56	MG	DA	3253	1/1	0.90	0.12	26,26,26,26	0
56	MG	CA	3025	1/1	0.90	0.09	48,48,48,48	0
56	MG	BA	3246	1/1	0.90	0.18	56,56,56,56	0
56	MG	DA	3271	1/1	0.90	0.09	55,55,55,55	0
56	MG	DA	3274	1/1	0.90	0.10	56,56,56,56	0
56	MG	CA	3032	1/1	0.90	0.16	68,68,68,68	0
56	MG	DA	3281	1/1	0.90	0.14	56,56,56,56	0
56	MG	AA	3038	1/1	0.90	0.14	53,53,53,53	0
56	MG	DA	3302	1/1	0.90	0.10	43,43,43,43	0
56	MG	DA	3030	1/1	0.90	0.14	30,30,30,30	0
56	MG	DA	3325	1/1	0.90	0.13	54,54,54,54	0
56	MG	DA	3326	1/1	0.90	0.12	41,41,41,41	0
56	MG	DA	3329	1/1	0.90	0.07	48,48,48,48	0
56	MG	AA	3124	1/1	0.90	0.19	30,30,30,30	0
56	MG	BA	3263	1/1	0.90	0.21	64,64,64,64	0
56	MG	BA	3653	1/1	0.90	0.14	33,33,33,33	0
56	MG	AA	3185	1/1	0.90	0.05	64,64,64,64	0
56	MG	BA	3268	1/1	0.90	0.26	39,39,39,39	0
56	MG	DA	3381	1/1	0.90	0.24	56,56,56,56	0
56	MG	DA	3067	1/1	0.90	0.17	53,53,53,53	0
56	MG	BA	3164	1/1	0.90	0.11	37,37,37,37	0
56	MG	BA	3087	1/1	0.90	0.18	36,36,36,36	0
56	MG	CA	3078	1/1	0.90	0.07	66,66,66,66	0
56	MG	DA	3087	1/1	0.90	0.29	35,35,35,35	0
56	MG	DA	3088	1/1	0.90	0.12	39,39,39,39	0
56	MG	DA	3469	1/1	0.90	0.18	33,33,33,33	0
56	MG	BA	3559	1/1	0.90	0.13	52,52,52,52	0
56	MG	BA	3562	1/1	0.90	0.09	46,46,46,46	0
56	MG	DA	3094	1/1	0.90	0.23	35,35,35,35	0
56	MG	BA	3036	1/1	0.90	0.11	56,56,56,56	0
56	MG	DA	3109	1/1	0.90	0.13	50,50,50,50	0
56	MG	BA	3092	1/1	0.90	0.22	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	3176	1/1	0.90	0.12	60,60,60,60	0
56	MG	DA	3122	1/1	0.90	0.17	45,45,45,45	0
56	MG	DA	3491	1/1	0.90	0.13	40,40,40,40	0
56	MG	DA	3492	1/1	0.90	0.09	44,44,44,44	0
56	MG	DA	3496	1/1	0.90	0.05	46,46,46,46	0
56	MG	DA	3125	1/1	0.90	0.35	47,47,47,47	0
56	MG	BA	3345	1/1	0.90	0.18	41,41,41,41	0
56	MG	BA	3187	1/1	0.90	0.13	37,37,37,37	0
56	MG	CA	3105	1/1	0.90	0.08	84,84,84,84	0
56	MG	CA	3110	1/1	0.90	0.17	64,64,64,64	0
56	MG	DA	3148	1/1	0.90	0.10	47,47,47,47	0
56	MG	DA	3534	1/1	0.90	0.14	54,54,54,54	0
56	MG	AA	3073	1/1	0.90	0.19	50,50,50,50	0
56	MG	CA	3119	1/1	0.90	0.09	48,48,48,48	0
56	MG	DA	3554	1/1	0.90	0.09	68,68,68,68	0
56	MG	DA	3557	1/1	0.90	0.16	62,62,62,62	0
56	MG	DA	3152	1/1	0.90	0.17	34,34,34,34	0
56	MG	DA	3564	1/1	0.90	0.07	36,36,36,36	0
56	MG	DA	3566	1/1	0.90	0.14	61,61,61,61	0
56	MG	BA	3596	1/1	0.90	0.14	56,56,56,56	0
56	MG	CA	3123	1/1	0.90	0.19	66,66,66,66	0
56	MG	DA	3173	1/1	0.90	0.12	54,54,54,54	0
56	MG	DB	3002	1/1	0.90	0.13	50,50,50,50	0
56	MG	DA	3186	1/1	0.90	0.14	41,41,41,41	0
56	MG	AA	3044	1/1	0.90	0.19	50,50,50,50	0
56	MG	DD	302	1/1	0.90	0.25	39,39,39,39	0
56	MG	DE	3001	1/1	0.90	0.20	43,43,43,43	0
56	MG	DA	3192	1/1	0.90	0.09	51,51,51,51	0
56	MG	DN	5001	1/1	0.90	0.14	65,65,65,65	0
56	MG	BA	3119	1/1	0.90	0.09	29,29,29,29	0
56	MG	BA	3061	1/1	0.90	0.21	44,44,44,44	0
56	MG	DA	3222	1/1	0.91	0.12	36,36,36,36	0
56	MG	BA	3054	1/1	0.91	0.14	42,42,42,42	0
56	MG	AA	3112	1/1	0.91	0.18	94,94,94,94	0
56	MG	CF	3001	1/1	0.91	0.13	45,45,45,45	0
56	MG	AA	3120	1/1	0.91	0.12	47,47,47,47	0
56	MG	CA	3005	1/1	0.91	0.10	42,42,42,42	0
56	MG	DA	3009	1/1	0.91	0.19	42,42,42,42	0
56	MG	DA	3017	1/1	0.91	0.20	46,46,46,46	0
56	MG	DA	3265	1/1	0.91	0.28	51,51,51,51	0
56	MG	BA	3060	1/1	0.91	0.14	42,42,42,42	0
56	MG	BA	3165	1/1	0.91	0.25	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	3339	1/1	0.91	0.11	34,34,34,34	0
56	MG	DA	3278	1/1	0.91	0.14	50,50,50,50	0
56	MG	BA	3599	1/1	0.91	0.15	46,46,46,46	0
56	MG	CA	3021	1/1	0.91	0.21	52,52,52,52	0
56	MG	DA	3047	1/1	0.91	0.13	41,41,41,41	0
56	MG	AA	3122	1/1	0.91	0.11	58,58,58,58	0
56	MG	AA	3034	1/1	0.91	0.20	54,54,54,54	0
56	MG	AA	3020	1/1	0.91	0.18	49,49,49,49	0
56	MG	DA	3060	1/1	0.91	0.10	45,45,45,45	0
56	MG	DA	3340	1/1	0.91	0.10	47,47,47,47	0
56	MG	DA	3063	1/1	0.91	0.11	31,31,31,31	0
56	MG	CA	3033	1/1	0.91	0.13	52,52,52,52	0
56	MG	BA	3180	1/1	0.91	0.32	33,33,33,33	0
56	MG	DA	3068	1/1	0.91	0.14	35,35,35,35	0
56	MG	DA	3366	1/1	0.91	0.17	43,43,43,43	0
56	MG	BA	3362	1/1	0.91	0.15	30,30,30,30	0
56	MG	AA	3001	1/1	0.91	0.18	57,57,57,57	0
56	MG	DA	3389	1/1	0.91	0.08	42,42,42,42	0
56	MG	CA	3047	1/1	0.91	0.17	51,51,51,51	0
56	MG	AA	3042	1/1	0.91	0.13	54,54,54,54	0
56	MG	DA	3416	1/1	0.91	0.16	44,44,44,44	0
56	MG	BA	3626	1/1	0.91	0.17	50,50,50,50	0
56	MG	DA	3428	1/1	0.91	0.18	33,33,33,33	0
56	MG	DA	3429	1/1	0.91	0.12	35,35,35,35	0
56	MG	BA	3188	1/1	0.91	0.17	39,39,39,39	0
56	MG	CA	3058	1/1	0.91	0.11	56,56,56,56	0
56	MG	CA	3065	1/1	0.91	0.07	55,55,55,55	0
56	MG	DA	3096	1/1	0.91	0.12	29,29,29,29	0
56	MG	DA	3472	1/1	0.91	0.16	53,53,53,53	0
56	MG	DA	3097	1/1	0.91	0.14	46,46,46,46	0
56	MG	DA	3099	1/1	0.91	0.14	37,37,37,37	0
56	MG	DA	3102	1/1	0.91	0.17	51,51,51,51	0
56	MG	DA	3105	1/1	0.91	0.09	36,36,36,36	0
56	MG	BA	3189	1/1	0.91	0.22	26,26,26,26	0
56	MG	BA	3086	1/1	0.91	0.18	39,39,39,39	0
56	MG	DA	3113	1/1	0.91	0.12	41,41,41,41	0
56	MG	DA	3115	1/1	0.91	0.14	36,36,36,36	0
56	MG	DA	3117	1/1	0.91	0.19	43,43,43,43	0
56	MG	CA	3072	1/1	0.91	0.14	57,57,57,57	0
56	MG	BA	3222	1/1	0.91	0.20	45,45,45,45	0
56	MG	BA	3224	1/1	0.91	0.17	45,45,45,45	0
56	MG	AA	3064	1/1	0.91	0.15	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DA	3515	1/1	0.91	0.09	64,64,64,64	0
56	MG	BA	3495	1/1	0.91	0.33	48,48,48,48	0
56	MG	BA	3513	1/1	0.91	0.14	60,60,60,60	0
56	MG	BB	3004	1/1	0.91	0.11	49,49,49,49	0
56	MG	BB	3005	1/1	0.91	0.20	30,30,30,30	0
56	MG	DA	3533	1/1	0.91	0.08	60,60,60,60	0
56	MG	BA	3515	1/1	0.91	0.16	25,25,25,25	0
56	MG	AA	3012	1/1	0.91	0.10	64,64,64,64	0
56	MG	BA	3010	1/1	0.91	0.14	33,33,33,33	0
56	MG	DA	3549	1/1	0.91	0.09	41,41,41,41	0
56	MG	BA	3240	1/1	0.91	0.21	43,43,43,43	0
56	MG	DA	3156	1/1	0.91	0.08	38,38,38,38	0
56	MG	DA	3158	1/1	0.91	0.16	36,36,36,36	0
56	MG	DA	3161	1/1	0.91	0.16	24,24,24,24	0
56	MG	AA	3097	1/1	0.91	0.11	49,49,49,49	0
56	MG	AA	3098	1/1	0.91	0.18	48,48,48,48	0
56	MG	AA	3045	1/1	0.91	0.13	60,60,60,60	0
56	MG	DA	3578	1/1	0.91	0.18	47,47,47,47	0
56	MG	BA	3118	1/1	0.91	0.31	45,45,45,45	0
56	MG	AA	3002	1/1	0.91	0.17	43,43,43,43	0
56	MG	DA	3191	1/1	0.91	0.14	53,53,53,53	0
56	MG	AA	3179	1/1	0.91	0.18	63,63,63,63	0
56	MG	DA	3194	1/1	0.91	0.09	47,47,47,47	0
56	MG	DA	3206	1/1	0.91	0.15	50,50,50,50	0
56	MG	DE	3002	1/1	0.91	0.23	35,35,35,35	0
56	MG	DE	3004	1/1	0.91	0.12	48,48,48,48	0
56	MG	CA	3132	1/1	0.91	0.18	73,73,73,73	0
56	MG	BA	3566	1/1	0.91	0.17	46,46,46,46	0
56	MG	DA	3218	1/1	0.91	0.12	33,33,33,33	0
56	MG	BA	3049	1/1	0.91	0.14	43,43,43,43	0
56	MG	D8	5002	1/1	0.91	0.23	64,64,64,64	0
56	MG	BA	3505	1/1	0.92	0.18	46,46,46,46	0
56	MG	BA	3158	1/1	0.92	0.13	33,33,33,33	0
56	MG	DA	3261	1/1	0.92	0.15	49,49,49,49	0
56	MG	DA	3020	1/1	0.92	0.44	50,50,50,50	0
56	MG	AA	3066	1/1	0.92	0.18	46,46,46,46	0
56	MG	BA	3518	1/1	0.92	0.19	41,41,41,41	0
56	MG	AA	3054	1/1	0.92	0.18	65,65,65,65	0
56	MG	BA	3254	1/1	0.92	0.17	45,45,45,45	0
56	MG	DA	3033	1/1	0.92	0.17	37,37,37,37	0
56	MG	AA	3094	1/1	0.92	0.20	49,49,49,49	0
56	MG	DA	3290	1/1	0.92	0.09	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	3069	1/1	0.92	0.12	50,50,50,50	0
56	MG	AA	3166	1/1	0.92	0.14	53,53,53,53	0
56	MG	BA	3096	1/1	0.92	0.10	44,44,44,44	0
56	MG	DA	3309	1/1	0.92	0.13	60,60,60,60	0
56	MG	DA	3318	1/1	0.92	0.12	43,43,43,43	0
56	MG	DA	3323	1/1	0.92	0.12	35,35,35,35	0
56	MG	CA	3009	1/1	0.92	0.13	55,55,55,55	0
56	MG	BA	3183	1/1	0.92	0.21	35,35,35,35	0
56	MG	BA	3306	1/1	0.92	0.13	54,54,54,54	0
56	MG	DA	3331	1/1	0.92	0.07	41,41,41,41	0
56	MG	DA	3338	1/1	0.92	0.13	36,36,36,36	0
56	MG	BA	3307	1/1	0.92	0.07	63,63,63,63	0
56	MG	DA	3346	1/1	0.92	0.11	33,33,33,33	0
56	MG	BA	3108	1/1	0.92	0.12	38,38,38,38	0
56	MG	DA	3351	1/1	0.92	0.15	46,46,46,46	0
56	MG	BA	3316	1/1	0.92	0.09	61,61,61,61	0
56	MG	BA	3317	1/1	0.92	0.15	35,35,35,35	0
56	MG	BA	3329	1/1	0.92	0.11	30,30,30,30	0
56	MG	DA	3361	1/1	0.92	0.13	38,38,38,38	0
56	MG	CA	3029	1/1	0.92	0.14	48,48,48,48	0
56	MG	DA	3368	1/1	0.92	0.07	25,25,25,25	0
56	MG	DA	3078	1/1	0.92	0.09	46,46,46,46	0
56	MG	DA	3375	1/1	0.92	0.14	49,49,49,49	0
56	MG	DA	3081	1/1	0.92	0.10	44,44,44,44	0
56	MG	BA	3066	1/1	0.92	0.18	48,48,48,48	0
56	MG	BA	3115	1/1	0.92	0.13	34,34,34,34	0
56	MG	DA	3399	1/1	0.92	0.17	40,40,40,40	0
56	MG	BA	3584	1/1	0.92	0.19	44,44,44,44	0
56	MG	BA	3023	1/1	0.92	0.17	40,40,40,40	0
56	MG	DA	3424	1/1	0.92	0.18	30,30,30,30	0
56	MG	DA	3093	1/1	0.92	0.22	46,46,46,46	0
56	MG	BA	3592	1/1	0.92	0.20	52,52,52,52	0
56	MG	CA	3045	1/1	0.92	0.16	52,52,52,52	0
56	MG	BA	3594	1/1	0.92	0.13	37,37,37,37	0
56	MG	DA	3098	1/1	0.92	0.10	46,46,46,46	0
56	MG	BA	3595	1/1	0.92	0.12	47,47,47,47	0
56	MG	BA	3193	1/1	0.92	0.20	48,48,48,48	0
56	MG	BA	3341	1/1	0.92	0.11	32,32,32,32	0
56	MG	AA	3008	1/1	0.92	0.62	55,55,55,55	0
56	MG	CA	3062	1/1	0.92	0.08	57,57,57,57	0
56	MG	DA	3111	1/1	0.92	0.21	39,39,39,39	0
56	MG	CA	3063	1/1	0.92	0.23	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
56	MG	CA	3064	1/1	0.92	0.08	60,60,60,60	0
56	MG	BA	3220	1/1	0.92	0.14	31,31,31,31	0
56	MG	BA	3079	1/1	0.92	0.12	46,46,46,46	0
56	MG	BA	3359	1/1	0.92	0.13	54,54,54,54	0
56	MG	AA	3102	1/1	0.92	0.13	60,60,60,60	0
56	MG	DA	3123	1/1	0.92	0.13	51,51,51,51	0
56	MG	BA	3228	1/1	0.92	0.14	40,40,40,40	0
56	MG	BA	3229	1/1	0.92	0.21	54,54,54,54	0
56	MG	BA	3387	1/1	0.92	0.23	49,49,49,49	0
56	MG	DA	3508	1/1	0.92	0.11	38,38,38,38	0
56	MG	BA	3394	1/1	0.92	0.18	35,35,35,35	0
56	MG	DA	3142	1/1	0.92	0.16	37,37,37,37	0
56	MG	AX	3003	1/1	0.92	0.23	50,50,50,50	0
56	MG	BA	3232	1/1	0.92	0.18	41,41,41,41	0
56	MG	BA	3234	1/1	0.92	0.15	57,57,57,57	0
56	MG	CA	3103	1/1	0.92	0.11	52,52,52,52	0
56	MG	BA	3428	1/1	0.92	0.08	58,58,58,58	0
56	MG	BA	3433	1/1	0.92	0.09	33,33,33,33	0
56	MG	BA	3655	1/1	0.92	0.13	18,18,18,18	0
56	MG	BA	3083	1/1	0.92	0.17	34,34,34,34	0
56	MG	AA	3072	1/1	0.92	0.10	39,39,39,39	0
56	MG	BA	3141	1/1	0.92	0.10	45,45,45,45	0
56	MG	BA	3469	1/1	0.92	0.17	28,28,28,28	0
56	MG	DA	3563	1/1	0.92	0.17	60,60,60,60	0
56	MG	DA	3179	1/1	0.92	0.14	20,20,20,20	0
56	MG	DA	3565	1/1	0.92	0.16	51,51,51,51	0
56	MG	BA	3483	1/1	0.92	0.13	47,47,47,47	0
56	MG	BA	3487	1/1	0.92	0.15	17,17,17,17	0
56	MG	DA	3572	1/1	0.92	0.08	51,51,51,51	0
56	MG	BB	3015	1/1	0.92	0.14	48,48,48,48	0
56	MG	BD	302	1/1	0.92	0.32	45,45,45,45	0
56	MG	BA	3488	1/1	0.92	0.27	36,36,36,36	0
56	MG	DA	3595	1/1	0.92	0.10	43,43,43,43	0
56	MG	DA	3199	1/1	0.92	0.09	52,52,52,52	0
56	MG	DB	3004	1/1	0.92	0.13	36,36,36,36	0
56	MG	BA	3153	1/1	0.92	0.29	39,39,39,39	0
56	MG	CA	3145	1/1	0.92	0.09	59,59,59,59	0
56	MG	DB	3010	1/1	0.92	0.20	60,60,60,60	0
56	MG	DB	3012	1/1	0.92	0.14	53,53,53,53	0
56	MG	CA	3149	1/1	0.92	0.23	66,66,66,66	0
56	MG	BA	3496	1/1	0.92	0.19	31,31,31,31	0
56	MG	BF	301	1/1	0.92	0.14	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	CE	201	1/1	0.92	0.14	52,52,52,52	0
56	MG	DF	303	1/1	0.92	0.13	57,57,57,57	0
56	MG	DA	3229	1/1	0.92	0.18	38,38,38,38	0
56	MG	BF	305	1/1	0.92	0.39	61,61,61,61	0
56	MG	DP	3001	1/1	0.92	0.30	44,44,44,44	0
56	MG	DQ	3002	1/1	0.92	0.21	38,38,38,38	0
56	MG	BG	3002	1/1	0.92	0.10	27,27,27,27	0
56	MG	DV	3002	1/1	0.92	0.16	43,43,43,43	0
56	MG	BA	3497	1/1	0.92	0.14	34,34,34,34	0
56	MG	DA	3004	1/1	0.92	0.15	51,51,51,51	0
56	MG	DA	3032	1/1	0.93	0.13	42,42,42,42	0
56	MG	BA	3163	1/1	0.93	0.12	31,31,31,31	0
56	MG	BA	3396	1/1	0.93	0.22	38,38,38,38	0
56	MG	DA	3300	1/1	0.93	0.18	58,58,58,58	0
56	MG	DA	3046	1/1	0.93	0.23	34,34,34,34	0
56	MG	BA	3400	1/1	0.93	0.28	45,45,45,45	0
56	MG	DA	3304	1/1	0.93	0.17	32,32,32,32	0
56	MG	AA	3170	1/1	0.93	0.14	54,54,54,54	0
56	MG	BA	3593	1/1	0.93	0.23	39,39,39,39	0
56	MG	BA	3403	1/1	0.93	0.14	18,18,18,18	0
56	MG	DA	3057	1/1	0.93	0.12	30,30,30,30	0
56	MG	DA	3058	1/1	0.93	0.22	45,45,45,45	0
56	MG	DA	3059	1/1	0.93	0.11	33,33,33,33	0
56	MG	CA	3030	1/1	0.93	0.10	41,41,41,41	0
56	MG	BA	3405	1/1	0.93	0.14	26,26,26,26	0
56	MG	DA	3332	1/1	0.93	0.07	43,43,43,43	0
56	MG	DA	3064	1/1	0.93	0.13	48,48,48,48	0
56	MG	BA	3247	1/1	0.93	0.19	48,48,48,48	0
56	MG	BA	3425	1/1	0.93	0.23	53,53,53,53	0
56	MG	BA	3427	1/1	0.93	0.21	49,49,49,49	0
56	MG	BA	3602	1/1	0.93	0.16	31,31,31,31	0
56	MG	AA	3110	1/1	0.93	0.10	60,60,60,60	0
56	MG	DA	3355	1/1	0.93	0.07	36,36,36,36	0
56	MG	AA	3085	1/1	0.93	0.11	63,63,63,63	0
56	MG	AA	3119	1/1	0.93	0.11	57,57,57,57	0
56	MG	AA	3043	1/1	0.93	0.08	53,53,53,53	0
56	MG	DA	3365	1/1	0.93	0.10	29,29,29,29	0
56	MG	BA	3451	1/1	0.93	0.08	48,48,48,48	0
56	MG	DA	3367	1/1	0.93	0.12	47,47,47,47	0
56	MG	CA	3056	1/1	0.93	0.21	40,40,40,40	0
56	MG	DA	3371	1/1	0.93	0.11	46,46,46,46	0
56	MG	BA	3458	1/1	0.93	0.07	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\AA^2$)	Q<0.9
56	MG	BA	3459	1/1	0.93	0.15	42,42,42,42	0
56	MG	BA	3629	1/1	0.93	0.08	60,60,60,60	0
56	MG	DA	3385	1/1	0.93	0.08	45,45,45,45	0
56	MG	BA	3463	1/1	0.93	0.12	43,43,43,43	0
56	MG	DA	3392	1/1	0.93	0.14	54,54,54,54	0
56	MG	DA	3393	1/1	0.93	0.09	48,48,48,48	0
56	MG	DA	3397	1/1	0.93	0.14	18,18,18,18	0
56	MG	AA	3029	1/1	0.93	0.11	52,52,52,52	0
56	MG	CA	3066	1/1	0.93	0.20	43,43,43,43	0
56	MG	DA	3401	1/1	0.93	0.12	55,55,55,55	0
56	MG	DA	3402	1/1	0.93	0.13	63,63,63,63	0
56	MG	AA	3030	1/1	0.93	0.10	47,47,47,47	0
56	MG	CA	3069	1/1	0.93	0.12	34,34,34,34	0
56	MG	DA	3419	1/1	0.93	0.22	59,59,59,59	0
56	MG	AA	3033	1/1	0.93	0.29	48,48,48,48	0
56	MG	BA	3642	1/1	0.93	0.19	47,47,47,47	0
56	MG	DA	3106	1/1	0.93	0.06	43,43,43,43	0
56	MG	CA	3073	1/1	0.93	0.13	57,57,57,57	0
56	MG	BA	3484	1/1	0.93	0.12	46,46,46,46	0
56	MG	CA	3080	1/1	0.93	0.13	41,41,41,41	0
56	MG	BA	3186	1/1	0.93	0.15	39,39,39,39	0
56	MG	AA	3016	1/1	0.93	0.19	49,49,49,49	0
56	MG	DA	3470	1/1	0.93	0.19	52,52,52,52	0
56	MG	DA	3471	1/1	0.93	0.16	50,50,50,50	0
56	MG	BA	3113	1/1	0.93	0.15	41,41,41,41	0
56	MG	BA	3675	1/1	0.93	0.39	33,33,33,33	0
56	MG	BB	3002	1/1	0.93	0.20	41,41,41,41	0
56	MG	AA	3006	1/1	0.93	0.28	67,67,67,67	0
56	MG	CA	3093	1/1	0.93	0.11	72,72,72,72	0
56	MG	CA	3095	1/1	0.93	0.16	56,56,56,56	0
56	MG	DA	3126	1/1	0.93	0.18	42,42,42,42	0
56	MG	CA	3096	1/1	0.93	0.13	61,61,61,61	0
56	MG	BA	3191	1/1	0.93	0.16	33,33,33,33	0
56	MG	DA	3488	1/1	0.93	0.12	41,41,41,41	0
56	MG	DA	3136	1/1	0.93	0.16	36,36,36,36	0
56	MG	BA	3324	1/1	0.93	0.12	53,53,53,53	0
56	MG	AK	3001	1/1	0.93	0.17	43,43,43,43	0
56	MG	CA	3107	1/1	0.93	0.15	56,56,56,56	0
56	MG	AA	3014	1/1	0.93	0.15	49,49,49,49	0
56	MG	BA	3124	1/1	0.93	0.17	58,58,58,58	0
56	MG	BA	3338	1/1	0.93	0.11	48,48,48,48	0
56	MG	BA	3069	1/1	0.93	0.10	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	BA	3525	1/1	0.93	0.09	46,46,46,46	0
56	MG	DA	3527	1/1	0.93	0.13	43,43,43,43	0
56	MG	CA	3124	1/1	0.93	0.12	52,52,52,52	0
56	MG	BA	3074	1/1	0.93	0.14	45,45,45,45	0
56	MG	AA	3159	1/1	0.93	0.08	56,56,56,56	0
56	MG	DA	3167	1/1	0.93	0.09	51,51,51,51	0
56	MG	DA	3535	1/1	0.93	0.15	22,22,22,22	0
56	MG	BA	3128	1/1	0.93	0.18	29,29,29,29	0
56	MG	BA	3536	1/1	0.93	0.15	53,53,53,53	0
56	MG	DA	3545	1/1	0.93	0.07	58,58,58,58	0
56	MG	DA	3547	1/1	0.93	0.17	41,41,41,41	0
56	MG	BA	3543	1/1	0.93	0.10	47,47,47,47	0
56	MG	DA	3183	1/1	0.93	0.09	37,37,37,37	0
56	MG	BO	5001	1/1	0.93	0.12	62,62,62,62	0
56	MG	CA	3139	1/1	0.93	0.10	67,67,67,67	0
56	MG	CA	3141	1/1	0.93	0.17	54,54,54,54	0
56	MG	BP	201	1/1	0.93	0.49	36,36,36,36	0
56	MG	BA	3545	1/1	0.93	0.08	54,54,54,54	0
56	MG	DA	3196	1/1	0.93	0.14	33,33,33,33	0
56	MG	BV	202	1/1	0.93	0.23	36,36,36,36	0
56	MG	AA	3060	1/1	0.93	0.14	55,55,55,55	0
56	MG	BA	3001	1/1	0.93	0.14	35,35,35,35	0
56	MG	DA	3576	1/1	0.93	0.15	36,36,36,36	0
56	MG	BA	3554	1/1	0.93	0.07	47,47,47,47	0
56	MG	AA	3028	1/1	0.93	0.18	39,39,39,39	0
56	MG	DA	3583	1/1	0.93	0.10	43,43,43,43	0
56	MG	DA	3587	1/1	0.93	0.11	53,53,53,53	0
56	MG	CK	3001	1/1	0.93	0.14	50,50,50,50	0
56	MG	AA	3083	1/1	0.93	0.07	59,59,59,59	0
56	MG	DA	3225	1/1	0.93	0.14	33,33,33,33	0
56	MG	CX	101	1/1	0.93	0.19	48,48,48,48	0
56	MG	DA	3232	1/1	0.93	0.13	38,38,38,38	0
56	MG	DB	3008	1/1	0.93	0.13	35,35,35,35	0
56	MG	DA	3236	1/1	0.93	0.14	47,47,47,47	0
56	MG	DA	3003	1/1	0.93	0.20	47,47,47,47	0
56	MG	BA	3565	1/1	0.93	0.12	51,51,51,51	0
56	MG	DA	3244	1/1	0.93	0.14	48,48,48,48	0
56	MG	DA	3245	1/1	0.93	0.13	46,46,46,46	0
56	MG	DE	3003	1/1	0.93	0.11	40,40,40,40	0
56	MG	DA	3008	1/1	0.93	0.14	38,38,38,38	0
56	MG	DF	301	1/1	0.93	0.31	44,44,44,44	0
56	MG	BA	3236	1/1	0.93	0.19	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DA	3010	1/1	0.93	0.16	36,36,36,36	0
56	MG	CA	3003	1/1	0.93	0.10	65,65,65,65	0
56	MG	BA	3154	1/1	0.93	0.30	40,40,40,40	0
56	MG	BA	3380	1/1	0.93	0.16	17,17,17,17	0
56	MG	BA	3575	1/1	0.93	0.15	55,55,55,55	0
56	MG	DV	3001	1/1	0.93	0.34	45,45,45,45	0
56	MG	DA	3024	1/1	0.93	0.16	36,36,36,36	0
56	MG	BA	3157	1/1	0.93	0.19	34,34,34,34	0
56	MG	D7	101	1/1	0.93	0.75	51,51,51,51	0
56	MG	AA	3084	1/1	0.93	0.10	43,43,43,43	0
58	ZN	B4	501	1/1	0.93	0.07	106,106,106,106	0
56	MG	BA	3376	1/1	0.94	0.12	39,39,39,39	0
56	MG	BA	3604	1/1	0.94	0.10	28,28,28,28	0
56	MG	DA	3190	1/1	0.94	0.14	34,34,34,34	0
56	MG	BA	3198	1/1	0.94	0.10	34,34,34,34	0
56	MG	BA	3607	1/1	0.94	0.14	51,51,51,51	0
56	MG	CA	3088	1/1	0.94	0.09	41,41,41,41	0
56	MG	CA	3089	1/1	0.94	0.12	40,40,40,40	0
56	MG	DA	3197	1/1	0.94	0.13	38,38,38,38	0
56	MG	BA	3611	1/1	0.94	0.40	59,59,59,59	0
56	MG	BA	3381	1/1	0.94	0.19	31,31,31,31	0
56	MG	BA	3201	1/1	0.94	0.11	41,41,41,41	0
56	MG	BA	3618	1/1	0.94	0.19	54,54,54,54	0
56	MG	DA	3216	1/1	0.94	0.12	37,37,37,37	0
56	MG	CA	3098	1/1	0.94	0.17	42,42,42,42	0
56	MG	BA	3393	1/1	0.94	0.12	49,49,49,49	0
56	MG	BA	3205	1/1	0.94	0.16	40,40,40,40	0
56	MG	BA	3095	1/1	0.94	0.09	33,33,33,33	0
56	MG	DA	3226	1/1	0.94	0.10	27,27,27,27	0
56	MG	BA	3218	1/1	0.94	0.18	38,38,38,38	0
56	MG	DA	3231	1/1	0.94	0.12	37,37,37,37	0
56	MG	BA	3399	1/1	0.94	0.12	42,42,42,42	0
56	MG	DA	3234	1/1	0.94	0.14	45,45,45,45	0
56	MG	CA	3112	1/1	0.94	0.14	55,55,55,55	0
56	MG	DA	3238	1/1	0.94	0.15	42,42,42,42	0
56	MG	CA	3116	1/1	0.94	0.08	59,59,59,59	0
56	MG	CA	3117	1/1	0.94	0.22	42,42,42,42	0
56	MG	BA	3018	1/1	0.94	0.21	47,47,47,47	0
56	MG	BA	3104	1/1	0.94	0.20	42,42,42,42	0
56	MG	AA	3117	1/1	0.94	0.09	47,47,47,47	0
56	MG	CA	3122	1/1	0.94	0.21	54,54,54,54	0
56	MG	BA	3225	1/1	0.94	0.11	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	3407	1/1	0.94	0.12	43,43,43,43	0
56	MG	DA	3257	1/1	0.94	0.17	55,55,55,55	0
56	MG	CA	3125	1/1	0.94	0.21	71,71,71,71	0
56	MG	BA	3643	1/1	0.94	0.12	42,42,42,42	0
56	MG	BA	3226	1/1	0.94	0.45	32,32,32,32	0
56	MG	BA	3422	1/1	0.94	0.11	46,46,46,46	0
56	MG	BA	3423	1/1	0.94	0.14	47,47,47,47	0
56	MG	CA	3135	1/1	0.94	0.09	62,62,62,62	0
56	MG	BA	3657	1/1	0.94	0.13	24,24,24,24	0
56	MG	BA	3661	1/1	0.94	0.22	38,38,38,38	0
56	MG	BA	3227	1/1	0.94	0.17	32,32,32,32	0
56	MG	DA	3296	1/1	0.94	0.09	28,28,28,28	0
56	MG	DA	3298	1/1	0.94	0.09	32,32,32,32	0
56	MG	CA	3140	1/1	0.94	0.19	61,61,61,61	0
56	MG	BA	3426	1/1	0.94	0.12	43,43,43,43	0
56	MG	BA	3110	1/1	0.94	0.18	31,31,31,31	0
56	MG	CA	3146	1/1	0.94	0.05	42,42,42,42	0
56	MG	AA	3059	1/1	0.94	0.12	54,54,54,54	0
56	MG	AA	3047	1/1	0.94	0.13	45,45,45,45	0
56	MG	DA	3311	1/1	0.94	0.13	43,43,43,43	0
56	MG	BA	3040	1/1	0.94	0.12	43,43,43,43	0
56	MG	BB	3006	1/1	0.94	0.18	49,49,49,49	0
56	MG	CE	202	1/1	0.94	0.12	68,68,68,68	0
56	MG	BA	3233	1/1	0.94	0.12	41,41,41,41	0
56	MG	DA	3328	1/1	0.94	0.14	48,48,48,48	0
56	MG	BA	3041	1/1	0.94	0.12	42,42,42,42	0
56	MG	AA	3013	1/1	0.94	0.09	58,58,58,58	0
56	MG	BB	3016	1/1	0.94	0.11	24,24,24,24	0
56	MG	BB	3017	1/1	0.94	0.11	40,40,40,40	0
56	MG	BA	3122	1/1	0.94	0.41	39,39,39,39	0
56	MG	AA	3177	1/1	0.94	0.15	32,32,32,32	0
56	MG	DA	3005	1/1	0.94	0.11	26,26,26,26	0
56	MG	DA	3348	1/1	0.94	0.13	25,25,25,25	0
56	MG	BA	3239	1/1	0.94	0.14	52,52,52,52	0
56	MG	DA	3353	1/1	0.94	0.13	32,32,32,32	0
56	MG	BA	3468	1/1	0.94	0.15	32,32,32,32	0
56	MG	BA	3051	1/1	0.94	0.19	41,41,41,41	0
56	MG	DA	3013	1/1	0.94	0.20	37,37,37,37	0
56	MG	BA	3470	1/1	0.94	0.15	48,48,48,48	0
56	MG	BA	3471	1/1	0.94	0.18	35,35,35,35	0
56	MG	BG	3003	1/1	0.94	0.10	41,41,41,41	0
56	MG	AA	3178	1/1	0.94	0.22	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\AA^2$)	Q<0.9
56	MG	BN	3002	1/1	0.94	0.13	27,27,27,27	0
56	MG	AA	3052	1/1	0.94	0.19	60,60,60,60	0
56	MG	DA	3029	1/1	0.94	0.11	40,40,40,40	0
56	MG	AA	3129	1/1	0.94	0.10	35,35,35,35	0
56	MG	AA	3134	1/1	0.94	0.24	52,52,52,52	0
56	MG	BQ	201	1/1	0.94	0.09	52,52,52,52	0
56	MG	DA	3034	1/1	0.94	0.18	46,46,46,46	0
56	MG	BA	3252	1/1	0.94	0.37	51,51,51,51	0
56	MG	DA	3039	1/1	0.94	0.27	51,51,51,51	0
56	MG	DA	3044	1/1	0.94	0.07	47,47,47,47	0
56	MG	DA	3045	1/1	0.94	0.12	48,48,48,48	0
56	MG	AA	3136	1/1	0.94	0.17	56,56,56,56	0
56	MG	BA	3062	1/1	0.94	0.16	46,46,46,46	0
56	MG	BA	3498	1/1	0.94	0.19	37,37,37,37	0
56	MG	BA	3142	1/1	0.94	0.11	40,40,40,40	0
56	MG	DA	3405	1/1	0.94	0.12	45,45,45,45	0
56	MG	DA	3406	1/1	0.94	0.10	50,50,50,50	0
56	MG	B0	101	1/1	0.94	0.14	71,71,71,71	0
56	MG	B0	102	1/1	0.94	0.23	42,42,42,42	0
56	MG	BA	3261	1/1	0.94	0.10	53,53,53,53	0
56	MG	DA	3420	1/1	0.94	0.16	46,46,46,46	0
56	MG	B3	101	1/1	0.94	0.27	35,35,35,35	0
56	MG	BA	3145	1/1	0.94	0.22	30,30,30,30	0
56	MG	DA	3062	1/1	0.94	0.22	42,42,42,42	0
56	MG	B7	3004	1/1	0.94	0.09	34,34,34,34	0
56	MG	AA	3137	1/1	0.94	0.07	79,79,79,79	0
56	MG	DA	3431	1/1	0.94	0.11	61,61,61,61	0
56	MG	DA	3435	1/1	0.94	0.20	33,33,33,33	0
56	MG	DA	3438	1/1	0.94	0.10	38,38,38,38	0
56	MG	B9	502	1/1	0.94	0.21	41,41,41,41	0
56	MG	BA	3067	1/1	0.94	0.16	34,34,34,34	0
56	MG	DA	3461	1/1	0.94	0.16	33,33,33,33	0
56	MG	BA	3271	1/1	0.94	0.10	49,49,49,49	0
56	MG	BA	3156	1/1	0.94	0.18	48,48,48,48	0
56	MG	DA	3071	1/1	0.94	0.18	36,36,36,36	0
56	MG	CA	3007	1/1	0.94	0.09	50,50,50,50	0
56	MG	DA	3074	1/1	0.94	0.14	29,29,29,29	0
56	MG	BA	3295	1/1	0.94	0.29	61,61,61,61	0
56	MG	BA	3297	1/1	0.94	0.12	39,39,39,39	0
56	MG	CA	3012	1/1	0.94	0.11	52,52,52,52	0
56	MG	DA	3082	1/1	0.94	0.13	58,58,58,58	0
56	MG	DA	3484	1/1	0.94	0.14	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\AA^2$)	Q<0.9
56	MG	DA	3083	1/1	0.94	0.08	48,48,48,48	0
56	MG	DA	3085	1/1	0.94	0.12	40,40,40,40	0
56	MG	BA	3301	1/1	0.94	0.13	46,46,46,46	0
56	MG	CA	3014	1/1	0.94	0.10	39,39,39,39	0
56	MG	DA	3089	1/1	0.94	0.34	33,33,33,33	0
56	MG	AA	3142	1/1	0.94	0.15	60,60,60,60	0
56	MG	CA	3017	1/1	0.94	0.10	41,41,41,41	0
56	MG	DA	3500	1/1	0.94	0.17	46,46,46,46	0
56	MG	DA	3092	1/1	0.94	0.18	45,45,45,45	0
56	MG	BA	3538	1/1	0.94	0.14	55,55,55,55	0
56	MG	DA	3507	1/1	0.94	0.08	54,54,54,54	0
56	MG	BA	3539	1/1	0.94	0.16	58,58,58,58	0
56	MG	BA	3070	1/1	0.94	0.11	30,30,30,30	0
56	MG	CA	3027	1/1	0.94	0.15	64,64,64,64	0
56	MG	BA	3308	1/1	0.94	0.17	52,52,52,52	0
56	MG	AD	502	1/1	0.94	0.20	55,55,55,55	0
56	MG	DA	3529	1/1	0.94	0.16	41,41,41,41	0
56	MG	DA	3100	1/1	0.94	0.11	34,34,34,34	0
56	MG	DA	3101	1/1	0.94	0.10	46,46,46,46	0
56	MG	AA	3145	1/1	0.94	0.12	35,35,35,35	0
56	MG	BA	3076	1/1	0.94	0.08	29,29,29,29	0
56	MG	BA	3557	1/1	0.94	0.14	42,42,42,42	0
56	MG	DA	3107	1/1	0.94	0.17	46,46,46,46	0
56	MG	DA	3539	1/1	0.94	0.12	52,52,52,52	0
56	MG	DA	3543	1/1	0.94	0.08	63,63,63,63	0
56	MG	BA	3318	1/1	0.94	0.16	44,44,44,44	0
56	MG	BA	3561	1/1	0.94	0.10	55,55,55,55	0
56	MG	BA	3077	1/1	0.94	0.17	37,37,37,37	0
56	MG	CA	3044	1/1	0.94	0.09	56,56,56,56	0
56	MG	DA	3550	1/1	0.94	0.14	46,46,46,46	0
56	MG	DA	3552	1/1	0.94	0.17	49,49,49,49	0
56	MG	AA	3053	1/1	0.94	0.07	50,50,50,50	0
56	MG	DA	3116	1/1	0.94	0.14	29,29,29,29	0
56	MG	DA	3560	1/1	0.94	0.12	51,51,51,51	0
56	MG	BA	3330	1/1	0.94	0.23	44,44,44,44	0
56	MG	DA	3118	1/1	0.94	0.19	49,49,49,49	0
56	MG	CA	3048	1/1	0.94	0.30	52,52,52,52	0
56	MG	BA	3174	1/1	0.94	0.08	29,29,29,29	0
56	MG	AA	3100	1/1	0.94	0.11	35,35,35,35	0
56	MG	CA	3052	1/1	0.94	0.10	39,39,39,39	0
56	MG	DA	3571	1/1	0.94	0.16	48,48,48,48	0
56	MG	BA	3573	1/1	0.94	0.18	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\AA^2$)	Q<0.9
56	MG	BA	3335	1/1	0.94	0.11	40,40,40,40	0
56	MG	DA	3575	1/1	0.94	0.11	49,49,49,49	0
56	MG	DA	3129	1/1	0.94	0.14	54,54,54,54	0
56	MG	AA	3065	1/1	0.94	0.13	48,48,48,48	0
56	MG	DA	3580	1/1	0.94	0.13	58,58,58,58	0
56	MG	DA	3581	1/1	0.94	0.19	53,53,53,53	0
56	MG	DA	3132	1/1	0.94	0.10	35,35,35,35	0
56	MG	DA	3134	1/1	0.94	0.23	33,33,33,33	0
56	MG	CA	3059	1/1	0.94	0.15	58,58,58,58	0
56	MG	DA	3588	1/1	0.94	0.16	21,21,21,21	0
56	MG	DA	3592	1/1	0.94	0.63	52,52,52,52	0
56	MG	DA	3593	1/1	0.94	0.32	51,51,51,51	0
56	MG	BA	3578	1/1	0.94	0.14	59,59,59,59	0
56	MG	DA	3139	1/1	0.94	0.22	39,39,39,39	0
56	MG	AA	3151	1/1	0.94	0.18	45,45,45,45	0
56	MG	AA	3017	1/1	0.94	0.13	63,63,63,63	0
56	MG	DA	3144	1/1	0.94	0.14	38,38,38,38	0
56	MG	BA	3583	1/1	0.94	0.10	37,37,37,37	0
56	MG	DA	3146	1/1	0.94	0.12	34,34,34,34	0
56	MG	AA	3108	1/1	0.94	0.14	54,54,54,54	0
56	MG	DD	301	1/1	0.94	0.15	43,43,43,43	0
56	MG	CA	3067	1/1	0.94	0.07	63,63,63,63	0
56	MG	BA	3344	1/1	0.94	0.14	35,35,35,35	0
56	MG	BA	3009	1/1	0.94	0.14	34,34,34,34	0
56	MG	AA	3067	1/1	0.94	0.13	42,42,42,42	0
56	MG	AA	3003	1/1	0.94	0.15	57,57,57,57	0
56	MG	BA	3190	1/1	0.94	0.26	31,31,31,31	0
56	MG	CA	3074	1/1	0.94	0.19	48,48,48,48	0
56	MG	DA	3163	1/1	0.94	0.26	31,31,31,31	0
56	MG	DA	3164	1/1	0.94	0.15	36,36,36,36	0
56	MG	DA	3165	1/1	0.94	0.12	34,34,34,34	0
56	MG	AA	3026	1/1	0.94	0.14	40,40,40,40	0
56	MG	DA	3171	1/1	0.94	0.24	51,51,51,51	0
56	MG	DU	201	1/1	0.94	0.29	41,41,41,41	0
56	MG	CA	3079	1/1	0.94	0.17	55,55,55,55	0
56	MG	BA	3192	1/1	0.94	0.13	58,58,58,58	0
56	MG	DA	3176	1/1	0.94	0.11	29,29,29,29	0
56	MG	DY	502	1/1	0.94	0.15	51,51,51,51	0
56	MG	BA	3017	1/1	0.94	0.15	40,40,40,40	0
56	MG	DA	3182	1/1	0.94	0.09	38,38,38,38	0
56	MG	CA	3082	1/1	0.94	0.17	62,62,62,62	0
59	K	AX	3001	1/1	0.94	0.07	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	K	DA	3001	1/1	0.94	0.10	48,48,48,48	0
56	MG	CA	3023	1/1	0.95	0.09	38,38,38,38	0
56	MG	BA	3356	1/1	0.95	0.10	46,46,46,46	0
56	MG	BA	3223	1/1	0.95	0.16	51,51,51,51	0
56	MG	BA	3572	1/1	0.95	0.11	59,59,59,59	0
56	MG	AA	3169	1/1	0.95	0.12	71,71,71,71	0
56	MG	BA	3365	1/1	0.95	0.11	41,41,41,41	0
56	MG	AA	3039	1/1	0.95	0.12	45,45,45,45	0
56	MG	AA	3171	1/1	0.95	0.10	62,62,62,62	0
56	MG	DA	3330	1/1	0.95	0.12	42,42,42,42	0
56	MG	DA	3070	1/1	0.95	0.20	49,49,49,49	0
56	MG	CA	3034	1/1	0.95	0.12	67,67,67,67	0
56	MG	DA	3333	1/1	0.95	0.18	38,38,38,38	0
56	MG	BA	3374	1/1	0.95	0.11	29,29,29,29	0
56	MG	DA	3339	1/1	0.95	0.14	32,32,32,32	0
56	MG	AA	3091	1/1	0.95	0.11	36,36,36,36	0
56	MG	DA	3341	1/1	0.95	0.13	25,25,25,25	0
56	MG	DA	3343	1/1	0.95	0.17	56,56,56,56	0
56	MG	DA	3344	1/1	0.95	0.16	31,31,31,31	0
56	MG	DA	3075	1/1	0.95	0.18	41,41,41,41	0
56	MG	AA	3173	1/1	0.95	0.15	32,32,32,32	0
56	MG	DA	3077	1/1	0.95	0.14	34,34,34,34	0
56	MG	CA	3043	1/1	0.95	0.14	60,60,60,60	0
56	MG	DA	3352	1/1	0.95	0.12	45,45,45,45	0
56	MG	BA	3130	1/1	0.95	0.28	40,40,40,40	0
56	MG	BA	3131	1/1	0.95	0.22	36,36,36,36	0
56	MG	BA	3590	1/1	0.95	0.13	55,55,55,55	0
56	MG	DA	3356	1/1	0.95	0.09	31,31,31,31	0
56	MG	BA	3390	1/1	0.95	0.09	47,47,47,47	0
56	MG	BA	3392	1/1	0.95	0.17	41,41,41,41	0
56	MG	DA	3360	1/1	0.95	0.09	39,39,39,39	0
56	MG	BA	3135	1/1	0.95	0.21	36,36,36,36	0
56	MG	BA	3073	1/1	0.95	0.18	14,14,14,14	0
56	MG	BA	3137	1/1	0.95	0.22	30,30,30,30	0
56	MG	BA	3597	1/1	0.95	0.15	43,43,43,43	0
56	MG	BA	3140	1/1	0.95	0.16	33,33,33,33	0
56	MG	DA	3369	1/1	0.95	0.11	45,45,45,45	0
56	MG	AA	3139	1/1	0.95	0.09	36,36,36,36	0
56	MG	AA	3046	1/1	0.95	0.11	42,42,42,42	0
56	MG	DA	3374	1/1	0.95	0.13	35,35,35,35	0
56	MG	BA	3238	1/1	0.95	0.21	47,47,47,47	0
56	MG	AA	3111	1/1	0.95	0.21	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DA	3383	1/1	0.95	0.08	47,47,47,47	0
56	MG	BA	3149	1/1	0.95	0.11	50,50,50,50	0
56	MG	DA	3386	1/1	0.95	0.13	48,48,48,48	0
56	MG	BA	3609	1/1	0.95	0.11	44,44,44,44	0
56	MG	DA	3391	1/1	0.95	0.06	42,42,42,42	0
56	MG	BA	3019	1/1	0.95	0.22	49,49,49,49	0
56	MG	BA	3415	1/1	0.95	0.21	54,54,54,54	0
56	MG	DA	3394	1/1	0.95	0.09	41,41,41,41	0
56	MG	DA	3396	1/1	0.95	0.10	45,45,45,45	0
56	MG	BA	3020	1/1	0.95	0.15	33,33,33,33	0
56	MG	BA	3417	1/1	0.95	0.17	24,24,24,24	0
56	MG	AA	3063	1/1	0.95	0.26	39,39,39,39	0
56	MG	BA	3621	1/1	0.95	0.15	30,30,30,30	0
56	MG	BA	3080	1/1	0.95	0.14	29,29,29,29	0
56	MG	BA	3248	1/1	0.95	0.21	21,21,21,21	0
56	MG	BA	3025	1/1	0.95	0.14	37,37,37,37	0
56	MG	DA	3408	1/1	0.95	0.16	28,28,28,28	0
56	MG	DA	3411	1/1	0.95	0.08	36,36,36,36	0
56	MG	BA	3161	1/1	0.95	0.10	39,39,39,39	0
56	MG	BA	3630	1/1	0.95	0.12	47,47,47,47	0
56	MG	DA	3418	1/1	0.95	0.13	29,29,29,29	0
56	MG	AA	3055	1/1	0.95	0.14	72,72,72,72	0
56	MG	BA	3430	1/1	0.95	0.12	29,29,29,29	0
56	MG	DA	3422	1/1	0.95	0.07	63,63,63,63	0
56	MG	BA	3256	1/1	0.95	0.22	41,41,41,41	0
56	MG	BA	3636	1/1	0.95	0.11	32,32,32,32	0
56	MG	DA	3426	1/1	0.95	0.22	35,35,35,35	0
56	MG	DA	3120	1/1	0.95	0.22	33,33,33,33	0
56	MG	BA	3638	1/1	0.95	0.10	32,32,32,32	0
56	MG	CA	3087	1/1	0.95	0.12	33,33,33,33	0
56	MG	BA	3030	1/1	0.95	0.62	43,43,43,43	0
56	MG	DA	3434	1/1	0.95	0.13	41,41,41,41	0
56	MG	BA	3443	1/1	0.95	0.11	44,44,44,44	0
56	MG	BA	3033	1/1	0.95	0.18	33,33,33,33	0
56	MG	BA	3644	1/1	0.95	0.08	41,41,41,41	0
56	MG	DA	3445	1/1	0.95	0.13	48,48,48,48	0
56	MG	BA	3447	1/1	0.95	0.12	55,55,55,55	0
56	MG	DA	3450	1/1	0.95	0.07	37,37,37,37	0
56	MG	BA	3449	1/1	0.95	0.08	47,47,47,47	0
56	MG	DA	3465	1/1	0.95	0.13	38,38,38,38	0
56	MG	DA	3467	1/1	0.95	0.12	47,47,47,47	0
56	MG	DA	3468	1/1	0.95	0.24	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
56	MG	AA	3009	1/1	0.95	0.11	54,54,54,54	0
56	MG	BA	3266	1/1	0.95	0.21	29,29,29,29	0
56	MG	BA	3660	1/1	0.95	0.08	49,49,49,49	0
56	MG	DA	3137	1/1	0.95	0.10	37,37,37,37	0
56	MG	DA	3473	1/1	0.95	0.06	50,50,50,50	0
56	MG	BA	3088	1/1	0.95	0.11	42,42,42,42	0
56	MG	BA	3666	1/1	0.95	0.29	35,35,35,35	0
56	MG	CA	3108	1/1	0.95	0.12	59,59,59,59	0
56	MG	CA	3109	1/1	0.95	0.17	50,50,50,50	0
56	MG	BA	3668	1/1	0.95	0.17	26,26,26,26	0
56	MG	DA	3480	1/1	0.95	0.08	32,32,32,32	0
56	MG	DA	3482	1/1	0.95	0.10	46,46,46,46	0
56	MG	DA	3483	1/1	0.95	0.13	54,54,54,54	0
56	MG	BA	3460	1/1	0.95	0.14	57,57,57,57	0
56	MG	DA	3147	1/1	0.95	0.19	47,47,47,47	0
56	MG	AA	3057	1/1	0.95	0.23	67,67,67,67	0
56	MG	BB	3001	1/1	0.95	0.15	36,36,36,36	0
56	MG	BA	3464	1/1	0.95	0.08	41,41,41,41	0
56	MG	BA	3269	1/1	0.95	0.08	34,34,34,34	0
56	MG	AA	3099	1/1	0.95	0.26	33,33,33,33	0
56	MG	BA	3274	1/1	0.95	0.28	47,47,47,47	0
56	MG	BA	3277	1/1	0.95	0.22	32,32,32,32	0
56	MG	DA	3501	1/1	0.95	0.09	55,55,55,55	0
56	MG	DA	3503	1/1	0.95	0.07	38,38,38,38	0
56	MG	BA	3042	1/1	0.95	0.17	33,33,33,33	0
56	MG	BA	3476	1/1	0.95	0.07	51,51,51,51	0
56	MG	BA	3478	1/1	0.95	0.13	47,47,47,47	0
56	MG	BA	3480	1/1	0.95	0.21	43,43,43,43	0
56	MG	DA	3514	1/1	0.95	0.07	40,40,40,40	0
56	MG	CA	3130	1/1	0.95	0.12	57,57,57,57	0
56	MG	BA	3280	1/1	0.95	0.10	48,48,48,48	0
56	MG	BA	3182	1/1	0.95	0.18	30,30,30,30	0
56	MG	DA	3519	1/1	0.95	0.08	42,42,42,42	0
56	MG	DA	3525	1/1	0.95	0.08	44,44,44,44	0
56	MG	BA	3485	1/1	0.95	0.14	64,64,64,64	0
56	MG	DA	3528	1/1	0.95	0.06	37,37,37,37	0
56	MG	BD	306	1/1	0.95	0.18	36,36,36,36	0
56	MG	BA	3486	1/1	0.95	0.17	21,21,21,21	0
56	MG	BA	3043	1/1	0.95	0.17	36,36,36,36	0
56	MG	BA	3298	1/1	0.95	0.11	28,28,28,28	0
56	MG	DA	3184	1/1	0.95	0.19	30,30,30,30	0
56	MG	BF	303	1/1	0.95	0.28	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	BA	3492	1/1	0.95	0.15	42,42,42,42	0
56	MG	BA	3044	1/1	0.95	0.15	30,30,30,30	0
56	MG	CA	3148	1/1	0.95	0.10	57,57,57,57	0
56	MG	BA	3302	1/1	0.95	0.12	55,55,55,55	0
56	MG	CA	3151	1/1	0.95	0.13	50,50,50,50	0
56	MG	BA	3305	1/1	0.95	0.15	28,28,28,28	0
56	MG	BA	3046	1/1	0.95	0.21	29,29,29,29	0
56	MG	BA	3499	1/1	0.95	0.16	35,35,35,35	0
56	MG	DA	3551	1/1	0.95	0.17	52,52,52,52	0
56	MG	DA	3200	1/1	0.95	0.12	28,28,28,28	0
56	MG	DA	3205	1/1	0.95	0.16	32,32,32,32	0
56	MG	DA	3555	1/1	0.95	0.13	51,51,51,51	0
56	MG	BA	3097	1/1	0.95	0.12	53,53,53,53	0
56	MG	BA	3507	1/1	0.95	0.12	53,53,53,53	0
56	MG	BA	3510	1/1	0.95	0.22	25,25,25,25	0
56	MG	BU	202	1/1	0.95	0.09	40,40,40,40	0
56	MG	DA	3217	1/1	0.95	0.12	39,39,39,39	0
56	MG	BU	205	1/1	0.95	0.24	53,53,53,53	0
56	MG	BA	3512	1/1	0.95	0.14	45,45,45,45	0
56	MG	BA	3103	1/1	0.95	0.13	42,42,42,42	0
56	MG	DA	3569	1/1	0.95	0.25	55,55,55,55	0
56	MG	BA	3047	1/1	0.95	0.22	41,41,41,41	0
56	MG	BA	3516	1/1	0.95	0.14	43,43,43,43	0
56	MG	DA	3573	1/1	0.95	0.14	45,45,45,45	0
56	MG	DA	3007	1/1	0.95	0.08	39,39,39,39	0
56	MG	DA	3230	1/1	0.95	0.12	41,41,41,41	0
56	MG	BA	3107	1/1	0.95	0.16	21,21,21,21	0
56	MG	AA	3158	1/1	0.95	0.09	54,54,54,54	0
56	MG	AA	3037	1/1	0.95	0.14	51,51,51,51	0
56	MG	B0	103	1/1	0.95	0.12	33,33,33,33	0
56	MG	BA	3319	1/1	0.95	0.21	39,39,39,39	0
56	MG	AA	3126	1/1	0.95	0.12	54,54,54,54	0
56	MG	DA	3240	1/1	0.95	0.09	54,54,54,54	0
56	MG	BA	3328	1/1	0.95	0.13	39,39,39,39	0
56	MG	DA	3591	1/1	0.95	0.07	42,42,42,42	0
56	MG	BA	3195	1/1	0.95	0.13	47,47,47,47	0
56	MG	BA	3053	1/1	0.95	0.18	31,31,31,31	0
56	MG	DA	3594	1/1	0.95	0.12	48,48,48,48	0
56	MG	DA	3027	1/1	0.95	0.12	30,30,30,30	0
56	MG	DA	3249	1/1	0.95	0.09	34,34,34,34	0
56	MG	BA	3200	1/1	0.95	0.18	25,25,25,25	0
56	MG	DA	3252	1/1	0.95	0.15	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	CA	3001	1/1	0.95	0.07	72,72,72,72	0
56	MG	AA	3051	1/1	0.95	0.14	49,49,49,49	0
56	MG	DB	3009	1/1	0.95	0.14	60,60,60,60	0
56	MG	BA	3202	1/1	0.95	0.13	30,30,30,30	0
56	MG	AX	3002	1/1	0.95	0.08	56,56,56,56	0
56	MG	DA	3263	1/1	0.95	0.11	39,39,39,39	0
56	MG	AA	3165	1/1	0.95	0.07	43,43,43,43	0
56	MG	DA	3036	1/1	0.95	0.09	38,38,38,38	0
56	MG	DA	3266	1/1	0.95	0.10	46,46,46,46	0
56	MG	DA	3268	1/1	0.95	0.13	38,38,38,38	0
56	MG	CA	3008	1/1	0.95	0.30	31,31,31,31	0
56	MG	DA	3272	1/1	0.95	0.08	57,57,57,57	0
56	MG	DA	3273	1/1	0.95	0.19	31,31,31,31	0
56	MG	BA	3210	1/1	0.95	0.23	24,24,24,24	0
56	MG	DA	3043	1/1	0.95	0.10	30,30,30,30	0
56	MG	CA	3010	1/1	0.95	0.14	53,53,53,53	0
56	MG	DA	3280	1/1	0.95	0.12	50,50,50,50	0
56	MG	BA	3553	1/1	0.95	0.67	48,48,48,48	0
56	MG	BA	3211	1/1	0.95	0.27	29,29,29,29	0
56	MG	BA	3213	1/1	0.95	0.23	21,21,21,21	0
56	MG	BA	3120	1/1	0.95	0.18	44,44,44,44	0
56	MG	DA	3299	1/1	0.95	0.12	50,50,50,50	0
56	MG	CA	3015	1/1	0.95	0.15	43,43,43,43	0
56	MG	D3	3001	1/1	0.95	0.69	70,70,70,70	0
56	MG	AA	3131	1/1	0.95	0.12	55,55,55,55	0
56	MG	BA	3349	1/1	0.95	0.08	46,46,46,46	0
56	MG	AA	3032	1/1	0.95	0.15	42,42,42,42	0
56	MG	DA	3306	1/1	0.95	0.11	38,38,38,38	0
56	MG	BA	3353	1/1	0.95	0.13	39,39,39,39	0
56	MG	AA	3163	1/1	0.96	0.06	49,49,49,49	0
56	MG	BV	203	1/1	0.96	0.09	24,24,24,24	0
56	MG	BW	3001	1/1	0.96	0.14	25,25,25,25	0
56	MG	AA	3125	1/1	0.96	0.19	41,41,41,41	0
56	MG	BA	3217	1/1	0.96	0.28	29,29,29,29	0
56	MG	DA	3308	1/1	0.96	0.13	29,29,29,29	0
56	MG	BX	102	1/1	0.96	0.28	38,38,38,38	0
56	MG	DA	3310	1/1	0.96	0.09	41,41,41,41	0
56	MG	BX	103	1/1	0.96	0.21	25,25,25,25	0
56	MG	DA	3314	1/1	0.96	0.14	54,54,54,54	0
56	MG	DA	3316	1/1	0.96	0.15	57,57,57,57	0
56	MG	BY	502	1/1	0.96	0.17	35,35,35,35	0
56	MG	DA	3321	1/1	0.96	0.10	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
56	MG	BA	3063	1/1	0.96	0.09	47,47,47,47	0
56	MG	BA	3219	1/1	0.96	0.10	20,20,20,20	0
56	MG	BA	3005	1/1	0.96	0.16	29,29,29,29	0
56	MG	DA	3327	1/1	0.96	0.18	34,34,34,34	0
56	MG	BA	3006	1/1	0.96	0.40	36,36,36,36	0
56	MG	BA	3528	1/1	0.96	0.19	38,38,38,38	0
56	MG	BA	3529	1/1	0.96	0.17	33,33,33,33	0
56	MG	DA	3048	1/1	0.96	0.15	41,41,41,41	0
56	MG	DA	3050	1/1	0.96	0.09	41,41,41,41	0
56	MG	DA	3051	1/1	0.96	0.11	50,50,50,50	0
56	MG	DA	3337	1/1	0.96	0.09	42,42,42,42	0
56	MG	B0	105	1/1	0.96	0.10	43,43,43,43	0
56	MG	BA	3007	1/1	0.96	0.12	32,32,32,32	0
56	MG	BA	3342	1/1	0.96	0.15	35,35,35,35	0
56	MG	B7	3001	1/1	0.96	0.25	45,45,45,45	0
56	MG	BA	3133	1/1	0.96	0.11	33,33,33,33	0
56	MG	BA	3537	1/1	0.96	0.10	58,58,58,58	0
56	MG	DA	3345	1/1	0.96	0.16	33,33,33,33	0
56	MG	BA	3134	1/1	0.96	0.28	40,40,40,40	0
56	MG	BA	3008	1/1	0.96	0.09	27,27,27,27	0
56	MG	CA	3002	1/1	0.96	0.09	43,43,43,43	0
56	MG	BA	3540	1/1	0.96	0.16	46,46,46,46	0
56	MG	BA	3348	1/1	0.96	0.13	31,31,31,31	0
56	MG	BA	3071	1/1	0.96	0.13	32,32,32,32	0
56	MG	AA	3022	1/1	0.96	0.10	39,39,39,39	0
56	MG	BA	3138	1/1	0.96	0.19	35,35,35,35	0
56	MG	BA	3551	1/1	0.96	0.09	48,48,48,48	0
56	MG	BA	3552	1/1	0.96	0.08	31,31,31,31	0
56	MG	AA	3127	1/1	0.96	0.04	68,68,68,68	0
56	MG	BA	3357	1/1	0.96	0.13	30,30,30,30	0
56	MG	BA	3555	1/1	0.96	0.20	42,42,42,42	0
56	MG	BA	3231	1/1	0.96	0.21	41,41,41,41	0
56	MG	BA	3558	1/1	0.96	0.12	59,59,59,59	0
56	MG	AA	3128	1/1	0.96	0.10	57,57,57,57	0
56	MG	BA	3363	1/1	0.96	0.20	29,29,29,29	0
56	MG	CA	3018	1/1	0.96	0.14	43,43,43,43	0
56	MG	AA	3104	1/1	0.96	0.07	56,56,56,56	0
56	MG	CA	3020	1/1	0.96	0.27	46,46,46,46	0
56	MG	DA	3086	1/1	0.96	0.08	41,41,41,41	0
56	MG	BA	3563	1/1	0.96	0.17	47,47,47,47	0
56	MG	DA	3376	1/1	0.96	0.05	38,38,38,38	0
56	MG	DA	3378	1/1	0.96	0.15	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\AA^2$)	Q<0.9
56	MG	DA	3379	1/1	0.96	0.08	26,26,26,26	0
56	MG	BA	3367	1/1	0.96	0.17	49,49,49,49	0
56	MG	DA	3382	1/1	0.96	0.12	50,50,50,50	0
56	MG	BA	3015	1/1	0.96	0.13	27,27,27,27	0
56	MG	BA	3147	1/1	0.96	0.24	35,35,35,35	0
56	MG	BA	3148	1/1	0.96	0.19	25,25,25,25	0
56	MG	BA	3571	1/1	0.96	0.14	50,50,50,50	0
56	MG	DA	3390	1/1	0.96	0.07	41,41,41,41	0
56	MG	BA	3375	1/1	0.96	0.20	51,51,51,51	0
56	MG	BA	3016	1/1	0.96	0.15	50,50,50,50	0
56	MG	BA	3150	1/1	0.96	0.13	32,32,32,32	0
56	MG	AA	3105	1/1	0.96	0.15	44,44,44,44	0
56	MG	AA	3018	1/1	0.96	0.13	50,50,50,50	0
56	MG	BA	3388	1/1	0.96	0.06	54,54,54,54	0
56	MG	CA	3040	1/1	0.96	0.25	52,52,52,52	0
56	MG	BA	3242	1/1	0.96	0.26	46,46,46,46	0
56	MG	CA	3042	1/1	0.96	0.11	56,56,56,56	0
56	MG	DA	3103	1/1	0.96	0.07	56,56,56,56	0
56	MG	DA	3403	1/1	0.96	0.08	39,39,39,39	0
56	MG	BA	3581	1/1	0.96	0.10	34,34,34,34	0
56	MG	BA	3582	1/1	0.96	0.11	31,31,31,31	0
56	MG	BA	3391	1/1	0.96	0.10	37,37,37,37	0
56	MG	CA	3046	1/1	0.96	0.09	41,41,41,41	0
56	MG	AA	3090	1/1	0.96	0.18	28,28,28,28	0
56	MG	DA	3415	1/1	0.96	0.17	40,40,40,40	0
56	MG	DA	3110	1/1	0.96	0.14	42,42,42,42	0
56	MG	AA	3074	1/1	0.96	0.15	38,38,38,38	0
56	MG	DA	3112	1/1	0.96	0.14	24,24,24,24	0
56	MG	BA	3586	1/1	0.96	0.17	45,45,45,45	0
56	MG	BA	3021	1/1	0.96	0.10	37,37,37,37	0
56	MG	DA	3423	1/1	0.96	0.15	40,40,40,40	0
56	MG	BA	3160	1/1	0.96	0.15	29,29,29,29	0
56	MG	AA	3175	1/1	0.96	0.12	53,53,53,53	0
56	MG	BA	3397	1/1	0.96	0.11	30,30,30,30	0
56	MG	BA	3398	1/1	0.96	0.15	41,41,41,41	0
56	MG	BA	3249	1/1	0.96	0.15	48,48,48,48	0
56	MG	CA	3060	1/1	0.96	0.19	50,50,50,50	0
56	MG	BA	3250	1/1	0.96	0.18	33,33,33,33	0
56	MG	BA	3251	1/1	0.96	0.28	37,37,37,37	0
56	MG	BA	3162	1/1	0.96	0.18	39,39,39,39	0
56	MG	DA	3437	1/1	0.96	0.26	48,48,48,48	0
56	MG	AA	3075	1/1	0.96	0.16	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	DA	3440	1/1	0.96	0.16	52,52,52,52	0
56	MG	DA	3442	1/1	0.96	0.19	42,42,42,42	0
56	MG	DA	3128	1/1	0.96	0.21	42,42,42,42	0
56	MG	AA	3140	1/1	0.96	0.12	31,31,31,31	0
56	MG	BA	3410	1/1	0.96	0.14	43,43,43,43	0
56	MG	DA	3447	1/1	0.96	0.08	33,33,33,33	0
56	MG	DA	3449	1/1	0.96	0.15	29,29,29,29	0
56	MG	BA	3412	1/1	0.96	0.17	48,48,48,48	0
56	MG	DA	3452	1/1	0.96	0.14	56,56,56,56	0
56	MG	DA	3454	1/1	0.96	0.08	64,64,64,64	0
56	MG	DA	3456	1/1	0.96	0.13	34,34,34,34	0
56	MG	DA	3457	1/1	0.96	0.12	38,38,38,38	0
56	MG	DA	3460	1/1	0.96	0.18	50,50,50,50	0
56	MG	BA	3255	1/1	0.96	0.21	32,32,32,32	0
56	MG	BA	3610	1/1	0.96	0.17	47,47,47,47	0
56	MG	AA	3036	1/1	0.96	0.07	41,41,41,41	0
56	MG	BA	3612	1/1	0.96	0.19	51,51,51,51	0
56	MG	BA	3615	1/1	0.96	0.12	42,42,42,42	0
56	MG	DA	3140	1/1	0.96	0.10	37,37,37,37	0
56	MG	BA	3258	1/1	0.96	0.23	30,30,30,30	0
56	MG	BA	3418	1/1	0.96	0.12	46,46,46,46	0
56	MG	BA	3420	1/1	0.96	0.10	24,24,24,24	0
56	MG	BA	3167	1/1	0.96	0.12	46,46,46,46	0
56	MG	AA	3005	1/1	0.96	0.18	37,37,37,37	0
56	MG	AA	3146	1/1	0.96	0.15	41,41,41,41	0
56	MG	BA	3265	1/1	0.96	0.29	47,47,47,47	0
56	MG	AA	3114	1/1	0.96	0.14	56,56,56,56	0
56	MG	BA	3175	1/1	0.96	0.14	33,33,33,33	0
56	MG	BA	3429	1/1	0.96	0.18	41,41,41,41	0
56	MG	AA	3182	1/1	0.96	0.14	57,57,57,57	0
56	MG	BA	3431	1/1	0.96	0.10	44,44,44,44	0
56	MG	AA	3116	1/1	0.96	0.12	51,51,51,51	0
56	MG	CA	3092	1/1	0.96	0.12	54,54,54,54	0
56	MG	BA	3635	1/1	0.96	0.19	63,63,63,63	0
56	MG	CA	3094	1/1	0.96	0.10	67,67,67,67	0
56	MG	DA	3489	1/1	0.96	0.16	49,49,49,49	0
56	MG	AA	3015	1/1	0.96	0.13	56,56,56,56	0
56	MG	BA	3273	1/1	0.96	0.09	29,29,29,29	0
56	MG	DA	3494	1/1	0.96	0.17	49,49,49,49	0
56	MG	CA	3097	1/1	0.96	0.19	67,67,67,67	0
56	MG	BA	3101	1/1	0.96	0.14	30,30,30,30	0
56	MG	CA	3100	1/1	0.96	0.14	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DA	3174	1/1	0.96	0.10	44,44,44,44	0
56	MG	BA	3641	1/1	0.96	0.21	33,33,33,33	0
56	MG	BA	3102	1/1	0.96	0.06	49,49,49,49	0
56	MG	DA	3180	1/1	0.96	0.11	30,30,30,30	0
56	MG	DA	3181	1/1	0.96	0.10	40,40,40,40	0
56	MG	DA	3511	1/1	0.96	0.08	53,53,53,53	0
56	MG	AA	3021	1/1	0.96	0.09	41,41,41,41	0
56	MG	BA	3450	1/1	0.96	0.15	45,45,45,45	0
56	MG	BA	3645	1/1	0.96	0.10	66,66,66,66	0
56	MG	BA	3646	1/1	0.96	0.15	23,23,23,23	0
56	MG	AA	3187	1/1	0.96	0.14	33,33,33,33	0
56	MG	DA	3524	1/1	0.96	0.08	51,51,51,51	0
56	MG	DA	3188	1/1	0.96	0.14	25,25,25,25	0
56	MG	BA	3651	1/1	0.96	0.14	42,42,42,42	0
56	MG	CA	3115	1/1	0.96	0.09	62,62,62,62	0
56	MG	BA	3454	1/1	0.96	0.17	21,21,21,21	0
56	MG	DA	3193	1/1	0.96	0.23	49,49,49,49	0
56	MG	BA	3284	1/1	0.96	0.10	41,41,41,41	0
56	MG	DA	3195	1/1	0.96	0.14	38,38,38,38	0
56	MG	BA	3286	1/1	0.96	0.12	32,32,32,32	0
56	MG	BA	3288	1/1	0.96	0.32	48,48,48,48	0
56	MG	CA	3120	1/1	0.96	0.13	51,51,51,51	0
56	MG	BA	3292	1/1	0.96	0.12	43,43,43,43	0
56	MG	DA	3203	1/1	0.96	0.16	21,21,21,21	0
56	MG	BA	3662	1/1	0.96	0.24	36,36,36,36	0
56	MG	BA	3665	1/1	0.96	0.11	30,30,30,30	0
56	MG	DA	3546	1/1	0.96	0.07	40,40,40,40	0
56	MG	DA	3207	1/1	0.96	0.13	39,39,39,39	0
56	MG	DA	3208	1/1	0.96	0.10	43,43,43,43	0
56	MG	BA	3293	1/1	0.96	0.13	17,17,17,17	0
56	MG	BA	3667	1/1	0.96	0.50	38,38,38,38	0
56	MG	DA	3215	1/1	0.96	0.13	31,31,31,31	0
56	MG	BA	3465	1/1	0.96	0.10	37,37,37,37	0
56	MG	CA	3128	1/1	0.96	0.09	39,39,39,39	0
56	MG	BA	3105	1/1	0.96	0.13	32,32,32,32	0
56	MG	DA	3558	1/1	0.96	0.09	39,39,39,39	0
56	MG	BA	3674	1/1	0.96	0.22	54,54,54,54	0
56	MG	DA	3221	1/1	0.96	0.10	33,33,33,33	0
56	MG	BA	3296	1/1	0.96	0.08	25,25,25,25	0
56	MG	AA	3086	1/1	0.96	0.25	61,61,61,61	0
56	MG	CA	3133	1/1	0.96	0.11	68,68,68,68	0
56	MG	DA	3227	1/1	0.96	0.15	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DA	3567	1/1	0.96	0.10	41,41,41,41	0
56	MG	DA	3228	1/1	0.96	0.07	51,51,51,51	0
56	MG	AA	3156	1/1	0.96	0.15	61,61,61,61	0
56	MG	DA	3570	1/1	0.96	0.14	52,52,52,52	0
56	MG	BA	3299	1/1	0.96	0.13	36,36,36,36	0
56	MG	BA	3474	1/1	0.96	0.18	53,53,53,53	0
56	MG	BA	3300	1/1	0.96	0.15	39,39,39,39	0
56	MG	BA	3477	1/1	0.96	0.10	50,50,50,50	0
56	MG	BB	3007	1/1	0.96	0.14	35,35,35,35	0
56	MG	DA	3237	1/1	0.96	0.29	39,39,39,39	0
56	MG	DA	3577	1/1	0.96	0.17	35,35,35,35	0
56	MG	CA	3142	1/1	0.96	0.12	42,42,42,42	0
56	MG	DA	3579	1/1	0.96	0.08	54,54,54,54	0
56	MG	CA	3143	1/1	0.96	0.15	42,42,42,42	0
56	MG	AA	3157	1/1	0.96	0.09	55,55,55,55	0
56	MG	DA	3241	1/1	0.96	0.15	36,36,36,36	0
56	MG	DA	3242	1/1	0.96	0.14	60,60,60,60	0
56	MG	DA	3584	1/1	0.96	0.17	61,61,61,61	0
56	MG	BA	3050	1/1	0.96	0.17	44,44,44,44	0
56	MG	BA	3303	1/1	0.96	0.13	31,31,31,31	0
56	MG	DA	3589	1/1	0.96	0.17	33,33,33,33	0
56	MG	BA	3304	1/1	0.96	0.08	43,43,43,43	0
56	MG	AA	3048	1/1	0.96	0.21	42,42,42,42	0
56	MG	DA	3248	1/1	0.96	0.28	52,52,52,52	0
56	MG	BA	3052	1/1	0.96	0.14	27,27,27,27	0
56	MG	DA	3250	1/1	0.96	0.17	37,37,37,37	0
56	MG	BA	3197	1/1	0.96	0.16	19,19,19,19	0
56	MG	BA	3116	1/1	0.96	0.19	50,50,50,50	0
56	MG	BA	3490	1/1	0.96	0.11	38,38,38,38	0
56	MG	DB	3006	1/1	0.96	0.15	55,55,55,55	0
56	MG	DA	3254	1/1	0.96	0.07	46,46,46,46	0
56	MG	BE	304	1/1	0.96	0.15	13,13,13,13	0
56	MG	AA	3123	1/1	0.96	0.16	38,38,38,38	0
56	MG	DA	3258	1/1	0.96	0.18	49,49,49,49	0
56	MG	DA	3259	1/1	0.96	0.19	42,42,42,42	0
56	MG	BA	3493	1/1	0.96	0.14	40,40,40,40	0
56	MG	BA	3494	1/1	0.96	0.17	34,34,34,34	0
56	MG	BA	3311	1/1	0.96	0.11	39,39,39,39	0
56	MG	DA	3002	1/1	0.96	0.13	33,33,33,33	0
56	MG	AX	3004	1/1	0.96	0.17	39,39,39,39	0
56	MG	BA	3055	1/1	0.96	0.16	13,13,13,13	0
56	MG	DA	3269	1/1	0.96	0.21	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	3203	1/1	0.96	0.14	35,35,35,35	0
56	MG	BA	3204	1/1	0.96	0.16	35,35,35,35	0
56	MG	BA	3323	1/1	0.96	0.07	61,61,61,61	0
56	MG	AX	3005	1/1	0.96	0.26	42,42,42,42	0
56	MG	BP	202	1/1	0.96	0.47	31,31,31,31	0
56	MG	BA	3327	1/1	0.96	0.14	44,44,44,44	0
56	MG	BA	3511	1/1	0.96	0.14	38,38,38,38	0
56	MG	DA	3019	1/1	0.96	0.13	40,40,40,40	0
56	MG	DA	3286	1/1	0.96	0.07	35,35,35,35	0
56	MG	DA	3287	1/1	0.96	0.11	38,38,38,38	0
56	MG	BR	3001	1/1	0.96	0.12	31,31,31,31	0
56	MG	DA	3291	1/1	0.96	0.07	38,38,38,38	0
56	MG	DA	3293	1/1	0.96	0.13	34,34,34,34	0
56	MG	BR	3002	1/1	0.96	0.13	23,23,23,23	0
56	MG	AA	3101	1/1	0.96	0.13	53,53,53,53	0
58	ZN	D4	501	1/1	0.96	0.05	141,141,141,141	0
56	MG	AA	3161	1/1	0.96	0.10	66,66,66,66	0
56	MG	BV	201	1/1	0.96	0.44	36,36,36,36	0
56	MG	CA	3070	1/1	0.97	0.08	39,39,39,39	0
56	MG	AA	3070	1/1	0.97	0.17	33,33,33,33	0
56	MG	BA	3285	1/1	0.97	0.10	48,48,48,48	0
56	MG	BA	3215	1/1	0.97	0.14	32,32,32,32	0
56	MG	BA	3664	1/1	0.97	0.16	30,30,30,30	0
56	MG	CA	3076	1/1	0.97	0.23	48,48,48,48	0
56	MG	BA	3014	1/1	0.97	0.29	35,35,35,35	0
56	MG	BA	3517	1/1	0.97	0.12	40,40,40,40	0
56	MG	DA	3114	1/1	0.97	0.10	37,37,37,37	0
56	MG	BA	3291	1/1	0.97	0.14	14,14,14,14	0
56	MG	AA	3095	1/1	0.97	0.16	55,55,55,55	0
56	MG	BA	3669	1/1	0.97	0.17	29,29,29,29	0
56	MG	DA	3363	1/1	0.97	0.09	36,36,36,36	0
56	MG	BA	3671	1/1	0.97	0.27	48,48,48,48	0
56	MG	AA	3007	1/1	0.97	0.14	30,30,30,30	0
56	MG	BA	3673	1/1	0.97	0.10	37,37,37,37	0
56	MG	BA	3294	1/1	0.97	0.10	32,32,32,32	0
56	MG	BA	3151	1/1	0.97	0.12	34,34,34,34	0
56	MG	DA	3370	1/1	0.97	0.11	44,44,44,44	0
56	MG	BA	3152	1/1	0.97	0.20	39,39,39,39	0
56	MG	DA	3372	1/1	0.97	0.10	21,21,21,21	0
56	MG	AA	3050	1/1	0.97	0.12	24,24,24,24	0
56	MG	BA	3530	1/1	0.97	0.14	36,36,36,36	0
56	MG	DA	3127	1/1	0.97	0.13	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\AA^2$)	Q<0.9
56	MG	CA	3091	1/1	0.97	0.15	66,66,66,66	0
56	MG	BA	3057	1/1	0.97	0.16	38,38,38,38	0
56	MG	DA	3130	1/1	0.97	0.26	47,47,47,47	0
56	MG	DA	3380	1/1	0.97	0.10	33,33,33,33	0
56	MG	BA	3155	1/1	0.97	0.29	27,27,27,27	0
56	MG	AL	201	1/1	0.97	0.08	63,63,63,63	0
56	MG	DA	3133	1/1	0.97	0.11	53,53,53,53	0
56	MG	DA	3384	1/1	0.97	0.17	52,52,52,52	0
56	MG	BA	3402	1/1	0.97	0.23	28,28,28,28	0
56	MG	BB	3008	1/1	0.97	0.15	21,21,21,21	0
56	MG	DA	3388	1/1	0.97	0.05	35,35,35,35	0
56	MG	AM	3001	1/1	0.97	0.13	54,54,54,54	0
56	MG	AA	3025	1/1	0.97	0.16	37,37,37,37	0
56	MG	DA	3138	1/1	0.97	0.12	33,33,33,33	0
56	MG	CA	3099	1/1	0.97	0.14	57,57,57,57	0
56	MG	BB	3011	1/1	0.97	0.08	45,45,45,45	0
56	MG	CA	3101	1/1	0.97	0.13	53,53,53,53	0
56	MG	DA	3395	1/1	0.97	0.10	41,41,41,41	0
56	MG	BB	3012	1/1	0.97	0.14	44,44,44,44	0
56	MG	DA	3143	1/1	0.97	0.21	27,27,27,27	0
56	MG	BB	3014	1/1	0.97	0.17	35,35,35,35	0
56	MG	AA	3150	1/1	0.97	0.19	51,51,51,51	0
56	MG	DA	3400	1/1	0.97	0.17	38,38,38,38	0
56	MG	BA	3541	1/1	0.97	0.11	26,26,26,26	0
56	MG	BA	3408	1/1	0.97	0.13	56,56,56,56	0
56	MG	AA	3004	1/1	0.97	0.15	67,67,67,67	0
56	MG	BA	3411	1/1	0.97	0.16	25,25,25,25	0
56	MG	CA	3111	1/1	0.97	0.12	43,43,43,43	0
56	MG	BD	305	1/1	0.97	0.15	38,38,38,38	0
56	MG	DA	3409	1/1	0.97	0.17	53,53,53,53	0
56	MG	DA	3153	1/1	0.97	0.14	42,42,42,42	0
56	MG	DA	3155	1/1	0.97	0.24	45,45,45,45	0
56	MG	CA	3114	1/1	0.97	0.09	80,80,80,80	0
56	MG	BA	3547	1/1	0.97	0.06	60,60,60,60	0
56	MG	DA	3159	1/1	0.97	0.17	31,31,31,31	0
56	MG	DA	3160	1/1	0.97	0.15	44,44,44,44	0
56	MG	BD	307	1/1	0.97	0.20	27,27,27,27	0
56	MG	BD	308	1/1	0.97	0.17	35,35,35,35	0
56	MG	BA	3548	1/1	0.97	0.11	30,30,30,30	0
56	MG	BA	3549	1/1	0.97	0.12	57,57,57,57	0
56	MG	BA	3065	1/1	0.97	0.15	29,29,29,29	0
56	MG	DA	3166	1/1	0.97	0.15	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	DA	3427	1/1	0.97	0.15	25,25,25,25	0
56	MG	BE	306	1/1	0.97	0.08	32,32,32,32	0
56	MG	DA	3170	1/1	0.97	0.14	38,38,38,38	0
56	MG	BA	3414	1/1	0.97	0.15	31,31,31,31	0
56	MG	BA	3111	1/1	0.97	0.14	27,27,27,27	0
56	MG	DA	3432	1/1	0.97	0.18	33,33,33,33	0
56	MG	BF	304	1/1	0.97	0.25	37,37,37,37	0
56	MG	BA	3024	1/1	0.97	0.31	32,32,32,32	0
56	MG	DA	3175	1/1	0.97	0.13	47,47,47,47	0
56	MG	AA	3174	1/1	0.97	0.09	55,55,55,55	0
56	MG	DA	3178	1/1	0.97	0.24	46,46,46,46	0
56	MG	CA	3127	1/1	0.97	0.08	49,49,49,49	0
56	MG	BA	3166	1/1	0.97	0.12	35,35,35,35	0
56	MG	BA	3556	1/1	0.97	0.07	41,41,41,41	0
56	MG	BN	3001	1/1	0.97	0.12	57,57,57,57	0
56	MG	BA	3419	1/1	0.97	0.13	20,20,20,20	0
56	MG	DA	3448	1/1	0.97	0.21	29,29,29,29	0
56	MG	BA	3068	1/1	0.97	0.09	39,39,39,39	0
56	MG	DA	3185	1/1	0.97	0.22	32,32,32,32	0
56	MG	BA	3312	1/1	0.97	0.13	18,18,18,18	0
56	MG	BA	3560	1/1	0.97	0.18	55,55,55,55	0
56	MG	BA	3314	1/1	0.97	0.18	36,36,36,36	0
56	MG	DA	3189	1/1	0.97	0.27	31,31,31,31	0
56	MG	DA	3459	1/1	0.97	0.24	38,38,38,38	0
56	MG	BA	3027	1/1	0.97	0.21	28,28,28,28	0
56	MG	BQ	202	1/1	0.97	0.08	14,14,14,14	0
56	MG	DA	3462	1/1	0.97	0.12	35,35,35,35	0
56	MG	DA	3464	1/1	0.97	0.11	46,46,46,46	0
56	MG	BA	3117	1/1	0.97	0.38	40,40,40,40	0
56	MG	DA	3466	1/1	0.97	0.12	38,38,38,38	0
56	MG	BA	3172	1/1	0.97	0.15	54,54,54,54	0
56	MG	BR	3003	1/1	0.97	0.15	39,39,39,39	0
56	MG	AA	3130	1/1	0.97	0.11	50,50,50,50	0
56	MG	CA	3144	1/1	0.97	0.12	56,56,56,56	0
56	MG	BU	203	1/1	0.97	0.38	32,32,32,32	0
56	MG	DA	3198	1/1	0.97	0.16	54,54,54,54	0
56	MG	BA	3029	1/1	0.97	0.15	12,12,12,12	0
56	MG	CA	3147	1/1	0.97	0.17	52,52,52,52	0
56	MG	BA	3568	1/1	0.97	0.12	42,42,42,42	0
56	MG	DA	3204	1/1	0.97	0.07	37,37,37,37	0
56	MG	BA	3072	1/1	0.97	0.16	24,24,24,24	0
56	MG	CA	3150	1/1	0.97	0.15	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\AA^2$)	Q<0.9
56	MG	BA	3570	1/1	0.97	0.07	36,36,36,36	0
56	MG	DA	3481	1/1	0.97	0.09	41,41,41,41	0
56	MG	BA	3325	1/1	0.97	0.16	42,42,42,42	0
56	MG	BA	3121	1/1	0.97	0.48	43,43,43,43	0
56	MG	DA	3210	1/1	0.97	0.10	37,37,37,37	0
56	MG	DA	3211	1/1	0.97	0.15	35,35,35,35	0
56	MG	BA	3434	1/1	0.97	0.12	43,43,43,43	0
56	MG	DA	3213	1/1	0.97	0.11	34,34,34,34	0
56	MG	BA	3574	1/1	0.97	0.12	55,55,55,55	0
56	MG	BA	3435	1/1	0.97	0.17	36,36,36,36	0
56	MG	BA	3436	1/1	0.97	0.10	35,35,35,35	0
56	MG	BA	3577	1/1	0.97	0.08	57,57,57,57	0
56	MG	BA	3437	1/1	0.97	0.13	58,58,58,58	0
56	MG	DA	3495	1/1	0.97	0.28	45,45,45,45	0
56	MG	BA	3439	1/1	0.97	0.20	30,30,30,30	0
56	MG	DA	3498	1/1	0.97	0.13	48,48,48,48	0
56	MG	DA	3499	1/1	0.97	0.13	45,45,45,45	0
56	MG	AA	3154	1/1	0.97	0.18	51,51,51,51	0
56	MG	DA	3224	1/1	0.97	0.15	22,22,22,22	0
56	MG	BA	3123	1/1	0.97	0.21	36,36,36,36	0
56	MG	BA	3444	1/1	0.97	0.11	34,34,34,34	0
56	MG	BA	3184	1/1	0.97	0.10	37,37,37,37	0
56	MG	BA	3032	1/1	0.97	0.24	40,40,40,40	0
56	MG	BA	3448	1/1	0.97	0.12	42,42,42,42	0
56	MG	DA	3509	1/1	0.97	0.08	36,36,36,36	0
56	MG	BA	3332	1/1	0.97	0.07	61,61,61,61	0
56	MG	B7	3002	1/1	0.97	0.23	35,35,35,35	0
56	MG	DA	3011	1/1	0.97	0.15	38,38,38,38	0
56	MG	B7	3003	1/1	0.97	0.21	28,28,28,28	0
56	MG	DA	3016	1/1	0.97	0.18	31,31,31,31	0
56	MG	BA	3587	1/1	0.97	0.14	42,42,42,42	0
56	MG	DA	3521	1/1	0.97	0.19	51,51,51,51	0
56	MG	DA	3522	1/1	0.97	0.10	44,44,44,44	0
56	MG	DA	3523	1/1	0.97	0.14	40,40,40,40	0
56	MG	DA	3018	1/1	0.97	0.12	39,39,39,39	0
56	MG	BA	3588	1/1	0.97	0.10	51,51,51,51	0
56	MG	BA	3589	1/1	0.97	0.12	27,27,27,27	0
56	MG	AX	3008	1/1	0.97	0.15	23,23,23,23	0
56	MG	BA	3035	1/1	0.97	0.20	21,21,21,21	0
56	MG	BA	3452	1/1	0.97	0.17	38,38,38,38	0
56	MG	BA	3336	1/1	0.97	0.09	43,43,43,43	0
56	MG	AA	3040	1/1	0.97	0.16	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	3006	1/1	0.97	0.28	37,37,37,37	0
56	MG	AA	3079	1/1	0.97	0.33	49,49,49,49	0
56	MG	DA	3537	1/1	0.97	0.12	47,47,47,47	0
56	MG	BA	3003	1/1	0.97	0.10	49,49,49,49	0
56	MG	BA	3598	1/1	0.97	0.16	48,48,48,48	0
56	MG	DA	3540	1/1	0.97	0.11	46,46,46,46	0
56	MG	DA	3541	1/1	0.97	0.15	57,57,57,57	0
56	MG	BA	3461	1/1	0.97	0.24	52,52,52,52	0
56	MG	DA	3035	1/1	0.97	0.14	46,46,46,46	0
56	MG	BA	3600	1/1	0.97	0.13	68,68,68,68	0
56	MG	BA	3004	1/1	0.97	0.13	23,23,23,23	0
56	MG	DA	3255	1/1	0.97	0.20	32,32,32,32	0
56	MG	DA	3548	1/1	0.97	0.20	40,40,40,40	0
56	MG	AA	3103	1/1	0.97	0.13	51,51,51,51	0
56	MG	DA	3040	1/1	0.97	0.23	34,34,34,34	0
56	MG	DA	3041	1/1	0.97	0.08	35,35,35,35	0
56	MG	BA	3343	1/1	0.97	0.16	27,27,27,27	0
56	MG	DA	3553	1/1	0.97	0.12	46,46,46,46	0
56	MG	DA	3260	1/1	0.97	0.20	36,36,36,36	0
56	MG	BA	3257	1/1	0.97	0.08	29,29,29,29	0
56	MG	BA	3606	1/1	0.97	0.15	32,32,32,32	0
56	MG	AA	3041	1/1	0.97	0.20	52,52,52,52	0
56	MG	BA	3608	1/1	0.97	0.13	45,45,45,45	0
56	MG	BA	3346	1/1	0.97	0.08	43,43,43,43	0
56	MG	DA	3562	1/1	0.97	0.13	42,42,42,42	0
56	MG	DA	3049	1/1	0.97	0.06	40,40,40,40	0
56	MG	BA	3259	1/1	0.97	0.17	35,35,35,35	0
56	MG	DA	3270	1/1	0.97	0.08	37,37,37,37	0
56	MG	BA	3045	1/1	0.97	0.13	34,34,34,34	0
56	MG	CA	3022	1/1	0.97	0.14	34,34,34,34	0
56	MG	BA	3085	1/1	0.97	0.16	27,27,27,27	0
56	MG	DA	3055	1/1	0.97	0.09	34,34,34,34	0
56	MG	CA	3024	1/1	0.97	0.07	64,64,64,64	0
56	MG	DA	3277	1/1	0.97	0.10	48,48,48,48	0
56	MG	AA	3138	1/1	0.97	0.15	50,50,50,50	0
56	MG	DA	3279	1/1	0.97	0.12	27,27,27,27	0
56	MG	CA	3026	1/1	0.97	0.22	44,44,44,44	0
56	MG	BA	3351	1/1	0.97	0.06	33,33,33,33	0
56	MG	DA	3282	1/1	0.97	0.12	30,30,30,30	0
56	MG	DA	3283	1/1	0.97	0.11	38,38,38,38	0
56	MG	DA	3285	1/1	0.97	0.13	52,52,52,52	0
56	MG	BA	3199	1/1	0.97	0.17	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DA	3061	1/1	0.97	0.08	35,35,35,35	0
56	MG	AA	3121	1/1	0.97	0.09	40,40,40,40	0
56	MG	BA	3481	1/1	0.97	0.14	31,31,31,31	0
56	MG	DA	3292	1/1	0.97	0.17	45,45,45,45	0
56	MG	CA	3031	1/1	0.97	0.13	52,52,52,52	0
56	MG	DA	3585	1/1	0.97	0.08	37,37,37,37	0
56	MG	DA	3586	1/1	0.97	0.09	47,47,47,47	0
56	MG	DA	3294	1/1	0.97	0.13	37,37,37,37	0
56	MG	DA	3295	1/1	0.97	0.25	61,61,61,61	0
56	MG	AA	3082	1/1	0.97	0.10	57,57,57,57	0
56	MG	DA	3590	1/1	0.97	0.35	38,38,38,38	0
56	MG	DA	3066	1/1	0.97	0.23	49,49,49,49	0
56	MG	BA	3622	1/1	0.97	0.13	45,45,45,45	0
56	MG	BA	3139	1/1	0.97	0.19	31,31,31,31	0
56	MG	BA	3089	1/1	0.97	0.14	37,37,37,37	0
56	MG	BA	3270	1/1	0.97	0.16	21,21,21,21	0
56	MG	CA	3038	1/1	0.97	0.12	44,44,44,44	0
56	MG	DB	3003	1/1	0.97	0.11	29,29,29,29	0
56	MG	DA	3305	1/1	0.97	0.16	30,30,30,30	0
56	MG	DA	3072	1/1	0.97	0.10	33,33,33,33	0
56	MG	BA	3628	1/1	0.97	0.12	38,38,38,38	0
56	MG	AA	3141	1/1	0.97	0.07	47,47,47,47	0
56	MG	BA	3366	1/1	0.97	0.07	34,34,34,34	0
56	MG	BA	3011	1/1	0.97	0.10	30,30,30,30	0
56	MG	BA	3632	1/1	0.97	0.14	54,54,54,54	0
56	MG	BA	3491	1/1	0.97	0.11	39,39,39,39	0
56	MG	DA	3315	1/1	0.97	0.16	43,43,43,43	0
56	MG	BA	3369	1/1	0.97	0.16	33,33,33,33	0
56	MG	BA	3370	1/1	0.97	0.15	29,29,29,29	0
56	MG	BA	3143	1/1	0.97	0.33	36,36,36,36	0
56	MG	BA	3207	1/1	0.97	0.16	36,36,36,36	0
56	MG	BA	3144	1/1	0.97	0.33	44,44,44,44	0
56	MG	BA	3640	1/1	0.97	0.25	33,33,33,33	0
56	MG	DF	302	1/1	0.97	0.18	41,41,41,41	0
56	MG	CA	3053	1/1	0.97	0.15	44,44,44,44	0
56	MG	CA	3054	1/1	0.97	0.09	44,44,44,44	0
56	MG	BA	3279	1/1	0.97	0.10	38,38,38,38	0
56	MG	AA	3011	1/1	0.97	0.08	24,24,24,24	0
56	MG	DQ	3001	1/1	0.97	0.13	48,48,48,48	0
56	MG	CA	3057	1/1	0.97	0.14	41,41,41,41	0
56	MG	BA	3378	1/1	0.97	0.16	16,16,16,16	0
56	MG	DR	201	1/1	0.97	0.24	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	DR	202	1/1	0.97	0.14	32,32,32,32	0
56	MG	DT	5001	1/1	0.97	0.07	42,42,42,42	0
56	MG	BA	3500	1/1	0.97	0.11	35,35,35,35	0
56	MG	DA	3335	1/1	0.97	0.15	36,36,36,36	0
56	MG	DA	3336	1/1	0.97	0.18	22,22,22,22	0
56	MG	DW	3001	1/1	0.97	0.31	38,38,38,38	0
56	MG	BA	3503	1/1	0.97	0.13	30,30,30,30	0
56	MG	BA	3504	1/1	0.97	0.18	39,39,39,39	0
56	MG	BA	3282	1/1	0.97	0.23	31,31,31,31	0
56	MG	BA	3283	1/1	0.97	0.11	57,57,57,57	0
56	MG	D8	5001	1/1	0.97	0.13	50,50,50,50	0
56	MG	BA	3652	1/1	0.97	0.14	49,49,49,49	0
56	MG	BA	3509	1/1	0.97	0.16	23,23,23,23	0
58	ZN	CN	501	1/1	0.97	0.11	82,82,82,82	0
58	ZN	DY	501	1/1	0.97	0.12	92,92,92,92	0
56	MG	BA	3383	1/1	0.97	0.11	33,33,33,33	0
58	ZN	D6	501	1/1	0.97	0.19	68,68,68,68	0
58	ZN	D9	501	1/1	0.97	0.10	54,54,54,54	0
56	MG	BA	3386	1/1	0.97	0.22	32,32,32,32	0
56	MG	BA	3658	1/1	0.97	0.13	27,27,27,27	0
56	MG	BA	3361	1/1	0.98	0.10	45,45,45,45	0
56	MG	BA	3534	1/1	0.98	0.14	20,20,20,20	0
56	MG	DA	3262	1/1	0.98	0.12	39,39,39,39	0
56	MG	BA	3637	1/1	0.98	0.21	24,24,24,24	0
56	MG	BA	3159	1/1	0.98	0.17	27,27,27,27	0
56	MG	BA	3438	1/1	0.98	0.12	33,33,33,33	0
56	MG	AA	3135	1/1	0.98	0.09	46,46,46,46	0
56	MG	DA	3453	1/1	0.98	0.13	31,31,31,31	0
56	MG	DA	3267	1/1	0.98	0.07	47,47,47,47	0
56	MG	DA	3455	1/1	0.98	0.16	45,45,45,45	0
56	MG	BA	3440	1/1	0.98	0.06	38,38,38,38	0
56	MG	BA	3364	1/1	0.98	0.18	29,29,29,29	0
56	MG	DA	3458	1/1	0.98	0.13	34,34,34,34	0
56	MG	BA	3442	1/1	0.98	0.15	20,20,20,20	0
56	MG	BA	3542	1/1	0.98	0.05	51,51,51,51	0
56	MG	CA	3134	1/1	0.98	0.12	53,53,53,53	0
56	MG	AA	3077	1/1	0.98	0.14	39,39,39,39	0
56	MG	DA	3463	1/1	0.98	0.13	28,28,28,28	0
56	MG	BA	3544	1/1	0.98	0.18	25,25,25,25	0
56	MG	CA	3137	1/1	0.98	0.13	66,66,66,66	0
56	MG	DA	3276	1/1	0.98	0.17	50,50,50,50	0
56	MG	BA	3647	1/1	0.98	0.10	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\AA^2$)	Q<0.9
56	MG	BA	3648	1/1	0.98	0.11	28,28,28,28	0
56	MG	BA	3031	1/1	0.98	0.47	46,46,46,46	0
56	MG	BA	3445	1/1	0.98	0.09	22,22,22,22	0
56	MG	BA	3132	1/1	0.98	0.15	25,25,25,25	0
56	MG	BA	3368	1/1	0.98	0.09	42,42,42,42	0
56	MG	BA	3654	1/1	0.98	0.10	64,64,64,64	0
56	MG	DA	3284	1/1	0.98	0.10	23,23,23,23	0
56	MG	AN	502	1/1	0.98	0.20	53,53,53,53	0
56	MG	DA	3476	1/1	0.98	0.06	32,32,32,32	0
56	MG	BA	3656	1/1	0.98	0.09	12,12,12,12	0
56	MG	AA	3162	1/1	0.98	0.12	40,40,40,40	0
56	MG	DA	3288	1/1	0.98	0.11	64,64,64,64	0
56	MG	BA	3106	1/1	0.98	0.14	40,40,40,40	0
56	MG	BA	3659	1/1	0.98	0.14	28,28,28,28	0
56	MG	BA	3372	1/1	0.98	0.19	29,29,29,29	0
56	MG	AA	3107	1/1	0.98	0.24	36,36,36,36	0
56	MG	BA	3208	1/1	0.98	0.24	25,25,25,25	0
56	MG	CA	3153	1/1	0.98	0.13	37,37,37,37	0
56	MG	BA	3663	1/1	0.98	0.08	20,20,20,20	0
56	MG	BA	3456	1/1	0.98	0.13	33,33,33,33	0
56	MG	BA	3457	1/1	0.98	0.14	29,29,29,29	0
56	MG	BA	3168	1/1	0.98	0.16	47,47,47,47	0
56	MG	DA	3490	1/1	0.98	0.15	34,34,34,34	0
56	MG	AA	3113	1/1	0.98	0.18	53,53,53,53	0
56	MG	BA	3212	1/1	0.98	0.16	28,28,28,28	0
56	MG	BA	3379	1/1	0.98	0.14	31,31,31,31	0
56	MG	BA	3462	1/1	0.98	0.08	44,44,44,44	0
56	MG	BA	3170	1/1	0.98	0.12	34,34,34,34	0
56	MG	DA	3497	1/1	0.98	0.08	45,45,45,45	0
56	MG	BA	3214	1/1	0.98	0.22	28,28,28,28	0
56	MG	DA	3149	1/1	0.98	0.23	41,41,41,41	0
56	MG	BA	3564	1/1	0.98	0.16	29,29,29,29	0
56	MG	BA	3382	1/1	0.98	0.14	27,27,27,27	0
56	MG	DA	3006	1/1	0.98	0.14	33,33,33,33	0
56	MG	DA	3313	1/1	0.98	0.09	40,40,40,40	0
56	MG	DA	3505	1/1	0.98	0.10	44,44,44,44	0
56	MG	BA	3109	1/1	0.98	0.09	36,36,36,36	0
56	MG	CA	3037	1/1	0.98	0.09	45,45,45,45	0
56	MG	BA	3467	1/1	0.98	0.17	20,20,20,20	0
56	MG	DA	3317	1/1	0.98	0.09	53,53,53,53	0
56	MG	DA	3510	1/1	0.98	0.09	53,53,53,53	0
56	MG	DA	3157	1/1	0.98	0.10	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	DA	3512	1/1	0.98	0.11	36,36,36,36	0
56	MG	DA	3319	1/1	0.98	0.20	38,38,38,38	0
56	MG	DA	3320	1/1	0.98	0.08	46,46,46,46	0
56	MG	CA	3039	1/1	0.98	0.18	50,50,50,50	0
56	MG	DA	3322	1/1	0.98	0.17	23,23,23,23	0
56	MG	BA	3384	1/1	0.98	0.11	28,28,28,28	0
56	MG	DA	3520	1/1	0.98	0.09	34,34,34,34	0
56	MG	DA	3324	1/1	0.98	0.12	52,52,52,52	0
56	MG	BA	3262	1/1	0.98	0.17	24,24,24,24	0
56	MG	DA	3014	1/1	0.98	0.10	33,33,33,33	0
56	MG	AA	3031	1/1	0.98	0.12	60,60,60,60	0
56	MG	BA	3264	1/1	0.98	0.19	35,35,35,35	0
56	MG	DA	3526	1/1	0.98	0.07	64,64,64,64	0
56	MG	BA	3472	1/1	0.98	0.10	34,34,34,34	0
56	MG	BA	3473	1/1	0.98	0.10	37,37,37,37	0
56	MG	BA	3320	1/1	0.98	0.13	44,44,44,44	0
56	MG	BA	3321	1/1	0.98	0.07	53,53,53,53	0
56	MG	DA	3168	1/1	0.98	0.14	39,39,39,39	0
56	MG	DA	3169	1/1	0.98	0.10	38,38,38,38	0
56	MG	BA	3173	1/1	0.98	0.19	45,45,45,45	0
56	MG	DA	3023	1/1	0.98	0.14	37,37,37,37	0
56	MG	DA	3536	1/1	0.98	0.11	56,56,56,56	0
56	MG	AA	3152	1/1	0.98	0.11	57,57,57,57	0
56	MG	DA	3026	1/1	0.98	0.11	34,34,34,34	0
56	MG	BB	3013	1/1	0.98	0.16	57,57,57,57	0
56	MG	CA	3051	1/1	0.98	0.13	66,66,66,66	0
56	MG	DA	3342	1/1	0.98	0.21	37,37,37,37	0
56	MG	DA	3542	1/1	0.98	0.12	30,30,30,30	0
56	MG	BA	3479	1/1	0.98	0.15	45,45,45,45	0
56	MG	BA	3084	1/1	0.98	0.23	34,34,34,34	0
56	MG	DA	3031	1/1	0.98	0.13	21,21,21,21	0
56	MG	BA	3326	1/1	0.98	0.20	28,28,28,28	0
56	MG	BA	3482	1/1	0.98	0.12	23,23,23,23	0
56	MG	BB	3018	1/1	0.98	0.16	30,30,30,30	0
56	MG	DA	3350	1/1	0.98	0.12	36,36,36,36	0
56	MG	BA	3176	1/1	0.98	0.10	47,47,47,47	0
56	MG	BD	303	1/1	0.98	0.42	37,37,37,37	0
56	MG	AA	3096	1/1	0.98	0.18	53,53,53,53	0
56	MG	DA	3038	1/1	0.98	0.11	30,30,30,30	0
56	MG	BA	3178	1/1	0.98	0.24	26,26,26,26	0
56	MG	CA	3061	1/1	0.98	0.13	45,45,45,45	0
56	MG	DA	3556	1/1	0.98	0.15	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	BA	3114	1/1	0.98	0.21	34,34,34,34	0
56	MG	DA	3358	1/1	0.98	0.23	45,45,45,45	0
56	MG	DA	3559	1/1	0.98	0.09	55,55,55,55	0
56	MG	BA	3272	1/1	0.98	0.10	37,37,37,37	0
56	MG	BA	3181	1/1	0.98	0.16	37,37,37,37	0
56	MG	BE	302	1/1	0.98	0.77	36,36,36,36	0
56	MG	DA	3362	1/1	0.98	0.08	43,43,43,43	0
56	MG	BA	3333	1/1	0.98	0.19	35,35,35,35	0
56	MG	DA	3364	1/1	0.98	0.06	37,37,37,37	0
56	MG	BA	3064	1/1	0.98	0.19	30,30,30,30	0
56	MG	BA	3404	1/1	0.98	0.17	38,38,38,38	0
56	MG	BA	3591	1/1	0.98	0.08	36,36,36,36	0
56	MG	BA	3276	1/1	0.98	0.12	42,42,42,42	0
56	MG	BF	302	1/1	0.98	0.08	45,45,45,45	0
56	MG	BA	3406	1/1	0.98	0.22	39,39,39,39	0
56	MG	AA	3168	1/1	0.98	0.10	56,56,56,56	0
56	MG	DA	3201	1/1	0.98	0.11	51,51,51,51	0
56	MG	DA	3202	1/1	0.98	0.17	24,24,24,24	0
56	MG	BA	3337	1/1	0.98	0.12	37,37,37,37	0
56	MG	CA	3075	1/1	0.98	0.15	53,53,53,53	0
56	MG	BG	3001	1/1	0.98	0.12	71,71,71,71	0
56	MG	DA	3377	1/1	0.98	0.14	37,37,37,37	0
56	MG	CA	3077	1/1	0.98	0.14	44,44,44,44	0
56	MG	BA	3146	1/1	0.98	0.18	31,31,31,31	0
56	MG	AA	3076	1/1	0.98	0.10	52,52,52,52	0
56	MG	AA	3155	1/1	0.98	0.09	61,61,61,61	0
56	MG	BA	3413	1/1	0.98	0.16	26,26,26,26	0
56	MG	BA	3501	1/1	0.98	0.13	44,44,44,44	0
56	MG	BA	3502	1/1	0.98	0.16	33,33,33,33	0
56	MG	BA	3281	1/1	0.98	0.22	51,51,51,51	0
56	MG	DA	3214	1/1	0.98	0.21	30,30,30,30	0
56	MG	DA	3387	1/1	0.98	0.07	53,53,53,53	0
56	MG	BA	3603	1/1	0.98	0.05	49,49,49,49	0
56	MG	AA	3186	1/1	0.98	0.13	55,55,55,55	0
56	MG	BP	204	1/1	0.98	0.16	31,31,31,31	0
56	MG	BA	3022	1/1	0.98	0.14	26,26,26,26	0
56	MG	DA	3219	1/1	0.98	0.12	33,33,33,33	0
56	MG	BA	3506	1/1	0.98	0.09	39,39,39,39	0
56	MG	BQ	203	1/1	0.98	0.34	33,33,33,33	0
56	MG	DA	3596	1/1	0.98	0.28	54,54,54,54	0
56	MG	DB	3001	1/1	0.98	0.17	40,40,40,40	0
56	MG	AA	3132	1/1	0.98	0.25	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	3223	1/1	0.98	0.09	47,47,47,47	0
56	MG	BA	3508	1/1	0.98	0.13	25,25,25,25	0
56	MG	AA	3144	1/1	0.98	0.19	42,42,42,42	0
56	MG	BU	201	1/1	0.98	0.31	32,32,32,32	0
56	MG	AE	3001	1/1	0.98	0.09	71,71,71,71	0
56	MG	BA	3287	1/1	0.98	0.13	46,46,46,46	0
56	MG	BA	3421	1/1	0.98	0.18	36,36,36,36	0
56	MG	DA	3080	1/1	0.98	0.21	29,29,29,29	0
56	MG	DB	3011	1/1	0.98	0.08	29,29,29,29	0
56	MG	DA	3404	1/1	0.98	0.10	46,46,46,46	0
56	MG	BA	3613	1/1	0.98	0.15	45,45,45,45	0
56	MG	BA	3614	1/1	0.98	0.05	55,55,55,55	0
56	MG	DA	3233	1/1	0.98	0.41	36,36,36,36	0
56	MG	AA	3133	1/1	0.98	0.08	38,38,38,38	0
56	MG	DA	3410	1/1	0.98	0.14	64,64,64,64	0
56	MG	DA	3235	1/1	0.98	0.18	42,42,42,42	0
56	MG	DE	3005	1/1	0.98	0.12	20,20,20,20	0
56	MG	AA	3118	1/1	0.98	0.15	36,36,36,36	0
56	MG	DA	3414	1/1	0.98	0.05	42,42,42,42	0
56	MG	CA	3102	1/1	0.98	0.19	30,30,30,30	0
56	MG	BA	3194	1/1	0.98	0.15	23,23,23,23	0
56	MG	DA	3417	1/1	0.98	0.15	40,40,40,40	0
56	MG	BA	3098	1/1	0.98	0.12	56,56,56,56	0
56	MG	BX	101	1/1	0.98	0.22	46,46,46,46	0
56	MG	BA	3352	1/1	0.98	0.14	32,32,32,32	0
56	MG	DA	3421	1/1	0.98	0.15	52,52,52,52	0
56	MG	BA	3519	1/1	0.98	0.25	53,53,53,53	0
56	MG	BA	3520	1/1	0.98	0.14	24,24,24,24	0
56	MG	BA	3196	1/1	0.98	0.18	17,17,17,17	0
56	MG	BA	3522	1/1	0.98	0.10	52,52,52,52	0
56	MG	DA	3246	1/1	0.98	0.36	38,38,38,38	0
56	MG	DA	3095	1/1	0.98	0.33	47,47,47,47	0
56	MG	BA	3354	1/1	0.98	0.11	42,42,42,42	0
56	MG	BA	3627	1/1	0.98	0.10	54,54,54,54	0
56	MG	BA	3524	1/1	0.98	0.07	57,57,57,57	0
56	MG	D0	5001	1/1	0.98	0.06	39,39,39,39	0
56	MG	BA	3099	1/1	0.98	0.20	32,32,32,32	0
56	MG	BA	3100	1/1	0.98	0.11	29,29,29,29	0
56	MG	DA	3433	1/1	0.98	0.16	33,33,33,33	0
56	MG	BA	3432	1/1	0.98	0.11	37,37,37,37	0
58	ZN	BY	501	1/1	0.98	0.15	51,51,51,51	0
56	MG	BA	3358	1/1	0.98	0.17	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	DA	3436	1/1	0.98	0.10	27,27,27,27	0
56	MG	B5	502	1/1	0.98	0.32	34,34,34,34	0
56	MG	DA	3104	1/1	0.98	0.11	35,35,35,35	0
56	MG	B5	503	1/1	0.98	0.21	47,47,47,47	0
56	MG	DA	3441	1/1	0.98	0.12	45,45,45,45	0
56	MG	BA	3245	1/1	0.98	0.17	27,27,27,27	0
56	MG	BA	3360	1/1	0.98	0.15	21,21,21,21	0
56	MG	DA	3502	1/1	0.99	0.12	39,39,39,39	0
56	MG	BA	3290	1/1	0.99	0.15	36,36,36,36	0
56	MG	DA	3025	1/1	0.99	0.09	41,41,41,41	0
56	MG	BA	3026	1/1	0.99	0.22	46,46,46,46	0
56	MG	DA	3079	1/1	0.99	0.12	54,54,54,54	0
56	MG	BA	3526	1/1	0.99	0.23	25,25,25,25	0
56	MG	BA	3377	1/1	0.99	0.17	31,31,31,31	0
56	MG	DA	3439	1/1	0.99	0.13	28,28,28,28	0
56	MG	BA	3310	1/1	0.99	0.18	35,35,35,35	0
56	MG	DA	3312	1/1	0.99	0.04	47,47,47,47	0
56	MG	BA	3355	1/1	0.99	0.09	31,31,31,31	0
56	MG	DA	3513	1/1	0.99	0.12	32,32,32,32	0
56	MG	DA	3084	1/1	0.99	0.30	39,39,39,39	0
56	MG	DA	3444	1/1	0.99	0.19	53,53,53,53	0
56	MG	BA	3059	1/1	0.99	0.11	27,27,27,27	0
56	MG	DA	3517	1/1	0.99	0.15	47,47,47,47	0
56	MG	BA	3275	1/1	0.99	0.18	39,39,39,39	0
56	MG	BA	3532	1/1	0.99	0.04	53,53,53,53	0
56	MG	BA	3313	1/1	0.99	0.12	17,17,17,17	0
56	MG	BA	3409	1/1	0.99	0.16	28,28,28,28	0
56	MG	BA	3535	1/1	0.99	0.10	47,47,47,47	0
56	MG	DA	3451	1/1	0.99	0.11	30,30,30,30	0
56	MG	AA	3143	1/1	0.99	0.10	32,32,32,32	0
56	MG	BA	3315	1/1	0.99	0.17	31,31,31,31	0
56	MG	BA	3385	1/1	0.99	0.09	20,20,20,20	0
56	MG	BA	3216	1/1	0.99	0.24	33,33,33,33	0
56	MG	BA	3650	1/1	0.99	0.08	31,31,31,31	0
56	MG	DA	3042	1/1	0.99	0.10	32,32,32,32	0
56	MG	BU	204	1/1	0.99	0.16	29,29,29,29	0
56	MG	CA	3106	1/1	0.99	0.15	40,40,40,40	0
56	MG	DA	3532	1/1	0.99	0.06	51,51,51,51	0
56	MG	DA	3154	1/1	0.99	0.13	24,24,24,24	0
56	MG	BA	3179	1/1	0.99	0.20	27,27,27,27	0
56	MG	BA	3091	1/1	0.99	0.14	19,19,19,19	0
56	MG	BA	3389	1/1	0.99	0.19	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	BD	301	1/1	0.99	0.16	30,30,30,30	0
56	MG	DA	3334	1/1	0.99	0.11	24,24,24,24	0
56	MG	BA	3475	1/1	0.99	0.10	45,45,45,45	0
56	MG	AA	3080	1/1	0.99	0.24	39,39,39,39	0
56	MG	CA	3113	1/1	0.99	0.11	57,57,57,57	0
56	MG	BW	3003	1/1	0.99	0.15	27,27,27,27	0
56	MG	DA	3053	1/1	0.99	0.13	41,41,41,41	0
56	MG	BA	3034	1/1	0.99	0.18	24,24,24,24	0
56	MG	AE	3002	1/1	0.99	0.13	38,38,38,38	0
56	MG	BA	3322	1/1	0.99	0.13	40,40,40,40	0
56	MG	BA	3620	1/1	0.99	0.16	41,41,41,41	0
56	MG	DA	3407	1/1	0.99	0.05	40,40,40,40	0
56	MG	AA	3078	1/1	0.99	0.12	34,34,34,34	0
56	MG	BE	301	1/1	0.99	0.08	45,45,45,45	0
56	MG	BA	3209	1/1	0.99	0.19	26,26,26,26	0
56	MG	BA	3514	1/1	0.99	0.08	32,32,32,32	0
56	MG	BA	3037	1/1	0.99	0.13	24,24,24,24	0
56	MG	DA	3413	1/1	0.99	0.17	24,24,24,24	0
56	MG	DA	3349	1/1	0.99	0.15	46,46,46,46	0
56	MG	BA	3625	1/1	0.99	0.12	25,25,25,25	0
56	MG	DA	3012	1/1	0.99	0.12	30,30,30,30	0
56	MG	DA	3289	1/1	0.99	0.16	26,26,26,26	0
56	MG	BA	3424	1/1	0.99	0.20	38,38,38,38	0
56	MG	BA	3453	1/1	0.99	0.09	27,27,27,27	0
56	MG	DA	3177	1/1	0.99	0.11	52,52,52,52	0
56	MG	DA	3015	1/1	0.99	0.26	41,41,41,41	0
56	MG	D5	502	1/1	0.99	0.34	36,36,36,36	0
56	MG	BA	3038	1/1	0.99	0.14	30,30,30,30	0
56	MG	B3	102	1/1	0.99	0.23	22,22,22,22	0
56	MG	DA	3124	1/1	0.99	0.15	29,29,29,29	0
57	SF4	AD	501	8/8	0.99	0.16	50,63,78,83	0
57	SF4	CD	501	8/8	0.99	0.14	58,71,82,82	0
58	ZN	AN	501	1/1	0.99	0.14	67,67,67,67	0
56	MG	DA	3493	1/1	0.99	0.06	45,45,45,45	0
56	MG	DA	3297	1/1	0.99	0.15	38,38,38,38	0
58	ZN	B5	501	1/1	0.99	0.16	42,42,42,42	0
58	ZN	B6	501	1/1	0.99	0.16	45,45,45,45	0
58	ZN	B9	501	1/1	0.99	0.17	45,45,45,45	0
56	MG	BA	3455	1/1	0.99	0.11	21,21,21,21	0
56	MG	BA	3241	1/1	0.99	0.29	26,26,26,26	0
56	MG	BA	3670	1/1	0.99	0.32	34,34,34,34	0
58	ZN	D5	501	1/1	0.99	0.16	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
56	MG	BA	3039	1/1	0.99	0.08	31,31,31,31	0
56	MG	BA	3489	1/1	0.99	0.25	41,41,41,41	0
56	MG	DA	3303	1/1	0.99	0.07	43,43,43,43	0
56	MG	BA	3289	1/1	0.99	0.15	28,28,28,28	0
56	MG	BA	3221	1/1	1.00	0.24	41,41,41,41	0
56	MG	AA	3115	1/1	1.00	0.07	35,35,35,35	0

6.5 Other polymers ⓘ

There are no such residues in this entry.