wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 9, 2023 – 09:56 AM EDT

PDB ID	:	4V9R
Title	:	Crystal structure of antibiotic DITYROMYCIN bound to 70S ribosome
Authors	:	Bulkley, D.P.; Brandi, L.; Polikanov, Y.S.; Fabbretti, A.; O'Connor, M.; Gualerzi, C.O.; Steitz, T.A.
Deposited on	:	2013-12-05
Resolution	:	3.00 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

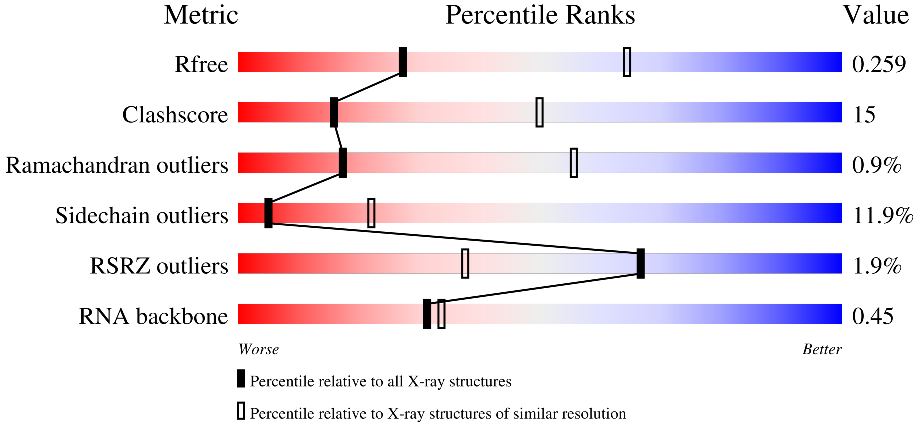
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance ⓘ

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

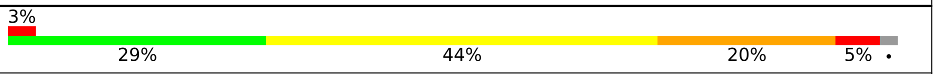
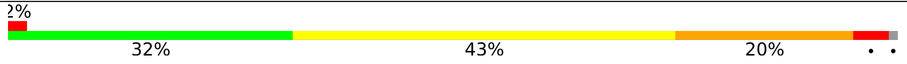
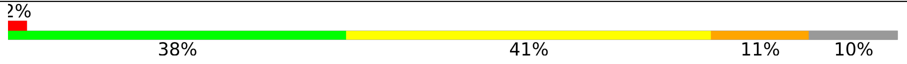
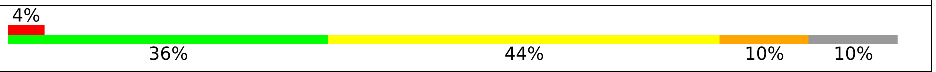
The reported resolution of this entry is 3.00 Å.

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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)
RNA backbone	3102	1173 (3.30-2.70)

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	1522	
1	CA	1522	
2	AB	256	
2	CB	256	

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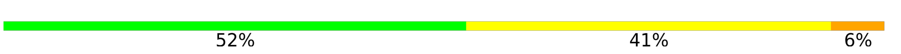
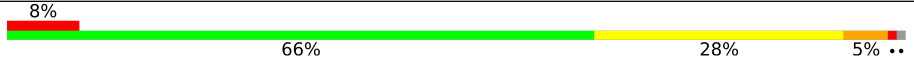
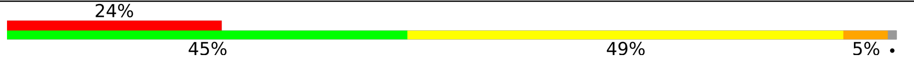
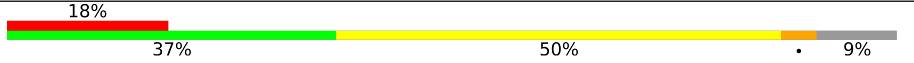
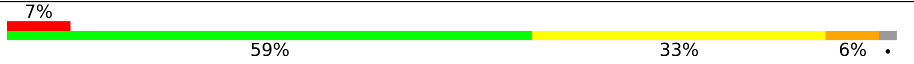
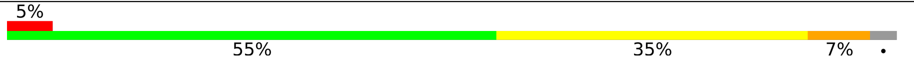
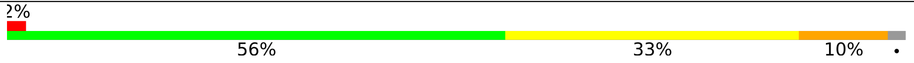
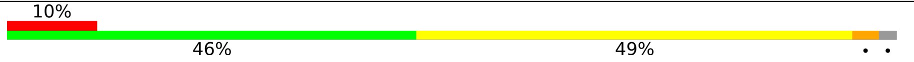
Mol	Chain	Length	Quality of chain
3	AC	239	
3	CC	239	
4	AD	209	
4	CD	209	
5	AE	162	
5	CE	162	
6	AF	101	
6	CF	101	
7	AG	156	
7	CG	156	
8	AH	138	
8	CH	138	
9	AI	128	
9	CI	128	
10	AJ	105	
10	CJ	105	
11	AK	129	
11	CK	129	
12	AL	132	
12	CL	132	
13	AM	126	
13	CM	126	
14	AN	61	
14	CN	61	
15	AO	89	

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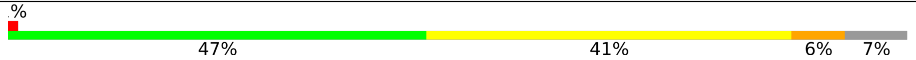
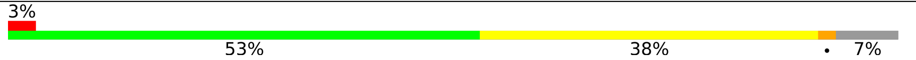
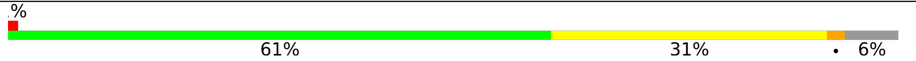
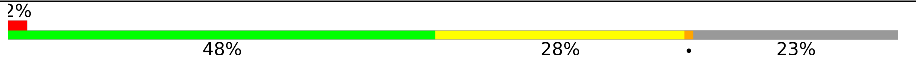
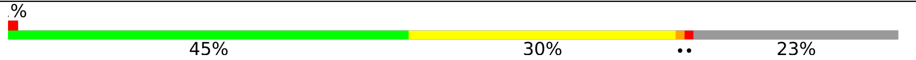
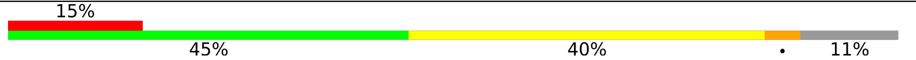
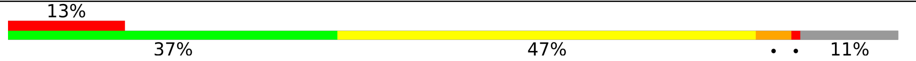
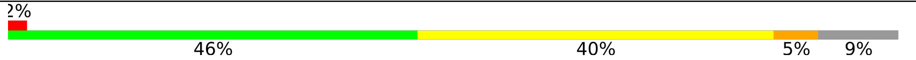
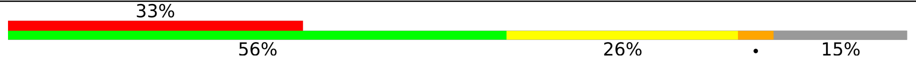
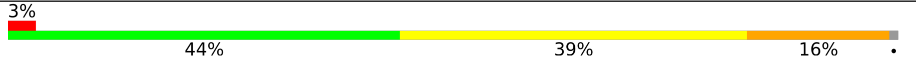
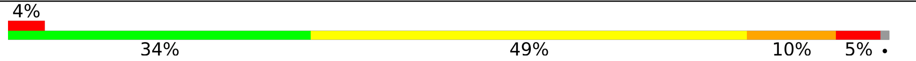
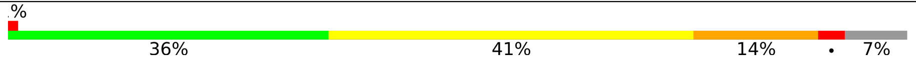
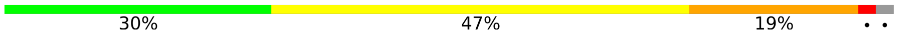
Mol	Chain	Length	Quality of chain
15	CO	89	
16	AP	88	
16	CP	88	
17	AQ	105	
17	CQ	105	
18	AR	88	
18	CR	88	
19	AS	93	
19	CS	93	
20	AT	106	
20	CT	106	
21	AU	27	
21	CU	27	
22	AV	24	
22	CV	24	
23	AX	77	
23	CX	77	
24	AW	10	
24	CW	10	
25	BA	2915	
25	DA	2915	
26	BB	122	
26	DB	122	
27	BD	276	
27	DD	276	

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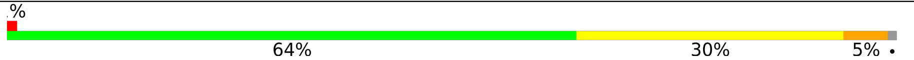
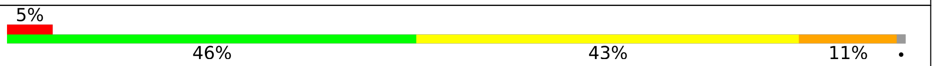
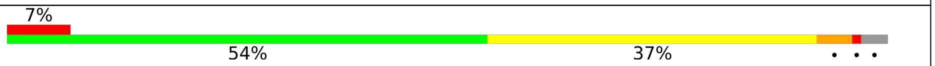
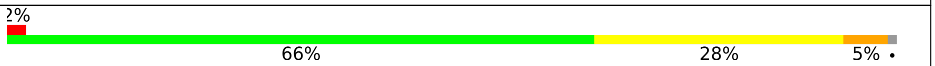
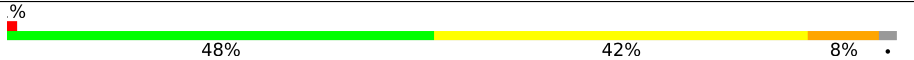
Mol	Chain	Length	Quality of chain
28	BE	206	
28	DE	206	
29	BF	210	
29	DF	210	
30	BG	182	
30	DG	182	
31	BH	180	
31	DH	180	
32	BI	148	
32	DI	148	
33	BN	140	
33	DN	140	
34	BO	122	
34	DO	122	
35	BP	150	
35	DP	150	
36	BQ	141	
36	DQ	141	
37	BR	118	
37	DR	118	
38	BS	112	
38	DS	112	
39	BT	146	
39	DT	146	
40	BU	118	

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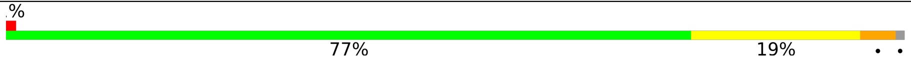
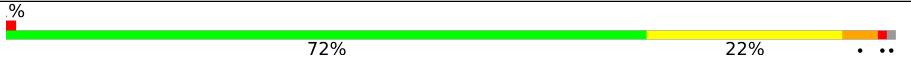
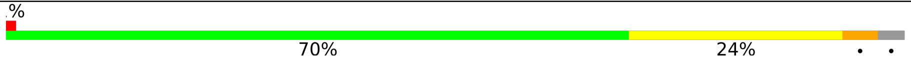
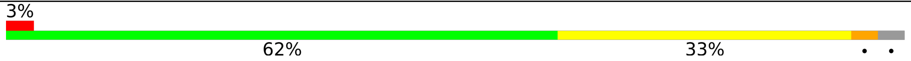
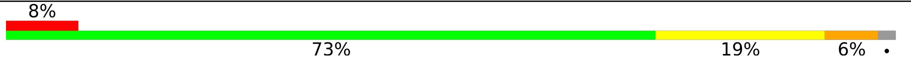
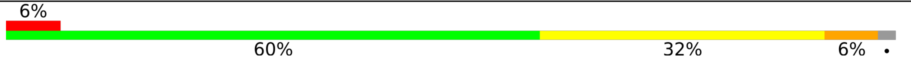
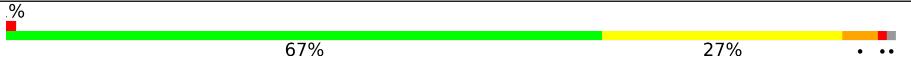
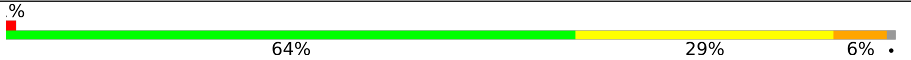
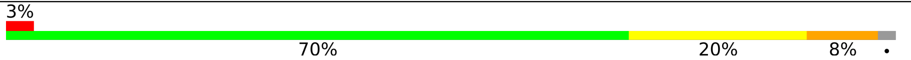
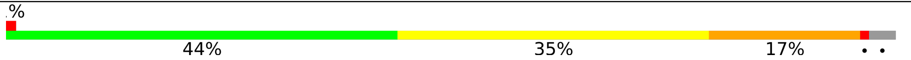
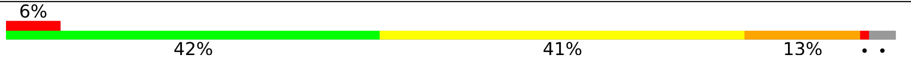
Mol	Chain	Length	Quality of chain
40	DU	118	
41	BV	101	
41	DV	101	
42	BW	113	
42	DW	113	
43	BX	96	
43	DX	96	
44	BY	110	
44	DY	110	
45	BZ	206	
45	DZ	206	
46	B0	85	
46	D0	85	
47	B1	98	
47	D1	98	
48	B2	72	
48	D2	72	
49	B3	60	
49	D3	60	
50	B4	71	
50	D4	71	
51	B5	60	
51	D5	60	
52	B6	54	
52	D6	54	

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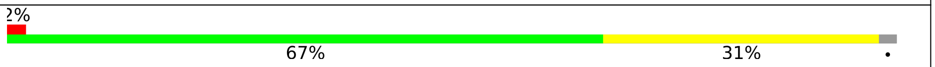
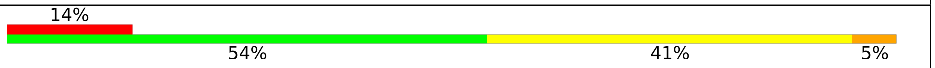
Mol	Chain	Length	Quality of chain
53	B7	49	
53	D7	49	
54	B8	65	
54	D8	65	
55	B9	37	
55	D9	37	

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	AA	3029	-	-	-	X
56	MG	AA	3030	-	-	-	X
56	MG	AA	3038	-	-	-	X
56	MG	AA	3079	-	-	-	X
56	MG	AA	3086	-	-	-	X
56	MG	AA	3147	-	-	-	X
56	MG	AA	3180	-	-	-	X
56	MG	AX	105	-	-	-	X
56	MG	BA	3139	-	-	-	X
56	MG	BA	3143	-	-	-	X
56	MG	BA	3154	-	-	-	X
56	MG	BA	3178	-	-	-	X
56	MG	BA	3230	-	-	-	X
56	MG	BA	3252	-	-	-	X
56	MG	BA	3296	-	-	-	X
56	MG	BA	3625	-	-	-	X
56	MG	BA	3740	-	-	-	X
56	MG	BD	311	-	-	-	X
56	MG	BF	306	-	-	-	X
56	MG	CA	3016	-	-	-	X
56	MG	CA	3039	-	-	-	X
56	MG	CA	3053	-	-	-	X
56	MG	CA	3054	-	-	-	X
56	MG	CA	3144	-	-	-	X
56	MG	DA	3024	-	-	-	X
56	MG	DA	3064	-	-	-	X
56	MG	DA	3113	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	DA	3356	-	-	-	X
56	MG	DA	3431	-	-	-	X
56	MG	DA	3568	-	-	-	X

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 286321 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1498	Total	C	N	O	P	0	0	0
			32196	14328	5966	10404	1498			
1	CA	1503	Total	C	N	O	P	0	0	0
			32312	14381	5990	10438	1503			

- Molecule 2 is a protein called 30S Ribosomal Protein S2.

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

- Molecule 3 is a protein called 30S Ribosomal Protein S3.

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

- Molecule 4 is a protein called 30S Ribosomal Protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AD	208	Total	C	N	O	S	0	0	0
			1659	1040	326	286	7			
4	CD	208	Total	C	N	O	S	0	0	0
			1674	1050	333	284	7			

- 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
			Total	C	N	O			
10	CJ	96	714	445	138	131	0	0	0

- Molecule 11 is a protein called 30S Ribosomal Protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	AK	114	829	516	155	155	3	0	0	0
11	CK	114	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
			Total	C	N	O	S			
12	AL	122	930	585	185	159	1	0	0	0
12	CL	122	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
			Total	C	N	O	S			
13	AM	123	958	592	198	166	2	0	0	0
13	CM	122	950	586	197	165	2	0	0	0

- Molecule 14 is a protein called 30S Ribosomal Protein S14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
14	AN	60	492	312	104	72	4	0	0	0
14	CN	60	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
			Total	C	N	O	S			
15	AO	88	728	456	144	126	2	0	0	0
15	CO	88	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
			Total	C	N	O	S			
16	AP	82	681	433	134	113	1	0	0	0
16	CP	82	677	430	133	113	1	0	0	0

- Molecule 17 is a protein called 30S Ribosomal Protein S17.

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

- Molecule 18 is a protein called 30S Ribosomal Protein S18.

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

- Molecule 19 is a protein called 30S Ribosomal Protein S19.

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

- Molecule 20 is a protein called 30S Ribosomal Protein S20.

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

- 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	7	Total C N O P 114 49 22 37 6	0	0	1
22	CV	6	Total C N O P 113 49 22 36 6	0	0	0

- Molecule 23 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
23	AX	76	Total C N O P 1623 723 294 530 76	0	0	0
23	CX	76	Total C N O P 1623 723 294 530 76	0	0	0

- Molecule 24 is a protein called Dityromycin.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
24	AW	10	Total C N O 93 67 10 16	0	0	0
24	CW	10	Total C N O 93 67 10 16	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
25	BA	2731	Total C N O P 58834 26185 11020 18899 2730	0	0	0
25	DA	2714	Total C N O P 58458 26018 10942 18786 2712	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 C N O S 1085 693 189 202 1	0	0	0
32	DI	146	Total C N O S 1061 680 186 194 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 C N O S 1117 719 207 187 4	0	0	0
33	DN	140	Total C N O S 1117 719 207 187 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 C N O S 933 588 171 170 4	0	0	0
34	DO	122	Total C N O S 933 588 171 170 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 C N O S 1135 706 230 196 3	0	0	0
35	DP	149	Total C N O S 1135 706 230 196 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 C N O S 1122 715 212 188 7	0	0	0
36	DQ	141	Total C N O S 1122 715 212 188 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 886 557 174 153 2	0	0	0

- 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 750 488 135 126 1	0	0	0
43	DX	95	Total C N O S 750 488 135 126 1	0	0	0

- 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 806 517 152 131 6	0	0	0
44	DY	107	Total C N O S 806 517 152 131 6	0	0	0

- 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 1349 862 243 242 2	0	0	0
45	DZ	174	Total C N O S 1360 870 243 245 2	0	0	0

- 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 653 404 139 109 1	0	0	0
46	D0	83	Total C N O S 653 404 139 109 1	0	0	0

- 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 755 475 148 131 1	0	0	0
47	D1	97	Total C N O S 755 475 148 131 1	0	0	0

- 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 551 348 99 99 5	0	0	0
50	D4	69	Total C N O S 531 338 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 C N O S 418 257 104 55 2	0	0	0
53	D7	48	Total C N O S 418 257 104 55 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 C N O S 511 328 99 82 2	0	0	0
54	D8	64	Total C N O S 517 331 102 82 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 C N O S 307 188 68 47 4	0	0	0
55	D9	37	Total C N O S 307 188 68 47 4	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	AA	222	Total Mg 222 222	0	0
56	AD	1	Total Mg 1 1	0	0
56	AF	1	Total Mg 1 1	0	0
56	AK	1	Total Mg 1 1	0	0
56	AL	1	Total Mg 1 1	0	0
56	AM	2	Total Mg 2 2	0	0
56	AN	1	Total Mg 1 1	0	0
56	AS	1	Total Mg 1 1	0	0
56	AV	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	AX	9	Total Mg 9 9	0	0
56	BA	739	Total Mg 739 739	0	0
56	BB	18	Total Mg 18 18	0	0
56	BD	12	Total Mg 12 12	0	0
56	BE	9	Total Mg 9 9	0	0
56	BF	6	Total Mg 6 6	0	0
56	BG	4	Total Mg 4 4	0	0
56	BN	6	Total Mg 6 6	0	0
56	BO	1	Total Mg 1 1	0	0
56	BP	4	Total Mg 4 4	0	0
56	BQ	4	Total Mg 4 4	0	0
56	BR	3	Total Mg 3 3	0	0
56	BU	9	Total Mg 9 9	0	0
56	BV	3	Total Mg 3 3	0	0
56	BW	5	Total Mg 5 5	0	0
56	BX	2	Total Mg 2 2	0	0
56	BZ	1	Total Mg 1 1	0	0
56	B0	6	Total Mg 6 6	0	0
56	B1	2	Total Mg 2 2	0	0
56	B2	1	Total Mg 1 1	0	0
56	B3	3	Total Mg 3 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	B5	1	Total Mg 1 1	0	0
56	B7	4	Total Mg 4 4	0	0
56	B8	2	Total Mg 2 2	0	0
56	B9	1	Total Mg 1 1	0	0
56	CA	172	Total Mg 172 172	0	0
56	CE	2	Total Mg 2 2	0	0
56	CF	1	Total Mg 1 1	0	0
56	CN	1	Total Mg 1 1	0	0
56	CT	1	Total Mg 1 1	0	0
56	CX	3	Total Mg 3 3	0	0
56	DA	657	Total Mg 657 657	0	0
56	DB	12	Total Mg 12 12	0	0
56	DD	5	Total Mg 5 5	0	0
56	DE	6	Total Mg 6 6	0	0
56	DF	5	Total Mg 5 5	0	0
56	DG	1	Total Mg 1 1	0	0
56	DN	1	Total Mg 1 1	0	0
56	DO	1	Total Mg 1 1	0	0
56	DP	2	Total Mg 2 2	0	0
56	DQ	4	Total Mg 4 4	0	0
56	DR	1	Total Mg 1 1	0	0

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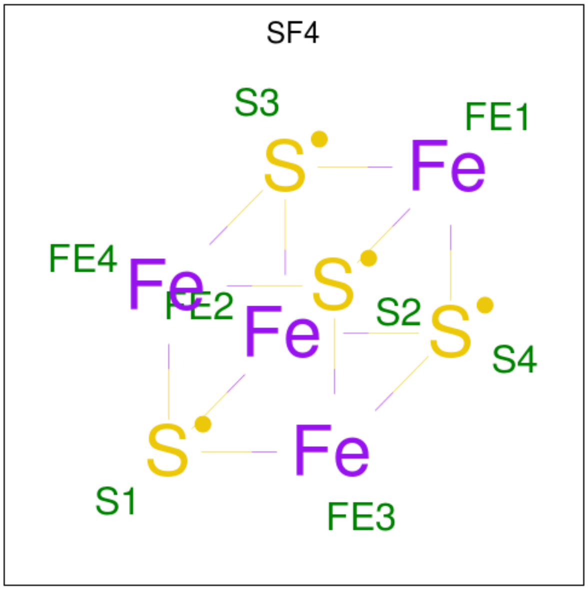
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	DU	2	Total Mg 2 2	0	0
56	DV	3	Total Mg 3 3	0	0
56	DW	2	Total Mg 2 2	0	0
56	DY	1	Total Mg 1 1	0	0
56	D3	1	Total Mg 1 1	0	0
56	D5	2	Total Mg 2 2	0	0
56	D8	1	Total Mg 1 1	0	0

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

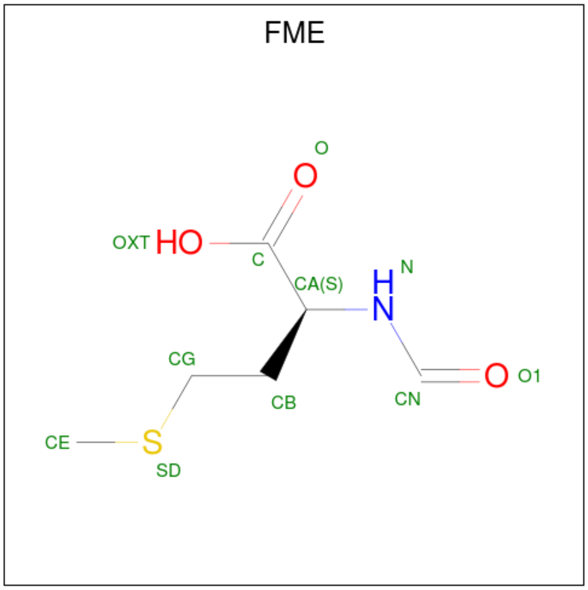


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	AD	1	Total Fe S 8 4 4	0	0
57	CD	1	Total Fe S 8 4 4	0	0

- 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 N-FORMYLMETHIONINE (three-letter code: FME) (formula: $C_6H_{11}NO_3S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
59	AX	1	Total 10	C 6	N 1	O 2	S 1	0	0
59	CX	1	Total 10	C 6	N 1	O 2	S 1	0	0

- Molecule 60 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	BA	1	Total 1	K 1	0	0
60	DA	1	Total 1	K 1	0	0

- Molecule 61 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	AA	147	Total 147	O 147	0	0
61	AD	1	Total 1	O 1	0	0
61	AE	2	Total 2	O 2	0	0
61	AJ	1	Total 1	O 1	0	0
61	AL	2	Total 2	O 2	0	0
61	AO	2	Total 2	O 2	0	0
61	AU	1	Total 1	O 1	0	0
61	AV	2	Total 2	O 2	0	0
61	AX	1	Total 1	O 1	0	0
61	BA	1086	Total 1086	O 1086	0	0
61	BB	26	Total 26	O 26	0	0
61	BD	6	Total 6	O 6	0	0
61	BE	13	Total 13	O 13	0	0
61	BF	5	Total 5	O 5	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	BG	1	Total O 1 1	0	0
61	BN	3	Total O 3 3	0	0
61	BO	2	Total O 2 2	0	0
61	BP	15	Total O 15 15	0	0
61	BQ	3	Total O 3 3	0	0
61	BR	1	Total O 1 1	0	0
61	BT	2	Total O 2 2	0	0
61	BU	5	Total O 5 5	0	0
61	BV	2	Total O 2 2	0	0
61	BW	4	Total O 4 4	0	0
61	BX	4	Total O 4 4	0	0
61	B0	4	Total O 4 4	0	0
61	B1	2	Total O 2 2	0	0
61	B5	2	Total O 2 2	0	0
61	B7	1	Total O 1 1	0	0
61	B8	7	Total O 7 7	0	0
61	CA	186	Total O 186 186	0	0
61	CE	2	Total O 2 2	0	0
61	CN	1	Total O 1 1	0	0
61	CT	1	Total O 1 1	0	0
61	CX	2	Total O 2 2	0	0

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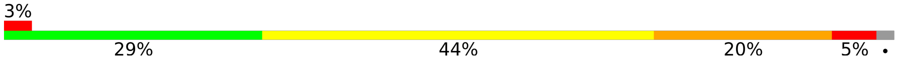
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	DA	906	Total O 906 906	0	0
61	DB	7	Total O 7 7	0	0
61	DD	10	Total O 10 10	0	0
61	DE	11	Total O 11 11	0	0
61	DF	4	Total O 4 4	0	0
61	DO	1	Total O 1 1	0	0
61	DP	14	Total O 14 14	0	0
61	DQ	3	Total O 3 3	0	0
61	DR	1	Total O 1 1	0	0
61	DU	4	Total O 4 4	0	0
61	DV	1	Total O 1 1	0	0
61	DX	2	Total O 2 2	0	0
61	DY	1	Total O 1 1	0	0
61	D0	3	Total O 3 3	0	0
61	D1	1	Total O 1 1	0	0
61	D3	1	Total O 1 1	0	0
61	D7	1	Total O 1 1	0	0
61	D8	4	Total O 4 4	0	0

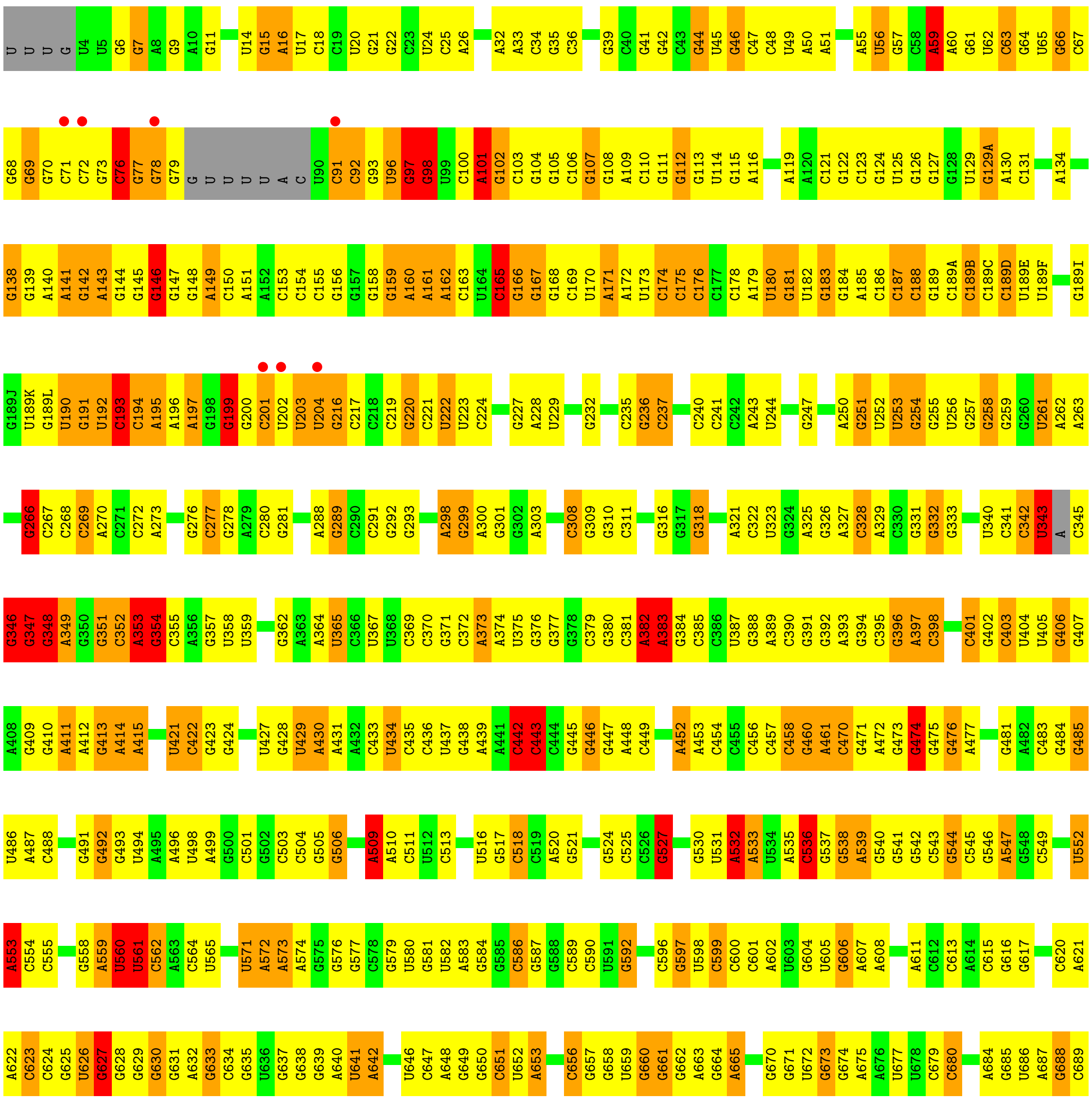
3 Residue-property plots (i)

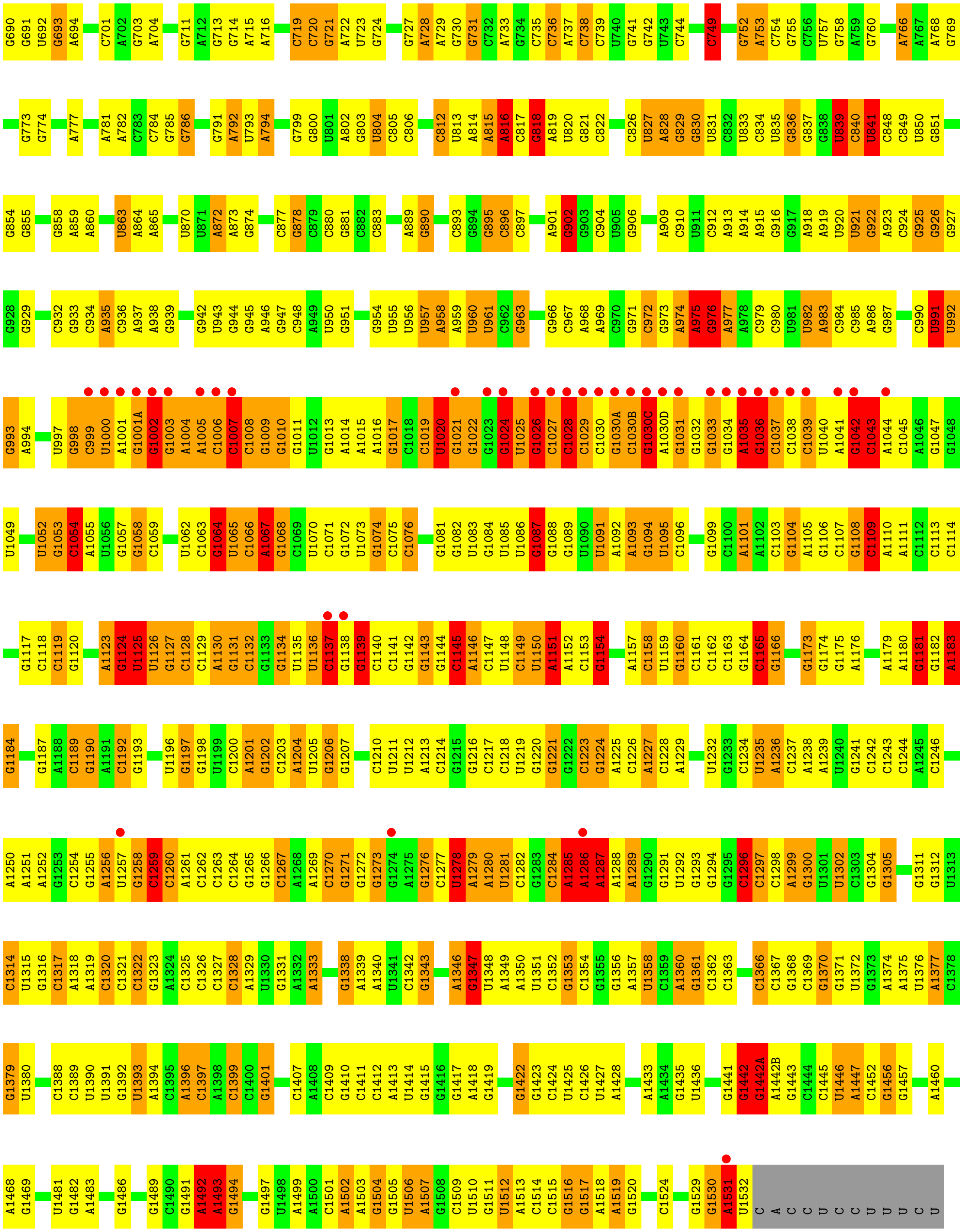
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: 16S Ribosomal RNA

Chain AA:

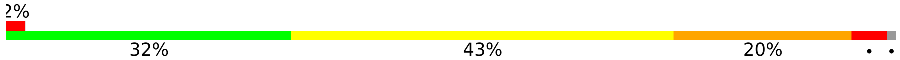


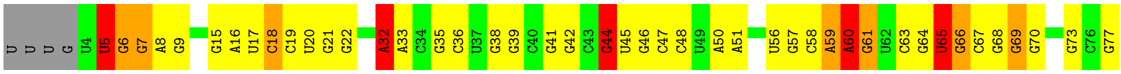


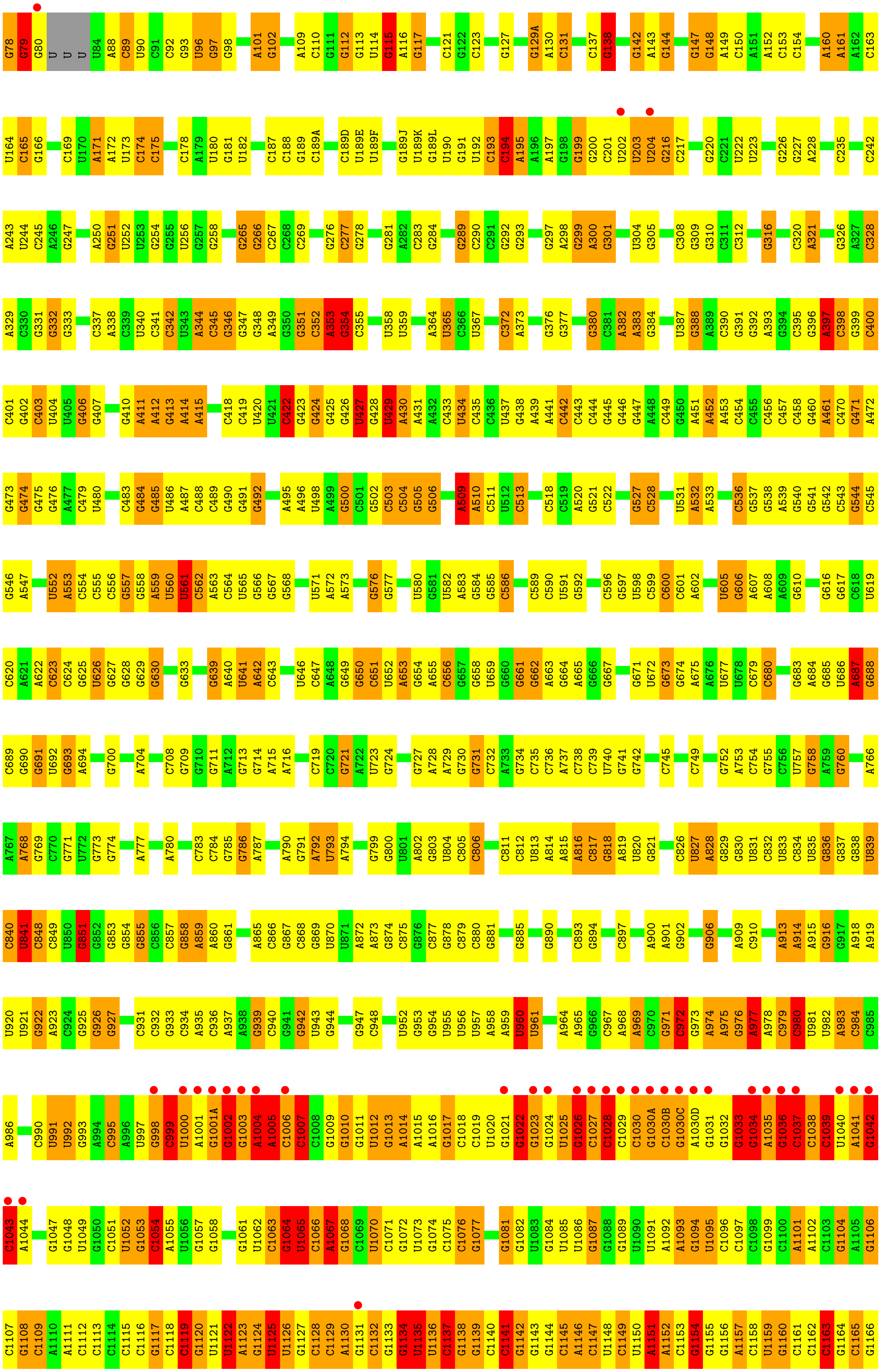


- Molecule 1: 16S Ribosomal RNA

Chain CA:



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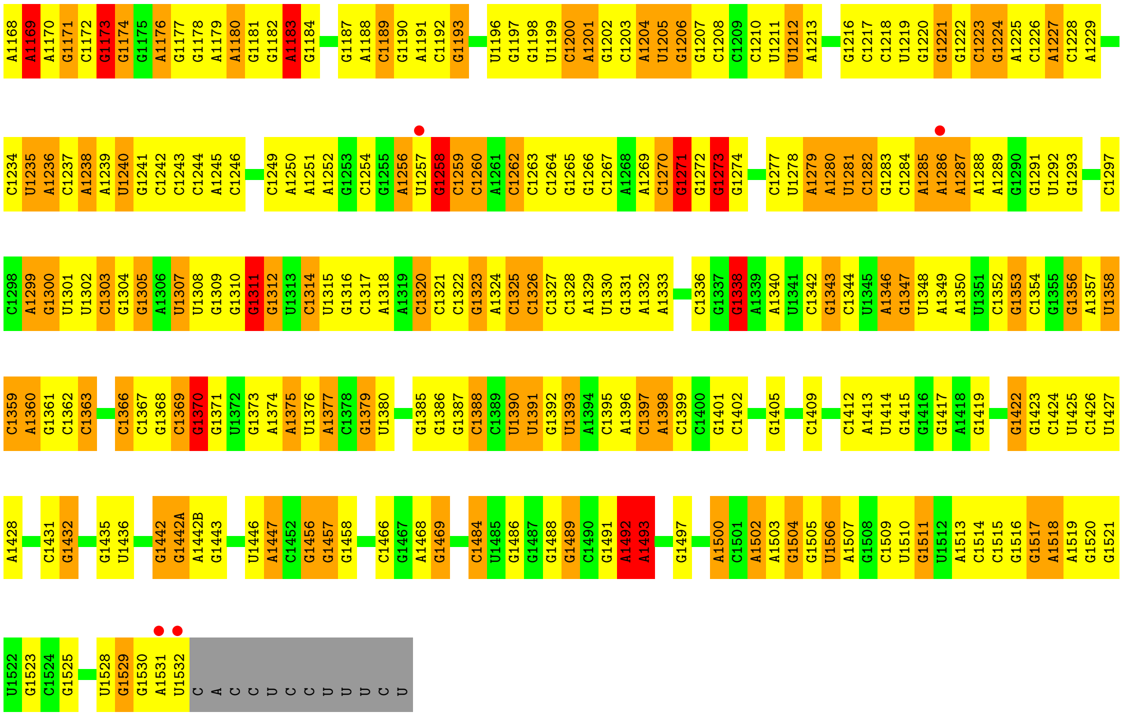

- Molecule 2: 30S Ribosomal Protein S2

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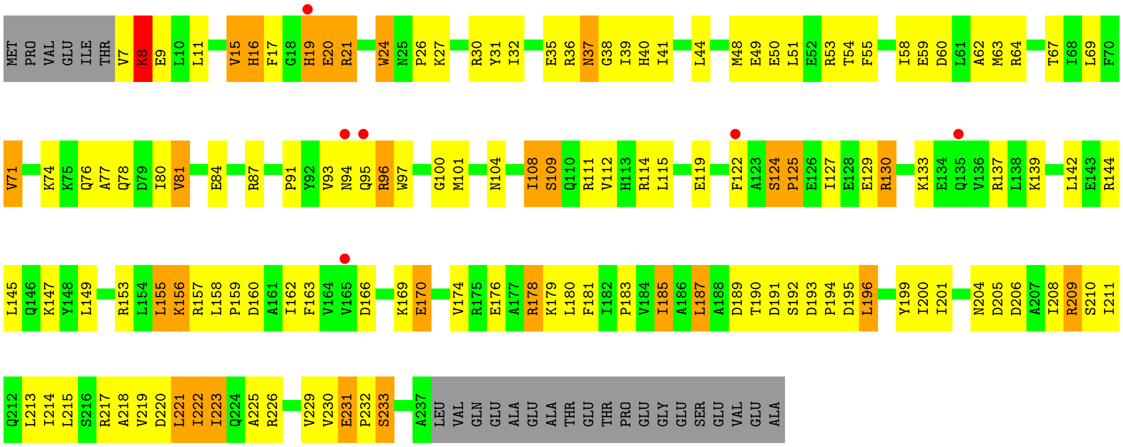

- Molecule 2: 30S Ribosomal Protein S2

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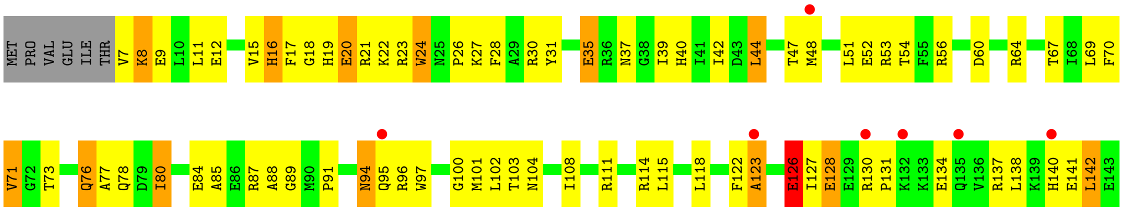

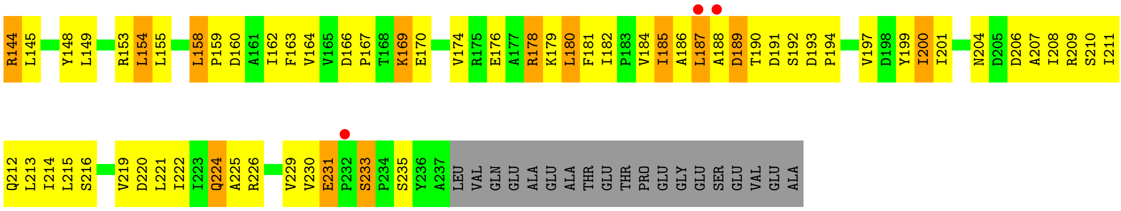

- Molecule 3: 30S Ribosomal Protein S3

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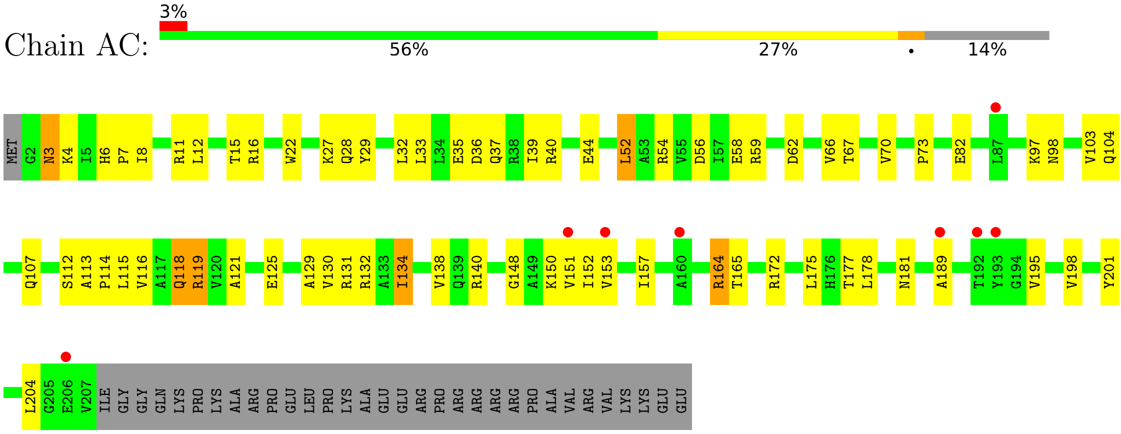

- Molecule 3: 30S Ribosomal Protein S3

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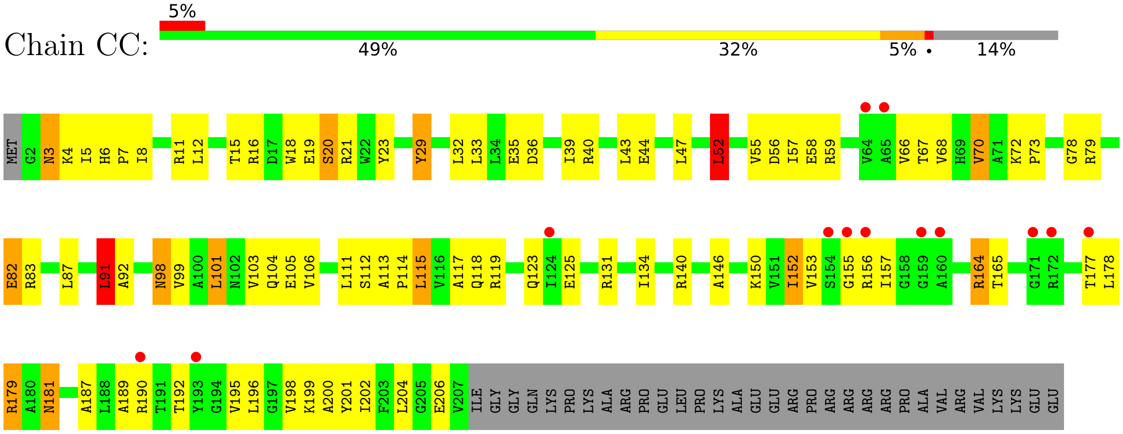

- Molecule 4: 30S Ribosomal Protein S4

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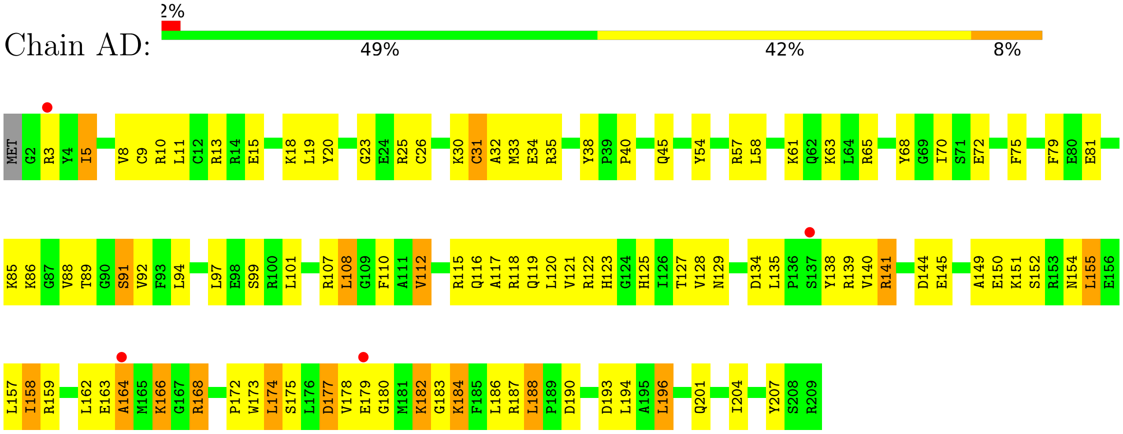

- Molecule 4: 30S Ribosomal Protein S4

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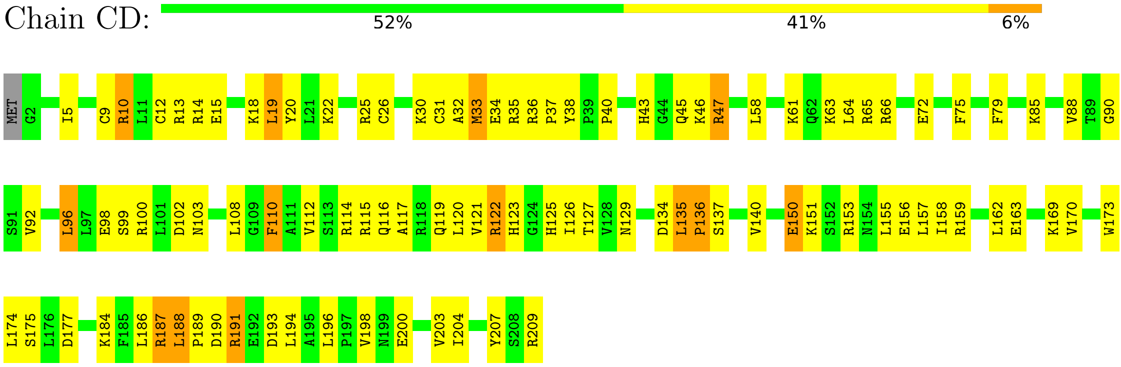

- Molecule 5: 30S Ribosomal Protein S5

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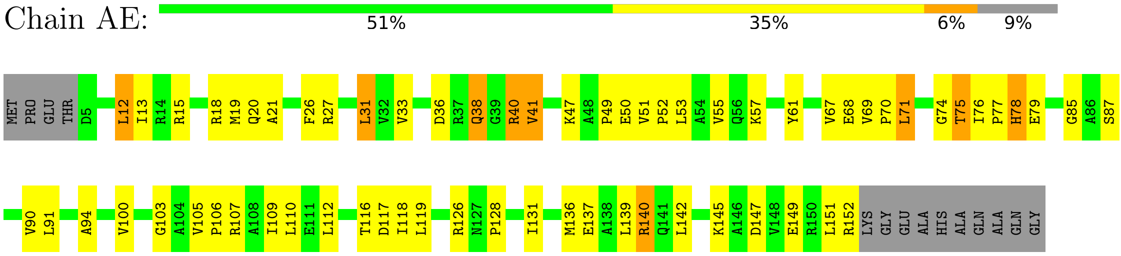

- Molecule 5: 30S Ribosomal Protein S5

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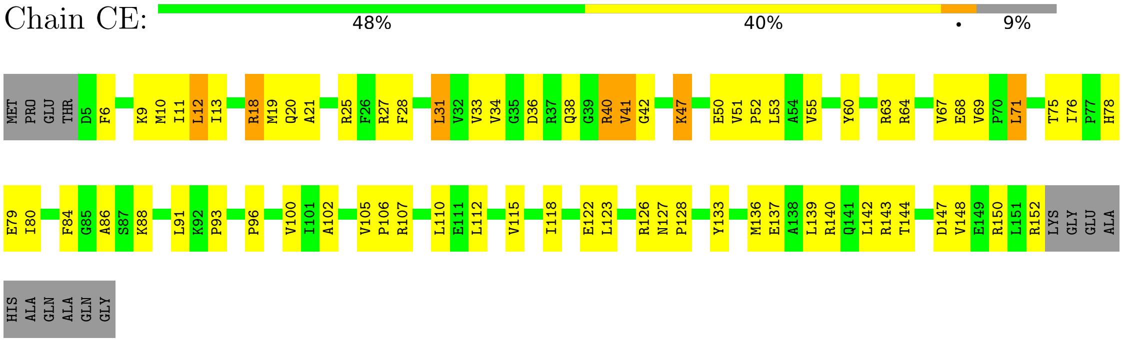
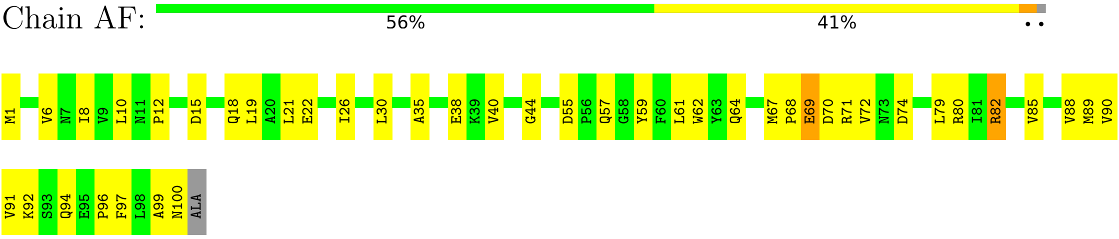


- Molecule 6: 30S Ribosomal Protein S6

Chain AF:



- Molecule 6: 30S Ribosomal Protein S6

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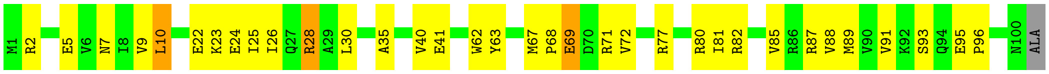
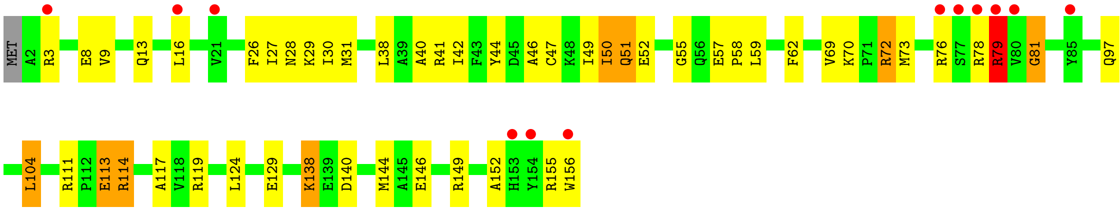


- Molecule 7: 30S Ribosomal Protein S7

Chain AG:



- Molecule 7: 30S Ribosomal Protein S7

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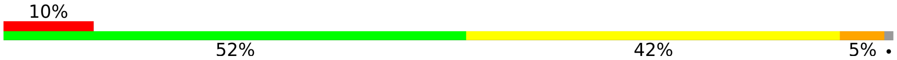

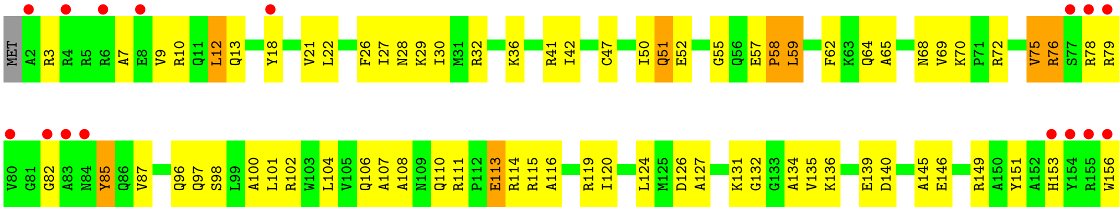

- Molecule 8: 30S Ribosomal Protein S8

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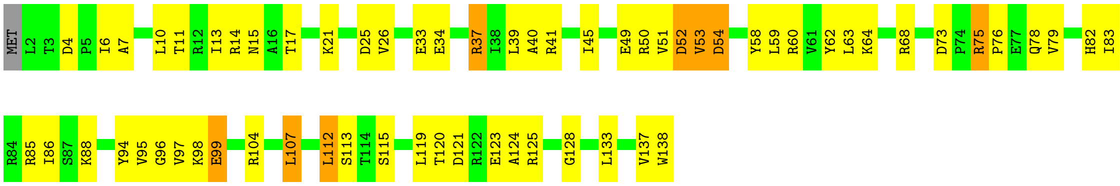

- Molecule 8: 30S Ribosomal Protein S8

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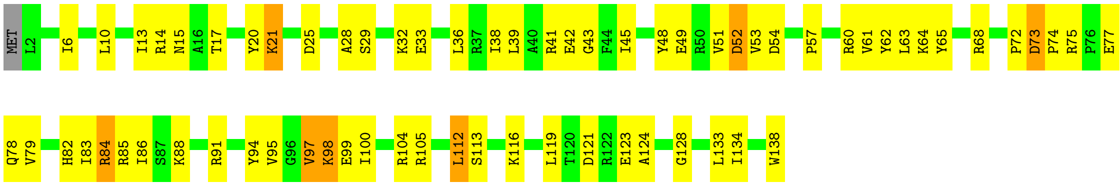

- Molecule 9: 30S Ribosomal Protein S9

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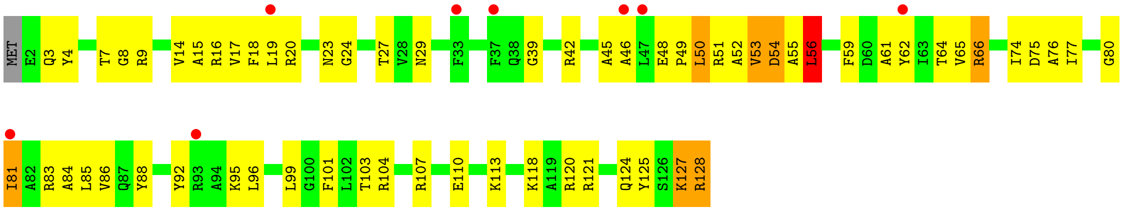

- Molecule 9: 30S Ribosomal Protein S9

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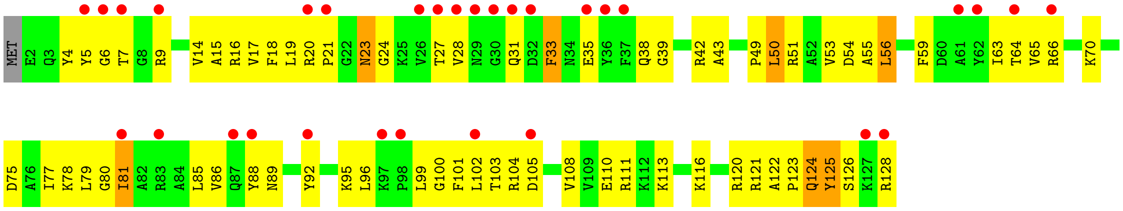

- Molecule 10: 30S Ribosomal Protein S10

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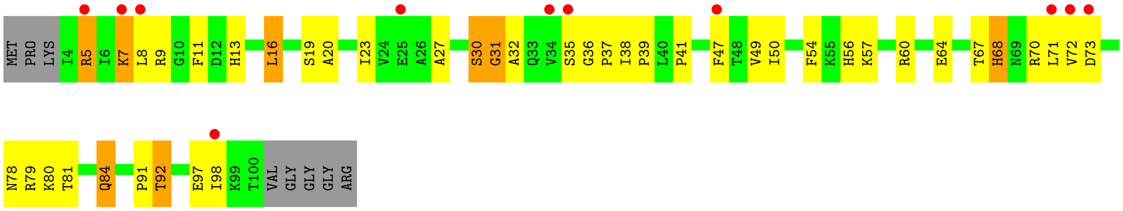

- Molecule 10: 30S Ribosomal Protein S10

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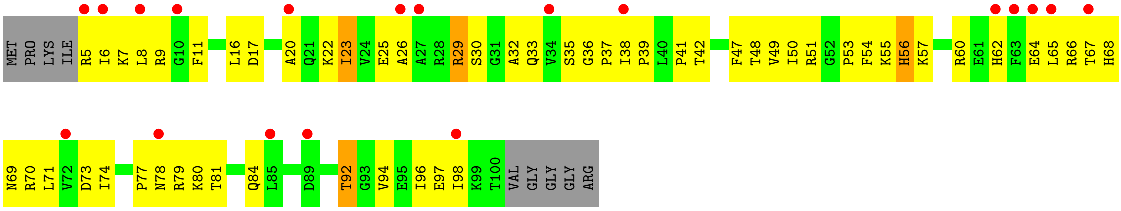

- Molecule 11: 30S Ribosomal Protein S11

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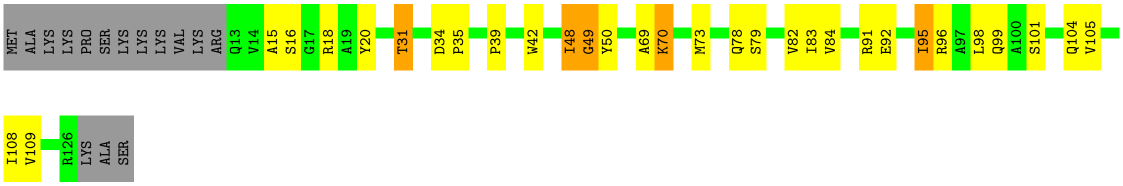
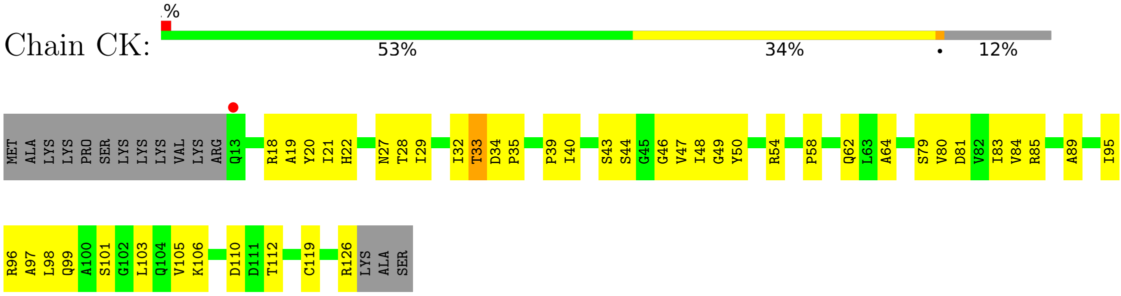
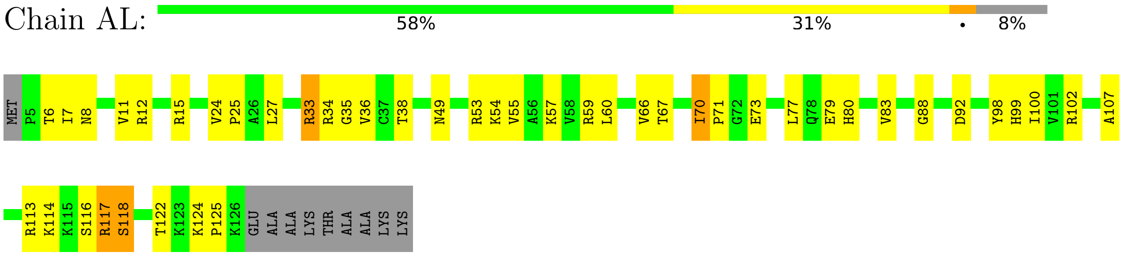


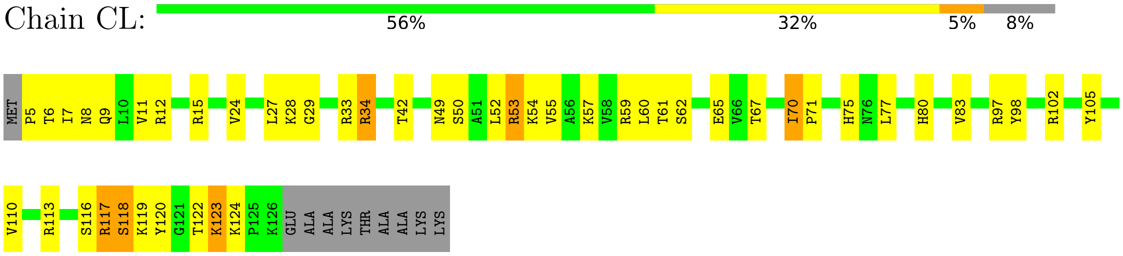
- Molecule 11: 30S Ribosomal Protein S11



• Molecule 12: 30S Ribosomal Protein S12



• Molecule 12: 30S Ribosomal Protein S12



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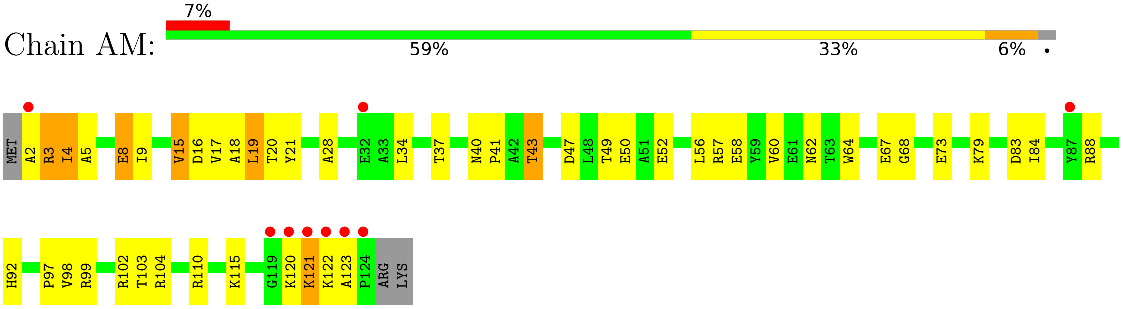
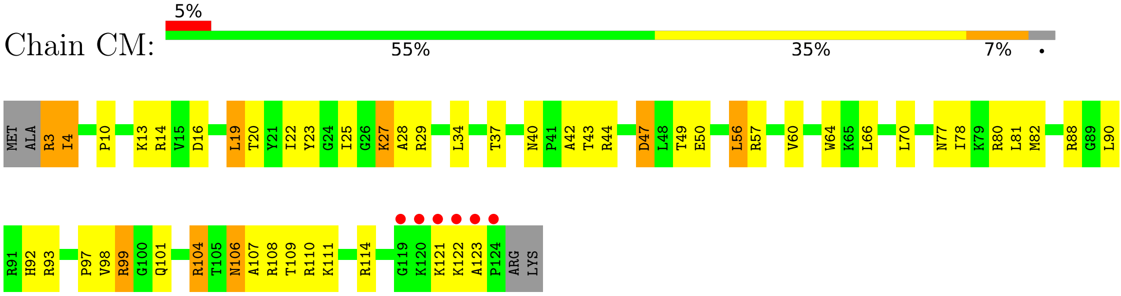


• Molecule 13: 30S Ribosomal Protein S13



- Molecule 14: 30S Ribosomal Protein S14

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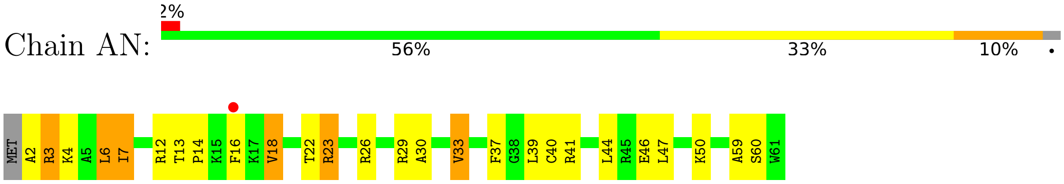

- Molecule 14: 30S Ribosomal Protein S14

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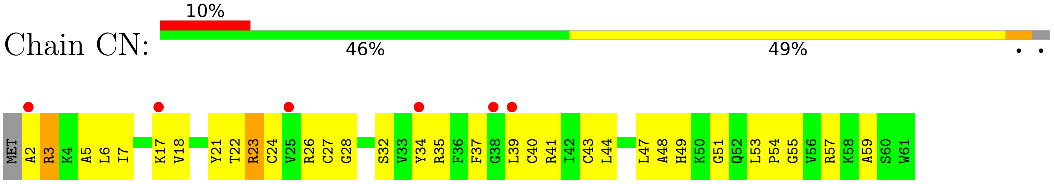

- Molecule 15: 30S Ribosomal Protein S15

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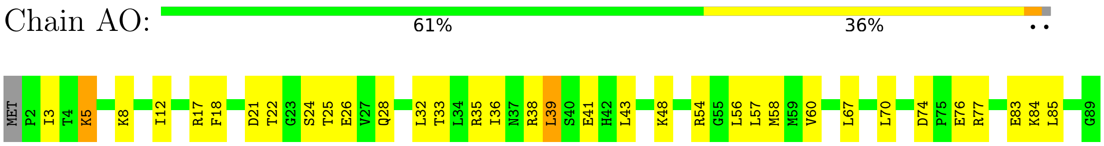

- Molecule 15: 30S Ribosomal Protein S15

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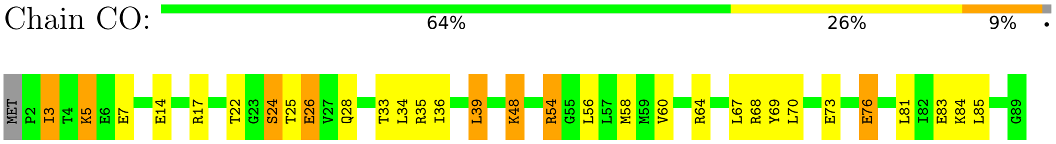
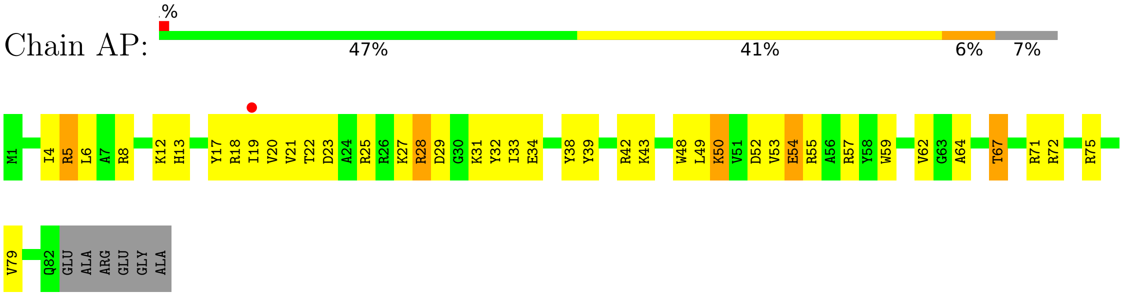


- Molecule 16: 30S Ribosomal Protein S16

Chain AP:



- Molecule 16: 30S Ribosomal Protein S16

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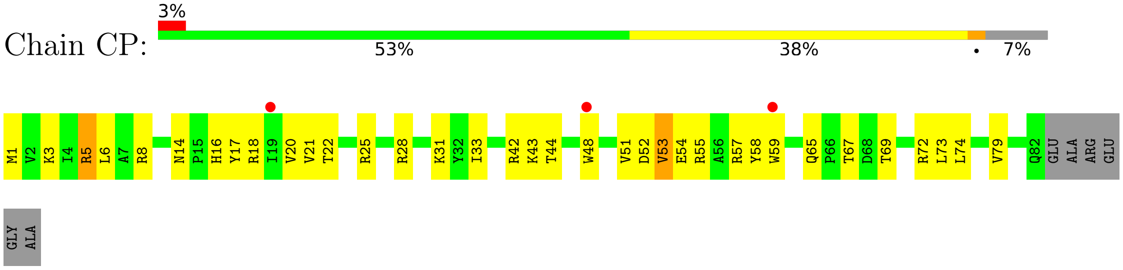

- Molecule 17: 30S Ribosomal Protein S17

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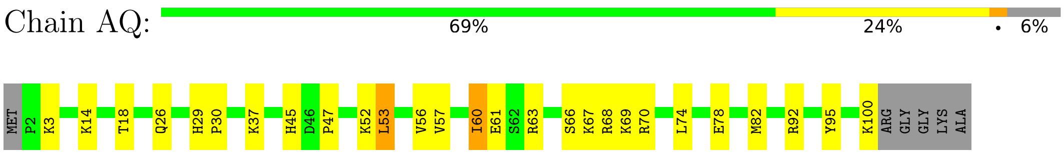

- Molecule 17: 30S Ribosomal Protein S17

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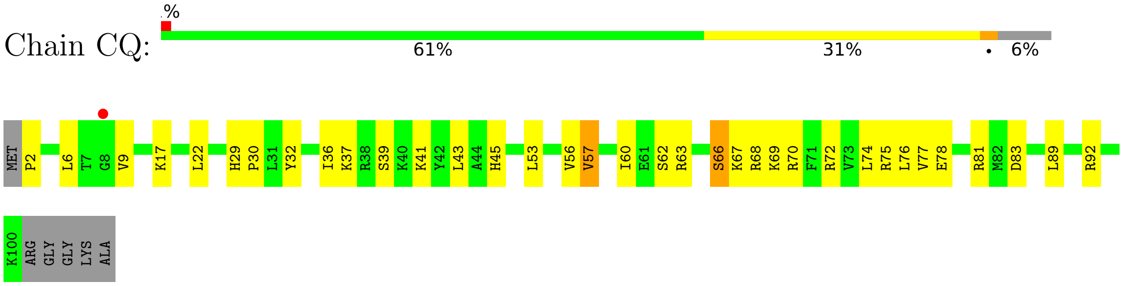

- Molecule 18: 30S Ribosomal Protein S18

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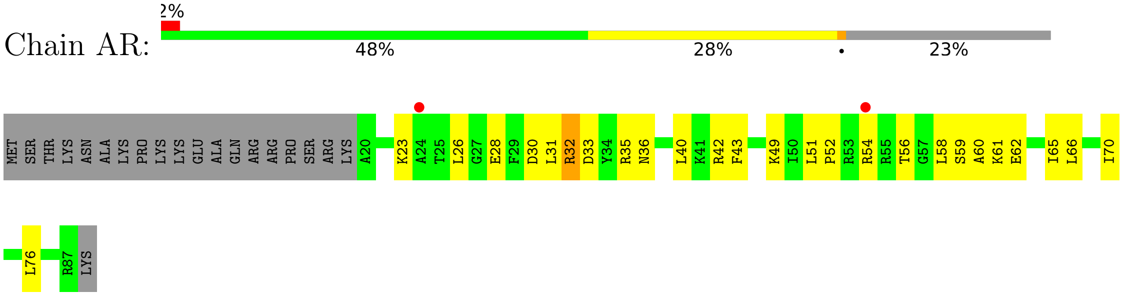

- Molecule 18: 30S Ribosomal Protein S18

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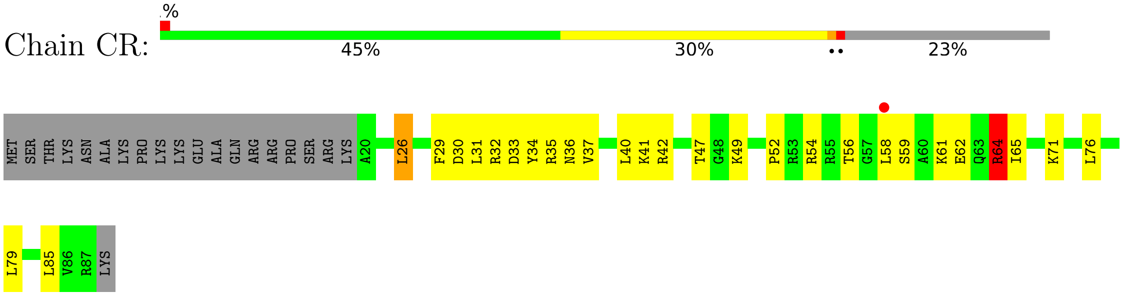
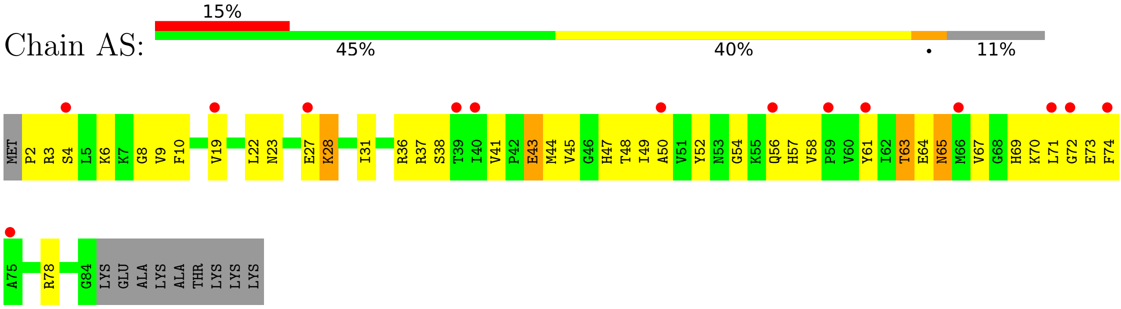


- Molecule 19: 30S Ribosomal Protein S19

Chain AS:



- Molecule 19: 30S Ribosomal Protein S19

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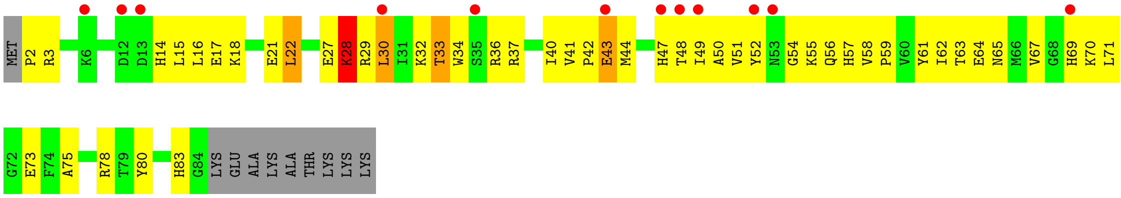

- Molecule 20: 30S Ribosomal Protein S20

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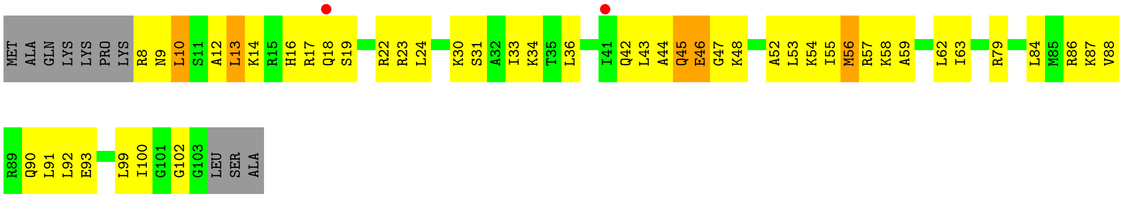

- Molecule 20: 30S Ribosomal Protein S20

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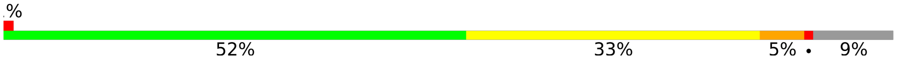
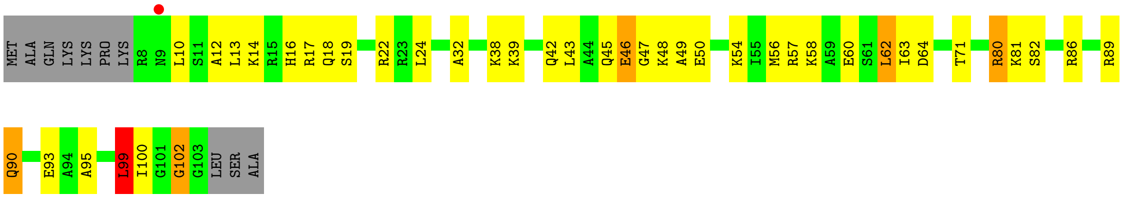
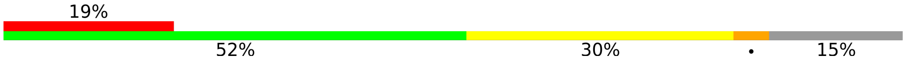
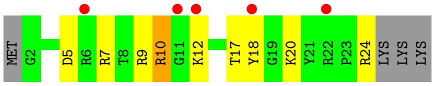




- Molecule 21: 30S Ribosomal Protein THX

Chain AU:





- Molecule 21: 30S Ribosomal Protein THX

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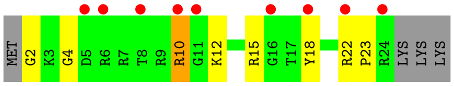
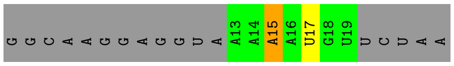


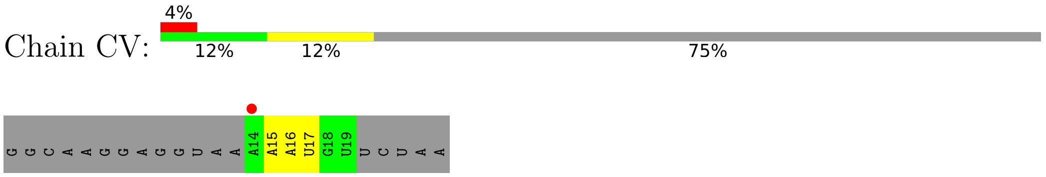
- Molecule 22: mRNA

Chain AV:



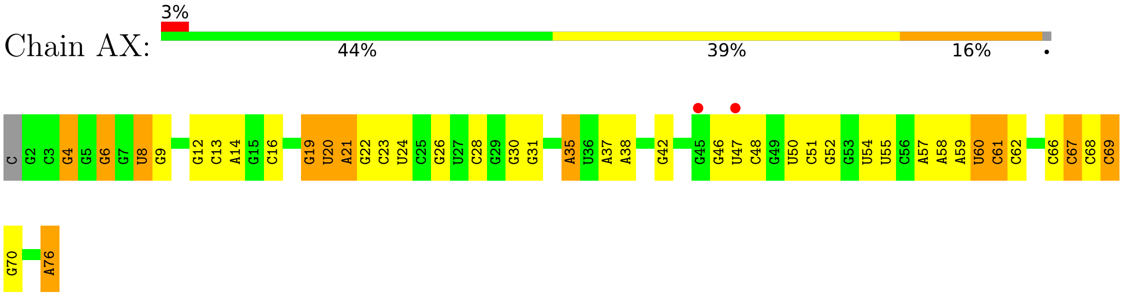
- Molecule 22: mRNA

Chain CV:



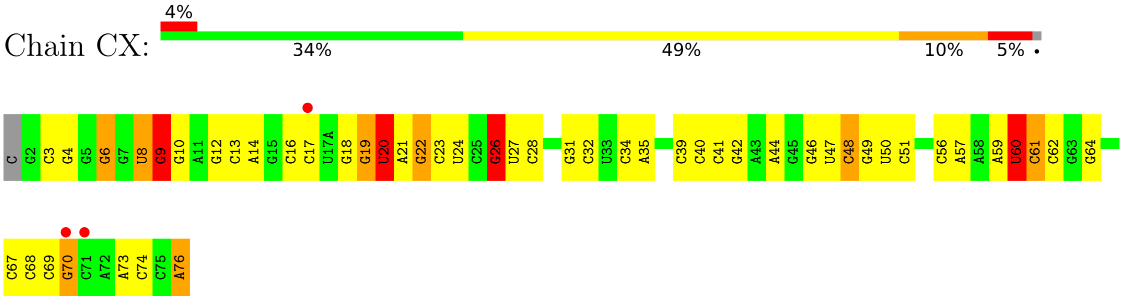
- Molecule 23: P-site tRNA

Chain AX:



- Molecule 23: P-site tRNA

Chain CX:



- Molecule 24: Dityromycin

Chain AW:

- Molecule 24: Dityromycin

Chain CW:

- Molecule 25: 23S Ribosomal RNA

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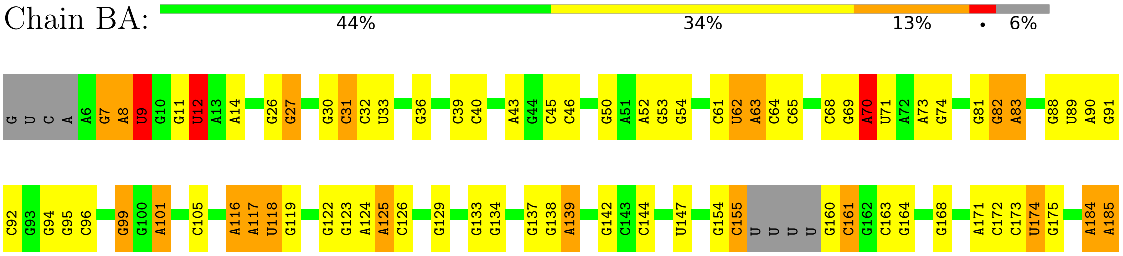

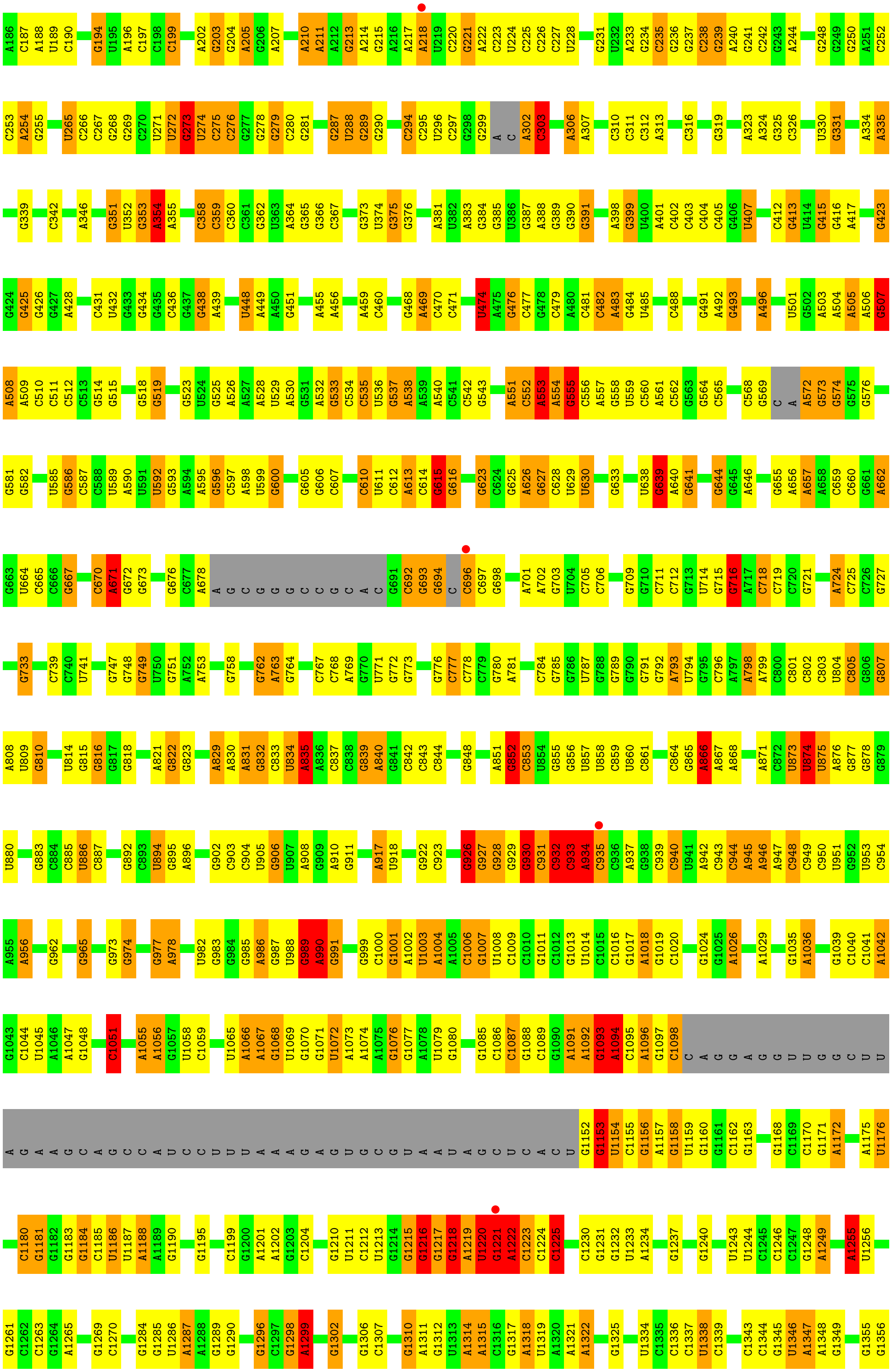
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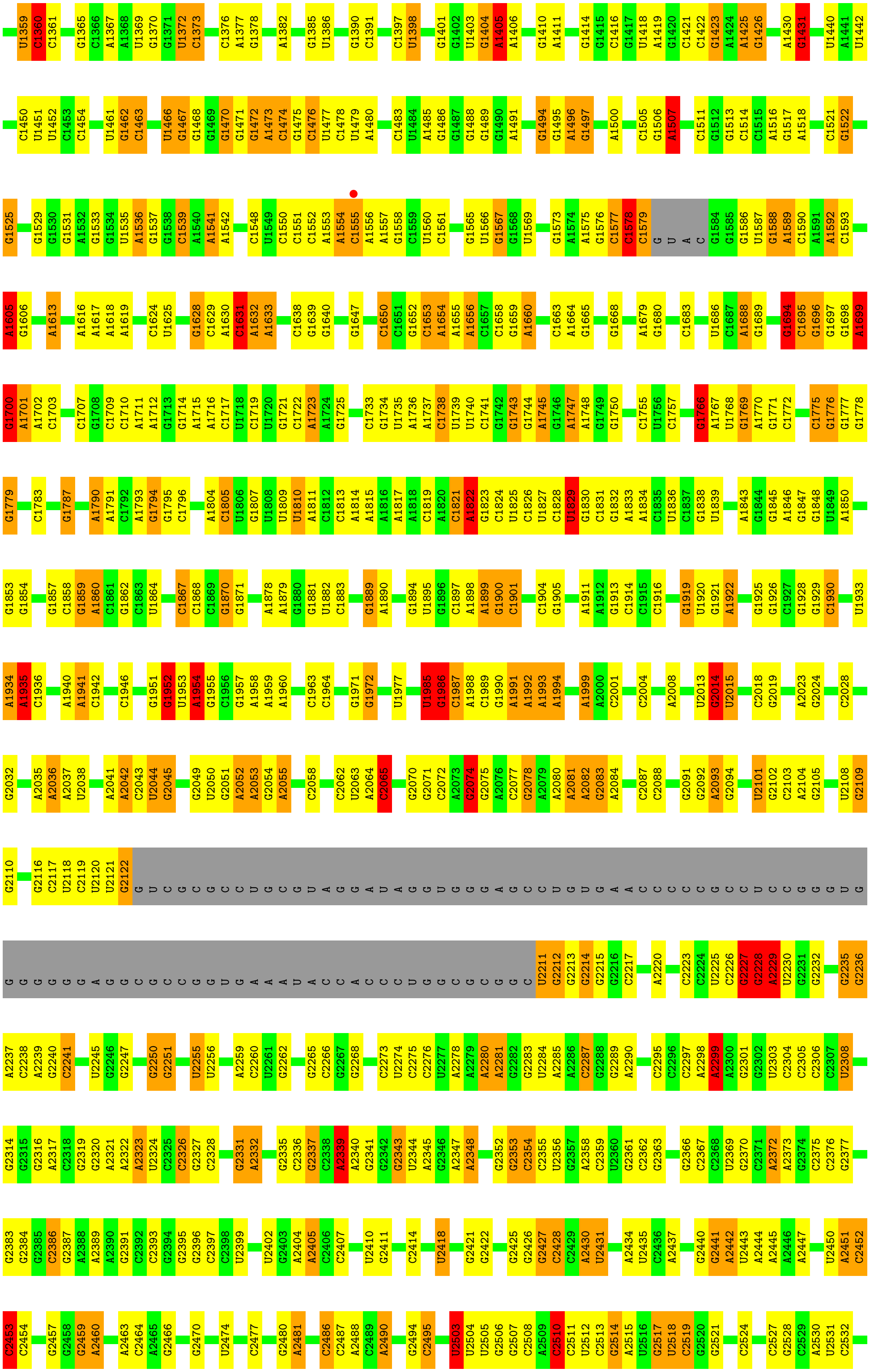
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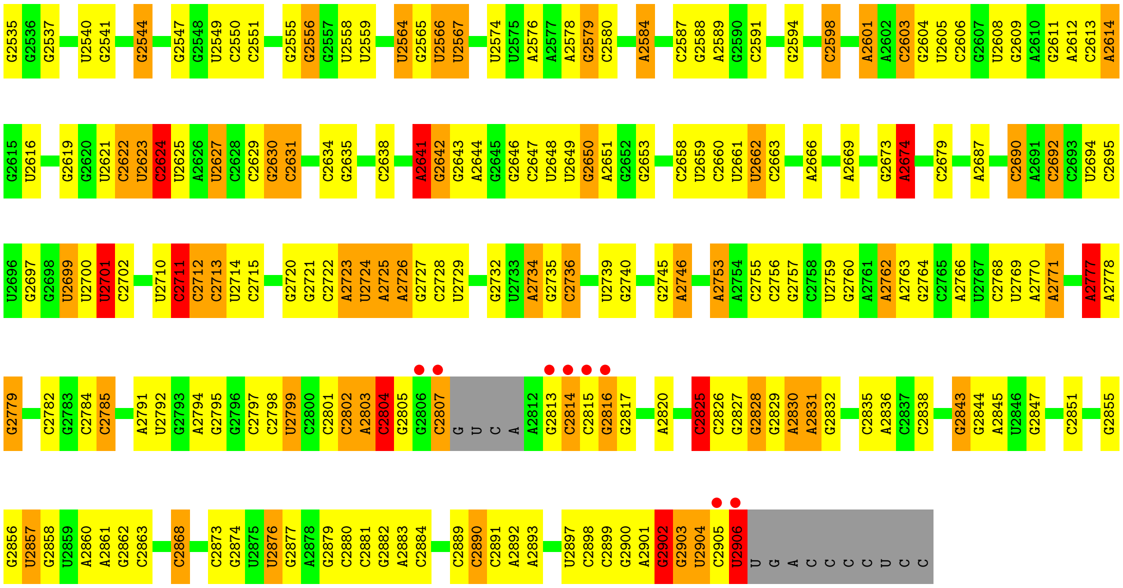

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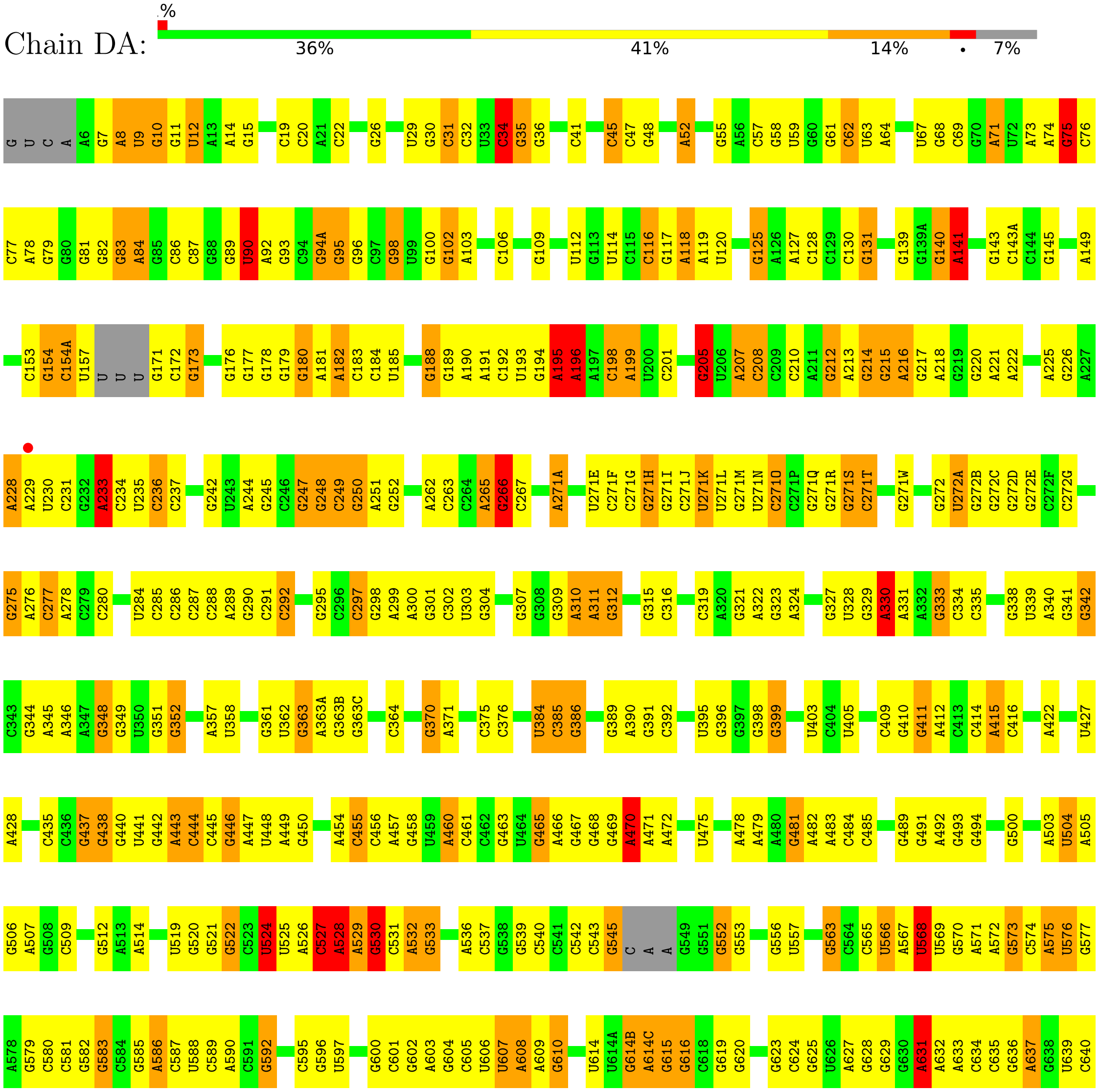

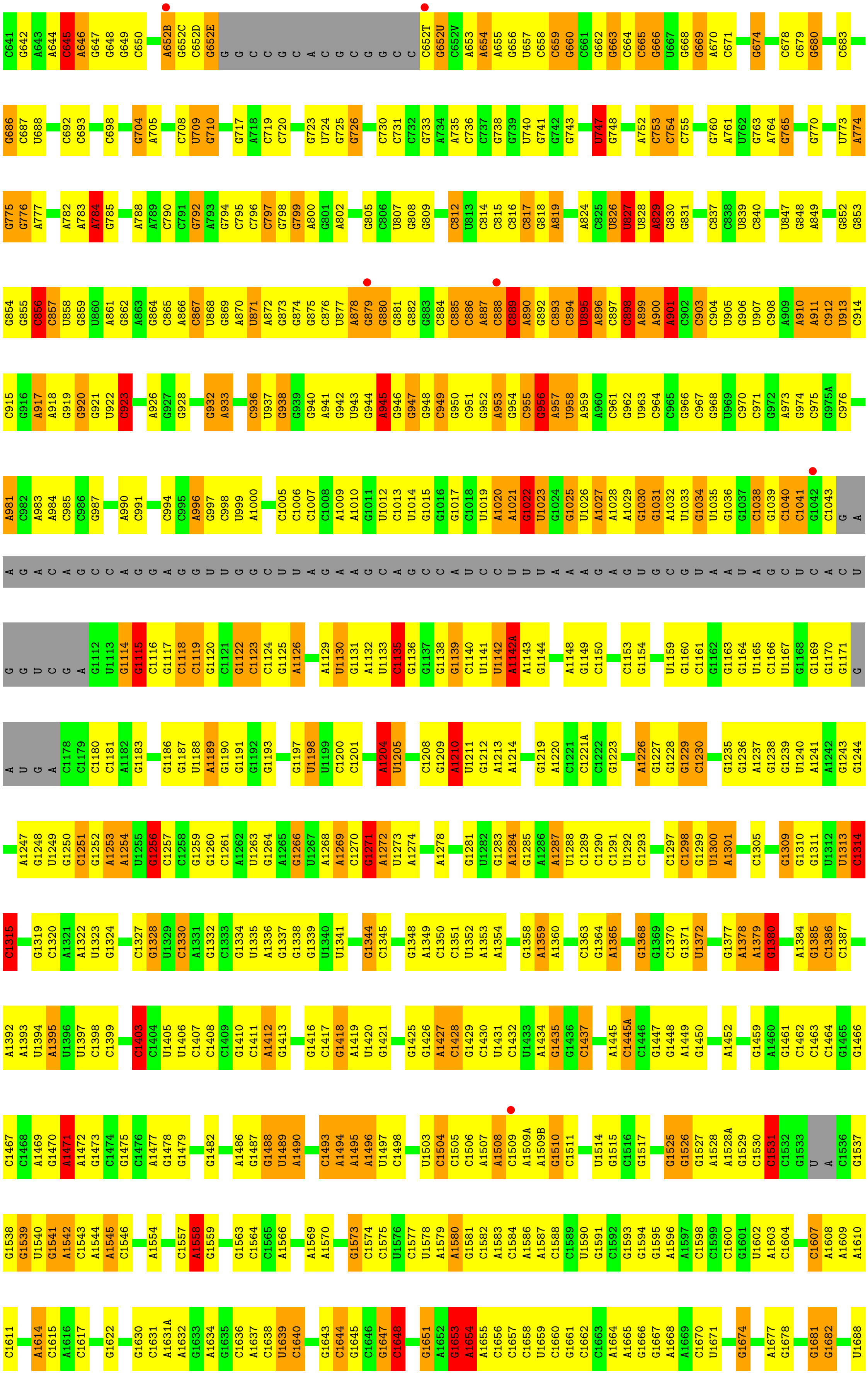
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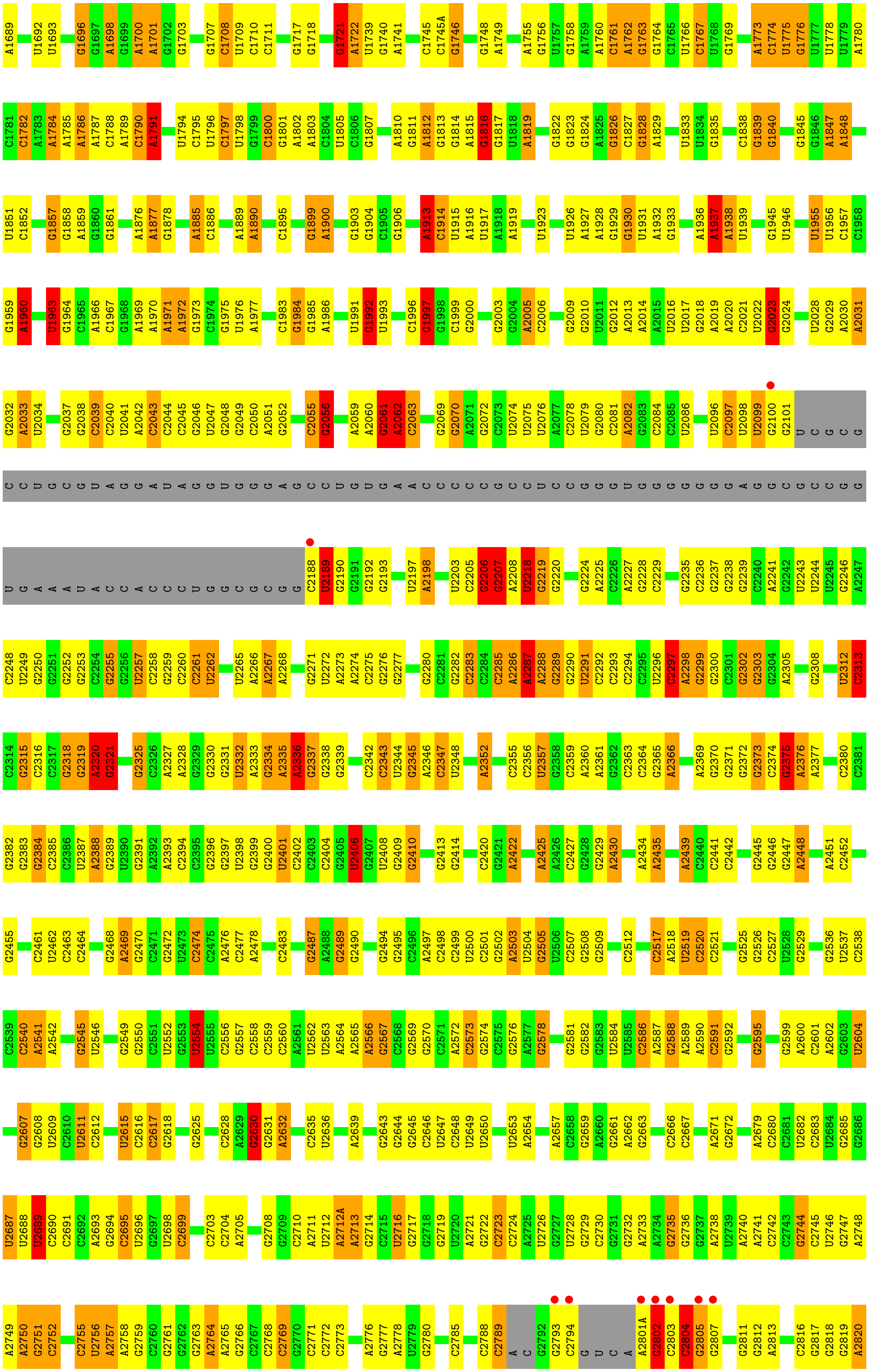
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G2455 C2461 U2462 C2463 C2464 G2468 A2469 G2470 C2471 G2472 U2473 C2474 C2475 A2476 C2477 A2478 C2483 G2487 A2488 G2489 G2490 G2494 G2495 C2496 A2497 C2498 C2499 U2500 C2501 G2502 A2503 U2504 G2505 U2506 C2507 G2508 G2509 C2512 C2517 A2518 U2519 C2520 C2521 G2525 G2526 C2527 U2528 G2529 G2536 U2537 C2538
C2539 C2540 A2541 A2542 G2545 U2546 G2549 G2550 C2551 U2552 G2553 U2554 U2555 C2556 G2557 C2558 C2559 C2560 A2561 U2562 U2563 A2564 A2565 A2566 G2567 C2568 G2569 G2570 C2571 A2572 C2573 G2574 C2575 G2576 A2577 G2578 G2581 G2582 G2583 U2584 U2585 C2586 A2587 G2588 A2589 A2590 C2591 G2592 G2595 G2599 A2600 C2601 A2602 G2603 U2604
G2607 G2608 U2609 C2610 U2611 C2612 U2615 C2616 C2617 G2618 G2625 C2628 A2629 G2630 G2631 A2632 C2635 U2636 A2639 G2643 G2644 G2645 C2646 U2647 C2648 U2649 U2650 U2653 A2654 A2657 C2658 G2659 A2660 G2661 A2662 G2663 C2666 C2667 A2671 G2672 A2679 C2680 C2681 U2682 C2683 U2684 G2685 G2686
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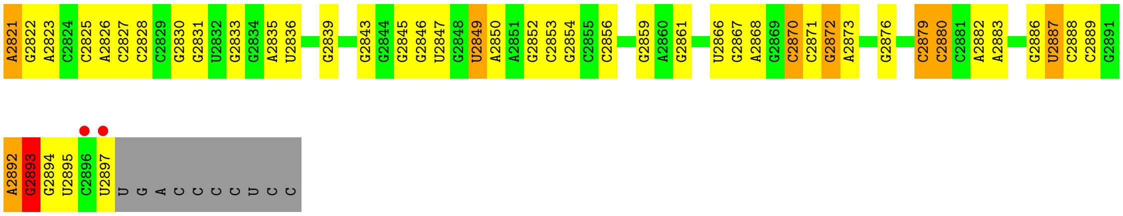
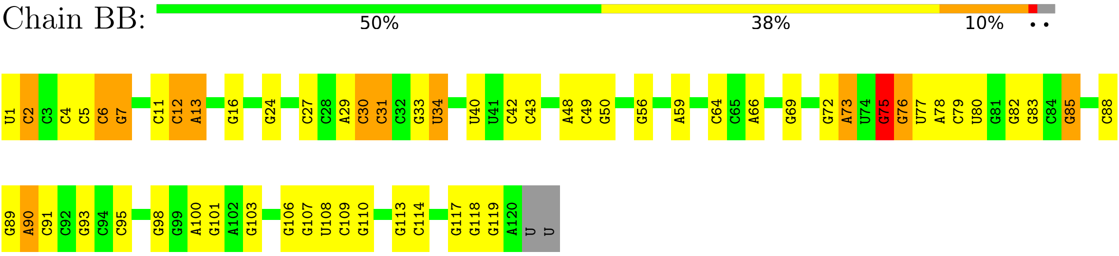
A2749 A2750 G2751 C2752 C2755 U2756 A2757 A2758 G2759 C2760 G2761 G2762 G2763 A2764 A2765 G2766 C2767 C2768 C2769 G2770 C2771 C2772 C2773 A2776 G2777 A2778 U2779 G2780 C2785 C2788 C2789 A C G2792 G2793 C2794 G U C A A2801A G2802 C2803 C2804 G2805 G2807 G2811 G2812 A2813 C2816 G2817 G2818 G2819 A2820



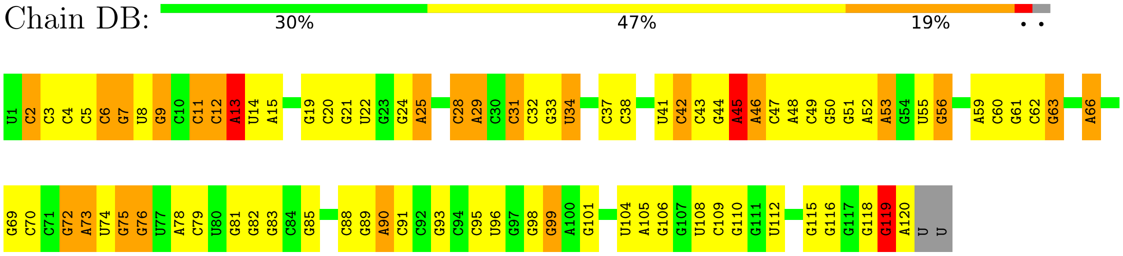
- Molecule 26: 5S Ribosomal RNA

Chain BB:



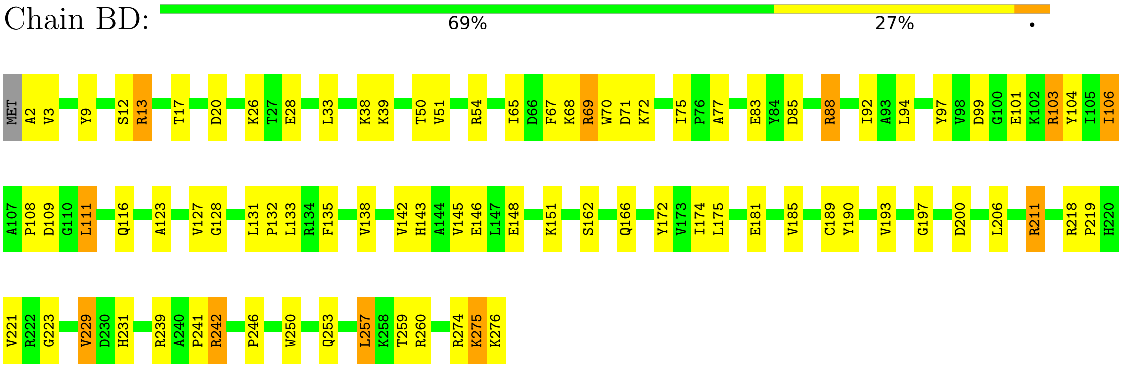
- Molecule 26: 5S Ribosomal RNA

Chain DB:



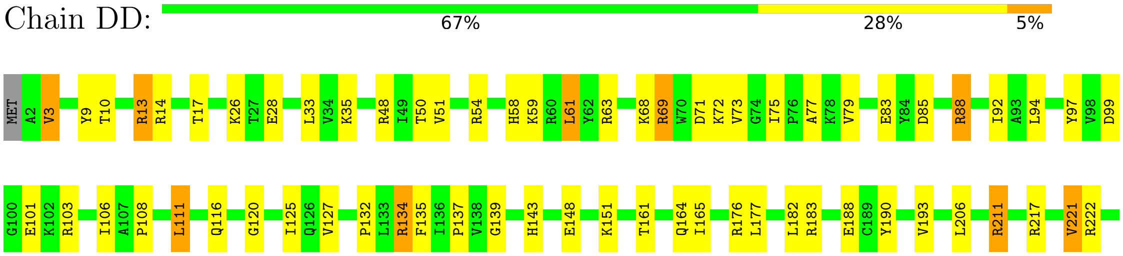
- Molecule 27: 50S Ribosomal Protein L2

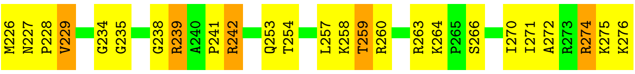
Chain BD:



- Molecule 27: 50S Ribosomal Protein L2

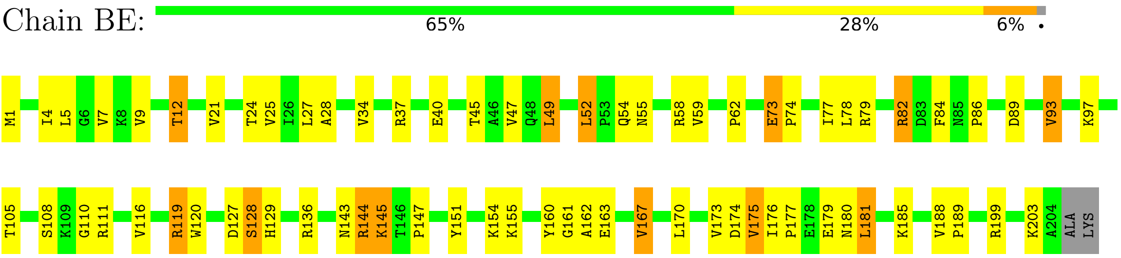
Chain DD:





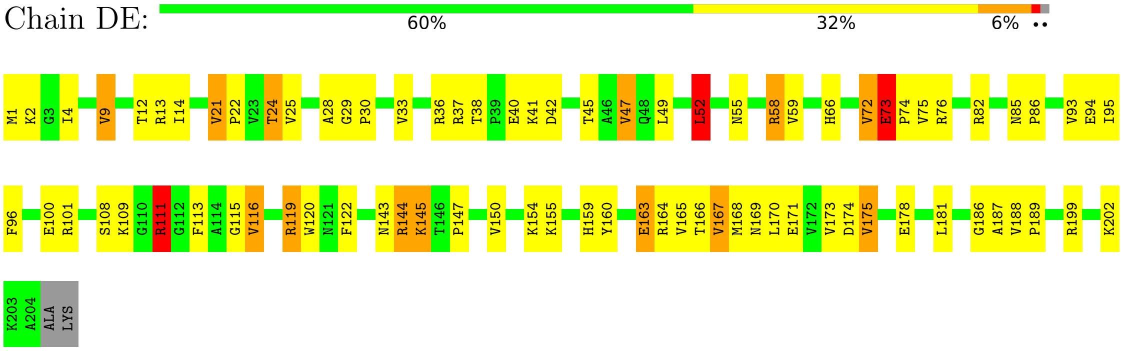
- Molecule 28: 50S Ribosomal Protein L3

Chain BE:



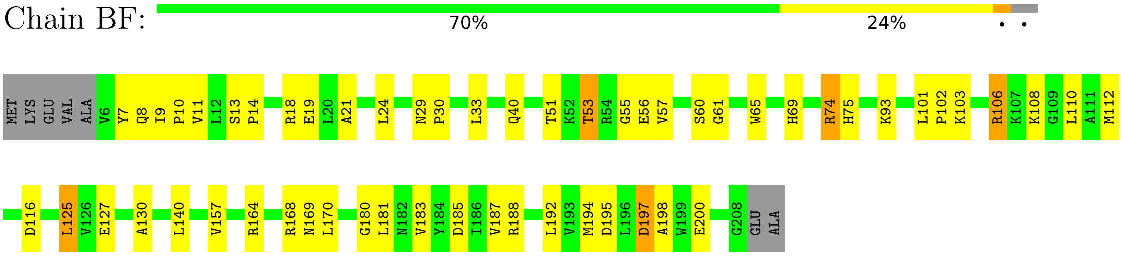
- Molecule 28: 50S Ribosomal Protein L3

Chain DE:



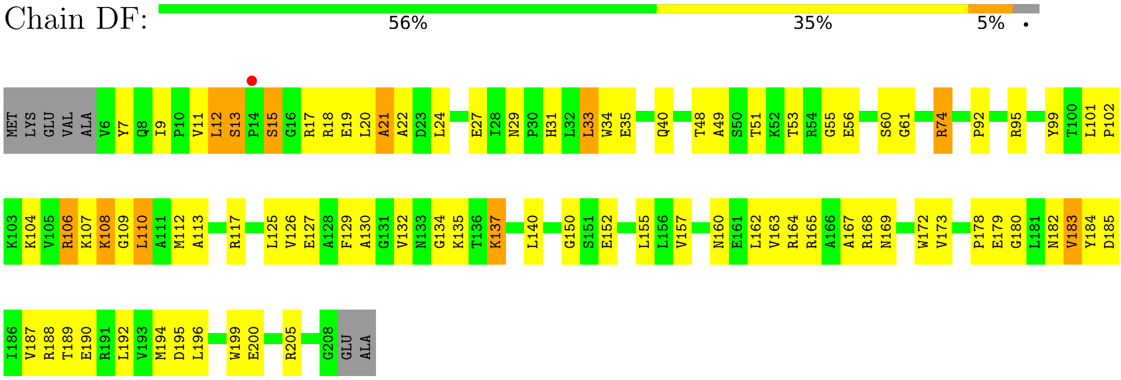
- Molecule 29: 50S Ribosomal Protein L4

Chain BF:

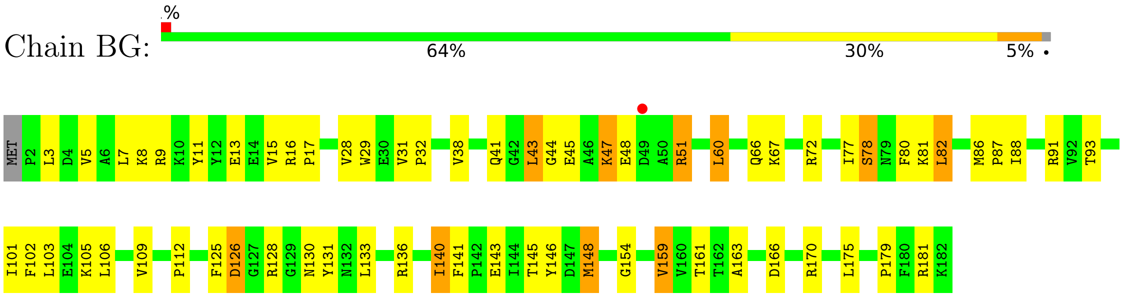


- Molecule 29: 50S Ribosomal Protein L4

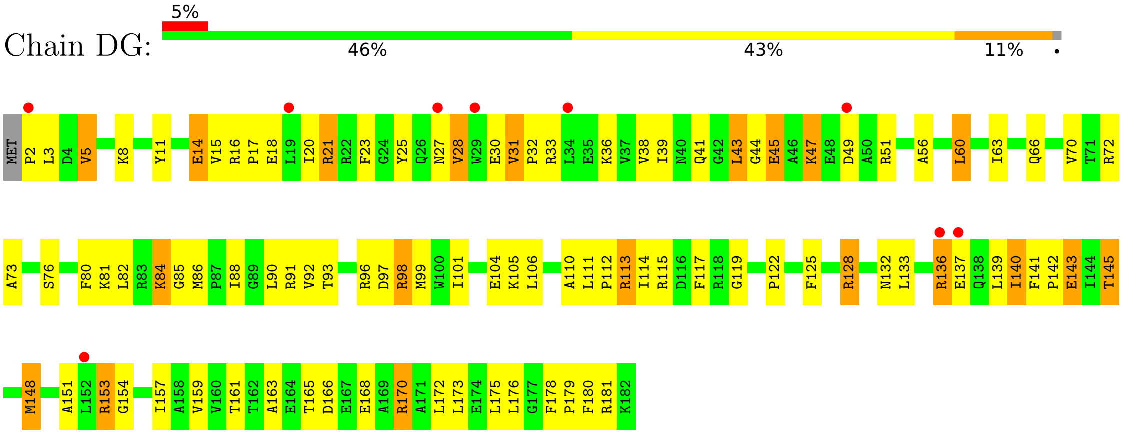
Chain DF:



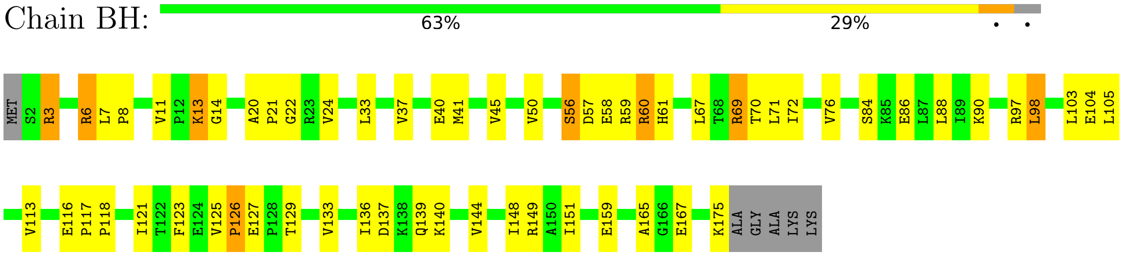
- Molecule 30: 50S Ribosomal Protein L5



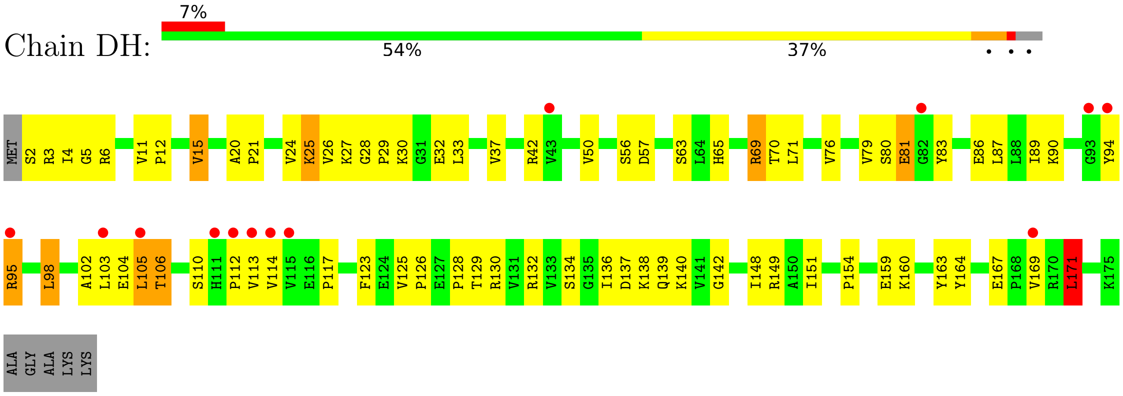
- Molecule 30: 50S Ribosomal Protein L5



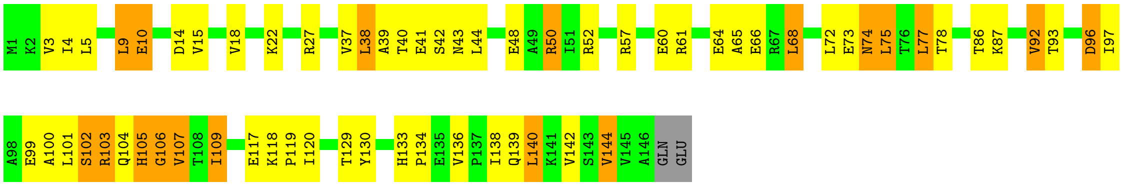
- Molecule 31: 50S Ribosomal Protein L6



- Molecule 31: 50S Ribosomal Protein L6

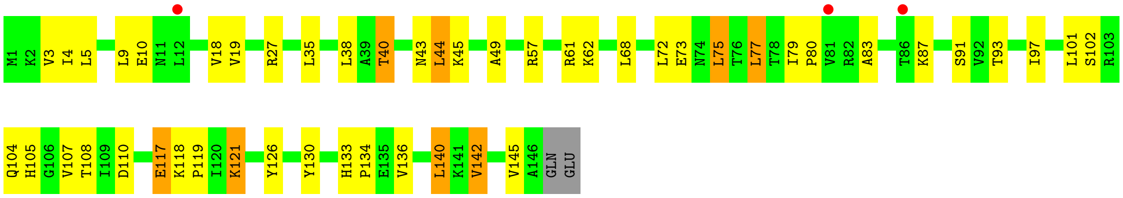


- Molecule 32: 50S Ribosomal Protein L9



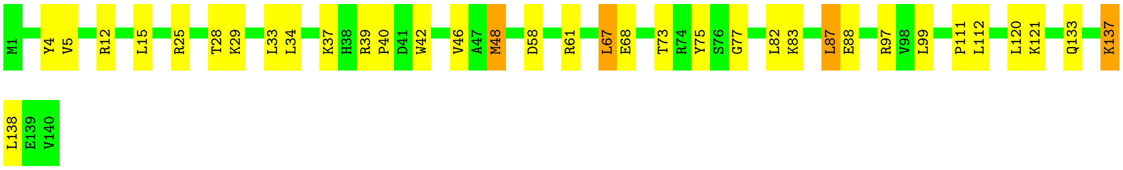
- Molecule 32: 50S Ribosomal Protein L9

Chain DI:



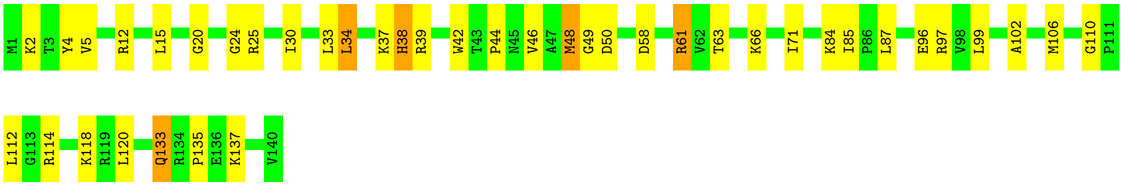
- Molecule 33: 50S Ribosomal Protein L13

Chain BN:



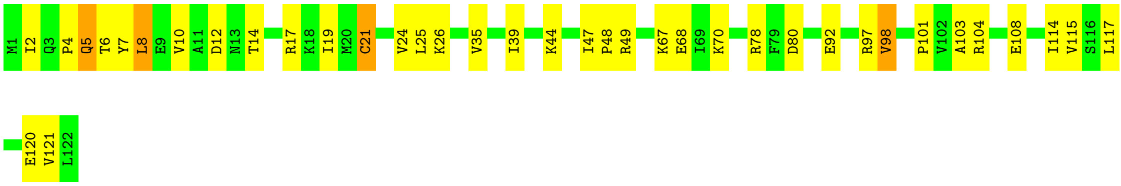
- Molecule 33: 50S Ribosomal Protein L13

Chain DN:



- Molecule 34: 50S Ribosomal Protein L14

Chain BO:

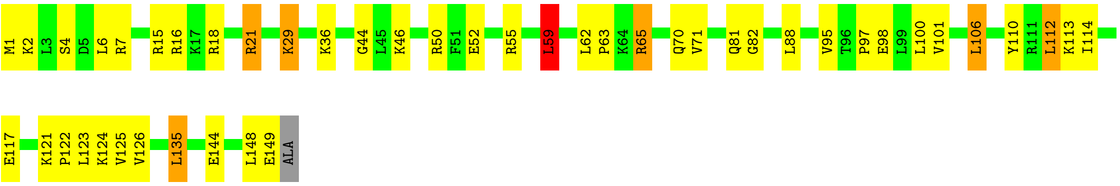


- Molecule 34: 50S Ribosomal Protein L14

Chain DO:

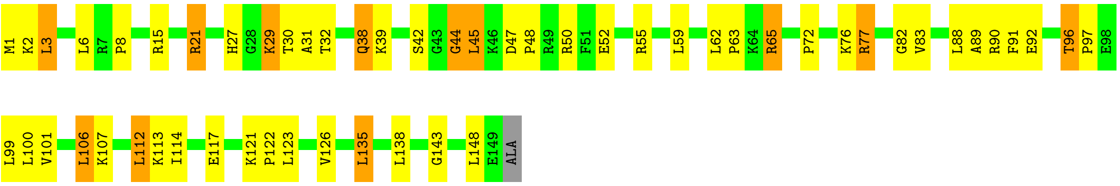
- Molecule 35: 50S Ribosomal Protein L15

Chain BP:



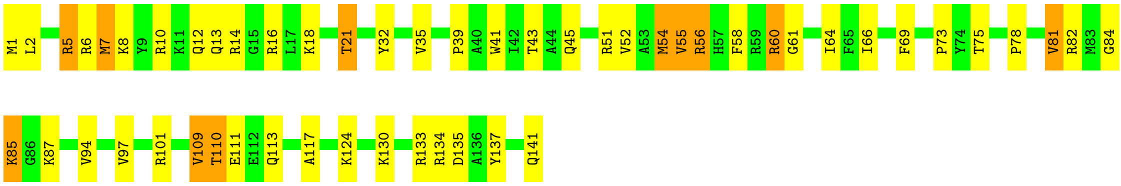
- Molecule 35: 50S Ribosomal Protein L15

Chain DP:



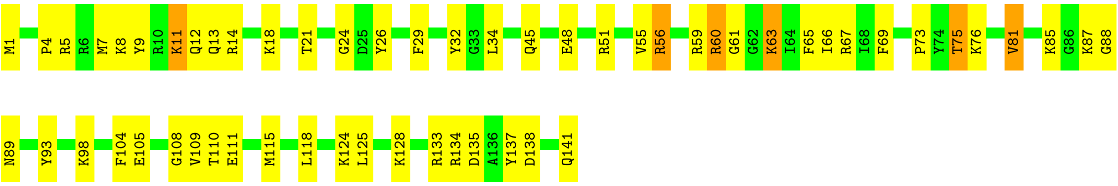
- Molecule 36: 50S Ribosomal Protein L16

Chain BQ:



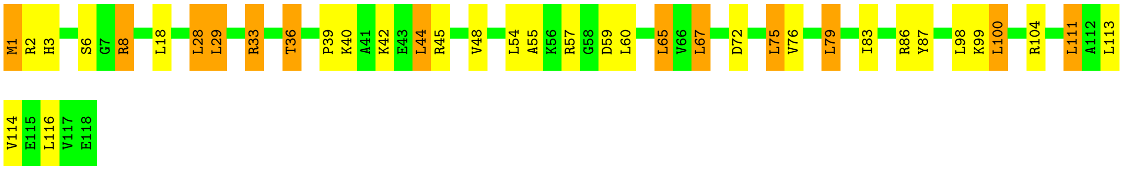
- Molecule 36: 50S Ribosomal Protein L16

Chain DQ:

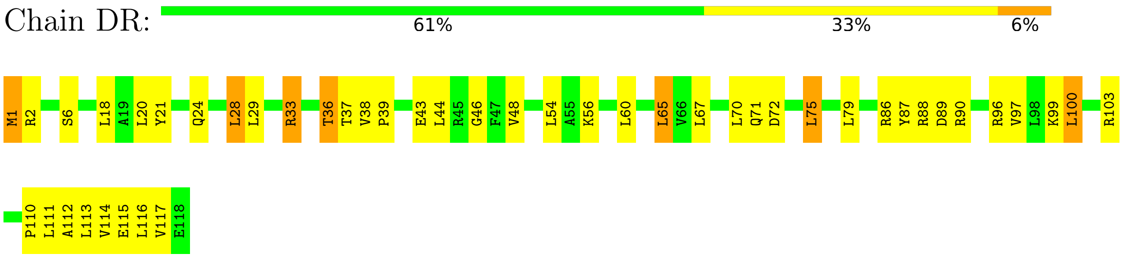


- Molecule 37: 50S Ribosomal Protein L17

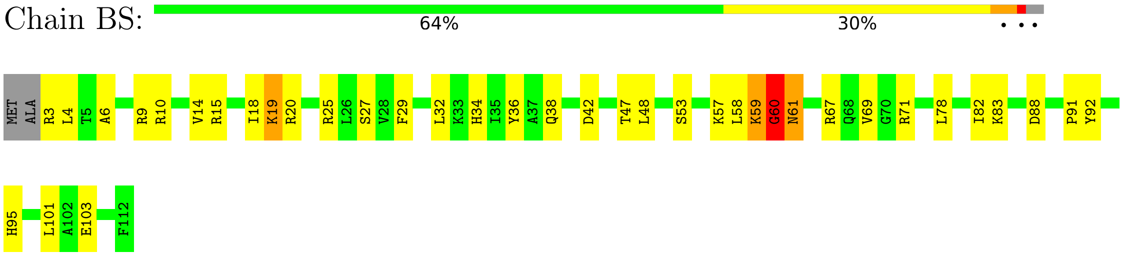
Chain BR:



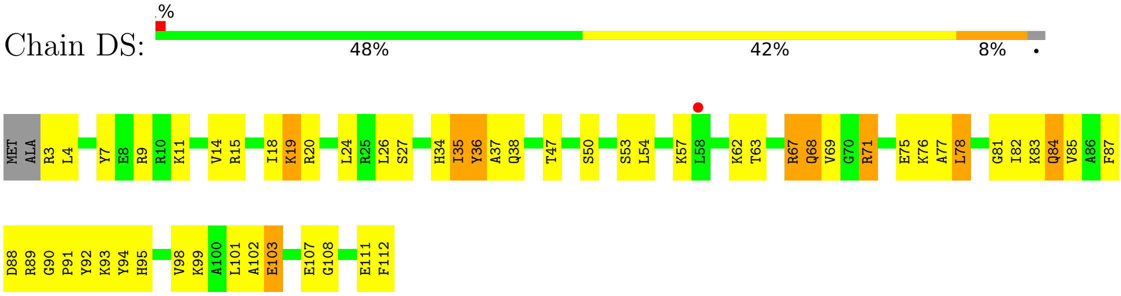
- Molecule 37: 50S Ribosomal Protein L17



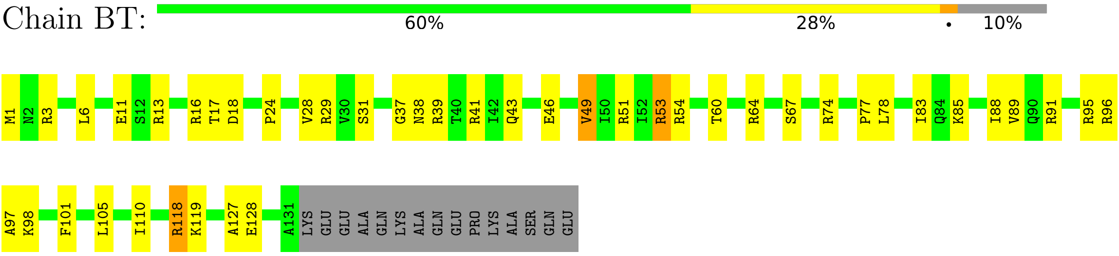
- Molecule 38: 50S Ribosomal Protein L18



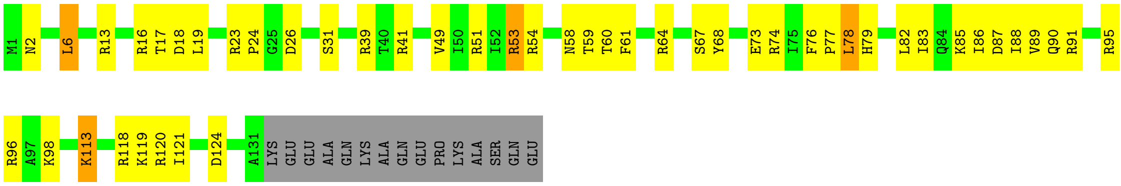
- Molecule 38: 50S Ribosomal Protein L18



- Molecule 39: 50S Ribosomal Protein L19

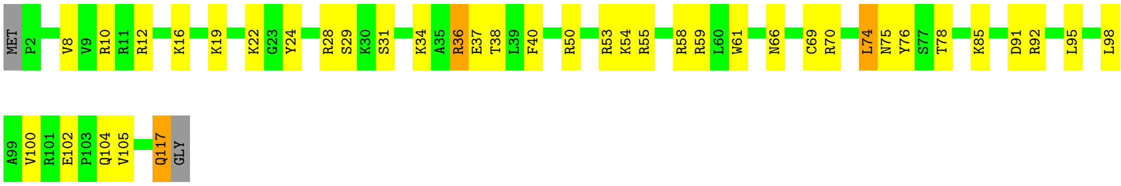


- Molecule 39: 50S Ribosomal Protein L19



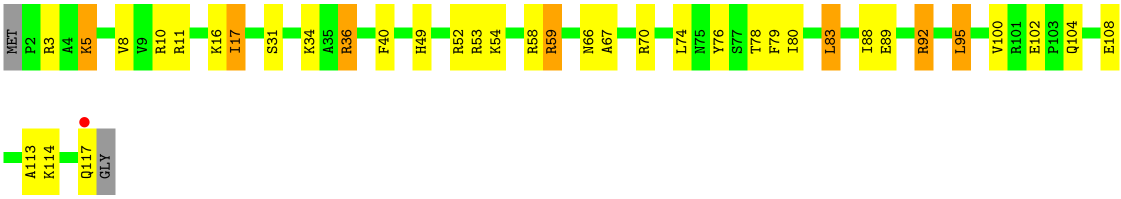
- Molecule 40: 50S Ribosomal Protein L20

Chain BU:



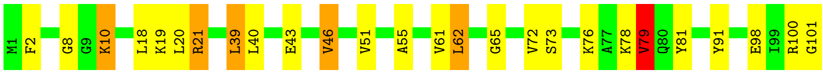
- Molecule 40: 50S Ribosomal Protein L20

Chain DU:



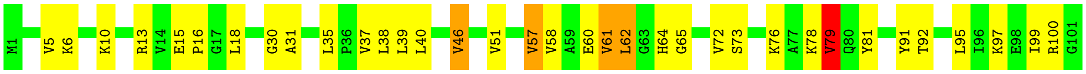
- Molecule 41: 50S Ribosomal Protein L21

Chain BV:



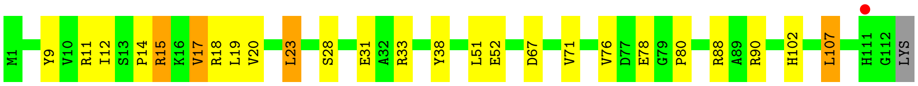
- Molecule 41: 50S Ribosomal Protein L21

Chain DV:

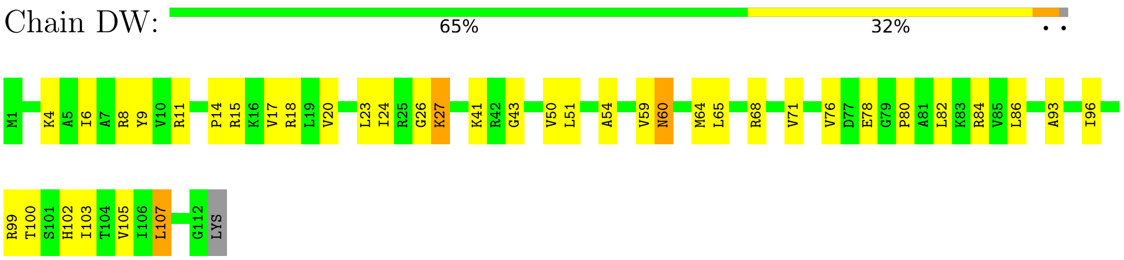


- Molecule 42: 50S Ribosomal Protein L22

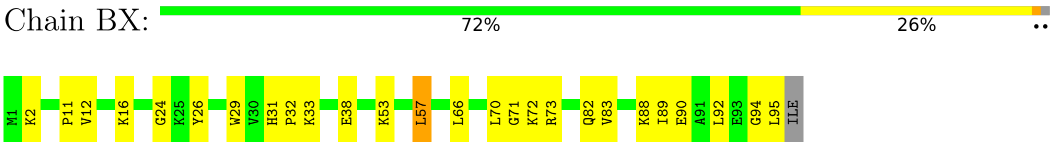
Chain BW:



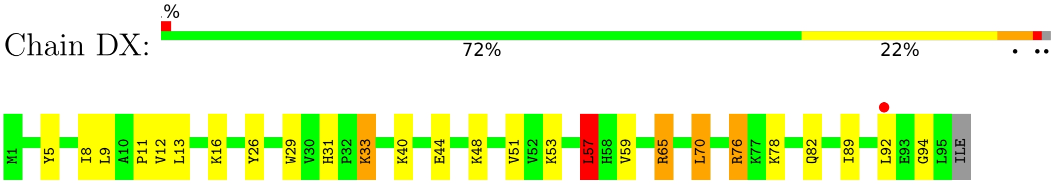
- Molecule 42: 50S Ribosomal Protein L22



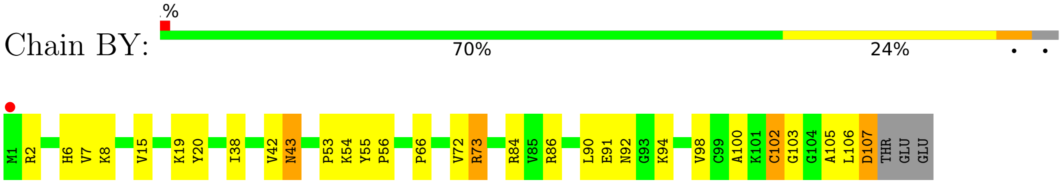
- Molecule 43: 50S Ribosomal Protein L23



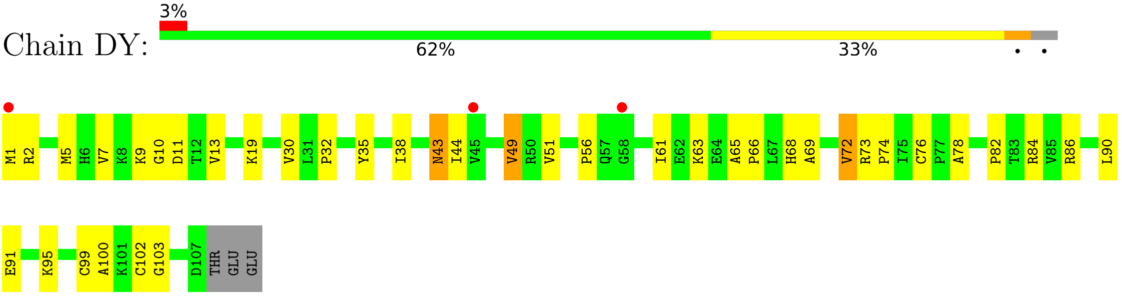
- Molecule 43: 50S Ribosomal Protein L23



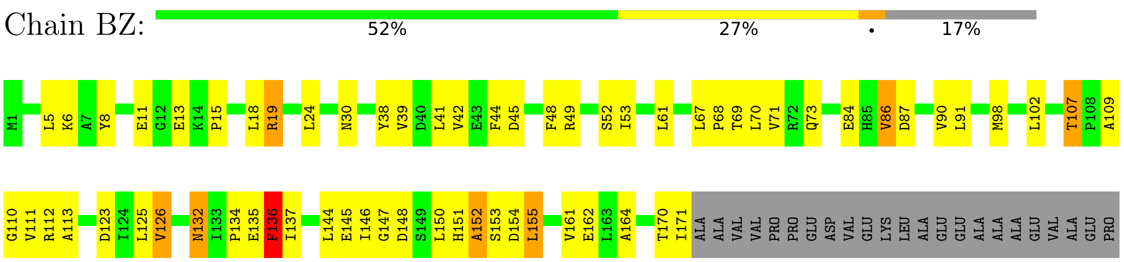
- Molecule 44: 50S Ribosomal Protein L24



- Molecule 44: 50S Ribosomal Protein L24

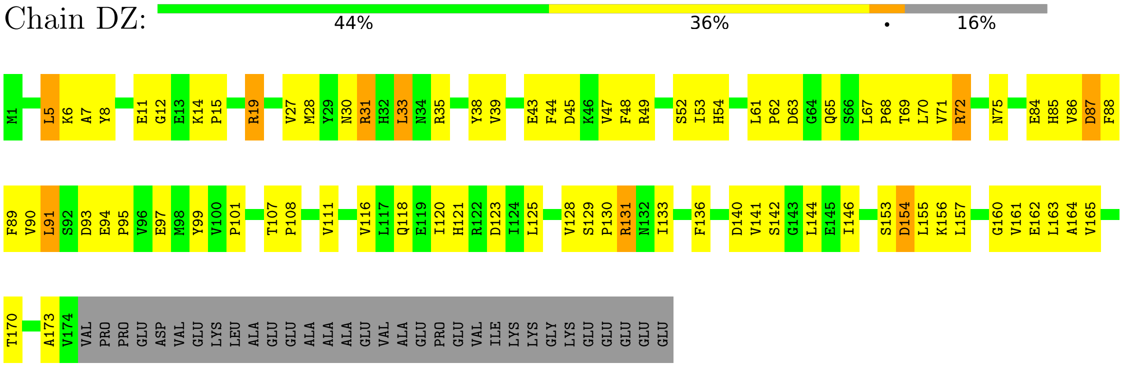


- Molecule 45: 50S Ribosomal Protein L25



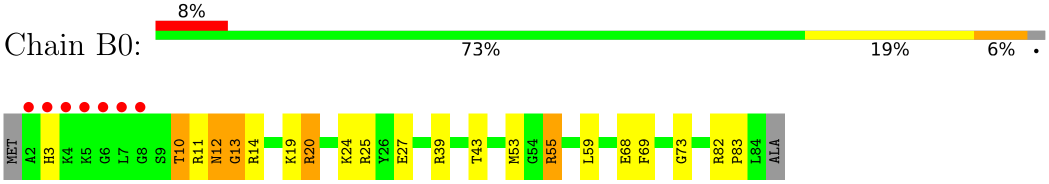
- Molecule 45: 50S Ribosomal Protein L25

Chain DZ:



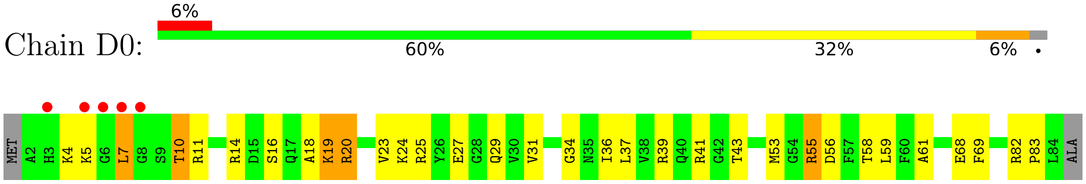
- Molecule 46: 50S Ribosomal Protein L27

Chain B0:



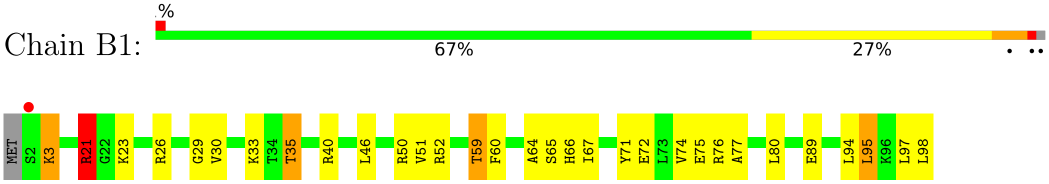
- Molecule 46: 50S Ribosomal Protein L27

Chain D0:



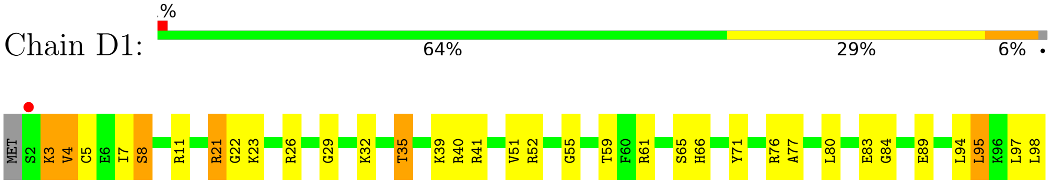
- Molecule 47: 50S Ribosomal Protein L28

Chain B1:



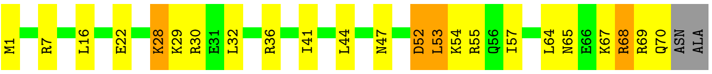
- Molecule 47: 50S Ribosomal Protein L28

Chain D1:



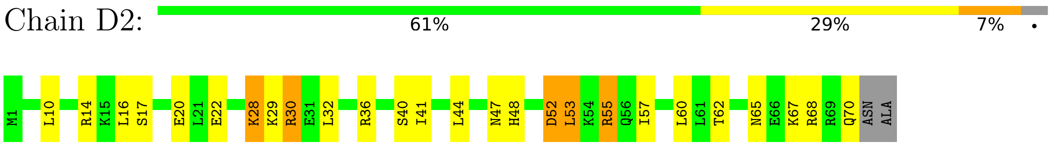
- Molecule 48: 50S Ribosomal Protein L29

Chain B2:



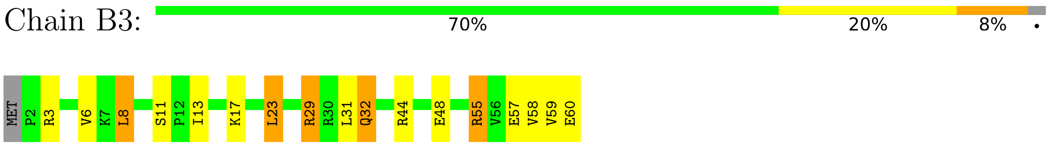
- Molecule 48: 50S Ribosomal Protein L29

Chain D2:



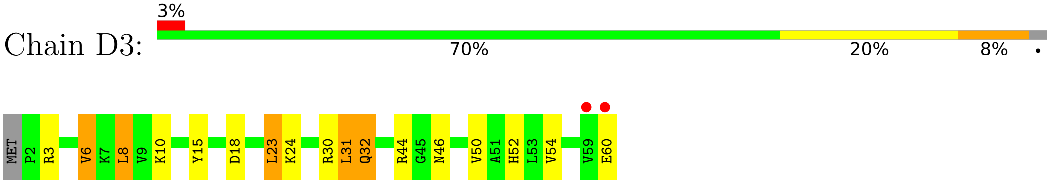
- Molecule 49: 50S Ribosomal Protein L30

Chain B3:



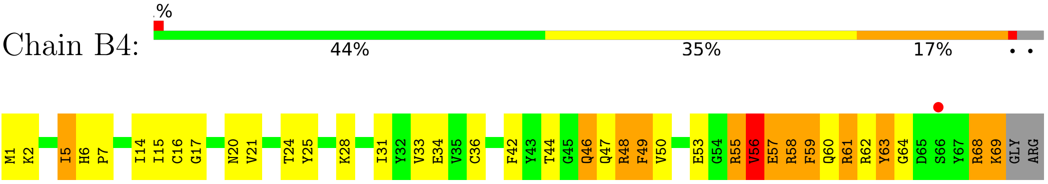
- Molecule 49: 50S Ribosomal Protein L30

Chain D3:



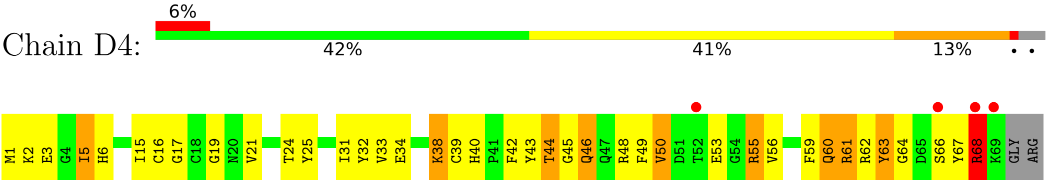
- Molecule 50: 50S Ribosomal Protein L31

Chain B4:



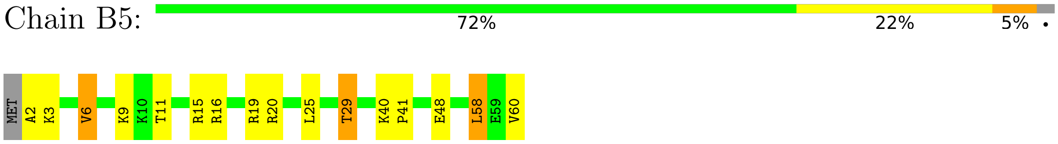
- Molecule 50: 50S Ribosomal Protein L31

Chain D4:



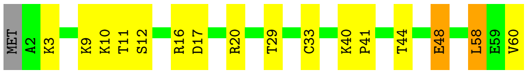
- Molecule 51: 50S Ribosomal Protein L32

Chain B5:



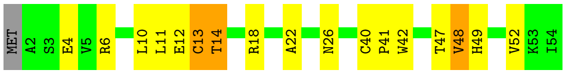
- Molecule 51: 50S Ribosomal Protein L32

Chain D5:



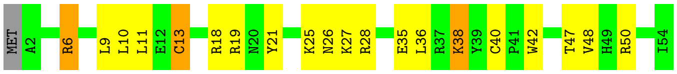
- Molecule 52: 50S Ribosomal Protein L33

Chain B6:



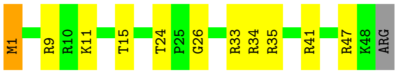
- Molecule 52: 50S Ribosomal Protein L33

Chain D6:



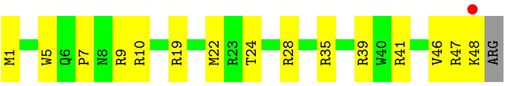
- Molecule 53: 50S Ribosomal Protein L34

Chain B7:



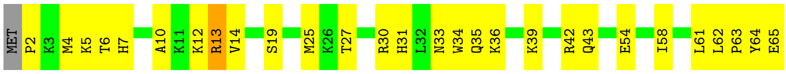
- Molecule 53: 50S Ribosomal Protein L34

Chain D7:



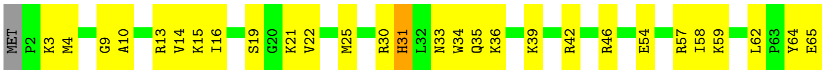
- Molecule 54: 50S Ribosomal Protein L35

Chain B8:



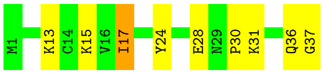
- Molecule 54: 50S Ribosomal Protein L35

Chain D8:



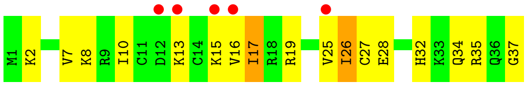
- Molecule 55: 50S Ribosomal Protein L36

Chain B9:



- Molecule 55: 50S Ribosomal Protein L36

Chain D9:



4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	210.08Å 449.83Å 619.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.74 – 3.00 49.75 – 3.00	Depositor EDS
% Data completeness (in resolution range)	98.8 (49.74-3.00) 98.8 (49.75-3.00)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	0.24	Depositor
$< I/\sigma(I) >$ [1]	1.26 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.203 , 0.259 0.203 , 0.259	Depositor DCC
R_{free} test set	57319 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	66.8	Xtriage
Anisotropy	0.228	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 66.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	286321	wwPDB-VP
Average B, all atoms (Å^2)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.70% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: FME, K, MG, 2R3, 2R1, ZN, 2QY, 004, MVA, SF4, 2QZ

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	0.77	7/36038 (0.0%)	1.39	355/56244 (0.6%)
1	CA	0.76	13/36170 (0.0%)	1.43	365/56452 (0.6%)
2	AB	0.49	0/1881	0.77	0/2542
2	CB	0.56	0/1860	0.81	2/2518 (0.1%)
3	AC	0.48	0/1576	0.64	0/2130
3	CC	0.50	0/1566	0.72	2/2119 (0.1%)
4	AD	0.49	0/1689	0.76	1/2267 (0.0%)
4	CD	0.50	0/1704	0.71	0/2284
5	AE	0.47	0/1145	0.71	0/1543
5	CE	0.50	0/1149	0.76	0/1548
6	AF	0.48	0/819	0.69	0/1111
6	CF	0.53	0/829	0.76	0/1123
7	AG	0.48	0/1250	0.66	1/1679 (0.1%)
7	CG	0.50	0/1254	0.72	1/1683 (0.1%)
8	AH	0.46	0/1108	0.69	0/1494
8	CH	0.47	0/1108	0.71	0/1494
9	AI	0.47	0/1002	0.73	1/1346 (0.1%)
9	CI	0.56	0/997	0.75	2/1343 (0.1%)
10	AJ	0.47	0/722	0.67	0/982
10	CJ	0.53	0/727	0.69	0/988
11	AK	0.44	0/844	0.65	1/1145 (0.1%)
11	CK	0.46	0/848	0.67	0/1149
12	AL	0.50	0/946	0.73	0/1274
12	CL	0.52	0/946	0.74	0/1274
13	AM	0.48	0/969	0.68	0/1302
13	CM	0.48	0/961	0.66	0/1291
14	AN	0.48	0/501	0.71	0/664
14	CN	0.55	0/501	0.71	0/664
15	AO	0.49	0/739	0.76	0/985
15	CO	0.47	0/739	0.70	0/985
16	AP	0.47	0/697	0.73	0/939
16	CP	0.49	0/693	0.70	0/935

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	AQ	0.51	0/836	0.68	0/1117
17	CQ	0.51	0/836	0.70	0/1117
18	AR	0.48	0/560	0.73	0/746
18	CR	0.50	0/560	0.75	1/746 (0.1%)
19	AS	0.47	0/667	0.66	0/900
19	CS	0.50	0/661	0.80	1/893 (0.1%)
20	AT	0.48	0/730	0.77	0/965
20	CT	0.43	0/729	0.68	0/965
21	AU	0.47	0/203	0.62	0/266
21	CU	0.51	0/203	0.64	0/266
22	AV	0.99	0/127	1.42	2/198 (1.0%)
22	CV	0.82	0/126	1.39	1/195 (0.5%)
23	AX	0.88	8/1813 (0.4%)	1.62	47/2825 (1.7%)
23	CX	0.94	6/1813 (0.3%)	1.87	57/2825 (2.0%)
24	AW	0.46	0/20	0.84	0/23
24	CW	0.34	0/20	0.64	0/23
25	BA	1.07	33/65892 (0.1%)	1.49	877/102850 (0.9%)
25	DA	0.82	13/65466 (0.0%)	1.46	741/102184 (0.7%)
26	BB	0.83	0/2878	1.31	13/4490 (0.3%)
26	DB	0.93	2/2878 (0.1%)	1.50	45/4490 (1.0%)
27	BD	0.71	2/2186 (0.1%)	0.82	0/2944
27	DD	0.63	2/2186 (0.1%)	0.77	0/2944
28	BE	0.72	0/1592	0.77	0/2149
28	DE	0.57	0/1592	0.79	2/2149 (0.1%)
29	BF	0.73	0/1619	0.75	0/2193
29	DF	0.53	0/1615	0.80	2/2188 (0.1%)
30	BG	0.46	0/1450	0.71	0/1959
30	DG	0.54	0/1449	0.76	0/1958
31	BH	0.61	0/1356	0.72	0/1834
31	DH	0.54	0/1356	0.71	1/1834 (0.1%)
32	BI	0.51	0/1100	0.70	0/1501
32	DI	0.51	0/1076	0.74	0/1471
33	BN	0.67	0/1144	0.75	0/1543
33	DN	0.54	0/1144	0.74	0/1543
34	BO	0.66	0/943	0.78	1/1269 (0.1%)
34	DO	0.56	0/943	0.78	1/1269 (0.1%)
35	BP	0.64	0/1152	0.82	1/1533 (0.1%)
35	DP	0.55	0/1152	0.83	2/1533 (0.1%)
36	BQ	0.69	0/1143	0.81	0/1527
36	DQ	0.59	0/1143	0.77	0/1527
37	BR	0.62	0/982	0.86	0/1312
37	DR	0.51	0/982	0.70	0/1312
38	BS	0.55	0/887	0.78	1/1180 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
38	DS	0.51	0/880	0.74	0/1172
39	BT	0.59	0/1105	0.79	0/1477
39	DT	0.53	0/1097	0.74	0/1468
40	BU	0.70	0/977	0.76	0/1301
40	DU	0.52	0/977	0.71	0/1301
41	BV	0.67	0/782	0.72	0/1049
41	DV	0.57	0/782	0.75	0/1049
42	BW	0.73	0/897	0.76	0/1205
42	DW	0.59	0/897	0.74	0/1205
43	BX	0.71	0/764	0.75	1/1025 (0.1%)
43	DX	0.56	0/764	0.80	2/1025 (0.2%)
44	BY	0.70	0/819	0.78	0/1095
44	DY	0.57	0/819	0.75	0/1095
45	BZ	0.55	0/1379	0.74	0/1873
45	DZ	0.54	0/1390	0.70	0/1890
46	B0	0.63	0/662	0.81	2/881 (0.2%)
46	D0	0.55	0/662	0.78	0/881
47	B1	0.66	0/762	0.81	3/1014 (0.3%)
47	D1	0.55	0/762	0.74	0/1014
48	B2	0.61	0/590	0.81	0/781
48	D2	0.47	0/590	0.67	0/781
49	B3	0.67	0/474	0.78	0/635
49	D3	0.50	0/469	0.70	0/630
50	B4	0.57	0/564	0.81	0/759
50	D4	0.59	0/544	0.89	1/735 (0.1%)
51	B5	0.72	0/469	0.84	1/635 (0.2%)
51	D5	0.59	0/469	0.73	1/635 (0.2%)
52	B6	0.66	0/460	0.66	0/613
52	D6	0.58	0/456	0.72	0/608
53	B7	0.74	0/426	0.82	0/561
53	D7	0.60	0/426	0.78	1/561 (0.2%)
54	B8	0.68	0/519	0.72	0/684
54	D8	0.58	0/525	0.73	0/691
55	B9	0.74	0/310	0.73	0/407
55	D9	0.61	0/310	0.80	0/407
All	All	0.81	86/305966 (0.0%)	1.30	2539/457396 (0.6%)

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	3
4	CD	0	1
7	AG	0	1
9	AI	0	1
19	CS	0	1
23	CX	1	0
24	AW	0	1
24	CW	0	1
27	DD	0	1
38	BS	0	1
44	BY	0	1
45	BZ	0	1
50	B4	0	1
50	D4	0	1
All	All	1	15

The worst 5 of 86 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	CA	1154	G	C6-N1	-13.21	1.30	1.39
1	CA	1119	C	N3-C4	-13.12	1.24	1.33
1	AA	343	U	C4-O4	12.79	1.33	1.23
1	CA	1154	G	N1-C2	-12.44	1.27	1.37
23	CX	76	A	N7-C5	-12.26	1.31	1.39

The worst 5 of 2539 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	CA	1119	C	N1-C2-O2	40.38	143.13	118.90
1	CA	1154	G	C5-C6-O6	34.47	149.28	128.60
23	CX	76	A	O4'-C1'-N9	33.86	135.29	108.20
1	CA	1154	G	N3-C2-N2	29.11	140.27	119.90
1	CA	1154	G	N1-C2-N2	-27.03	91.87	116.20

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	CX	76	A	C1'

5 of 15 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	AB	231	GLU	Peptide

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Mol	Chain	Res	Type	Group
2	AB	8	LYS	Peptide
2	AB	9	GLU	Peptide
7	AG	79	ARG	Peptide
9	AI	52	ALA	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	32196	0	16250	907	0
1	CA	32312	0	16307	1000	0
2	AB	1846	0	1867	106	0
2	CB	1825	0	1828	118	0
3	AC	1552	0	1546	51	0
3	CC	1542	0	1517	81	0
4	AD	1659	0	1676	86	0
4	CD	1674	0	1714	83	0
5	AE	1129	0	1185	44	0
5	CE	1133	0	1191	57	0
6	AF	806	0	793	34	0
6	CF	816	0	808	24	0
7	AG	1231	0	1238	33	0
7	CG	1235	0	1249	53	0
8	AH	1088	0	1126	43	0
8	CH	1088	0	1126	56	0
9	AI	983	0	986	47	0
9	CI	978	0	966	55	0
10	AJ	709	0	650	41	0
10	CJ	714	0	672	58	0
11	AK	829	0	825	17	0
11	CK	833	0	836	27	0
12	AL	930	0	980	35	0
12	CL	930	0	980	40	0
13	AM	958	0	1002	35	0
13	CM	950	0	988	50	0
14	AN	492	0	529	27	0
14	CN	492	0	529	31	0
15	AO	728	0	760	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	CO	728	0	760	26	0
16	AP	681	0	697	35	0
16	CP	677	0	686	30	0
17	AQ	823	0	891	21	0
17	CQ	823	0	891	27	0
18	AR	555	0	618	24	0
18	CR	555	0	618	19	0
19	AS	652	0	662	42	0
19	CS	646	0	644	49	0
20	AT	728	0	798	36	0
20	CT	727	0	796	26	0
21	AU	199	0	208	6	0
21	CU	199	0	208	8	0
22	AV	114	0	54	1	0
22	CV	113	0	54	1	0
23	AX	1623	0	823	23	0
23	CX	1623	0	823	22	0
24	AW	93	0	84	10	0
24	CW	93	0	84	10	0
25	BA	58834	0	29666	828	0
25	DA	58458	0	29481	1163	0
26	BB	2573	0	1306	33	0
26	DB	2573	0	1306	65	0
27	BD	2136	0	2218	62	0
27	DD	2136	0	2218	74	0
28	BE	1559	0	1618	55	0
28	DE	1559	0	1618	65	0
29	BF	1584	0	1625	38	0
29	DF	1580	0	1619	65	0
30	BG	1425	0	1443	41	0
30	DG	1424	0	1434	89	0
31	BH	1330	0	1407	37	0
31	DH	1330	0	1407	50	0
32	BI	1085	0	1114	42	0
32	DI	1061	0	1080	27	0
33	BN	1117	0	1183	18	0
33	DN	1117	0	1184	25	0
34	BO	933	0	996	26	0
34	DO	933	0	996	30	0
35	BP	1135	0	1212	42	0
35	DP	1135	0	1212	52	0
36	BQ	1122	0	1179	38	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	DQ	1122	0	1179	38	0
37	BR	968	0	1033	24	0
37	DR	968	0	1032	28	0
38	BS	877	0	938	30	0
38	DS	870	0	923	45	0
39	BT	1091	0	1151	36	0
39	DT	1083	0	1136	38	0
40	BU	959	0	1019	28	0
40	DU	959	0	1019	26	0
41	BV	771	0	830	15	0
41	DV	771	0	830	23	0
42	BW	886	0	940	15	0
42	DW	886	0	940	25	0
43	BX	750	0	814	19	0
43	DX	750	0	814	22	0
44	BY	806	0	881	22	0
44	DY	806	0	881	27	0
45	BZ	1349	0	1355	44	0
45	DZ	1360	0	1363	55	0
46	B0	653	0	674	19	0
46	D0	653	0	674	31	0
47	B1	755	0	826	19	0
47	D1	755	0	826	20	0
48	B2	588	0	643	13	0
48	D2	588	0	643	18	0
49	B3	469	0	518	12	0
49	D3	464	0	514	10	0
50	B4	551	0	532	38	0
50	D4	531	0	502	38	0
51	B5	455	0	465	14	0
51	D5	455	0	465	8	0
52	B6	453	0	473	10	0
52	D6	449	0	469	13	0
53	B7	418	0	467	11	0
53	D7	418	0	467	8	0
54	B8	511	0	571	31	0
54	D8	517	0	582	24	0
55	B9	307	0	335	7	0
55	D9	307	0	335	14	0
56	AA	222	0	0	0	0
56	AD	1	0	0	0	0
56	AF	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	AK	1	0	0	0	0
56	AL	1	0	0	0	0
56	AM	2	0	0	0	0
56	AN	1	0	0	0	0
56	AS	1	0	0	0	0
56	AV	1	0	0	0	0
56	AX	9	0	0	0	0
56	B0	6	0	0	0	0
56	B1	2	0	0	0	0
56	B2	1	0	0	0	0
56	B3	3	0	0	0	0
56	B5	1	0	0	0	0
56	B7	4	0	0	0	0
56	B8	2	0	0	0	0
56	B9	1	0	0	0	0
56	BA	739	0	0	0	0
56	BB	18	0	0	0	0
56	BD	12	0	0	0	0
56	BE	9	0	0	0	0
56	BF	6	0	0	0	0
56	BG	4	0	0	0	0
56	BN	6	0	0	0	0
56	BO	1	0	0	0	0
56	BP	4	0	0	0	0
56	BQ	4	0	0	0	0
56	BR	3	0	0	0	0
56	BU	9	0	0	0	0
56	BV	3	0	0	0	0
56	BW	5	0	0	0	0
56	BX	2	0	0	0	0
56	BZ	1	0	0	0	0
56	CA	172	0	0	0	0
56	CE	2	0	0	0	0
56	CF	1	0	0	0	0
56	CN	1	0	0	0	0
56	CT	1	0	0	0	0
56	CX	3	0	0	0	0
56	D3	1	0	0	0	0
56	D5	2	0	0	0	0
56	D8	1	0	0	0	0
56	DA	657	0	0	0	0
56	DB	12	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	DD	5	0	0	0	0
56	DE	6	0	0	0	0
56	DF	5	0	0	0	0
56	DG	1	0	0	0	0
56	DN	1	0	0	0	0
56	DO	1	0	0	0	0
56	DP	2	0	0	0	0
56	DQ	4	0	0	0	0
56	DR	1	0	0	0	0
56	DU	2	0	0	0	0
56	DV	3	0	0	0	0
56	DW	2	0	0	0	0
56	DY	1	0	0	0	0
57	AD	8	0	0	1	0
57	CD	8	0	0	1	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	10	0	10	1	0
59	CX	10	0	10	2	0
60	BA	1	0	0	0	0
60	DA	1	0	0	0	0
61	AA	147	0	0	23	0
61	AD	1	0	0	0	0
61	AE	2	0	0	0	0
61	AJ	1	0	0	0	0
61	AL	2	0	0	0	0
61	AO	2	0	0	0	0
61	AU	1	0	0	1	0
61	AV	2	0	0	0	0
61	AX	1	0	0	0	0
61	B0	4	0	0	0	0
61	B1	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	B5	2	0	0	0	0
61	B7	1	0	0	1	0
61	B8	7	0	0	1	0
61	BA	1086	0	0	94	0
61	BB	26	0	0	2	0
61	BD	6	0	0	0	0
61	BE	13	0	0	3	0
61	BF	5	0	0	0	0
61	BG	1	0	0	0	0
61	BN	3	0	0	0	0
61	BO	2	0	0	0	0
61	BP	15	0	0	2	0
61	BQ	3	0	0	1	0
61	BR	1	0	0	0	0
61	BT	2	0	0	0	0
61	BU	5	0	0	0	0
61	BV	2	0	0	0	0
61	BW	4	0	0	0	0
61	BX	4	0	0	1	0
61	CA	186	0	0	24	0
61	CE	2	0	0	0	0
61	CN	1	0	0	0	0
61	CT	1	0	0	0	0
61	CX	2	0	0	0	0
61	D0	3	0	0	1	0
61	D1	1	0	0	0	0
61	D3	1	0	0	0	0
61	D7	1	0	0	0	0
61	D8	4	0	0	0	0
61	DA	906	0	0	116	0
61	DB	7	0	0	0	0
61	DD	10	0	0	0	0
61	DE	11	0	0	1	0
61	DF	4	0	0	0	0
61	DO	1	0	0	0	0
61	DP	14	0	0	2	0
61	DQ	3	0	0	1	0
61	DR	1	0	0	0	0
61	DU	4	0	0	0	0
61	DV	1	0	0	0	0
61	DX	2	0	0	1	0
61	DY	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	286321	0	191124	6684	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 15.

The worst 5 of 6684 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1129:C:N4	1:AA:1143:G:H1	1.46	1.12
1:CA:1002:G:H1	1:CA:1038:C:N4	1.48	1.09
1:AA:348:G:H2'	1:AA:349:A:H5'	1.30	1.06
2:AB:185:ILE:HG22	2:AB:199:TYR:HB2	1.39	1.04
2:CB:16:HIS:HB2	2:CB:204:ASN:HB3	1.36	1.03

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%)	201 (88%)	23 (10%)	5 (2%)	6	31
2	CB	229/256 (90%)	201 (88%)	21 (9%)	7 (3%)	4	23
3	AC	204/239 (85%)	182 (89%)	20 (10%)	2 (1%)	15	53
3	CC	204/239 (85%)	181 (89%)	21 (10%)	2 (1%)	15	53
4	AD	206/209 (99%)	184 (89%)	20 (10%)	2 (1%)	15	53
4	CD	206/209 (99%)	185 (90%)	18 (9%)	3 (2%)	10	42
5	AE	146/162 (90%)	136 (93%)	8 (6%)	2 (1%)	11	43
5	CE	146/162 (90%)	134 (92%)	12 (8%)	0	100	100
6	AF	98/101 (97%)	94 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	CF	98/101 (97%)	94 (96%)	4 (4%)	0	100	100
7	AG	153/156 (98%)	137 (90%)	15 (10%)	1 (1%)	22	60
7	CG	153/156 (98%)	139 (91%)	13 (8%)	1 (1%)	22	60
8	AH	135/138 (98%)	131 (97%)	4 (3%)	0	100	100
8	CH	135/138 (98%)	131 (97%)	3 (2%)	1 (1%)	22	60
9	AI	125/128 (98%)	112 (90%)	10 (8%)	3 (2%)	6	29
9	CI	125/128 (98%)	115 (92%)	8 (6%)	2 (2%)	9	40
10	AJ	95/105 (90%)	84 (88%)	8 (8%)	3 (3%)	4	22
10	CJ	94/105 (90%)	84 (89%)	8 (8%)	2 (2%)	7	33
11	AK	112/129 (87%)	101 (90%)	10 (9%)	1 (1%)	17	55
11	CK	112/129 (87%)	101 (90%)	10 (9%)	1 (1%)	17	55
12	AL	120/132 (91%)	117 (98%)	3 (2%)	0	100	100
12	CL	120/132 (91%)	113 (94%)	7 (6%)	0	100	100
13	AM	121/126 (96%)	113 (93%)	7 (6%)	1 (1%)	19	57
13	CM	120/126 (95%)	113 (94%)	6 (5%)	1 (1%)	19	57
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%)	80 (93%)	6 (7%)	0	100	100
15	CO	86/89 (97%)	81 (94%)	5 (6%)	0	100	100
16	AP	80/88 (91%)	74 (92%)	6 (8%)	0	100	100
16	CP	80/88 (91%)	73 (91%)	6 (8%)	1 (1%)	12	45
17	AQ	97/105 (92%)	92 (95%)	5 (5%)	0	100	100
17	CQ	97/105 (92%)	93 (96%)	4 (4%)	0	100	100
18	AR	66/88 (75%)	60 (91%)	5 (8%)	1 (2%)	10	42
18	CR	66/88 (75%)	61 (92%)	5 (8%)	0	100	100
19	AS	81/93 (87%)	76 (94%)	5 (6%)	0	100	100
19	CS	81/93 (87%)	74 (91%)	7 (9%)	0	100	100
20	AT	94/106 (89%)	84 (89%)	9 (10%)	1 (1%)	14	50
20	CT	94/106 (89%)	86 (92%)	5 (5%)	3 (3%)	4	22
21	AU	21/27 (78%)	17 (81%)	4 (19%)	0	100	100
21	CU	21/27 (78%)	18 (86%)	3 (14%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
24	AW	3/10 (30%)	0	2 (67%)	1 (33%)	0	0
24	CW	3/10 (30%)	1 (33%)	1 (33%)	1 (33%)	0	0
27	BD	273/276 (99%)	260 (95%)	12 (4%)	1 (0%)	34	72
27	DD	273/276 (99%)	258 (94%)	13 (5%)	2 (1%)	22	60
28	BE	202/206 (98%)	194 (96%)	7 (4%)	1 (0%)	29	68
28	DE	202/206 (98%)	195 (96%)	4 (2%)	3 (2%)	10	42
29	BF	201/210 (96%)	195 (97%)	5 (2%)	1 (0%)	29	68
29	DF	201/210 (96%)	195 (97%)	4 (2%)	2 (1%)	15	53
30	BG	179/182 (98%)	167 (93%)	9 (5%)	3 (2%)	9	39
30	DG	179/182 (98%)	161 (90%)	14 (8%)	4 (2%)	6	31
31	BH	172/180 (96%)	165 (96%)	6 (4%)	1 (1%)	25	64
31	DH	172/180 (96%)	164 (95%)	7 (4%)	1 (1%)	25	64
32	BI	144/148 (97%)	124 (86%)	14 (10%)	6 (4%)	3	16
32	DI	144/148 (97%)	124 (86%)	17 (12%)	3 (2%)	7	33
33	BN	138/140 (99%)	133 (96%)	5 (4%)	0	100	100
33	DN	138/140 (99%)	132 (96%)	5 (4%)	1 (1%)	22	60
34	BO	120/122 (98%)	116 (97%)	3 (2%)	1 (1%)	19	57
34	DO	120/122 (98%)	117 (98%)	2 (2%)	1 (1%)	19	57
35	BP	147/150 (98%)	138 (94%)	8 (5%)	1 (1%)	22	60
35	DP	147/150 (98%)	135 (92%)	9 (6%)	3 (2%)	7	34
36	BQ	139/141 (99%)	131 (94%)	7 (5%)	1 (1%)	22	60
36	DQ	139/141 (99%)	129 (93%)	9 (6%)	1 (1%)	22	60
37	BR	116/118 (98%)	110 (95%)	5 (4%)	1 (1%)	17	55
37	DR	116/118 (98%)	111 (96%)	5 (4%)	0	100	100
38	BS	108/112 (96%)	103 (95%)	4 (4%)	1 (1%)	17	55
38	DS	108/112 (96%)	102 (94%)	5 (5%)	1 (1%)	17	55
39	BT	129/146 (88%)	123 (95%)	6 (5%)	0	100	100
39	DT	129/146 (88%)	127 (98%)	2 (2%)	0	100	100
40	BU	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
40	DU	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
41	BV	99/101 (98%)	93 (94%)	5 (5%)	1 (1%)	15	53

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
41	DV	99/101 (98%)	94 (95%)	4 (4%)	1 (1%)	15	53
42	BW	110/113 (97%)	108 (98%)	2 (2%)	0	100	100
42	DW	110/113 (97%)	108 (98%)	2 (2%)	0	100	100
43	BX	93/96 (97%)	91 (98%)	2 (2%)	0	100	100
43	DX	93/96 (97%)	89 (96%)	4 (4%)	0	100	100
44	BY	105/110 (96%)	98 (93%)	7 (7%)	0	100	100
44	DY	105/110 (96%)	97 (92%)	8 (8%)	0	100	100
45	BZ	169/206 (82%)	150 (89%)	18 (11%)	1 (1%)	25	64
45	DZ	172/206 (84%)	162 (94%)	10 (6%)	0	100	100
46	B0	81/85 (95%)	76 (94%)	4 (5%)	1 (1%)	13	48
46	D0	81/85 (95%)	76 (94%)	4 (5%)	1 (1%)	13	48
47	B1	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	14	50
47	D1	95/98 (97%)	92 (97%)	2 (2%)	1 (1%)	14	50
48	B2	68/72 (94%)	68 (100%)	0	0	100	100
48	D2	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
49	B3	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
49	D3	57/60 (95%)	57 (100%)	0	0	100	100
50	B4	67/71 (94%)	53 (79%)	9 (13%)	5 (8%)	1	5
50	D4	67/71 (94%)	52 (78%)	8 (12%)	7 (10%)	0	2
51	B5	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
51	D5	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
52	B6	51/54 (94%)	48 (94%)	3 (6%)	0	100	100
52	D6	51/54 (94%)	47 (92%)	4 (8%)	0	100	100
53	B7	46/49 (94%)	46 (100%)	0	0	100	100
53	D7	46/49 (94%)	44 (96%)	1 (2%)	1 (2%)	6	31
54	B8	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
54	D8	62/65 (95%)	61 (98%)	1 (2%)	0	100	100
55	B9	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
55	D9	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
All	All	11415/12148 (94%)	10659 (93%)	648 (6%)	108 (1%)	17	55

5 of 108 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	125	PRO
3	AC	107	GLN
4	AD	166	LYS
9	AI	54	ASP
10	AJ	31	GLY

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%)	154 (80%)	38 (20%)	1	7
2	CB	187/220 (85%)	155 (83%)	32 (17%)	2	10
3	AC	143/188 (76%)	128 (90%)	15 (10%)	7	27
3	CC	140/188 (74%)	123 (88%)	17 (12%)	5	21
4	AD	170/181 (94%)	146 (86%)	24 (14%)	3	16
4	CD	173/181 (96%)	152 (88%)	21 (12%)	5	21
5	AE	113/123 (92%)	102 (90%)	11 (10%)	8	31
5	CE	114/123 (93%)	104 (91%)	10 (9%)	10	36
6	AF	83/90 (92%)	76 (92%)	7 (8%)	11	38
6	CF	85/90 (94%)	79 (93%)	6 (7%)	14	46
7	AG	119/127 (94%)	100 (84%)	19 (16%)	2	12
7	CG	120/127 (94%)	102 (85%)	18 (15%)	3	14
8	AH	114/119 (96%)	97 (85%)	17 (15%)	3	14
8	CH	114/119 (96%)	102 (90%)	12 (10%)	7	27
9	AI	90/99 (91%)	78 (87%)	12 (13%)	4	17
9	CI	89/99 (90%)	75 (84%)	14 (16%)	2	13
10	AJ	66/92 (72%)	59 (89%)	7 (11%)	6	26
10	CJ	69/92 (75%)	65 (94%)	4 (6%)	20	55
11	AK	82/99 (83%)	75 (92%)	7 (8%)	10	38
11	CK	83/99 (84%)	77 (93%)	6 (7%)	14	45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	AL	97/109 (89%)	87 (90%)	10 (10%)	7	28
12	CL	97/109 (89%)	83 (86%)	14 (14%)	3	15
13	AM	93/101 (92%)	81 (87%)	12 (13%)	4	19
13	CM	92/101 (91%)	78 (85%)	14 (15%)	3	14
14	AN	49/50 (98%)	41 (84%)	8 (16%)	2	11
14	CN	49/50 (98%)	41 (84%)	8 (16%)	2	11
15	AO	78/80 (98%)	68 (87%)	10 (13%)	4	19
15	CO	78/80 (98%)	66 (85%)	12 (15%)	2	13
16	AP	69/74 (93%)	61 (88%)	8 (12%)	5	23
16	CP	68/74 (92%)	64 (94%)	4 (6%)	19	54
17	AQ	94/97 (97%)	88 (94%)	6 (6%)	17	51
17	CQ	94/97 (97%)	86 (92%)	8 (8%)	10	38
18	AR	59/77 (77%)	56 (95%)	3 (5%)	24	60
18	CR	59/77 (77%)	53 (90%)	6 (10%)	7	28
19	AS	69/80 (86%)	63 (91%)	6 (9%)	10	37
19	CS	67/80 (84%)	59 (88%)	8 (12%)	5	22
20	AT	70/82 (85%)	60 (86%)	10 (14%)	3	15
20	CT	70/82 (85%)	61 (87%)	9 (13%)	4	19
21	AU	18/22 (82%)	15 (83%)	3 (17%)	2	11
21	CU	18/22 (82%)	16 (89%)	2 (11%)	6	25
24	AW	3/3 (100%)	2 (67%)	1 (33%)	0	1
24	CW	3/3 (100%)	2 (67%)	1 (33%)	0	1
27	BD	215/218 (99%)	193 (90%)	22 (10%)	7	28
27	DD	215/218 (99%)	195 (91%)	20 (9%)	9	33
28	BE	164/166 (99%)	140 (85%)	24 (15%)	3	15
28	DE	164/166 (99%)	140 (85%)	24 (15%)	3	15
29	BF	160/166 (96%)	145 (91%)	15 (9%)	8	32
29	DF	159/166 (96%)	142 (89%)	17 (11%)	6	26
30	BG	143/156 (92%)	124 (87%)	19 (13%)	4	17
30	DG	142/156 (91%)	117 (82%)	25 (18%)	2	10
31	BH	144/148 (97%)	128 (89%)	16 (11%)	6	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	DH	144/148 (97%)	131 (91%)	13 (9%)	9	35
32	BI	110/124 (89%)	85 (77%)	25 (23%)	1	4
32	DI	104/124 (84%)	90 (86%)	14 (14%)	4	17
33	BN	118/119 (99%)	100 (85%)	18 (15%)	2	13
33	DN	118/119 (99%)	102 (86%)	16 (14%)	3	17
34	BO	100/100 (100%)	95 (95%)	5 (5%)	24	60
34	DO	100/100 (100%)	92 (92%)	8 (8%)	12	40
35	BP	115/116 (99%)	103 (90%)	12 (10%)	7	27
35	DP	115/116 (99%)	102 (89%)	13 (11%)	6	24
36	BQ	111/111 (100%)	96 (86%)	15 (14%)	4	17
36	DQ	111/111 (100%)	97 (87%)	14 (13%)	4	20
37	BR	101/101 (100%)	83 (82%)	18 (18%)	2	9
37	DR	101/101 (100%)	84 (83%)	17 (17%)	2	11
38	BS	87/88 (99%)	78 (90%)	9 (10%)	7	28
38	DS	85/88 (97%)	73 (86%)	12 (14%)	3	16
39	BT	115/127 (91%)	103 (90%)	12 (10%)	7	27
39	DT	113/127 (89%)	103 (91%)	10 (9%)	10	36
40	BU	93/94 (99%)	85 (91%)	8 (9%)	10	37
40	DU	93/94 (99%)	79 (85%)	14 (15%)	3	14
41	BV	80/82 (98%)	68 (85%)	12 (15%)	3	14
41	DV	80/82 (98%)	70 (88%)	10 (12%)	4	20
42	BW	90/92 (98%)	83 (92%)	7 (8%)	12	42
42	DW	90/92 (98%)	82 (91%)	8 (9%)	9	35
43	BX	77/78 (99%)	74 (96%)	3 (4%)	32	69
43	DX	77/78 (99%)	73 (95%)	4 (5%)	23	59
44	BY	85/91 (93%)	76 (89%)	9 (11%)	6	26
44	DY	85/91 (93%)	77 (91%)	8 (9%)	8	32
45	BZ	145/179 (81%)	127 (88%)	18 (12%)	4	20
45	DZ	145/179 (81%)	128 (88%)	17 (12%)	5	22
46	B0	65/67 (97%)	62 (95%)	3 (5%)	27	64
46	D0	65/67 (97%)	60 (92%)	5 (8%)	13	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
47	B1	80/83 (96%)	70 (88%)	10 (12%)	4	20
47	D1	80/83 (96%)	69 (86%)	11 (14%)	3	17
48	B2	65/67 (97%)	56 (86%)	9 (14%)	3	17
48	D2	65/67 (97%)	57 (88%)	8 (12%)	4	21
49	B3	51/52 (98%)	44 (86%)	7 (14%)	3	17
49	D3	50/52 (96%)	42 (84%)	8 (16%)	2	12
50	B4	59/63 (94%)	47 (80%)	12 (20%)	1	6
50	D4	53/63 (84%)	44 (83%)	9 (17%)	2	10
51	B5	50/52 (96%)	45 (90%)	5 (10%)	7	29
51	D5	50/52 (96%)	45 (90%)	5 (10%)	7	29
52	B6	51/52 (98%)	47 (92%)	4 (8%)	12	42
52	D6	50/52 (96%)	43 (86%)	7 (14%)	3	16
53	B7	41/42 (98%)	39 (95%)	2 (5%)	25	61
53	D7	41/42 (98%)	38 (93%)	3 (7%)	14	44
54	B8	53/55 (96%)	50 (94%)	3 (6%)	20	56
54	D8	54/55 (98%)	52 (96%)	2 (4%)	34	70
55	B9	34/34 (100%)	33 (97%)	1 (3%)	42	76
55	D9	34/34 (100%)	31 (91%)	3 (9%)	10	36
All	All	9325/10072 (93%)	8217 (88%)	1108 (12%)	5	22

5 of 1108 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
35	DP	65	ARG
37	DR	36	THR
35	DP	55	ARG
45	DZ	131	ARG
35	BP	135	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 115 such sidechains are listed below:

Mol	Chain	Res	Type
55	B9	36	GLN
44	DY	43	ASN
5	CE	141	GLN

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Mol	Chain	Res	Type
43	DX	31	HIS
32	DI	133	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1495/1522 (98%)	421 (28%)	24 (1%)
1	CA	1501/1522 (98%)	421 (28%)	30 (1%)
22	AV	4/24 (16%)	1 (25%)	0
22	CV	4/24 (16%)	1 (25%)	0
23	AX	75/77 (97%)	18 (24%)	0
23	CX	75/77 (97%)	19 (25%)	0
25	BA	2722/2915 (93%)	527 (19%)	41 (1%)
25	DA	2704/2915 (92%)	526 (19%)	35 (1%)
26	BB	119/122 (97%)	21 (17%)	0
26	DB	119/122 (97%)	23 (19%)	1 (0%)
All	All	8818/9320 (94%)	1978 (22%)	131 (1%)

5 of 1978 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	7	G
1	AA	9	G
1	AA	15	G
1	AA	16	A
1	AA	22	G

5 of 131 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	DA	1427	A
25	DA	1608	A
26	DB	45	A
25	BA	1466	U
25	BA	1321	A

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

14 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	$\#\|Z\|>2$
24	MVA	AW	5	24	6,7,8	0.57	0	7,8,10	1.61	1 (14%)
24	2QZ	CW	1	24	7,8,9	0.79	0	8,10,12	3.63	3 (37%)
24	2R1	AW	6	24	10,10,11	2.03	4 (40%)	6,13,15	4.80	2 (33%)
24	004	AW	3	24	9,10,11	1.09	1 (11%)	9,12,14	1.05	0
24	004	CW	3	24	9,10,11	1.24	1 (11%)	9,12,14	0.77	0
24	MVA	CW	9	24	6,7,8	0.88	0	7,8,10	1.00	0
24	2QY	CW	10	24	12,13,14	2.26	2 (16%)	13,16,18	3.21	2 (15%)
24	2R3	CW	8	24	12,14,15	0.66	0	16,18,20	2.17	5 (31%)
24	2R1	CW	6	24	10,10,11	1.77	3 (30%)	6,13,15	4.10	2 (33%)
24	2R3	AW	8	24	12,14,15	0.78	0	16,18,20	2.05	6 (37%)
24	2QY	AW	10	24	12,13,14	2.14	2 (16%)	13,16,18	3.12	4 (30%)
24	2QZ	AW	1	24	7,8,9	0.42	0	8,10,12	2.37	1 (12%)
24	MVA	AW	9	24	6,7,8	0.38	0	7,8,10	0.86	1 (14%)
24	MVA	CW	5	24	6,7,8	0.79	0	7,8,10	1.44	2 (28%)

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
24	MVA	AW	5	24	-	2/6/8/10	-
24	2QZ	CW	1	24	-	1/6/10/12	-
24	2R1	AW	6	24	-	1/2/14/16	0/1/1/1
24	004	AW	3	24	-	1/4/6/8	0/1/1/1
24	004	CW	3	24	-	0/4/6/8	0/1/1/1
24	MVA	CW	9	24	-	5/6/8/10	-
24	2QY	CW	10	24	-	1/4/8/10	0/1/1/1
24	2R3	CW	8	24	-	6/11/12/14	0/1/1/1
24	2R1	CW	6	24	-	1/2/14/16	0/1/1/1
24	2R3	AW	8	24	-	6/11/12/14	0/1/1/1
24	2QY	AW	10	24	-	3/4/8/10	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	2QZ	AW	1	24	-	3/6/10/12	-
24	MVA	AW	9	24	-	5/6/8/10	-
24	MVA	CW	5	24	-	5/6/8/10	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	CW	10	2QY	C-CA	7.00	1.53	1.43
24	AW	10	2QY	C-CA	6.63	1.53	1.43
24	AW	6	2R1	CA-N	3.98	1.46	1.36
24	CW	6	2R1	CA-N	3.70	1.45	1.36
24	CW	3	004	CB-CA	-3.18	1.49	1.52

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	AW	6	2R1	OD2-CG2-CB	-11.05	92.15	112.24
24	CW	10	2QY	CN-N-CA	-9.39	109.17	123.45
24	AW	10	2QY	CN-N-CA	-9.29	109.33	123.45
24	CW	1	2QZ	OG1-CB-CG2	9.27	137.20	109.74
24	CW	6	2R1	OD2-CG2-CB	-9.26	95.40	112.24

There are no chirality outliers.

5 of 40 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	AW	1	2QZ	N-CA-CB-OG1
24	AW	1	2QZ	N-CA-CB-CG2
24	AW	5	MVA	CB-CA-N-CN
24	AW	8	2R3	N-CA-CB-OB
24	AW	8	2R3	N-CA-CB-CG

There are no ring outliers.

14 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	AW	5	MVA	1	0
24	CW	1	2QZ	3	0
24	AW	6	2R1	3	0
24	AW	3	004	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	CW	3	004	1	0
24	CW	9	MVA	3	0
24	CW	10	2QY	4	0
24	CW	8	2R3	2	0
24	CW	6	2R1	1	0
24	AW	8	2R3	4	0
24	AW	10	2QY	3	0
24	AW	1	2QZ	2	0
24	AW	9	MVA	3	0
24	CW	5	MVA	1	0

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 1991 ligands modelled in this entry, 1987 are monoatomic - leaving 4 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	$\#\|Z\| > 2$
59	FME	CX	101	23	8,9,10	0.87	0	7,9,11	1.38	1 (14%)
57	SF4	AD	501	4	0,12,12	-	-	-		
59	FME	AX	101	23	8,9,10	1.01	1 (12%)	7,9,11	1.33	1 (14%)
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
59	FME	CX	101	23	-	1/7/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	SF4	AD	501	4	-	-	0/6/5/5
59	FME	AX	101	23	-	2/7/9/11	-
57	SF4	CD	501	4	-	-	0/6/5/5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	AX	101	FME	CA-N	2.16	1.49	1.46

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	AX	101	FME	CA-N-CN	-2.47	119.03	122.82
59	CX	101	FME	CA-N-CN	-2.33	119.25	122.82

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
59	AX	101	FME	O1-CN-N-CA
59	CX	101	FME	O1-CN-N-CA
59	AX	101	FME	CB-CG-SD-CE

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
59	CX	101	FME	2	0
57	AD	501	SF4	1	0
59	AX	101	FME	1	0
57	CD	501	SF4	1	0

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	1498/1522 (98%)	-0.06	45 (3%)	50	22	39, 80, 103, 118	0
1	CA	1503/1522 (98%)	-0.11	38 (2%)	57	29	41, 80, 103, 119	0
2	AB	231/256 (90%)	-0.03	6 (2%)	56	27	69, 86, 97, 105	0
2	CB	231/256 (90%)	0.20	10 (4%)	35	13	70, 88, 98, 107	0
3	AC	206/239 (86%)	0.20	8 (3%)	39	15	73, 87, 95, 104	0
3	CC	206/239 (86%)	0.34	13 (6%)	20	6	72, 89, 97, 104	0
4	AD	208/209 (99%)	-0.07	4 (1%)	66	37	61, 80, 90, 97	0
4	CD	208/209 (99%)	-0.22	0	100	100	61, 79, 89, 97	0
5	AE	148/162 (91%)	-0.34	0	100	100	51, 73, 82, 93	0
5	CE	148/162 (91%)	-0.28	0	100	100	53, 75, 84, 96	0
6	AF	100/101 (99%)	-0.29	0	100	100	63, 77, 87, 94	0
6	CF	100/101 (99%)	-0.39	0	100	100	62, 78, 87, 95	0
7	AG	155/156 (99%)	0.38	12 (7%)	13	4	74, 86, 99, 106	0
7	CG	155/156 (99%)	0.46	16 (10%)	6	2	75, 86, 99, 105	0
8	AH	137/138 (99%)	-0.11	0	100	100	60, 74, 82, 89	0
8	CH	137/138 (99%)	-0.15	0	100	100	62, 75, 83, 89	0
9	AI	127/128 (99%)	0.44	8 (6%)	20	6	73, 91, 99, 101	0
9	CI	127/128 (99%)	1.08	31 (24%)	0	0	72, 93, 100, 102	0
10	AJ	97/105 (92%)	0.72	11 (11%)	5	1	73, 91, 100, 105	0
10	CJ	96/105 (91%)	0.98	19 (19%)	1	0	77, 93, 100, 104	0
11	AK	114/129 (88%)	-0.28	0	100	100	53, 74, 87, 91	0
11	CK	114/129 (88%)	0.02	1 (0%)	84	63	55, 76, 87, 92	0
12	AL	122/132 (92%)	-0.26	0	100	100	53, 68, 80, 87	0
12	CL	122/132 (92%)	-0.22	0	100	100	53, 69, 80, 87	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
13	AM	123/126 (97%)	0.35	9 (7%)	15	4	67, 85, 95, 105	0
13	CM	122/126 (96%)	0.54	6 (4%)	29	11	77, 92, 100, 109	0
14	AN	60/61 (98%)	0.11	1 (1%)	70	41	75, 87, 94, 103	0
14	CN	60/61 (98%)	0.78	6 (10%)	7	2	77, 89, 94, 100	0
15	AO	88/89 (98%)	-0.18	0	100	100	55, 72, 85, 90	0
15	CO	88/89 (98%)	-0.15	0	100	100	55, 72, 85, 91	0
16	AP	82/88 (93%)	0.47	1 (1%)	79	54	67, 78, 89, 94	0
16	CP	82/88 (93%)	0.18	3 (3%)	41	17	66, 76, 88, 94	0
17	AQ	99/105 (94%)	-0.25	0	100	100	59, 72, 83, 90	0
17	CQ	99/105 (94%)	-0.15	1 (1%)	82	59	58, 72, 83, 89	0
18	AR	68/88 (77%)	0.16	2 (2%)	51	23	65, 73, 87, 91	0
18	CR	68/88 (77%)	0.24	1 (1%)	73	46	64, 75, 87, 91	0
19	AS	83/93 (89%)	0.94	14 (16%)	1	0	77, 92, 99, 106	0
19	CS	83/93 (89%)	1.14	12 (14%)	2	1	79, 92, 101, 106	0
20	AT	96/106 (90%)	0.10	2 (2%)	63	34	62, 76, 86, 90	0
20	CT	96/106 (90%)	0.11	1 (1%)	82	59	62, 74, 86, 92	0
21	AU	23/27 (85%)	1.37	5 (21%)	0	0	73, 88, 93, 94	0
21	CU	23/27 (85%)	1.48	9 (39%)	0	0	73, 89, 92, 94	0
22	AV	7/24 (29%)	0.60	0	100	100	65, 77, 102, 104	0
22	CV	6/24 (25%)	0.79	1 (16%)	1	0	67, 78, 103, 103	0
23	AX	76/77 (98%)	0.47	2 (2%)	56	27	52, 80, 97, 105	0
23	CX	76/77 (98%)	0.35	3 (3%)	39	15	52, 82, 100, 106	0
24	AW	3/10 (30%)	-0.30	0	100	100	67, 67, 82, 98	0
24	CW	3/10 (30%)	-0.44	0	100	100	67, 67, 78, 82	0
25	BA	2731/2915 (93%)	-0.24	13 (0%)	91	75	23, 44, 85, 111	0
25	DA	2714/2915 (93%)	-0.45	18 (0%)	87	69	26, 47, 85, 118	0
26	BB	120/122 (98%)	-0.37	0	100	100	42, 68, 80, 95	0
26	DB	120/122 (98%)	-0.26	0	100	100	48, 74, 84, 97	0
27	BD	275/276 (99%)	-0.48	0	100	100	22, 42, 58, 77	0
27	DD	275/276 (99%)	-0.53	0	100	100	23, 44, 60, 79	0
28	BE	204/206 (99%)	-0.39	0	100	100	23, 45, 67, 88	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
28	DE	204/206 (99%)	-0.47	0 100 100	24, 47, 70, 88	0
29	BF	203/210 (96%)	-0.36	0 100 100	20, 51, 77, 94	0
29	DF	203/210 (96%)	-0.50	1 (0%) 91 75	22, 54, 78, 93	0
30	BG	181/182 (99%)	-0.35	1 (0%) 89 72	59, 77, 90, 103	0
30	DG	181/182 (99%)	0.13	9 (4%) 28 10	63, 80, 92, 102	0
31	BH	174/180 (96%)	-0.37	0 100 100	50, 66, 78, 84	0
31	DH	174/180 (96%)	0.29	13 (7%) 14 4	54, 71, 82, 87	0
32	BI	146/148 (98%)	-0.36	0 100 100	45, 75, 87, 92	0
32	DI	146/148 (98%)	0.04	3 (2%) 63 34	48, 76, 86, 91	0
33	BN	140/140 (100%)	-0.43	0 100 100	32, 49, 68, 80	0
33	DN	140/140 (100%)	-0.48	0 100 100	34, 53, 72, 81	0
34	BO	122/122 (100%)	-0.50	0 100 100	25, 39, 60, 78	0
34	DO	122/122 (100%)	-0.49	0 100 100	34, 52, 68, 79	0
35	BP	149/150 (99%)	-0.35	0 100 100	26, 54, 76, 84	0
35	DP	149/150 (99%)	-0.18	0 100 100	30, 57, 79, 86	0
36	BQ	141/141 (100%)	-0.36	0 100 100	33, 51, 65, 79	0
36	DQ	141/141 (100%)	-0.46	0 100 100	35, 54, 70, 80	0
37	BR	118/118 (100%)	-0.54	0 100 100	22, 35, 51, 64	0
37	DR	118/118 (100%)	-0.42	0 100 100	36, 50, 64, 80	0
38	BS	110/112 (98%)	-0.34	0 100 100	38, 55, 69, 81	0
38	DS	110/112 (98%)	0.15	1 (0%) 84 63	66, 78, 90, 100	0
39	BT	131/146 (89%)	-0.48	0 100 100	33, 45, 75, 91	0
39	DT	131/146 (89%)	-0.53	0 100 100	44, 56, 80, 86	0
40	BU	116/118 (98%)	-0.64	0 100 100	19, 30, 50, 63	0
40	DU	116/118 (98%)	-0.36	1 (0%) 84 63	39, 61, 79, 88	0
41	BV	101/101 (100%)	-0.39	0 100 100	29, 52, 70, 77	0
41	DV	101/101 (100%)	-0.18	0 100 100	32, 58, 74, 79	0
42	BW	112/113 (99%)	-0.49	1 (0%) 84 63	27, 37, 61, 94	0
42	DW	112/113 (99%)	-0.44	0 100 100	31, 40, 63, 94	0
43	BX	95/96 (98%)	-0.41	0 100 100	32, 46, 69, 82	0
43	DX	95/96 (98%)	-0.33	1 (1%) 80 56	38, 50, 72, 83	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
44	BY	107/110 (97%)	-0.29	1 (0%)	84	63	44, 59, 77, 82	0
44	DY	107/110 (97%)	0.24	3 (2%)	53	25	46, 63, 80, 85	0
45	BZ	171/206 (83%)	-0.45	0	100	100	52, 71, 85, 93	0
45	DZ	174/206 (84%)	-0.17	0	100	100	56, 74, 87, 95	0
46	B0	83/85 (97%)	-0.16	7 (8%)	11	3	22, 40, 75, 104	0
46	D0	83/85 (97%)	0.19	5 (6%)	21	7	45, 66, 87, 98	0
47	B1	97/98 (98%)	-0.26	1 (1%)	82	59	25, 42, 71, 77	0
47	D1	97/98 (98%)	-0.25	1 (1%)	82	59	35, 56, 79, 85	0
48	B2	70/72 (97%)	-0.52	0	100	100	31, 48, 64, 77	0
48	D2	70/72 (97%)	-0.35	0	100	100	56, 73, 84, 86	0
49	B3	59/60 (98%)	-0.33	0	100	100	26, 38, 63, 86	0
49	D3	59/60 (98%)	0.02	2 (3%)	45	19	49, 62, 80, 93	0
50	B4	69/71 (97%)	-0.03	1 (1%)	75	49	64, 87, 101, 104	0
50	D4	69/71 (97%)	0.51	4 (5%)	23	7	85, 95, 104, 107	0
51	B5	59/60 (98%)	-0.61	0	100	100	14, 35, 55, 71	0
51	D5	59/60 (98%)	-0.55	0	100	100	29, 51, 70, 77	0
52	B6	53/54 (98%)	-0.37	0	100	100	40, 54, 68, 74	0
52	D6	53/54 (98%)	-0.39	0	100	100	42, 58, 68, 74	0
53	B7	48/49 (97%)	-0.28	0	100	100	26, 32, 67, 78	0
53	D7	48/49 (97%)	-0.18	1 (2%)	63	34	27, 34, 66, 79	0
54	B8	64/65 (98%)	-0.34	0	100	100	33, 43, 51, 56	0
54	D8	64/65 (98%)	-0.29	0	100	100	34, 46, 56, 60	0
55	B9	37/37 (100%)	0.09	0	100	100	43, 52, 68, 77	0
55	D9	37/37 (100%)	0.84	5 (13%)	3	1	48, 57, 72, 78	0
All	All	20462/21468 (95%)	-0.17	394 (1%)	66	37	14, 65, 95, 119	0

The worst 5 of 394 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	CM	124	PRO	15.8
13	CM	123	ALA	11.8
13	AM	123	ALA	8.8
13	AM	124	PRO	7.8
7	CG	78	ARG	7.3

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\AA^2$)	Q<0.9
24	2R1	AW	6	10/11	0.91	0.14	66,72,84,91	0
24	2R3	AW	8	14/15	0.92	0.24	70,78,86,87	0
24	MVA	AW	5	8/9	0.92	0.19	69,82,86,91	0
24	2R1	CW	6	10/11	0.92	0.13	68,82,90,91	0
24	2QY	CW	10	13/14	0.92	0.16	60,72,80,86	0
24	004	AW	3	10/11	0.93	0.11	67,87,95,97	0
24	MVA	CW	9	8/9	0.94	0.22	70,73,84,91	0
24	MVA	CW	5	8/9	0.95	0.21	76,88,91,99	0
24	2QZ	AW	1	9/10	0.95	0.23	50,71,82,83	0
24	2R3	CW	8	14/15	0.96	0.14	62,69,77,78	0
24	2QY	AW	10	13/14	0.96	0.14	49,70,87,100	0
24	MVA	AW	9	8/9	0.96	0.28	63,74,87,88	0
24	2QZ	CW	1	9/10	0.97	0.27	63,71,80,101	0
24	004	CW	3	10/11	0.97	0.16	69,78,82,83	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\AA^2$)	Q<0.9
56	MG	CA	3147	1/1	0.27	0.37	77,77,77,77	0
56	MG	AA	3086	1/1	0.28	0.72	65,65,65,65	0
56	MG	CA	3053	1/1	0.41	1.38	87,87,87,87	0
56	MG	BA	3625	1/1	0.49	0.48	80,80,80,80	0
56	MG	BA	3252	1/1	0.51	0.59	65,65,65,65	0
56	MG	BA	3296	1/1	0.52	0.67	69,69,69,69	0
56	MG	AS	3001	1/1	0.56	0.17	79,79,79,79	0
56	MG	AA	3131	1/1	0.57	0.38	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DA	3064	1/1	0.61	0.43	55,55,55,55	0
56	MG	CA	3039	1/1	0.62	0.51	82,82,82,82	0
56	MG	CA	3065	1/1	0.63	0.33	81,81,81,81	0
56	MG	BA	3616	1/1	0.63	0.27	73,73,73,73	0
56	MG	BA	3143	1/1	0.63	0.82	41,41,41,41	0
56	MG	AA	3124	1/1	0.64	0.20	61,61,61,61	0
56	MG	BF	306	1/1	0.65	0.41	52,52,52,52	0
56	MG	DA	3568	1/1	0.65	0.43	58,58,58,58	0
56	MG	BA	3582	1/1	0.66	0.23	52,52,52,52	0
56	MG	AA	3093	1/1	0.66	0.39	90,90,90,90	0
56	MG	DA	3314	1/1	0.67	0.19	56,56,56,56	0
56	MG	DA	3113	1/1	0.67	1.16	61,61,61,61	0
56	MG	AA	3002	1/1	0.68	0.20	74,74,74,74	0
56	MG	BA	3021	1/1	0.68	0.36	62,62,62,62	0
56	MG	DA	3496	1/1	0.68	0.34	76,76,76,76	0
56	MG	BA	3103	1/1	0.68	0.33	58,58,58,58	0
56	MG	BA	3230	1/1	0.69	1.02	70,70,70,70	0
56	MG	AA	3079	1/1	0.69	0.91	65,65,65,65	0
56	MG	CA	3070	1/1	0.69	0.35	59,59,59,59	0
56	MG	DW	202	1/1	0.69	0.39	53,53,53,53	0
56	MG	CA	3016	1/1	0.70	0.43	72,72,72,72	0
56	MG	BA	3022	1/1	0.70	0.16	66,66,66,66	0
56	MG	CA	3161	1/1	0.70	0.20	71,71,71,71	0
56	MG	BA	3223	1/1	0.71	0.39	49,49,49,49	0
56	MG	CA	3071	1/1	0.71	0.12	64,64,64,64	0
56	MG	AA	3001	1/1	0.71	0.26	74,74,74,74	0
56	MG	DA	3135	1/1	0.71	0.31	58,58,58,58	0
56	MG	AA	3015	1/1	0.72	0.24	74,74,74,74	0
56	MG	BA	3185	1/1	0.72	0.22	40,40,40,40	0
56	MG	DA	3356	1/1	0.72	0.45	57,57,57,57	0
56	MG	DA	3024	1/1	0.72	0.61	59,59,59,59	0
56	MG	AA	3038	1/1	0.72	0.45	64,64,64,64	0
56	MG	DB	3006	1/1	0.72	0.17	54,54,54,54	0
56	MG	DQ	3004	1/1	0.72	0.20	52,52,52,52	0
56	MG	AA	3076	1/1	0.72	0.38	74,74,74,74	0
56	MG	DA	3122	1/1	0.73	0.14	60,60,60,60	0
56	MG	DA	3500	1/1	0.73	0.25	66,66,66,66	0
56	MG	AA	3114	1/1	0.73	0.18	73,73,73,73	0
56	MG	AA	3032	1/1	0.74	0.29	65,65,65,65	0
56	MG	AA	3045	1/1	0.74	0.23	71,71,71,71	0
56	MG	DA	3008	1/1	0.74	0.27	56,56,56,56	0
56	MG	AA	3130	1/1	0.74	0.19	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	AX	102	1/1	0.75	0.14	66,66,66,66	0
56	MG	BA	3178	1/1	0.75	0.50	51,51,51,51	0
56	MG	BA	3292	1/1	0.75	0.22	59,59,59,59	0
56	MG	DA	3096	1/1	0.75	0.34	68,68,68,68	0
56	MG	DA	3109	1/1	0.75	0.26	55,55,55,55	0
56	MG	AA	3067	1/1	0.75	0.36	76,76,76,76	0
56	MG	CA	3018	1/1	0.75	0.30	55,55,55,55	0
56	MG	BA	3139	1/1	0.75	0.74	50,50,50,50	0
58	ZN	B4	501	1/1	0.75	0.09	152,152,152,152	0
56	MG	CA	3144	1/1	0.76	0.96	84,84,84,84	0
56	MG	DA	3131	1/1	0.76	0.23	60,60,60,60	0
56	MG	AA	3030	1/1	0.76	0.63	66,66,66,66	0
56	MG	AA	3089	1/1	0.76	0.33	80,80,80,80	0
56	MG	CA	3033	1/1	0.76	0.18	64,64,64,64	0
56	MG	DA	3423	1/1	0.76	0.18	29,29,29,29	0
56	MG	DA	3441	1/1	0.76	0.20	46,46,46,46	0
56	MG	DA	3456	1/1	0.76	0.20	58,58,58,58	0
56	MG	DA	3011	1/1	0.76	0.35	42,42,42,42	0
56	MG	BA	3538	1/1	0.76	0.20	29,29,29,29	0
56	MG	AA	3128	1/1	0.76	0.15	64,64,64,64	0
56	MG	DA	3087	1/1	0.76	0.24	43,43,43,43	0
56	MG	AA	3072	1/1	0.76	0.24	69,69,69,69	0
56	MG	AA	3094	1/1	0.76	0.25	78,78,78,78	0
56	MG	AA	3180	1/1	0.76	0.47	75,75,75,75	0
56	MG	BA	3708	1/1	0.77	0.29	38,38,38,38	0
56	MG	DA	3591	1/1	0.77	0.14	67,67,67,67	0
56	MG	CA	3032	1/1	0.77	0.20	44,44,44,44	0
56	MG	DA	3163	1/1	0.77	0.20	52,52,52,52	0
56	MG	BA	3239	1/1	0.77	0.21	33,33,33,33	0
56	MG	AA	3218	1/1	0.77	0.21	73,73,73,73	0
56	MG	CA	3034	1/1	0.78	0.28	66,66,66,66	0
56	MG	BA	3740	1/1	0.78	1.13	57,57,57,57	0
56	MG	DA	3373	1/1	0.78	0.28	52,52,52,52	0
56	MG	BB	3004	1/1	0.78	0.27	57,57,57,57	0
56	MG	BD	311	1/1	0.78	0.84	53,53,53,53	0
56	MG	BA	3154	1/1	0.78	0.40	55,55,55,55	0
56	MG	DA	3464	1/1	0.78	0.20	51,51,51,51	0
56	MG	BA	3157	1/1	0.78	0.31	52,52,52,52	0
56	MG	CA	3074	1/1	0.78	0.24	56,56,56,56	0
56	MG	CA	3110	1/1	0.78	0.13	93,93,93,93	0
56	MG	CA	3114	1/1	0.78	0.19	67,67,67,67	0
56	MG	BA	3126	1/1	0.78	0.34	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	AX	105	1/1	0.78	0.47	72,72,72,72	0
56	MG	AA	3129	1/1	0.78	0.22	77,77,77,77	0
56	MG	DA	3241	1/1	0.78	0.10	74,74,74,74	0
56	MG	DA	3155	1/1	0.79	0.28	50,50,50,50	0
56	MG	BZ	3001	1/1	0.79	0.19	47,47,47,47	0
56	MG	DA	3170	1/1	0.79	0.24	45,45,45,45	0
56	MG	DA	3212	1/1	0.79	0.07	48,48,48,48	0
56	MG	CA	3127	1/1	0.79	0.20	72,72,72,72	0
56	MG	DA	3263	1/1	0.79	0.14	48,48,48,48	0
56	MG	DA	3295	1/1	0.79	0.23	31,31,31,31	0
56	MG	CA	3139	1/1	0.79	0.24	76,76,76,76	0
56	MG	BA	3098	1/1	0.79	0.25	42,42,42,42	0
56	MG	AA	3025	1/1	0.79	0.13	78,78,78,78	0
56	MG	AA	3029	1/1	0.79	1.02	60,60,60,60	0
56	MG	DA	3431	1/1	0.79	0.40	56,56,56,56	0
56	MG	BA	3137	1/1	0.79	0.20	59,59,59,59	0
56	MG	BA	3697	1/1	0.79	0.19	63,63,63,63	0
56	MG	AA	3147	1/1	0.79	0.41	51,51,51,51	0
56	MG	AX	108	1/1	0.79	0.14	66,66,66,66	0
56	MG	CA	3054	1/1	0.79	0.41	74,74,74,74	0
56	MG	DA	3549	1/1	0.79	0.37	73,73,73,73	0
56	MG	CA	3056	1/1	0.79	0.18	63,63,63,63	0
56	MG	AA	3009	1/1	0.79	0.22	71,71,71,71	0
56	MG	BB	3005	1/1	0.79	0.19	62,62,62,62	0
56	MG	AA	3065	1/1	0.79	0.25	50,50,50,50	0
56	MG	BA	3409	1/1	0.79	0.17	40,40,40,40	0
56	MG	BQ	3002	1/1	0.79	0.23	51,51,51,51	0
56	MG	AA	3120	1/1	0.80	0.44	53,53,53,53	0
56	MG	AA	3148	1/1	0.80	0.24	72,72,72,72	0
56	MG	CA	3027	1/1	0.80	0.27	64,64,64,64	0
56	MG	BA	3004	1/1	0.80	0.22	45,45,45,45	0
56	MG	BA	3530	1/1	0.80	0.23	72,72,72,72	0
56	MG	BA	3018	1/1	0.80	0.27	54,54,54,54	0
56	MG	AA	3115	1/1	0.80	0.19	67,67,67,67	0
56	MG	DA	3491	1/1	0.80	0.27	55,55,55,55	0
56	MG	DA	3141	1/1	0.80	0.19	63,63,63,63	0
56	MG	CA	3041	1/1	0.80	0.39	71,71,71,71	0
56	MG	CA	3042	1/1	0.80	0.28	69,69,69,69	0
56	MG	BA	3259	1/1	0.80	0.22	59,59,59,59	0
56	MG	CX	103	1/1	0.80	0.23	57,57,57,57	0
56	MG	BG	3002	1/1	0.80	0.11	51,51,51,51	0
56	MG	BA	3283	1/1	0.80	0.18	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
56	MG	CA	3063	1/1	0.80	0.12	57,57,57,57	0
56	MG	BA	3661	1/1	0.80	0.27	69,69,69,69	0
59	FME	CX	101	10/11	0.80	0.43	59,80,100,106	0
56	MG	BA	3188	1/1	0.81	0.29	49,49,49,49	0
56	MG	BA	3291	1/1	0.81	0.15	44,44,44,44	0
56	MG	BA	3155	1/1	0.81	0.46	56,56,56,56	0
56	MG	BB	3017	1/1	0.81	0.20	80,80,80,80	0
56	MG	DA	3053	1/1	0.81	0.19	47,47,47,47	0
56	MG	BA	3606	1/1	0.81	0.10	44,44,44,44	0
56	MG	DA	3531	1/1	0.81	0.12	44,44,44,44	0
56	MG	BA	3257	1/1	0.81	0.25	56,56,56,56	0
56	MG	DA	3557	1/1	0.81	0.26	74,74,74,74	0
56	MG	BA	3313	1/1	0.81	0.12	56,56,56,56	0
56	MG	BA	3358	1/1	0.81	0.15	78,78,78,78	0
56	MG	DB	3003	1/1	0.81	0.20	70,70,70,70	0
56	MG	DA	3346	1/1	0.81	0.20	64,64,64,64	0
56	MG	BA	3694	1/1	0.81	0.27	48,48,48,48	0
56	MG	BA	3405	1/1	0.81	0.25	57,57,57,57	0
56	MG	AA	3022	1/1	0.81	0.24	56,56,56,56	0
56	MG	CA	3167	1/1	0.81	0.08	68,68,68,68	0
56	MG	DA	3153	1/1	0.82	0.32	51,51,51,51	0
56	MG	BA	3307	1/1	0.82	0.16	35,35,35,35	0
56	MG	DA	3012	1/1	0.82	0.39	52,52,52,52	0
56	MG	AA	3084	1/1	0.82	0.32	71,71,71,71	0
56	MG	DA	3203	1/1	0.82	0.14	48,48,48,48	0
56	MG	AA	3135	1/1	0.82	0.31	49,49,49,49	0
56	MG	DA	3214	1/1	0.82	0.09	48,48,48,48	0
56	MG	DA	3232	1/1	0.82	0.12	39,39,39,39	0
56	MG	AA	3140	1/1	0.82	0.12	65,65,65,65	0
56	MG	BA	3674	1/1	0.82	0.30	67,67,67,67	0
56	MG	AA	3222	1/1	0.82	0.14	64,64,64,64	0
56	MG	DA	3596	1/1	0.82	0.13	68,68,68,68	0
56	MG	DA	3642	1/1	0.82	0.18	67,67,67,67	0
56	MG	BA	3485	1/1	0.82	0.19	67,67,67,67	0
56	MG	CA	3152	1/1	0.82	0.32	45,45,45,45	0
56	MG	DD	302	1/1	0.82	0.61	48,48,48,48	0
56	MG	BA	3107	1/1	0.82	0.15	60,60,60,60	0
56	MG	AA	3077	1/1	0.82	0.39	67,67,67,67	0
56	MG	BA	3248	1/1	0.82	0.37	68,68,68,68	0
56	MG	BA	3601	1/1	0.82	0.19	61,61,61,61	0
56	MG	BA	3006	1/1	0.83	0.27	46,46,46,46	0
56	MG	AA	3051	1/1	0.83	0.16	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	CA	3162	1/1	0.83	0.25	60,60,60,60	0
56	MG	DA	3296	1/1	0.83	0.46	65,65,65,65	0
56	MG	BA	3302	1/1	0.83	0.26	48,48,48,48	0
56	MG	DA	3068	1/1	0.83	0.22	52,52,52,52	0
56	MG	CA	3172	1/1	0.83	0.22	65,65,65,65	0
56	MG	DA	3603	1/1	0.83	0.23	66,66,66,66	0
56	MG	DA	3089	1/1	0.83	0.27	51,51,51,51	0
56	MG	BA	3163	1/1	0.83	0.37	50,50,50,50	0
56	MG	DA	3171	1/1	0.83	0.89	58,58,58,58	0
56	MG	DA	3098	1/1	0.83	1.02	45,45,45,45	0
56	MG	DA	3100	1/1	0.83	0.63	55,55,55,55	0
56	MG	DU	3001	1/1	0.83	0.90	61,61,61,61	0
56	MG	CA	3073	1/1	0.83	0.51	74,74,74,74	0
56	MG	DA	3227	1/1	0.83	0.17	40,40,40,40	0
58	ZN	D4	501	1/1	0.83	0.08	155,155,155,155	0
56	MG	CA	3024	1/1	0.83	0.34	57,57,57,57	0
56	MG	CA	3150	1/1	0.84	0.18	63,63,63,63	0
56	MG	DA	3468	1/1	0.84	0.28	47,47,47,47	0
56	MG	BA	3349	1/1	0.84	0.17	31,31,31,31	0
56	MG	AA	3028	1/1	0.84	0.47	72,72,72,72	0
56	MG	AA	3069	1/1	0.84	0.09	77,77,77,77	0
56	MG	DA	3220	1/1	0.84	0.36	61,61,61,61	0
56	MG	DA	3222	1/1	0.84	0.22	45,45,45,45	0
56	MG	AA	3127	1/1	0.84	0.21	50,50,50,50	0
56	MG	DA	3103	1/1	0.84	0.36	52,52,52,52	0
56	MG	BA	3067	1/1	0.84	0.46	55,55,55,55	0
56	MG	CA	3091	1/1	0.84	0.15	95,95,95,95	0
56	MG	DA	3005	1/1	0.84	0.40	50,50,50,50	0
56	MG	DA	3125	1/1	0.84	0.48	55,55,55,55	0
56	MG	CA	3103	1/1	0.84	0.50	101,101,101,101	0
56	MG	DA	3344	1/1	0.84	0.12	48,48,48,48	0
56	MG	BN	3003	1/1	0.84	0.42	67,67,67,67	0
56	MG	DD	304	1/1	0.84	0.53	40,40,40,40	0
56	MG	DF	304	1/1	0.84	0.51	39,39,39,39	0
56	MG	DG	3001	1/1	0.84	0.11	68,68,68,68	0
56	MG	BA	3517	1/1	0.84	0.12	52,52,52,52	0
56	MG	BA	3249	1/1	0.84	0.39	46,46,46,46	0
56	MG	AA	3027	1/1	0.84	0.27	67,67,67,67	0
56	MG	DA	3157	1/1	0.84	0.49	56,56,56,56	0
56	MG	BA	3255	1/1	0.84	0.21	53,53,53,53	0
56	MG	AA	3090	1/1	0.84	0.18	64,64,64,64	0
56	MG	BA	3156	1/1	0.85	0.42	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DA	3361	1/1	0.85	0.13	58,58,58,58	0
56	MG	AA	3189	1/1	0.85	0.15	74,74,74,74	0
56	MG	AX	104	1/1	0.85	0.25	62,62,62,62	0
56	MG	CA	3048	1/1	0.85	0.24	70,70,70,70	0
56	MG	AA	3088	1/1	0.85	0.34	53,53,53,53	0
56	MG	DA	3448	1/1	0.85	0.33	67,67,67,67	0
56	MG	CA	3157	1/1	0.85	0.18	56,56,56,56	0
56	MG	CA	3160	1/1	0.85	0.14	49,49,49,49	0
56	MG	BA	3110	1/1	0.85	0.24	43,43,43,43	0
56	MG	BA	3121	1/1	0.85	0.26	50,50,50,50	0
56	MG	CA	3057	1/1	0.85	0.22	40,40,40,40	0
56	MG	CA	3062	1/1	0.85	0.34	67,67,67,67	0
56	MG	BA	3596	1/1	0.85	0.25	79,79,79,79	0
56	MG	DA	3164	1/1	0.85	0.16	40,40,40,40	0
56	MG	DA	3554	1/1	0.85	0.27	62,62,62,62	0
56	MG	BA	3204	1/1	0.85	0.20	48,48,48,48	0
56	MG	CA	3067	1/1	0.85	0.27	66,66,66,66	0
56	MG	DA	3190	1/1	0.85	0.10	54,54,54,54	0
56	MG	BA	3299	1/1	0.85	0.32	56,56,56,56	0
56	MG	AA	3126	1/1	0.85	0.17	54,54,54,54	0
56	MG	DA	3627	1/1	0.85	0.24	52,52,52,52	0
56	MG	BA	3060	1/1	0.85	0.59	64,64,64,64	0
56	MG	DA	3041	1/1	0.85	0.41	54,54,54,54	0
56	MG	BA	3634	1/1	0.85	0.11	77,77,77,77	0
56	MG	DA	3225	1/1	0.85	0.12	64,64,64,64	0
56	MG	DA	3057	1/1	0.85	0.25	57,57,57,57	0
56	MG	AA	3050	1/1	0.85	0.31	50,50,50,50	0
56	MG	BA	3068	1/1	0.85	0.45	43,43,43,43	0
56	MG	DA	3077	1/1	0.85	0.32	48,48,48,48	0
56	MG	BA	3074	1/1	0.85	0.17	38,38,38,38	0
56	MG	BA	3397	1/1	0.85	0.07	44,44,44,44	0
56	MG	CA	3119	1/1	0.85	0.48	73,73,73,73	0
56	MG	BA	3092	1/1	0.85	0.26	28,28,28,28	0
56	MG	CA	3134	1/1	0.85	0.23	92,92,92,92	0
56	MG	AA	3023	1/1	0.86	0.12	56,56,56,56	0
56	MG	BA	3331	1/1	0.86	0.17	61,61,61,61	0
56	MG	BA	3203	1/1	0.86	0.22	45,45,45,45	0
56	MG	AA	3033	1/1	0.86	0.45	68,68,68,68	0
56	MG	DA	3221	1/1	0.86	0.27	56,56,56,56	0
56	MG	BA	3207	1/1	0.86	0.37	44,44,44,44	0
56	MG	BR	203	1/1	0.86	0.51	48,48,48,48	0
56	MG	BW	3001	1/1	0.86	0.29	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\AA^2$)	Q<0.9
56	MG	BA	3217	1/1	0.86	0.33	59,59,59,59	0
56	MG	B9	502	1/1	0.86	0.26	49,49,49,49	0
56	MG	AA	3071	1/1	0.86	0.23	60,60,60,60	0
56	MG	BA	3228	1/1	0.86	0.35	23,23,23,23	0
56	MG	BA	3506	1/1	0.86	0.25	33,33,33,33	0
56	MG	DA	3001	1/1	0.86	0.26	76,76,76,76	0
56	MG	DA	3003	1/1	0.86	0.18	43,43,43,43	0
56	MG	BA	3514	1/1	0.86	0.21	49,49,49,49	0
56	MG	CA	3028	1/1	0.86	0.56	62,62,62,62	0
56	MG	CA	3030	1/1	0.86	0.36	74,74,74,74	0
56	MG	DA	3371	1/1	0.86	0.24	37,37,37,37	0
56	MG	AA	3026	1/1	0.86	0.18	52,52,52,52	0
56	MG	BA	3238	1/1	0.86	0.17	48,48,48,48	0
56	MG	DA	3036	1/1	0.86	0.27	35,35,35,35	0
56	MG	AA	3203	1/1	0.86	0.15	76,76,76,76	0
56	MG	CA	3036	1/1	0.86	0.23	56,56,56,56	0
56	MG	BA	3571	1/1	0.86	0.20	48,48,48,48	0
56	MG	AA	3209	1/1	0.86	0.38	66,66,66,66	0
56	MG	DA	3066	1/1	0.86	0.31	59,59,59,59	0
56	MG	AA	3117	1/1	0.86	0.15	64,64,64,64	0
56	MG	BA	3250	1/1	0.86	0.28	61,61,61,61	0
56	MG	BA	3251	1/1	0.86	0.27	45,45,45,45	0
56	MG	BA	3028	1/1	0.86	0.31	59,59,59,59	0
56	MG	CA	3055	1/1	0.86	0.25	61,61,61,61	0
56	MG	BA	3029	1/1	0.86	0.66	53,53,53,53	0
56	MG	AA	3064	1/1	0.86	0.27	65,65,65,65	0
56	MG	BA	3636	1/1	0.86	0.13	54,54,54,54	0
56	MG	BA	3641	1/1	0.86	0.14	33,33,33,33	0
56	MG	DA	3110	1/1	0.86	0.17	46,46,46,46	0
56	MG	AA	3133	1/1	0.86	0.69	71,71,71,71	0
56	MG	DA	3621	1/1	0.86	0.17	46,46,46,46	0
56	MG	AA	3121	1/1	0.86	0.46	52,52,52,52	0
56	MG	BA	3071	1/1	0.86	0.22	55,55,55,55	0
56	MG	DA	3645	1/1	0.86	0.41	57,57,57,57	0
56	MG	AA	3042	1/1	0.86	0.28	50,50,50,50	0
56	MG	BA	3158	1/1	0.86	0.44	43,43,43,43	0
56	MG	BA	3717	1/1	0.86	0.11	51,51,51,51	0
56	MG	BA	3722	1/1	0.86	0.27	49,49,49,49	0
56	MG	BA	3733	1/1	0.86	0.42	40,40,40,40	0
56	MG	BA	3082	1/1	0.86	0.16	54,54,54,54	0
56	MG	BB	3003	1/1	0.86	0.23	40,40,40,40	0
56	MG	BA	3300	1/1	0.86	0.29	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	3122	1/1	0.86	0.20	70,70,70,70	0
56	MG	BA	3084	1/1	0.86	0.50	47,47,47,47	0
56	MG	DA	3188	1/1	0.86	0.51	52,52,52,52	0
59	FME	AX	101	10/11	0.86	0.45	55,74,92,107	0
56	MG	BA	3085	1/1	0.86	0.38	35,35,35,35	0
56	MG	DA	3458	1/1	0.87	0.22	47,47,47,47	0
56	MG	BA	3484	1/1	0.87	0.16	40,40,40,40	0
56	MG	DA	3208	1/1	0.87	0.19	46,46,46,46	0
56	MG	AA	3020	1/1	0.87	0.18	80,80,80,80	0
56	MG	DA	3213	1/1	0.87	0.08	48,48,48,48	0
56	MG	CA	3019	1/1	0.87	0.15	62,62,62,62	0
56	MG	DA	3528	1/1	0.87	0.15	33,33,33,33	0
56	MG	BA	3070	1/1	0.87	0.24	46,46,46,46	0
56	MG	AA	3142	1/1	0.87	0.37	60,60,60,60	0
56	MG	BA	3133	1/1	0.87	0.60	53,53,53,53	0
56	MG	DA	3112	1/1	0.87	0.31	49,49,49,49	0
56	MG	DA	3015	1/1	0.87	0.33	54,54,54,54	0
56	MG	DA	3115	1/1	0.87	0.08	64,64,64,64	0
56	MG	DA	3119	1/1	0.87	0.15	44,44,44,44	0
56	MG	CA	3029	1/1	0.87	0.17	54,54,54,54	0
56	MG	DA	3035	1/1	0.87	0.71	58,58,58,58	0
56	MG	DA	3626	1/1	0.87	0.17	63,63,63,63	0
56	MG	AA	3039	1/1	0.87	0.20	62,62,62,62	0
56	MG	BA	3224	1/1	0.87	0.40	48,48,48,48	0
56	MG	DA	3338	1/1	0.87	0.16	58,58,58,58	0
56	MG	BA	3099	1/1	0.87	0.31	55,55,55,55	0
56	MG	BA	3081	1/1	0.87	0.29	44,44,44,44	0
56	MG	AA	3063	1/1	0.87	0.14	57,57,57,57	0
56	MG	BA	3192	1/1	0.87	0.36	48,48,48,48	0
56	MG	CA	3084	1/1	0.87	0.18	80,80,80,80	0
56	MG	DA	3074	1/1	0.87	0.31	60,60,60,60	0
56	MG	DA	3165	1/1	0.87	0.32	48,48,48,48	0
56	MG	DA	3424	1/1	0.87	0.19	58,58,58,58	0
56	MG	DU	3002	1/1	0.87	0.58	52,52,52,52	0
56	MG	BA	3240	1/1	0.87	0.26	54,54,54,54	0
56	MG	DA	3079	1/1	0.87	0.28	44,44,44,44	0
56	MG	BA	3293	1/1	0.87	0.28	69,69,69,69	0
56	MG	CA	3007	1/1	0.87	0.41	63,63,63,63	0
56	MG	DA	3457	1/1	0.87	0.15	44,44,44,44	0
56	MG	BA	3675	1/1	0.88	0.26	68,68,68,68	0
56	MG	BA	3687	1/1	0.88	0.14	59,59,59,59	0
56	MG	AA	3037	1/1	0.88	0.28	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	3021	1/1	0.88	0.25	54,54,54,54	0
56	MG	DA	3029	1/1	0.88	0.12	62,62,62,62	0
56	MG	DA	3455	1/1	0.88	0.21	53,53,53,53	0
56	MG	BA	3105	1/1	0.88	0.19	54,54,54,54	0
56	MG	BA	3704	1/1	0.88	0.34	58,58,58,58	0
56	MG	BA	3707	1/1	0.88	0.17	57,57,57,57	0
56	MG	DA	3460	1/1	0.88	0.10	47,47,47,47	0
56	MG	DA	3462	1/1	0.88	0.22	71,71,71,71	0
56	MG	DA	3049	1/1	0.88	0.18	56,56,56,56	0
56	MG	DA	3465	1/1	0.88	0.17	41,41,41,41	0
56	MG	BA	3076	1/1	0.88	0.22	40,40,40,40	0
56	MG	DA	3180	1/1	0.88	0.20	47,47,47,47	0
56	MG	DA	3186	1/1	0.88	0.29	38,38,38,38	0
56	MG	DA	3187	1/1	0.88	0.67	52,52,52,52	0
56	MG	BA	3713	1/1	0.88	0.22	49,49,49,49	0
56	MG	DA	3062	1/1	0.88	0.39	58,58,58,58	0
56	MG	BA	3109	1/1	0.88	0.28	62,62,62,62	0
56	MG	DA	3205	1/1	0.88	0.26	41,41,41,41	0
56	MG	AN	101	1/1	0.88	0.17	64,64,64,64	0
56	MG	BA	3563	1/1	0.88	0.39	66,66,66,66	0
56	MG	BA	3172	1/1	0.88	0.12	54,54,54,54	0
56	MG	CA	3142	1/1	0.88	0.20	80,80,80,80	0
56	MG	BA	3242	1/1	0.88	0.18	45,45,45,45	0
56	MG	DA	3608	1/1	0.88	0.29	63,63,63,63	0
56	MG	DA	3086	1/1	0.88	0.30	43,43,43,43	0
56	MG	BA	3039	1/1	0.88	0.29	44,44,44,44	0
56	MG	BA	3122	1/1	0.88	0.65	68,68,68,68	0
56	MG	CA	3043	1/1	0.88	0.34	62,62,62,62	0
56	MG	AA	3143	1/1	0.88	0.20	67,67,67,67	0
56	MG	DA	3647	1/1	0.88	0.56	45,45,45,45	0
56	MG	DB	3002	1/1	0.88	0.20	72,72,72,72	0
56	MG	BA	3007	1/1	0.88	0.25	55,55,55,55	0
56	MG	DA	3243	1/1	0.88	0.41	49,49,49,49	0
56	MG	DB	3008	1/1	0.88	0.12	36,36,36,36	0
56	MG	BA	3135	1/1	0.88	0.26	57,57,57,57	0
56	MG	DA	3287	1/1	0.88	0.06	53,53,53,53	0
56	MG	BA	3626	1/1	0.88	0.13	50,50,50,50	0
56	MG	AA	3003	1/1	0.88	0.25	70,70,70,70	0
56	MG	BA	3094	1/1	0.88	0.47	62,62,62,62	0
56	MG	BA	3640	1/1	0.88	0.21	31,31,31,31	0
56	MG	AA	3125	1/1	0.88	0.14	56,56,56,56	0
56	MG	DA	3117	1/1	0.88	0.17	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\AA^2$)	Q<0.9
56	MG	BA	3649	1/1	0.88	0.25	43,43,43,43	0
56	MG	BA	3261	1/1	0.88	0.28	45,45,45,45	0
56	MG	DA	3006	1/1	0.88	0.08	41,41,41,41	0
56	MG	AA	3164	1/1	0.88	0.23	61,61,61,61	0
60	K	DA	3234	1/1	0.88	0.27	102,102,102,102	0
56	MG	DA	3121	1/1	0.89	0.26	46,46,46,46	0
56	MG	AA	3075	1/1	0.89	0.11	50,50,50,50	0
56	MG	DA	3392	1/1	0.89	0.14	60,60,60,60	0
56	MG	BA	3429	1/1	0.89	0.16	55,55,55,55	0
56	MG	BW	3002	1/1	0.89	0.18	34,34,34,34	0
56	MG	BA	3435	1/1	0.89	0.21	59,59,59,59	0
56	MG	DA	3434	1/1	0.89	0.19	51,51,51,51	0
56	MG	BA	3444	1/1	0.89	0.27	29,29,29,29	0
56	MG	DA	3143	1/1	0.89	0.20	53,53,53,53	0
56	MG	DA	3144	1/1	0.89	0.34	37,37,37,37	0
56	MG	BA	3225	1/1	0.89	0.40	42,42,42,42	0
56	MG	BA	3164	1/1	0.89	0.49	57,57,57,57	0
56	MG	BA	3289	1/1	0.89	0.13	53,53,53,53	0
56	MG	DA	3160	1/1	0.89	0.24	47,47,47,47	0
56	MG	BA	3680	1/1	0.89	0.24	62,62,62,62	0
56	MG	BA	3166	1/1	0.89	0.20	41,41,41,41	0
56	MG	BA	3167	1/1	0.89	0.46	50,50,50,50	0
56	MG	DA	3038	1/1	0.89	0.33	37,37,37,37	0
56	MG	BA	3524	1/1	0.89	0.13	50,50,50,50	0
56	MG	DA	3175	1/1	0.89	0.30	52,52,52,52	0
56	MG	AF	3001	1/1	0.89	0.16	62,62,62,62	0
56	MG	CA	3117	1/1	0.89	0.15	58,58,58,58	0
56	MG	AX	107	1/1	0.89	0.44	82,82,82,82	0
56	MG	BA	3561	1/1	0.89	0.25	39,39,39,39	0
56	MG	AA	3102	1/1	0.89	0.05	68,68,68,68	0
56	MG	BA	3567	1/1	0.89	0.10	54,54,54,54	0
56	MG	DA	3067	1/1	0.89	0.29	35,35,35,35	0
56	MG	CA	3135	1/1	0.89	0.37	61,61,61,61	0
56	MG	BA	3246	1/1	0.89	0.33	38,38,38,38	0
56	MG	CA	3035	1/1	0.89	0.26	49,49,49,49	0
56	MG	DA	3606	1/1	0.89	0.18	58,58,58,58	0
56	MG	BA	3247	1/1	0.89	0.21	58,58,58,58	0
56	MG	DA	3613	1/1	0.89	0.31	64,64,64,64	0
56	MG	DA	3618	1/1	0.89	0.25	61,61,61,61	0
56	MG	DA	3081	1/1	0.89	0.23	56,56,56,56	0
56	MG	AA	3017	1/1	0.89	0.29	57,57,57,57	0
56	MG	BA	3599	1/1	0.89	0.10	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	BA	3058	1/1	0.89	0.39	41,41,41,41	0
56	MG	CA	3156	1/1	0.89	0.26	80,80,80,80	0
56	MG	BA	3604	1/1	0.89	0.38	64,64,64,64	0
56	MG	DA	3099	1/1	0.89	0.34	39,39,39,39	0
56	MG	AV	101	1/1	0.89	0.24	51,51,51,51	0
56	MG	DB	3005	1/1	0.89	0.25	41,41,41,41	0
56	MG	DA	3102	1/1	0.89	0.27	49,49,49,49	0
56	MG	DA	3278	1/1	0.89	0.08	39,39,39,39	0
56	MG	DA	3282	1/1	0.89	0.31	58,58,58,58	0
56	MG	BA	3064	1/1	0.89	0.38	49,49,49,49	0
56	MG	DA	3289	1/1	0.89	0.17	64,64,64,64	0
56	MG	DA	3108	1/1	0.89	0.41	50,50,50,50	0
56	MG	AA	3082	1/1	0.89	0.16	52,52,52,52	0
56	MG	CA	3163	1/1	0.89	0.24	60,60,60,60	0
56	MG	DA	3318	1/1	0.89	0.19	47,47,47,47	0
56	MG	AX	103	1/1	0.89	0.10	57,57,57,57	0
56	MG	D3	101	1/1	0.89	0.55	54,54,54,54	0
56	MG	CA	3171	1/1	0.89	0.15	61,61,61,61	0
56	MG	BA	3629	1/1	0.89	0.14	51,51,51,51	0
56	MG	DA	3354	1/1	0.89	0.18	39,39,39,39	0
56	MG	BA	3161	1/1	0.89	0.13	50,50,50,50	0
56	MG	CA	3061	1/1	0.89	0.48	68,68,68,68	0
56	MG	CA	3009	1/1	0.90	0.13	55,55,55,55	0
56	MG	AA	3068	1/1	0.90	0.11	67,67,67,67	0
56	MG	AA	3087	1/1	0.90	0.21	87,87,87,87	0
56	MG	BA	3086	1/1	0.90	0.32	50,50,50,50	0
56	MG	DA	3353	1/1	0.90	0.17	54,54,54,54	0
56	MG	DA	3106	1/1	0.90	0.40	45,45,45,45	0
56	MG	BA	3265	1/1	0.90	0.23	39,39,39,39	0
56	MG	CA	3145	1/1	0.90	0.11	67,67,67,67	0
56	MG	BA	3269	1/1	0.90	0.11	32,32,32,32	0
56	MG	CA	3025	1/1	0.90	0.12	102,102,102,102	0
56	MG	DA	3391	1/1	0.90	0.14	54,54,54,54	0
56	MG	BA	3688	1/1	0.90	0.05	58,58,58,58	0
56	MG	DA	3396	1/1	0.90	0.14	37,37,37,37	0
56	MG	DA	3409	1/1	0.90	0.10	54,54,54,54	0
56	MG	DA	3418	1/1	0.90	0.22	57,57,57,57	0
56	MG	BA	3089	1/1	0.90	0.23	50,50,50,50	0
56	MG	DA	3116	1/1	0.90	0.39	43,43,43,43	0
56	MG	DA	3428	1/1	0.90	0.28	30,30,30,30	0
56	MG	BA	3146	1/1	0.90	0.39	56,56,56,56	0
56	MG	BA	3048	1/1	0.90	0.35	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	AA	3098	1/1	0.90	0.43	76,76,76,76	0
56	MG	DA	3447	1/1	0.90	0.18	56,56,56,56	0
56	MG	AA	3136	1/1	0.90	0.11	68,68,68,68	0
56	MG	AA	3139	1/1	0.90	0.20	58,58,58,58	0
56	MG	BA	3716	1/1	0.90	0.24	77,77,77,77	0
56	MG	BA	3066	1/1	0.90	0.24	49,49,49,49	0
56	MG	DA	3137	1/1	0.90	0.31	62,62,62,62	0
56	MG	DA	3139	1/1	0.90	0.22	47,47,47,47	0
56	MG	AA	3073	1/1	0.90	0.11	63,63,63,63	0
56	MG	CN	502	1/1	0.90	0.31	70,70,70,70	0
56	MG	BA	3723	1/1	0.90	0.17	25,25,25,25	0
56	MG	AD	502	1/1	0.90	0.63	56,56,56,56	0
56	MG	DA	3472	1/1	0.90	0.18	38,38,38,38	0
56	MG	DA	3485	1/1	0.90	0.20	44,44,44,44	0
56	MG	BA	3738	1/1	0.90	0.22	58,58,58,58	0
56	MG	BA	3739	1/1	0.90	0.38	50,50,50,50	0
56	MG	AA	3105	1/1	0.90	0.30	54,54,54,54	0
56	MG	DA	3517	1/1	0.90	0.28	47,47,47,47	0
56	MG	DA	3521	1/1	0.90	0.19	46,46,46,46	0
56	MG	AA	3049	1/1	0.90	0.39	46,46,46,46	0
56	MG	DA	3529	1/1	0.90	0.48	72,72,72,72	0
56	MG	BA	3602	1/1	0.90	0.16	44,44,44,44	0
56	MG	DA	3532	1/1	0.90	0.10	60,60,60,60	0
56	MG	BA	3244	1/1	0.90	0.19	46,46,46,46	0
56	MG	BB	3014	1/1	0.90	0.09	68,68,68,68	0
56	MG	DA	3017	1/1	0.90	0.25	51,51,51,51	0
56	MG	BA	3334	1/1	0.90	0.14	41,41,41,41	0
56	MG	DA	3584	1/1	0.90	0.15	47,47,47,47	0
56	MG	AA	3052	1/1	0.90	0.24	58,58,58,58	0
56	MG	AA	3092	1/1	0.90	0.50	59,59,59,59	0
56	MG	BA	3123	1/1	0.90	0.27	47,47,47,47	0
56	MG	BA	3180	1/1	0.90	0.33	48,48,48,48	0
56	MG	DA	3189	1/1	0.90	0.21	55,55,55,55	0
56	MG	BN	3005	1/1	0.90	1.02	63,63,63,63	0
56	MG	DA	3042	1/1	0.90	0.35	38,38,38,38	0
56	MG	BP	203	1/1	0.90	0.62	39,39,39,39	0
56	MG	BA	3182	1/1	0.90	0.36	43,43,43,43	0
56	MG	BA	3023	1/1	0.90	0.43	34,34,34,34	0
56	MG	DA	3630	1/1	0.90	0.09	67,67,67,67	0
56	MG	DA	3060	1/1	0.90	0.34	51,51,51,51	0
56	MG	DA	3061	1/1	0.90	0.27	47,47,47,47	0
56	MG	DA	3219	1/1	0.90	0.36	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	AA	3119	1/1	0.90	0.31	42,42,42,42	0
56	MG	BA	3190	1/1	0.90	0.25	42,42,42,42	0
56	MG	CA	3101	1/1	0.90	0.11	58,58,58,58	0
56	MG	BW	3005	1/1	0.90	0.44	38,38,38,38	0
56	MG	CA	3106	1/1	0.90	0.39	72,72,72,72	0
56	MG	DB	3010	1/1	0.90	0.19	66,66,66,66	0
56	MG	BA	3648	1/1	0.90	0.16	54,54,54,54	0
56	MG	B7	101	1/1	0.90	0.19	45,45,45,45	0
56	MG	DE	301	1/1	0.90	0.83	51,51,51,51	0
56	MG	DA	3078	1/1	0.90	0.15	49,49,49,49	0
56	MG	DA	3256	1/1	0.90	0.12	41,41,41,41	0
56	MG	B7	104	1/1	0.90	0.22	55,55,55,55	0
56	MG	BA	3460	1/1	0.90	0.18	66,66,66,66	0
56	MG	CA	3006	1/1	0.90	0.09	72,72,72,72	0
56	MG	DA	3283	1/1	0.90	0.19	47,47,47,47	0
56	MG	CA	3124	1/1	0.90	0.17	64,64,64,64	0
56	MG	CA	3126	1/1	0.90	0.25	56,56,56,56	0
56	MG	DA	3090	1/1	0.90	0.27	59,59,59,59	0
56	MG	BA	3654	1/1	0.90	0.15	49,49,49,49	0
56	MG	DA	3298	1/1	0.90	0.26	45,45,45,45	0
56	MG	CA	3131	1/1	0.90	0.14	48,48,48,48	0
56	MG	AA	3134	1/1	0.91	0.37	70,70,70,70	0
56	MG	CA	3146	1/1	0.91	0.18	61,61,61,61	0
56	MG	BA	3138	1/1	0.91	0.17	54,54,54,54	0
56	MG	CA	3015	1/1	0.91	0.33	53,53,53,53	0
56	MG	BA	3431	1/1	0.91	0.25	54,54,54,54	0
56	MG	DA	3374	1/1	0.91	0.14	40,40,40,40	0
56	MG	BA	3667	1/1	0.91	0.22	72,72,72,72	0
56	MG	BA	3432	1/1	0.91	0.14	27,27,27,27	0
56	MG	DA	3395	1/1	0.91	0.14	40,40,40,40	0
56	MG	CA	3159	1/1	0.91	0.74	76,76,76,76	0
56	MG	DA	3402	1/1	0.91	0.17	33,33,33,33	0
56	MG	DA	3405	1/1	0.91	0.33	53,53,53,53	0
56	MG	BA	3191	1/1	0.91	0.20	56,56,56,56	0
56	MG	BA	3676	1/1	0.91	0.17	63,63,63,63	0
56	MG	BA	3020	1/1	0.91	0.29	43,43,43,43	0
56	MG	BA	3686	1/1	0.91	0.29	65,65,65,65	0
56	MG	BA	3097	1/1	0.91	0.16	30,30,30,30	0
56	MG	BA	3467	1/1	0.91	0.15	44,44,44,44	0
56	MG	BA	3477	1/1	0.91	0.16	52,52,52,52	0
56	MG	DA	3436	1/1	0.91	0.32	61,61,61,61	0
56	MG	DA	3138	1/1	0.91	0.41	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	CE	3001	1/1	0.91	0.20	66,66,66,66	0
56	MG	AA	3204	1/1	0.91	0.17	70,70,70,70	0
56	MG	DA	3454	1/1	0.91	0.11	52,52,52,52	0
56	MG	BA	3702	1/1	0.91	0.24	56,56,56,56	0
56	MG	BA	3264	1/1	0.91	0.18	29,29,29,29	0
56	MG	BA	3499	1/1	0.91	0.18	50,50,50,50	0
56	MG	DA	3154	1/1	0.91	0.49	45,45,45,45	0
56	MG	BA	3153	1/1	0.91	0.32	47,47,47,47	0
56	MG	BA	3267	1/1	0.91	0.18	56,56,56,56	0
56	MG	BA	3213	1/1	0.91	0.14	63,63,63,63	0
56	MG	DA	3009	1/1	0.91	0.11	33,33,33,33	0
56	MG	BA	3271	1/1	0.91	0.32	40,40,40,40	0
56	MG	BA	3279	1/1	0.91	0.16	60,60,60,60	0
56	MG	DA	3475	1/1	0.91	0.12	35,35,35,35	0
56	MG	DA	3483	1/1	0.91	0.14	55,55,55,55	0
56	MG	BA	3281	1/1	0.91	0.23	45,45,45,45	0
56	MG	BA	3550	1/1	0.91	0.19	32,32,32,32	0
56	MG	DA	3172	1/1	0.91	0.33	46,46,46,46	0
56	MG	AA	3080	1/1	0.91	0.23	58,58,58,58	0
56	MG	BA	3284	1/1	0.91	0.72	76,76,76,76	0
56	MG	AA	3167	1/1	0.91	0.18	78,78,78,78	0
56	MG	AA	3219	1/1	0.91	0.18	54,54,54,54	0
56	MG	BA	3581	1/1	0.91	0.32	54,54,54,54	0
56	MG	DA	3530	1/1	0.91	0.16	57,57,57,57	0
56	MG	DA	3040	1/1	0.91	0.21	45,45,45,45	0
56	MG	AA	3173	1/1	0.91	0.15	37,37,37,37	0
56	MG	DA	3537	1/1	0.91	0.16	74,74,74,74	0
56	MG	DA	3540	1/1	0.91	0.13	76,76,76,76	0
56	MG	DA	3195	1/1	0.91	0.20	51,51,51,51	0
56	MG	DA	3202	1/1	0.91	0.21	39,39,39,39	0
56	MG	AA	3081	1/1	0.91	0.38	46,46,46,46	0
56	MG	DA	3560	1/1	0.91	0.07	57,57,57,57	0
56	MG	DA	3565	1/1	0.91	0.22	48,48,48,48	0
56	MG	DA	3043	1/1	0.91	0.54	56,56,56,56	0
56	MG	CA	3064	1/1	0.91	0.14	74,74,74,74	0
56	MG	DA	3210	1/1	0.91	0.28	46,46,46,46	0
56	MG	BA	3046	1/1	0.91	0.41	52,52,52,52	0
56	MG	DA	3598	1/1	0.91	0.17	45,45,45,45	0
56	MG	BD	304	1/1	0.91	0.44	41,41,41,41	0
56	MG	BA	3118	1/1	0.91	0.26	53,53,53,53	0
56	MG	BF	302	1/1	0.91	0.26	49,49,49,49	0
56	MG	BA	3119	1/1	0.91	0.11	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	3617	1/1	0.91	0.07	51,51,51,51	0
56	MG	AA	3182	1/1	0.91	0.13	48,48,48,48	0
56	MG	BN	3002	1/1	0.91	0.20	52,52,52,52	0
56	MG	DA	3623	1/1	0.91	0.12	63,63,63,63	0
56	MG	BA	3241	1/1	0.91	0.41	41,41,41,41	0
56	MG	BA	3053	1/1	0.91	0.19	52,52,52,52	0
56	MG	DA	3071	1/1	0.91	0.52	46,46,46,46	0
56	MG	DA	3637	1/1	0.91	0.20	59,59,59,59	0
56	MG	DA	3240	1/1	0.91	0.17	58,58,58,58	0
56	MG	DA	3073	1/1	0.91	0.16	50,50,50,50	0
56	MG	AA	3096	1/1	0.91	0.27	52,52,52,52	0
56	MG	DA	3654	1/1	0.91	0.29	50,50,50,50	0
56	MG	DA	3655	1/1	0.91	0.17	62,62,62,62	0
56	MG	DA	3249	1/1	0.91	0.20	25,25,25,25	0
56	MG	DA	3254	1/1	0.91	0.14	52,52,52,52	0
56	MG	BA	3059	1/1	0.91	0.37	35,35,35,35	0
56	MG	BQ	3004	1/1	0.91	0.33	41,41,41,41	0
56	MG	DA	3276	1/1	0.91	0.11	26,26,26,26	0
56	MG	BA	3346	1/1	0.91	0.17	33,33,33,33	0
56	MG	BU	204	1/1	0.91	0.33	49,49,49,49	0
56	MG	BU	205	1/1	0.91	0.36	39,39,39,39	0
56	MG	BA	3632	1/1	0.91	0.15	55,55,55,55	0
56	MG	BA	3088	1/1	0.91	0.25	55,55,55,55	0
56	MG	BW	3003	1/1	0.91	0.26	39,39,39,39	0
56	MG	DA	3091	1/1	0.91	0.50	50,50,50,50	0
56	MG	BA	3635	1/1	0.91	0.20	52,52,52,52	0
56	MG	DA	3299	1/1	0.91	0.12	35,35,35,35	0
56	MG	DW	201	1/1	0.91	0.33	45,45,45,45	0
56	MG	BX	102	1/1	0.91	0.23	60,60,60,60	0
56	MG	BA	3134	1/1	0.91	0.14	34,34,34,34	0
56	MG	DA	3328	1/1	0.91	0.28	33,33,33,33	0
56	MG	BA	3372	1/1	0.91	0.17	42,42,42,42	0
56	MG	BA	3184	1/1	0.91	0.81	51,51,51,51	0
56	MG	BA	3647	1/1	0.91	0.26	40,40,40,40	0
60	K	BA	3304	1/1	0.91	0.32	93,93,93,93	0
56	MG	AA	3197	1/1	0.91	0.19	64,64,64,64	0
56	MG	BB	3008	1/1	0.92	0.21	49,49,49,49	0
56	MG	BB	3009	1/1	0.92	0.12	49,49,49,49	0
56	MG	CA	3082	1/1	0.92	0.12	46,46,46,46	0
56	MG	BB	3011	1/1	0.92	0.16	45,45,45,45	0
56	MG	DA	3364	1/1	0.92	0.17	40,40,40,40	0
56	MG	AA	3215	1/1	0.92	0.94	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	BA	3001	1/1	0.92	0.33	52,52,52,52	0
56	MG	DA	3097	1/1	0.92	0.17	58,58,58,58	0
56	MG	BD	301	1/1	0.92	0.41	35,35,35,35	0
56	MG	BA	3568	1/1	0.92	0.22	68,68,68,68	0
56	MG	CA	3107	1/1	0.92	0.08	71,71,71,71	0
56	MG	BA	3294	1/1	0.92	0.16	59,59,59,59	0
56	MG	AA	3162	1/1	0.92	0.14	79,79,79,79	0
56	MG	AA	3044	1/1	0.92	0.13	60,60,60,60	0
56	MG	AA	3099	1/1	0.92	0.51	49,49,49,49	0
56	MG	BA	3008	1/1	0.92	0.14	30,30,30,30	0
56	MG	BA	3016	1/1	0.92	0.52	50,50,50,50	0
56	MG	DA	3111	1/1	0.92	0.20	67,67,67,67	0
56	MG	AA	3014	1/1	0.92	0.13	24,24,24,24	0
56	MG	BP	201	1/1	0.92	0.57	37,37,37,37	0
56	MG	BA	3317	1/1	0.92	0.24	40,40,40,40	0
56	MG	BA	3324	1/1	0.92	0.30	54,54,54,54	0
56	MG	BA	3612	1/1	0.92	0.17	41,41,41,41	0
56	MG	DA	3444	1/1	0.92	0.27	43,43,43,43	0
56	MG	CA	3138	1/1	0.92	0.12	59,59,59,59	0
56	MG	AA	3057	1/1	0.92	0.16	45,45,45,45	0
56	MG	CA	3141	1/1	0.92	0.31	85,85,85,85	0
56	MG	DA	3124	1/1	0.92	0.13	66,66,66,66	0
56	MG	BA	3174	1/1	0.92	0.21	52,52,52,52	0
56	MG	BA	3338	1/1	0.92	0.21	62,62,62,62	0
56	MG	AA	3106	1/1	0.92	0.27	68,68,68,68	0
56	MG	AA	3109	1/1	0.92	0.21	59,59,59,59	0
56	MG	BA	3354	1/1	0.92	0.29	45,45,45,45	0
56	MG	BA	3075	1/1	0.92	0.24	36,36,36,36	0
56	MG	AA	3194	1/1	0.92	0.18	50,50,50,50	0
56	MG	BA	3385	1/1	0.92	0.06	56,56,56,56	0
56	MG	B0	106	1/1	0.92	0.08	43,43,43,43	0
56	MG	DA	3473	1/1	0.92	0.17	50,50,50,50	0
56	MG	DA	3146	1/1	0.92	0.20	34,34,34,34	0
56	MG	DA	3151	1/1	0.92	0.33	48,48,48,48	0
56	MG	BA	3392	1/1	0.92	0.13	53,53,53,53	0
56	MG	BA	3644	1/1	0.92	0.10	38,38,38,38	0
56	MG	DA	3493	1/1	0.92	0.25	38,38,38,38	0
56	MG	BA	3646	1/1	0.92	0.24	39,39,39,39	0
56	MG	CA	3002	1/1	0.92	0.07	74,74,74,74	0
56	MG	DA	3502	1/1	0.92	0.18	48,48,48,48	0
56	MG	DA	3507	1/1	0.92	0.20	53,53,53,53	0
56	MG	DA	3509	1/1	0.92	0.09	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	BA	3026	1/1	0.92	0.15	36,36,36,36	0
56	MG	CA	3164	1/1	0.92	0.35	43,43,43,43	0
56	MG	DA	3523	1/1	0.92	0.12	47,47,47,47	0
56	MG	BA	3187	1/1	0.92	0.23	53,53,53,53	0
56	MG	CA	3008	1/1	0.92	1.01	59,59,59,59	0
56	MG	BA	3408	1/1	0.92	0.13	28,28,28,28	0
56	MG	CA	3012	1/1	0.92	0.13	50,50,50,50	0
56	MG	CA	3014	1/1	0.92	0.17	56,56,56,56	0
56	MG	CT	3001	1/1	0.92	0.21	57,57,57,57	0
56	MG	BA	3253	1/1	0.92	0.28	63,63,63,63	0
56	MG	DA	3542	1/1	0.92	0.23	44,44,44,44	0
56	MG	DA	3181	1/1	0.92	0.33	55,55,55,55	0
56	MG	BA	3415	1/1	0.92	0.14	28,28,28,28	0
56	MG	BA	3662	1/1	0.92	0.15	46,46,46,46	0
56	MG	BA	3416	1/1	0.92	0.17	25,25,25,25	0
56	MG	DA	3561	1/1	0.92	0.14	40,40,40,40	0
56	MG	BA	3423	1/1	0.92	0.35	45,45,45,45	0
56	MG	DA	3567	1/1	0.92	0.10	68,68,68,68	0
56	MG	BA	3254	1/1	0.92	0.30	40,40,40,40	0
56	MG	DA	3575	1/1	0.92	0.11	51,51,51,51	0
56	MG	BA	3027	1/1	0.92	0.19	53,53,53,53	0
56	MG	DA	3585	1/1	0.92	0.26	62,62,62,62	0
56	MG	DA	3586	1/1	0.92	0.12	57,57,57,57	0
56	MG	DA	3589	1/1	0.92	0.11	65,65,65,65	0
56	MG	DA	3201	1/1	0.92	0.24	43,43,43,43	0
56	MG	DA	3593	1/1	0.92	0.24	62,62,62,62	0
56	MG	AA	3058	1/1	0.92	0.36	59,59,59,59	0
56	MG	AA	3199	1/1	0.92	0.15	62,62,62,62	0
56	MG	DA	3602	1/1	0.92	0.17	63,63,63,63	0
56	MG	DA	3013	1/1	0.92	0.10	38,38,38,38	0
56	MG	BA	3260	1/1	0.92	0.12	47,47,47,47	0
56	MG	DA	3016	1/1	0.92	0.22	33,33,33,33	0
56	MG	BA	3447	1/1	0.92	0.12	76,76,76,76	0
56	MG	DA	3614	1/1	0.92	0.12	46,46,46,46	0
56	MG	DA	3018	1/1	0.92	0.28	41,41,41,41	0
56	MG	DA	3023	1/1	0.92	0.40	64,64,64,64	0
56	MG	CA	3031	1/1	0.92	0.31	55,55,55,55	0
56	MG	DA	3025	1/1	0.92	0.49	38,38,38,38	0
56	MG	DA	3027	1/1	0.92	0.63	49,49,49,49	0
56	MG	BA	3689	1/1	0.92	0.18	25,25,25,25	0
56	MG	DA	3629	1/1	0.92	0.14	30,30,30,30	0
56	MG	BA	3031	1/1	0.92	0.61	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	DA	3636	1/1	0.92	0.11	64,64,64,64	0
56	MG	BA	3465	1/1	0.92	0.09	51,51,51,51	0
56	MG	BA	3196	1/1	0.92	0.19	45,45,45,45	0
56	MG	BA	3473	1/1	0.92	0.15	55,55,55,55	0
56	MG	DA	3646	1/1	0.92	0.20	42,42,42,42	0
56	MG	CA	3037	1/1	0.92	0.23	45,45,45,45	0
56	MG	BA	3033	1/1	0.92	0.50	54,54,54,54	0
56	MG	BA	3481	1/1	0.92	0.20	41,41,41,41	0
56	MG	BA	3709	1/1	0.92	0.16	77,77,77,77	0
56	MG	BA	3266	1/1	0.92	0.19	47,47,47,47	0
56	MG	DA	3262	1/1	0.92	0.22	60,60,60,60	0
56	MG	BA	3714	1/1	0.92	0.15	72,72,72,72	0
56	MG	DA	3267	1/1	0.92	0.28	40,40,40,40	0
56	MG	BA	3141	1/1	0.92	0.55	43,43,43,43	0
56	MG	AA	3041	1/1	0.92	0.14	41,41,41,41	0
56	MG	BA	3718	1/1	0.92	0.16	52,52,52,52	0
56	MG	BA	3211	1/1	0.92	0.08	43,43,43,43	0
56	MG	DE	305	1/1	0.92	0.45	68,68,68,68	0
56	MG	BA	3278	1/1	0.92	0.19	53,53,53,53	0
56	MG	CA	3058	1/1	0.92	0.20	36,36,36,36	0
56	MG	DQ	3001	1/1	0.92	0.26	40,40,40,40	0
56	MG	BA	3212	1/1	0.92	0.16	47,47,47,47	0
56	MG	BA	3518	1/1	0.92	0.10	52,52,52,52	0
56	MG	DA	3072	1/1	0.92	0.14	40,40,40,40	0
56	MG	DV	202	1/1	0.92	0.61	45,45,45,45	0
56	MG	BA	3090	1/1	0.92	0.24	42,42,42,42	0
56	MG	DA	3306	1/1	0.92	0.16	51,51,51,51	0
56	MG	BA	3216	1/1	0.92	0.28	46,46,46,46	0
56	MG	D5	102	1/1	0.92	0.59	44,44,44,44	0
56	MG	BA	3044	1/1	0.92	0.37	32,32,32,32	0
56	MG	AA	3012	1/1	0.92	0.16	58,58,58,58	0
56	MG	AA	3097	1/1	0.92	0.41	53,53,53,53	0
56	MG	BB	3006	1/1	0.92	0.29	34,34,34,34	0
56	MG	DA	3084	1/1	0.92	0.18	55,55,55,55	0
56	MG	DA	3351	1/1	0.92	0.24	58,58,58,58	0
56	MG	BA	3005	1/1	0.93	0.17	43,43,43,43	0
56	MG	DA	3411	1/1	0.93	0.23	33,33,33,33	0
56	MG	BA	3055	1/1	0.93	0.31	44,44,44,44	0
56	MG	BA	3504	1/1	0.93	0.18	54,54,54,54	0
56	MG	CA	3153	1/1	0.93	0.10	85,85,85,85	0
56	MG	DA	3425	1/1	0.93	0.19	51,51,51,51	0
56	MG	DA	3426	1/1	0.93	0.14	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	DA	3427	1/1	0.93	0.14	29,29,29,29	0
56	MG	DA	3123	1/1	0.93	0.17	61,61,61,61	0
56	MG	BA	3505	1/1	0.93	0.26	45,45,45,45	0
56	MG	AA	3214	1/1	0.93	0.31	42,42,42,42	0
56	MG	DA	3130	1/1	0.93	0.09	34,34,34,34	0
56	MG	BA	3692	1/1	0.93	0.20	36,36,36,36	0
56	MG	BA	3693	1/1	0.93	0.27	57,57,57,57	0
56	MG	BA	3509	1/1	0.93	0.21	29,29,29,29	0
56	MG	BA	3696	1/1	0.93	0.27	36,36,36,36	0
56	MG	BA	3100	1/1	0.93	0.21	42,42,42,42	0
56	MG	BA	3101	1/1	0.93	0.42	47,47,47,47	0
56	MG	BA	3301	1/1	0.93	0.53	44,44,44,44	0
56	MG	CA	3017	1/1	0.93	0.17	54,54,54,54	0
56	MG	BA	3705	1/1	0.93	0.22	64,64,64,64	0
56	MG	AA	3006	1/1	0.93	0.09	84,84,84,84	0
56	MG	AA	3123	1/1	0.93	0.38	38,38,38,38	0
56	MG	CA	3023	1/1	0.93	0.20	37,37,37,37	0
56	MG	BA	3061	1/1	0.93	0.35	44,44,44,44	0
56	MG	BA	3549	1/1	0.93	0.30	49,49,49,49	0
56	MG	DA	3469	1/1	0.93	0.15	52,52,52,52	0
56	MG	CA	3026	1/1	0.93	0.18	52,52,52,52	0
56	MG	BA	3245	1/1	0.93	0.23	45,45,45,45	0
56	MG	BA	3171	1/1	0.93	0.40	42,42,42,42	0
56	MG	BA	3011	1/1	0.93	0.17	39,39,39,39	0
56	MG	DA	3484	1/1	0.93	0.05	47,47,47,47	0
56	MG	DA	3167	1/1	0.93	0.25	46,46,46,46	0
56	MG	DA	3168	1/1	0.93	0.67	46,46,46,46	0
56	MG	AA	3100	1/1	0.93	0.59	43,43,43,43	0
56	MG	BA	3175	1/1	0.93	0.50	40,40,40,40	0
56	MG	BA	3113	1/1	0.93	0.20	48,48,48,48	0
56	MG	BA	3725	1/1	0.93	0.11	29,29,29,29	0
56	MG	BA	3729	1/1	0.93	0.14	54,54,54,54	0
56	MG	BA	3732	1/1	0.93	0.48	56,56,56,56	0
56	MG	DA	3516	1/1	0.93	0.20	54,54,54,54	0
56	MG	DA	3185	1/1	0.93	0.33	42,42,42,42	0
56	MG	BA	3572	1/1	0.93	0.19	23,23,23,23	0
56	MG	BA	3179	1/1	0.93	0.32	53,53,53,53	0
56	MG	DA	3524	1/1	0.93	0.24	51,51,51,51	0
56	MG	BA	3117	1/1	0.93	0.27	37,37,37,37	0
56	MG	BA	3357	1/1	0.93	0.17	45,45,45,45	0
56	MG	AA	3048	1/1	0.93	0.10	52,52,52,52	0
56	MG	BA	3367	1/1	0.93	0.19	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
56	MG	DA	3197	1/1	0.93	0.34	43,43,43,43	0
56	MG	DA	3534	1/1	0.93	0.14	62,62,62,62	0
56	MG	DA	3536	1/1	0.93	0.15	57,57,57,57	0
56	MG	AA	3053	1/1	0.93	0.40	56,56,56,56	0
56	MG	DA	3033	1/1	0.93	0.22	41,41,41,41	0
56	MG	AA	3055	1/1	0.93	0.28	56,56,56,56	0
56	MG	BA	3256	1/1	0.93	0.12	60,60,60,60	0
56	MG	DA	3037	1/1	0.93	0.37	37,37,37,37	0
56	MG	BA	3611	1/1	0.93	0.11	61,61,61,61	0
56	MG	AM	3002	1/1	0.93	0.58	60,60,60,60	0
56	MG	BA	3258	1/1	0.93	0.17	35,35,35,35	0
56	MG	BA	3621	1/1	0.93	0.22	57,57,57,57	0
56	MG	DA	3566	1/1	0.93	0.12	55,55,55,55	0
56	MG	BA	3073	1/1	0.93	0.20	43,43,43,43	0
56	MG	BA	3189	1/1	0.93	0.17	39,39,39,39	0
56	MG	DA	3574	1/1	0.93	0.20	22,22,22,22	0
56	MG	DA	3050	1/1	0.93	0.48	30,30,30,30	0
56	MG	AA	3056	1/1	0.93	0.23	61,61,61,61	0
56	MG	DA	3054	1/1	0.93	0.09	34,34,34,34	0
56	MG	DA	3055	1/1	0.93	0.20	55,55,55,55	0
56	MG	DA	3230	1/1	0.93	0.18	61,61,61,61	0
56	MG	DA	3231	1/1	0.93	0.11	45,45,45,45	0
56	MG	DA	3056	1/1	0.93	0.38	37,37,37,37	0
56	MG	BD	312	1/1	0.93	0.97	72,72,72,72	0
56	MG	BE	302	1/1	0.93	0.17	29,29,29,29	0
56	MG	DA	3599	1/1	0.93	0.25	69,69,69,69	0
56	MG	CA	3066	1/1	0.93	0.08	47,47,47,47	0
56	MG	BA	3631	1/1	0.93	0.16	41,41,41,41	0
56	MG	BF	304	1/1	0.93	0.48	30,30,30,30	0
56	MG	DA	3255	1/1	0.93	0.15	46,46,46,46	0
56	MG	DA	3065	1/1	0.93	0.19	40,40,40,40	0
56	MG	DA	3261	1/1	0.93	0.24	44,44,44,44	0
56	MG	BF	305	1/1	0.93	0.31	38,38,38,38	0
56	MG	BA	3262	1/1	0.93	0.31	44,44,44,44	0
56	MG	AA	3110	1/1	0.93	0.13	41,41,41,41	0
56	MG	DA	3274	1/1	0.93	0.40	49,49,49,49	0
56	MG	CA	3076	1/1	0.93	0.28	48,48,48,48	0
56	MG	CA	3078	1/1	0.93	0.25	51,51,51,51	0
56	MG	BG	3003	1/1	0.93	0.21	53,53,53,53	0
56	MG	BG	3004	1/1	0.93	0.06	53,53,53,53	0
56	MG	CA	3089	1/1	0.93	0.17	54,54,54,54	0
56	MG	DA	3288	1/1	0.93	0.22	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	BN	3001	1/1	0.93	0.34	65,65,65,65	0
56	MG	DA	3644	1/1	0.93	0.63	50,50,50,50	0
56	MG	AA	3112	1/1	0.93	0.09	53,53,53,53	0
56	MG	AA	3113	1/1	0.93	0.11	56,56,56,56	0
56	MG	AA	3031	1/1	0.93	0.22	41,41,41,41	0
56	MG	AA	3035	1/1	0.93	0.27	59,59,59,59	0
56	MG	AA	3116	1/1	0.93	0.41	62,62,62,62	0
56	MG	DB	3001	1/1	0.93	0.19	80,80,80,80	0
56	MG	BA	3038	1/1	0.93	0.12	51,51,51,51	0
56	MG	BA	3454	1/1	0.93	0.24	20,20,20,20	0
56	MG	DA	3325	1/1	0.93	0.24	31,31,31,31	0
56	MG	BA	3455	1/1	0.93	0.38	47,47,47,47	0
56	MG	DA	3330	1/1	0.93	0.13	30,30,30,30	0
56	MG	DA	3092	1/1	0.93	0.30	48,48,48,48	0
56	MG	DB	3012	1/1	0.93	0.19	50,50,50,50	0
56	MG	DD	301	1/1	0.93	0.24	23,23,23,23	0
56	MG	AA	3059	1/1	0.93	0.70	49,49,49,49	0
56	MG	DA	3345	1/1	0.93	0.13	16,16,16,16	0
56	MG	BA	3144	1/1	0.93	0.13	52,52,52,52	0
56	MG	DE	302	1/1	0.93	0.33	46,46,46,46	0
56	MG	CA	3125	1/1	0.93	0.20	64,64,64,64	0
56	MG	DF	302	1/1	0.93	0.20	47,47,47,47	0
56	MG	BU	207	1/1	0.93	0.35	38,38,38,38	0
56	MG	BV	3003	1/1	0.93	0.26	27,27,27,27	0
56	MG	CA	3129	1/1	0.93	0.23	54,54,54,54	0
56	MG	DQ	3003	1/1	0.93	0.21	58,58,58,58	0
56	MG	AA	3138	1/1	0.93	0.39	38,38,38,38	0
56	MG	DA	3104	1/1	0.93	0.17	46,46,46,46	0
56	MG	BA	3472	1/1	0.93	0.12	53,53,53,53	0
56	MG	BA	3147	1/1	0.93	0.60	42,42,42,42	0
56	MG	BA	3669	1/1	0.93	0.21	61,61,61,61	0
56	MG	DA	3385	1/1	0.93	0.32	58,58,58,58	0
56	MG	DA	3390	1/1	0.93	0.20	58,58,58,58	0
56	MG	AA	3085	1/1	0.93	0.43	57,57,57,57	0
56	MG	AA	3062	1/1	0.93	0.15	30,30,30,30	0
58	ZN	DY	501	1/1	0.93	0.04	90,90,90,90	0
56	MG	B0	101	1/1	0.93	0.26	57,57,57,57	0
56	MG	B0	104	1/1	0.93	0.32	55,55,55,55	0
56	MG	BA	3051	1/1	0.93	0.30	34,34,34,34	0
56	MG	B2	101	1/1	0.93	0.28	34,34,34,34	0
56	MG	DA	3407	1/1	0.93	0.14	35,35,35,35	0
56	MG	BA	3015	1/1	0.94	0.28	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	BA	3710	1/1	0.94	0.06	57,57,57,57	0
56	MG	DA	3070	1/1	0.94	0.43	51,51,51,51	0
56	MG	AA	3217	1/1	0.94	0.42	64,64,64,64	0
56	MG	CA	3046	1/1	0.94	0.25	52,52,52,52	0
56	MG	CA	3047	1/1	0.94	0.18	56,56,56,56	0
56	MG	BA	3128	1/1	0.94	0.16	28,28,28,28	0
56	MG	DA	3075	1/1	0.94	0.21	45,45,45,45	0
56	MG	BA	3202	1/1	0.94	0.47	29,29,29,29	0
56	MG	BA	3132	1/1	0.94	0.21	28,28,28,28	0
56	MG	DA	3377	1/1	0.94	0.19	32,32,32,32	0
56	MG	DA	3380	1/1	0.94	0.09	40,40,40,40	0
56	MG	DA	3384	1/1	0.94	0.13	24,24,24,24	0
56	MG	BA	3017	1/1	0.94	0.32	38,38,38,38	0
56	MG	DA	3386	1/1	0.94	0.17	18,18,18,18	0
56	MG	BA	3720	1/1	0.94	0.17	51,51,51,51	0
56	MG	AA	3054	1/1	0.94	0.19	46,46,46,46	0
56	MG	BA	3208	1/1	0.94	0.13	50,50,50,50	0
56	MG	AA	3137	1/1	0.94	0.14	40,40,40,40	0
56	MG	BA	3726	1/1	0.94	0.32	29,29,29,29	0
56	MG	DA	3397	1/1	0.94	0.19	40,40,40,40	0
56	MG	AA	3175	1/1	0.94	0.14	70,70,70,70	0
56	MG	DA	3403	1/1	0.94	0.21	42,42,42,42	0
56	MG	DA	3404	1/1	0.94	0.17	57,57,57,57	0
56	MG	BA	3298	1/1	0.94	0.38	45,45,45,45	0
56	MG	DA	3406	1/1	0.94	0.07	48,48,48,48	0
56	MG	BA	3539	1/1	0.94	0.21	23,23,23,23	0
56	MG	BA	3737	1/1	0.94	0.22	39,39,39,39	0
56	MG	BA	3540	1/1	0.94	0.33	29,29,29,29	0
56	MG	DA	3417	1/1	0.94	0.19	54,54,54,54	0
56	MG	CA	3068	1/1	0.94	0.11	47,47,47,47	0
56	MG	AA	3178	1/1	0.94	0.17	63,63,63,63	0
56	MG	BA	3215	1/1	0.94	0.09	32,32,32,32	0
56	MG	AA	3179	1/1	0.94	0.24	34,34,34,34	0
56	MG	BA	3025	1/1	0.94	0.20	48,48,48,48	0
56	MG	BA	3142	1/1	0.94	0.23	57,57,57,57	0
56	MG	BA	3310	1/1	0.94	0.12	59,59,59,59	0
56	MG	CA	3079	1/1	0.94	0.10	37,37,37,37	0
56	MG	BA	3569	1/1	0.94	0.08	55,55,55,55	0
56	MG	AM	3001	1/1	0.94	0.08	76,76,76,76	0
56	MG	DA	3440	1/1	0.94	0.07	48,48,48,48	0
56	MG	AA	3060	1/1	0.94	0.38	52,52,52,52	0
56	MG	BA	3578	1/1	0.94	0.19	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	3580	1/1	0.94	0.17	58,58,58,58	0
56	MG	BA	3226	1/1	0.94	0.31	31,31,31,31	0
56	MG	DA	3452	1/1	0.94	0.19	64,64,64,64	0
56	MG	BA	3326	1/1	0.94	0.24	15,15,15,15	0
56	MG	BD	305	1/1	0.94	0.25	41,41,41,41	0
56	MG	BD	309	1/1	0.94	0.18	43,43,43,43	0
56	MG	BA	3583	1/1	0.94	0.18	57,57,57,57	0
56	MG	CA	3115	1/1	0.94	0.08	81,81,81,81	0
56	MG	CA	3116	1/1	0.94	0.15	76,76,76,76	0
56	MG	BA	3585	1/1	0.94	0.22	25,25,25,25	0
56	MG	BA	3588	1/1	0.94	0.20	41,41,41,41	0
56	MG	CA	3121	1/1	0.94	0.45	59,59,59,59	0
56	MG	BE	304	1/1	0.94	0.49	45,45,45,45	0
56	MG	DA	3132	1/1	0.94	0.64	47,47,47,47	0
56	MG	DA	3470	1/1	0.94	0.17	45,45,45,45	0
56	MG	DA	3134	1/1	0.94	0.22	37,37,37,37	0
56	MG	CA	3123	1/1	0.94	0.12	75,75,75,75	0
56	MG	BE	306	1/1	0.94	0.45	38,38,38,38	0
56	MG	DA	3478	1/1	0.94	0.10	58,58,58,58	0
56	MG	BA	3590	1/1	0.94	0.17	23,23,23,23	0
56	MG	BA	3593	1/1	0.94	0.13	51,51,51,51	0
56	MG	BA	3594	1/1	0.94	0.28	55,55,55,55	0
56	MG	CA	3128	1/1	0.94	0.28	55,55,55,55	0
56	MG	AA	3118	1/1	0.94	0.42	39,39,39,39	0
56	MG	DA	3494	1/1	0.94	0.12	50,50,50,50	0
56	MG	BA	3597	1/1	0.94	0.29	46,46,46,46	0
56	MG	DA	3499	1/1	0.94	0.22	44,44,44,44	0
56	MG	DA	3147	1/1	0.94	0.20	46,46,46,46	0
56	MG	DA	3148	1/1	0.94	0.13	41,41,41,41	0
56	MG	DA	3506	1/1	0.94	0.09	61,61,61,61	0
56	MG	DA	3150	1/1	0.94	0.09	57,57,57,57	0
56	MG	AA	3007	1/1	0.94	0.17	68,68,68,68	0
56	MG	BA	3232	1/1	0.94	0.19	32,32,32,32	0
56	MG	BA	3235	1/1	0.94	0.38	44,44,44,44	0
56	MG	DA	3520	1/1	0.94	0.11	38,38,38,38	0
56	MG	BA	3151	1/1	0.94	0.21	40,40,40,40	0
56	MG	BA	3605	1/1	0.94	0.10	35,35,35,35	0
56	MG	AA	3190	1/1	0.94	0.31	61,61,61,61	0
56	MG	BA	3610	1/1	0.94	1.00	49,49,49,49	0
56	MG	BP	202	1/1	0.94	0.41	47,47,47,47	0
56	MG	BA	3087	1/1	0.94	0.33	48,48,48,48	0
56	MG	AA	3078	1/1	0.94	0.32	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	BA	3614	1/1	0.94	0.20	48,48,48,48	0
56	MG	BA	3615	1/1	0.94	0.23	55,55,55,55	0
56	MG	BA	3359	1/1	0.94	0.15	63,63,63,63	0
56	MG	BA	3620	1/1	0.94	0.29	57,57,57,57	0
56	MG	DA	3539	1/1	0.94	0.20	35,35,35,35	0
56	MG	DA	3173	1/1	0.94	0.29	50,50,50,50	0
56	MG	BU	206	1/1	0.94	0.27	41,41,41,41	0
56	MG	BA	3037	1/1	0.94	0.56	39,39,39,39	0
56	MG	BU	208	1/1	0.94	0.18	42,42,42,42	0
56	MG	DA	3556	1/1	0.94	0.10	35,35,35,35	0
56	MG	DA	3184	1/1	0.94	0.17	54,54,54,54	0
56	MG	BA	3368	1/1	0.94	0.14	22,22,22,22	0
56	MG	AA	3005	1/1	0.94	0.28	66,66,66,66	0
56	MG	BA	3627	1/1	0.94	0.29	50,50,50,50	0
56	MG	BA	3375	1/1	0.94	0.17	44,44,44,44	0
56	MG	BA	3384	1/1	0.94	0.28	47,47,47,47	0
56	MG	AA	3198	1/1	0.94	0.16	73,73,73,73	0
56	MG	DA	3570	1/1	0.94	0.12	67,67,67,67	0
56	MG	DA	3192	1/1	0.94	0.47	48,48,48,48	0
56	MG	BA	3390	1/1	0.94	0.08	40,40,40,40	0
56	MG	DA	3583	1/1	0.94	0.24	35,35,35,35	0
56	MG	BA	3093	1/1	0.94	0.46	52,52,52,52	0
56	MG	CF	3001	1/1	0.94	0.19	56,56,56,56	0
56	MG	B0	103	1/1	0.94	0.17	46,46,46,46	0
56	MG	DA	3587	1/1	0.94	0.22	57,57,57,57	0
56	MG	BA	3042	1/1	0.94	0.14	50,50,50,50	0
56	MG	BA	3043	1/1	0.94	0.38	33,33,33,33	0
56	MG	CX	104	1/1	0.94	0.11	52,52,52,52	0
56	MG	DA	3595	1/1	0.94	0.22	53,53,53,53	0
56	MG	AA	3146	1/1	0.94	0.20	55,55,55,55	0
56	MG	DA	3211	1/1	0.94	0.20	46,46,46,46	0
56	MG	BA	3643	1/1	0.94	0.20	59,59,59,59	0
56	MG	DA	3601	1/1	0.94	0.23	50,50,50,50	0
56	MG	AA	3201	1/1	0.94	0.12	76,76,76,76	0
56	MG	B8	5002	1/1	0.94	0.23	48,48,48,48	0
56	MG	BA	3168	1/1	0.94	0.45	52,52,52,52	0
56	MG	BA	3047	1/1	0.94	0.35	30,30,30,30	0
56	MG	DA	3612	1/1	0.94	0.32	46,46,46,46	0
56	MG	DA	3010	1/1	0.94	0.25	42,42,42,42	0
56	MG	CA	3003	1/1	0.94	0.13	69,69,69,69	0
56	MG	CA	3004	1/1	0.94	0.34	88,88,88,88	0
56	MG	DA	3226	1/1	0.94	0.18	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	DA	3619	1/1	0.94	0.13	67,67,67,67	0
56	MG	DA	3620	1/1	0.94	0.20	66,66,66,66	0
56	MG	CA	3005	1/1	0.94	0.38	37,37,37,37	0
56	MG	AA	3132	1/1	0.94	0.21	59,59,59,59	0
56	MG	BA	3425	1/1	0.94	0.22	42,42,42,42	0
56	MG	BA	3650	1/1	0.94	0.13	44,44,44,44	0
56	MG	DA	3628	1/1	0.94	0.15	38,38,38,38	0
56	MG	DA	3235	1/1	0.94	0.41	46,46,46,46	0
56	MG	DA	3236	1/1	0.94	0.16	38,38,38,38	0
56	MG	DA	3237	1/1	0.94	0.34	37,37,37,37	0
56	MG	BA	3173	1/1	0.94	0.23	41,41,41,41	0
56	MG	DA	3639	1/1	0.94	0.14	55,55,55,55	0
56	MG	DA	3641	1/1	0.94	0.21	47,47,47,47	0
56	MG	DA	3019	1/1	0.94	0.21	32,32,32,32	0
56	MG	DA	3022	1/1	0.94	0.18	41,41,41,41	0
56	MG	DA	3244	1/1	0.94	0.19	23,23,23,23	0
56	MG	DA	3245	1/1	0.94	0.25	43,43,43,43	0
56	MG	DA	3246	1/1	0.94	0.16	55,55,55,55	0
56	MG	CA	3010	1/1	0.94	0.15	34,34,34,34	0
56	MG	BA	3660	1/1	0.94	0.15	58,58,58,58	0
56	MG	DA	3658	1/1	0.94	0.30	50,50,50,50	0
56	MG	CA	3013	1/1	0.94	0.09	46,46,46,46	0
56	MG	AA	3004	1/1	0.94	0.16	50,50,50,50	0
56	MG	BA	3104	1/1	0.94	0.39	34,34,34,34	0
56	MG	DB	3004	1/1	0.94	0.11	56,56,56,56	0
56	MG	BA	3433	1/1	0.94	0.29	46,46,46,46	0
56	MG	BA	3052	1/1	0.94	0.26	29,29,29,29	0
56	MG	BA	3672	1/1	0.94	0.25	63,63,63,63	0
56	MG	DB	3009	1/1	0.94	0.38	41,41,41,41	0
56	MG	DA	3268	1/1	0.94	0.18	42,42,42,42	0
56	MG	DB	3011	1/1	0.94	0.33	49,49,49,49	0
56	MG	DA	3270	1/1	0.94	0.28	55,55,55,55	0
56	MG	AA	3207	1/1	0.94	0.19	51,51,51,51	0
56	MG	BA	3446	1/1	0.94	0.21	25,25,25,25	0
56	MG	BA	3054	1/1	0.94	0.19	39,39,39,39	0
56	MG	BA	3453	1/1	0.94	0.31	54,54,54,54	0
56	MG	BA	3181	1/1	0.94	0.13	37,37,37,37	0
56	MG	AA	3043	1/1	0.94	0.32	63,63,63,63	0
56	MG	DE	306	1/1	0.94	0.13	44,44,44,44	0
56	MG	BA	3456	1/1	0.94	0.20	24,24,24,24	0
56	MG	BA	3183	1/1	0.94	0.25	40,40,40,40	0
56	MG	DA	3292	1/1	0.94	0.18	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DN	5001	1/1	0.94	0.12	71,71,71,71	0
56	MG	DP	202	1/1	0.94	0.22	54,54,54,54	0
56	MG	DA	3051	1/1	0.94	0.14	39,39,39,39	0
56	MG	BA	3056	1/1	0.94	0.25	39,39,39,39	0
56	MG	AA	3211	1/1	0.94	0.11	58,58,58,58	0
56	MG	BA	3468	1/1	0.94	0.18	45,45,45,45	0
56	MG	BA	3186	1/1	0.94	0.17	50,50,50,50	0
56	MG	AA	3213	1/1	0.94	0.12	74,74,74,74	0
56	MG	DV	203	1/1	0.94	0.31	41,41,41,41	0
56	MG	DA	3059	1/1	0.94	0.05	42,42,42,42	0
56	MG	DA	3319	1/1	0.94	0.13	31,31,31,31	0
56	MG	DA	3322	1/1	0.94	0.06	41,41,41,41	0
56	MG	D5	101	1/1	0.94	0.63	44,44,44,44	0
56	MG	AA	3074	1/1	0.94	0.30	40,40,40,40	0
56	MG	BA	3270	1/1	0.94	0.30	29,29,29,29	0
56	MG	AA	3166	1/1	0.94	0.21	55,55,55,55	0
56	MG	DA	3333	1/1	0.94	0.14	61,61,61,61	0
56	MG	BA	3012	1/1	0.94	0.11	34,34,34,34	0
56	MG	DA	3340	1/1	0.94	0.12	29,29,29,29	0
56	MG	CA	3038	1/1	0.94	0.26	54,54,54,54	0
56	MG	BA	3486	1/1	0.94	0.27	55,55,55,55	0
56	MG	AA	3176	1/1	0.95	0.11	60,60,60,60	0
56	MG	AA	3205	1/1	0.95	0.20	66,66,66,66	0
56	MG	BA	3564	1/1	0.95	0.17	26,26,26,26	0
56	MG	BA	3565	1/1	0.95	0.13	75,75,75,75	0
56	MG	BB	3002	1/1	0.95	0.19	49,49,49,49	0
56	MG	DA	3394	1/1	0.95	0.07	46,46,46,46	0
56	MG	BA	3350	1/1	0.95	0.27	36,36,36,36	0
56	MG	BA	3353	1/1	0.95	0.25	31,31,31,31	0
56	MG	AA	3206	1/1	0.95	0.12	79,79,79,79	0
56	MG	DA	3398	1/1	0.95	0.10	50,50,50,50	0
56	MG	DA	3105	1/1	0.95	0.16	56,56,56,56	0
56	MG	AX	106	1/1	0.95	0.09	64,64,64,64	0
56	MG	DA	3107	1/1	0.95	0.13	50,50,50,50	0
56	MG	BB	3007	1/1	0.95	0.15	49,49,49,49	0
56	MG	BA	3034	1/1	0.95	0.15	37,37,37,37	0
56	MG	BA	3573	1/1	0.95	0.14	53,53,53,53	0
56	MG	BA	3131	1/1	0.95	0.13	31,31,31,31	0
56	MG	CA	3087	1/1	0.95	0.14	40,40,40,40	0
56	MG	DA	3415	1/1	0.95	0.10	22,22,22,22	0
56	MG	BA	3361	1/1	0.95	0.12	39,39,39,39	0
56	MG	CA	3090	1/1	0.95	0.15	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	BB	3015	1/1	0.95	0.09	35,35,35,35	0
56	MG	CA	3100	1/1	0.95	0.18	72,72,72,72	0
56	MG	BA	3366	1/1	0.95	0.14	30,30,30,30	0
56	MG	CA	3102	1/1	0.95	0.06	55,55,55,55	0
56	MG	BA	3078	1/1	0.95	0.33	44,44,44,44	0
56	MG	CA	3105	1/1	0.95	0.07	59,59,59,59	0
56	MG	BD	302	1/1	0.95	0.60	44,44,44,44	0
56	MG	DA	3432	1/1	0.95	0.22	37,37,37,37	0
56	MG	AA	3177	1/1	0.95	0.13	58,58,58,58	0
56	MG	DA	3127	1/1	0.95	0.16	44,44,44,44	0
56	MG	DA	3437	1/1	0.95	0.21	46,46,46,46	0
56	MG	DA	3439	1/1	0.95	0.23	45,45,45,45	0
56	MG	DA	3128	1/1	0.95	0.33	54,54,54,54	0
56	MG	CA	3108	1/1	0.95	0.17	45,45,45,45	0
56	MG	DA	3443	1/1	0.95	0.23	30,30,30,30	0
56	MG	BA	3371	1/1	0.95	0.17	38,38,38,38	0
56	MG	DA	3445	1/1	0.95	0.44	60,60,60,60	0
56	MG	CA	3111	1/1	0.95	0.10	69,69,69,69	0
56	MG	AA	3016	1/1	0.95	0.10	70,70,70,70	0
56	MG	DA	3449	1/1	0.95	0.29	46,46,46,46	0
56	MG	AA	3061	1/1	0.95	0.09	57,57,57,57	0
56	MG	BA	3376	1/1	0.95	0.32	35,35,35,35	0
56	MG	BA	3377	1/1	0.95	0.14	27,27,27,27	0
56	MG	BA	3595	1/1	0.95	0.15	37,37,37,37	0
56	MG	DA	3140	1/1	0.95	0.31	55,55,55,55	0
56	MG	BE	305	1/1	0.95	0.68	44,44,44,44	0
56	MG	DA	3142	1/1	0.95	0.23	33,33,33,33	0
56	MG	AA	3160	1/1	0.95	0.29	52,52,52,52	0
56	MG	BE	307	1/1	0.95	0.29	51,51,51,51	0
56	MG	AA	3181	1/1	0.95	0.19	46,46,46,46	0
56	MG	DA	3467	1/1	0.95	0.37	48,48,48,48	0
56	MG	BA	3386	1/1	0.95	0.13	29,29,29,29	0
56	MG	BA	3388	1/1	0.95	0.26	30,30,30,30	0
56	MG	AA	3101	1/1	0.95	0.12	61,61,61,61	0
56	MG	BA	3391	1/1	0.95	0.20	39,39,39,39	0
56	MG	AA	3216	1/1	0.95	0.30	60,60,60,60	0
56	MG	BA	3193	1/1	0.95	0.48	53,53,53,53	0
56	MG	BA	3399	1/1	0.95	0.25	22,22,22,22	0
56	MG	DA	3482	1/1	0.95	0.18	45,45,45,45	0
56	MG	BA	3402	1/1	0.95	0.22	23,23,23,23	0
56	MG	CA	3136	1/1	0.95	0.23	70,70,70,70	0
56	MG	DA	3161	1/1	0.95	0.19	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\AA^2$)	Q<0.9
56	MG	DA	3162	1/1	0.95	0.06	69,69,69,69	0
56	MG	DA	3492	1/1	0.95	0.09	44,44,44,44	0
56	MG	BA	3404	1/1	0.95	0.10	42,42,42,42	0
56	MG	BA	3613	1/1	0.95	0.18	47,47,47,47	0
56	MG	BA	3194	1/1	0.95	0.52	43,43,43,43	0
56	MG	DA	3166	1/1	0.95	0.08	37,37,37,37	0
56	MG	AA	3184	1/1	0.95	0.14	81,81,81,81	0
56	MG	DA	3501	1/1	0.95	0.11	67,67,67,67	0
56	MG	BA	3199	1/1	0.95	0.31	31,31,31,31	0
56	MG	DA	3504	1/1	0.95	0.15	46,46,46,46	0
56	MG	BP	204	1/1	0.95	0.08	53,53,53,53	0
56	MG	BA	3618	1/1	0.95	0.23	37,37,37,37	0
56	MG	BA	3009	1/1	0.95	0.24	36,36,36,36	0
56	MG	DA	3513	1/1	0.95	0.18	58,58,58,58	0
56	MG	DA	3514	1/1	0.95	0.20	60,60,60,60	0
56	MG	BR	202	1/1	0.95	0.25	25,25,25,25	0
56	MG	BA	3010	1/1	0.95	0.09	35,35,35,35	0
56	MG	DA	3177	1/1	0.95	0.21	30,30,30,30	0
56	MG	DA	3178	1/1	0.95	0.20	43,43,43,43	0
56	MG	BU	201	1/1	0.95	0.64	33,33,33,33	0
56	MG	CA	3154	1/1	0.95	0.16	54,54,54,54	0
56	MG	DA	3525	1/1	0.95	0.10	56,56,56,56	0
56	MG	BA	3624	1/1	0.95	0.17	73,73,73,73	0
56	MG	AA	3185	1/1	0.95	0.28	47,47,47,47	0
56	MG	AA	3187	1/1	0.95	0.06	72,72,72,72	0
56	MG	BA	3428	1/1	0.95	0.42	36,36,36,36	0
56	MG	BA	3150	1/1	0.95	0.32	42,42,42,42	0
56	MG	DA	3533	1/1	0.95	0.14	59,59,59,59	0
56	MG	BV	3001	1/1	0.95	0.26	42,42,42,42	0
56	MG	BA	3096	1/1	0.95	0.22	35,35,35,35	0
56	MG	BA	3277	1/1	0.95	0.45	45,45,45,45	0
56	MG	DA	3193	1/1	0.95	0.20	42,42,42,42	0
56	MG	DA	3194	1/1	0.95	0.60	65,65,65,65	0
56	MG	DA	3541	1/1	0.95	0.16	55,55,55,55	0
56	MG	AA	3163	1/1	0.95	0.24	23,23,23,23	0
56	MG	DA	3543	1/1	0.95	0.20	52,52,52,52	0
56	MG	DA	3547	1/1	0.95	0.12	47,47,47,47	0
56	MG	DA	3548	1/1	0.95	0.16	60,60,60,60	0
56	MG	CA	3170	1/1	0.95	0.38	44,44,44,44	0
56	MG	DA	3552	1/1	0.95	0.13	42,42,42,42	0
56	MG	DA	3199	1/1	0.95	0.15	46,46,46,46	0
56	MG	DA	3200	1/1	0.95	0.93	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	AA	3011	1/1	0.95	0.64	44,44,44,44	0
56	MG	BW	3004	1/1	0.95	0.61	46,46,46,46	0
56	MG	BA	3442	1/1	0.95	0.18	33,33,33,33	0
56	MG	BA	3280	1/1	0.95	0.33	44,44,44,44	0
56	MG	DA	3206	1/1	0.95	0.42	36,36,36,36	0
56	MG	AA	3019	1/1	0.95	0.42	64,64,64,64	0
56	MG	DA	3209	1/1	0.95	0.10	44,44,44,44	0
56	MG	DA	3569	1/1	0.95	0.07	54,54,54,54	0
56	MG	AK	3001	1/1	0.95	0.13	48,48,48,48	0
56	MG	DA	3572	1/1	0.95	0.10	39,39,39,39	0
56	MG	BA	3449	1/1	0.95	0.10	59,59,59,59	0
56	MG	BA	3019	1/1	0.95	0.10	42,42,42,42	0
56	MG	DA	3578	1/1	0.95	0.15	68,68,68,68	0
56	MG	BA	3288	1/1	0.95	0.10	45,45,45,45	0
56	MG	DA	3002	1/1	0.95	0.23	47,47,47,47	0
56	MG	BA	3219	1/1	0.95	0.36	36,36,36,36	0
56	MG	B3	3402	1/1	0.95	0.08	49,49,49,49	0
56	MG	B3	3403	1/1	0.95	0.39	37,37,37,37	0
56	MG	DA	3588	1/1	0.95	0.13	47,47,47,47	0
56	MG	BA	3290	1/1	0.95	0.15	35,35,35,35	0
56	MG	DA	3590	1/1	0.95	0.18	39,39,39,39	0
56	MG	BA	3221	1/1	0.95	0.63	55,55,55,55	0
56	MG	B8	5001	1/1	0.95	0.16	62,62,62,62	0
56	MG	AL	3001	1/1	0.95	0.15	50,50,50,50	0
56	MG	BA	3656	1/1	0.95	0.27	70,70,70,70	0
56	MG	CA	3001	1/1	0.95	0.20	48,48,48,48	0
56	MG	BA	3657	1/1	0.95	0.19	29,29,29,29	0
56	MG	BA	3466	1/1	0.95	0.12	53,53,53,53	0
56	MG	AA	3070	1/1	0.95	0.19	68,68,68,68	0
56	MG	BA	3062	1/1	0.95	0.44	46,46,46,46	0
56	MG	BA	3471	1/1	0.95	0.11	28,28,28,28	0
56	MG	DA	3607	1/1	0.95	0.17	68,68,68,68	0
56	MG	BA	3668	1/1	0.95	0.21	42,42,42,42	0
56	MG	DA	3611	1/1	0.95	0.16	51,51,51,51	0
56	MG	BA	3106	1/1	0.95	0.32	52,52,52,52	0
56	MG	BA	3297	1/1	0.95	0.39	43,43,43,43	0
56	MG	BA	3475	1/1	0.95	0.07	42,42,42,42	0
56	MG	BA	3063	1/1	0.95	0.14	34,34,34,34	0
56	MG	BA	3108	1/1	0.95	0.17	32,32,32,32	0
56	MG	DA	3252	1/1	0.95	0.23	36,36,36,36	0
56	MG	DA	3030	1/1	0.95	0.26	49,49,49,49	0
56	MG	BA	3677	1/1	0.95	0.22	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	3679	1/1	0.95	0.12	39,39,39,39	0
56	MG	DA	3259	1/1	0.95	0.22	45,45,45,45	0
56	MG	AA	3170	1/1	0.95	0.16	83,83,83,83	0
56	MG	BA	3684	1/1	0.95	0.16	44,44,44,44	0
56	MG	BA	3234	1/1	0.95	0.36	48,48,48,48	0
56	MG	DA	3264	1/1	0.95	0.20	38,38,38,38	0
56	MG	DA	3635	1/1	0.95	0.12	39,39,39,39	0
56	MG	DA	3266	1/1	0.95	0.19	32,32,32,32	0
56	MG	DA	3039	1/1	0.95	0.60	46,46,46,46	0
56	MG	BA	3169	1/1	0.95	0.23	39,39,39,39	0
56	MG	DA	3640	1/1	0.95	0.19	53,53,53,53	0
56	MG	DA	3269	1/1	0.95	0.14	47,47,47,47	0
56	MG	BA	3492	1/1	0.95	0.18	48,48,48,48	0
56	MG	DA	3643	1/1	0.95	0.27	18,18,18,18	0
56	MG	BA	3236	1/1	0.95	0.33	37,37,37,37	0
56	MG	BA	3690	1/1	0.95	0.23	55,55,55,55	0
56	MG	BA	3502	1/1	0.95	0.21	59,59,59,59	0
56	MG	DA	3281	1/1	0.95	0.14	33,33,33,33	0
56	MG	DA	3651	1/1	0.95	0.14	48,48,48,48	0
56	MG	BA	3237	1/1	0.95	0.16	43,43,43,43	0
56	MG	BA	3312	1/1	0.95	0.11	43,43,43,43	0
56	MG	DA	3284	1/1	0.95	0.17	45,45,45,45	0
56	MG	DA	3285	1/1	0.95	0.12	41,41,41,41	0
56	MG	AA	3171	1/1	0.95	0.29	77,77,77,77	0
56	MG	BA	3507	1/1	0.95	0.21	37,37,37,37	0
56	MG	BA	3699	1/1	0.95	0.15	23,23,23,23	0
56	MG	DA	3290	1/1	0.95	0.20	59,59,59,59	0
56	MG	BA	3112	1/1	0.95	0.11	46,46,46,46	0
56	MG	BA	3510	1/1	0.95	0.16	66,66,66,66	0
56	MG	BA	3323	1/1	0.95	0.17	25,25,25,25	0
56	MG	AA	3200	1/1	0.95	0.30	79,79,79,79	0
56	MG	AA	3107	1/1	0.95	0.31	44,44,44,44	0
56	MG	BA	3519	1/1	0.95	0.07	57,57,57,57	0
56	MG	BA	3328	1/1	0.95	0.19	41,41,41,41	0
56	MG	DA	3316	1/1	0.95	0.27	47,47,47,47	0
56	MG	DD	303	1/1	0.95	0.62	48,48,48,48	0
56	MG	BA	3711	1/1	0.95	0.46	64,64,64,64	0
56	MG	DD	305	1/1	0.95	0.14	73,73,73,73	0
56	MG	BA	3712	1/1	0.95	0.24	47,47,47,47	0
56	MG	BA	3069	1/1	0.95	0.10	33,33,33,33	0
56	MG	BA	3532	1/1	0.95	0.21	42,42,42,42	0
56	MG	BA	3533	1/1	0.95	0.29	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DF	301	1/1	0.95	0.38	40,40,40,40	0
56	MG	BA	3536	1/1	0.95	0.17	37,37,37,37	0
56	MG	BA	3332	1/1	0.95	0.13	52,52,52,52	0
56	MG	BA	3719	1/1	0.95	0.07	63,63,63,63	0
56	MG	CA	3051	1/1	0.95	0.16	77,77,77,77	0
56	MG	DO	5001	1/1	0.95	0.10	33,33,33,33	0
56	MG	BA	3333	1/1	0.95	0.15	27,27,27,27	0
56	MG	DA	3076	1/1	0.95	0.46	38,38,38,38	0
56	MG	BA	3721	1/1	0.95	0.34	56,56,56,56	0
56	MG	DA	3348	1/1	0.95	0.10	39,39,39,39	0
56	MG	BA	3177	1/1	0.95	0.57	35,35,35,35	0
56	MG	DA	3352	1/1	0.95	0.26	24,24,24,24	0
56	MG	DV	201	1/1	0.95	0.30	56,56,56,56	0
56	MG	BA	3542	1/1	0.95	0.19	37,37,37,37	0
56	MG	BA	3545	1/1	0.95	0.19	20,20,20,20	0
56	MG	BA	3547	1/1	0.95	0.19	30,30,30,30	0
56	MG	CA	3059	1/1	0.95	0.18	51,51,51,51	0
56	MG	DA	3363	1/1	0.95	0.20	56,56,56,56	0
56	MG	CA	3060	1/1	0.95	0.35	59,59,59,59	0
56	MG	AA	3047	1/1	0.95	0.47	59,59,59,59	0
56	MG	BA	3341	1/1	0.95	0.17	31,31,31,31	0
58	ZN	CN	501	1/1	0.95	0.11	104,104,104,104	0
56	MG	BA	3558	1/1	0.95	0.19	47,47,47,47	0
56	MG	BA	3734	1/1	0.95	0.33	42,42,42,42	0
56	MG	DA	3379	1/1	0.95	0.13	63,63,63,63	0
56	MG	DA	3093	1/1	0.95	0.12	51,51,51,51	0
56	MG	DA	3381	1/1	0.95	0.24	68,68,68,68	0
56	MG	DA	3094	1/1	0.95	0.25	26,26,26,26	0
56	MG	AA	3195	1/1	0.96	0.21	58,58,58,58	0
56	MG	DA	3198	1/1	0.96	0.31	34,34,34,34	0
56	MG	BA	3479	1/1	0.96	0.15	44,44,44,44	0
56	MG	CA	3040	1/1	0.96	0.36	47,47,47,47	0
56	MG	BA	3111	1/1	0.96	0.17	43,43,43,43	0
56	MG	BA	3083	1/1	0.96	0.10	33,33,33,33	0
56	MG	DA	3028	1/1	0.96	0.07	34,34,34,34	0
56	MG	BA	3622	1/1	0.96	0.26	32,32,32,32	0
56	MG	CA	3044	1/1	0.96	0.12	52,52,52,52	0
56	MG	DA	3471	1/1	0.96	0.13	32,32,32,32	0
56	MG	DA	3032	1/1	0.96	0.10	36,36,36,36	0
56	MG	BA	3623	1/1	0.96	0.15	43,43,43,43	0
56	MG	DA	3474	1/1	0.96	0.09	49,49,49,49	0
56	MG	DA	3034	1/1	0.96	0.19	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	3476	1/1	0.96	0.13	35,35,35,35	0
56	MG	AA	3196	1/1	0.96	0.28	78,78,78,78	0
56	MG	BB	3018	1/1	0.96	0.27	54,54,54,54	0
56	MG	CA	3049	1/1	0.96	0.14	51,51,51,51	0
56	MG	BA	3114	1/1	0.96	0.25	46,46,46,46	0
56	MG	DA	3215	1/1	0.96	0.30	43,43,43,43	0
56	MG	DA	3489	1/1	0.96	0.08	36,36,36,36	0
56	MG	BA	3487	1/1	0.96	0.20	47,47,47,47	0
56	MG	BD	303	1/1	0.96	0.25	35,35,35,35	0
56	MG	BA	3373	1/1	0.96	0.08	48,48,48,48	0
56	MG	BA	3498	1/1	0.96	0.29	81,81,81,81	0
56	MG	BA	3630	1/1	0.96	0.13	48,48,48,48	0
56	MG	DA	3044	1/1	0.96	0.22	45,45,45,45	0
56	MG	BD	310	1/1	0.96	0.33	48,48,48,48	0
56	MG	DA	3228	1/1	0.96	0.19	49,49,49,49	0
56	MG	BA	3116	1/1	0.96	0.25	30,30,30,30	0
56	MG	DA	3503	1/1	0.96	0.09	41,41,41,41	0
56	MG	AA	3083	1/1	0.96	0.09	56,56,56,56	0
56	MG	BA	3195	1/1	0.96	0.12	37,37,37,37	0
56	MG	BA	3295	1/1	0.96	0.14	30,30,30,30	0
56	MG	BA	3024	1/1	0.96	0.13	31,31,31,31	0
56	MG	BA	3638	1/1	0.96	0.09	73,73,73,73	0
56	MG	DA	3239	1/1	0.96	0.11	54,54,54,54	0
56	MG	DA	3515	1/1	0.96	0.07	57,57,57,57	0
56	MG	AX	109	1/1	0.96	0.10	56,56,56,56	0
56	MG	DA	3058	1/1	0.96	0.16	56,56,56,56	0
56	MG	BE	308	1/1	0.96	0.26	27,27,27,27	0
56	MG	BA	3162	1/1	0.96	0.28	43,43,43,43	0
56	MG	AA	3095	1/1	0.96	0.19	54,54,54,54	0
56	MG	BA	3512	1/1	0.96	0.18	42,42,42,42	0
56	MG	DA	3248	1/1	0.96	0.20	30,30,30,30	0
56	MG	DA	3527	1/1	0.96	0.11	58,58,58,58	0
56	MG	BA	3513	1/1	0.96	0.31	51,51,51,51	0
56	MG	DA	3250	1/1	0.96	0.09	42,42,42,42	0
56	MG	CA	3072	1/1	0.96	0.23	57,57,57,57	0
56	MG	AA	3221	1/1	0.96	0.12	52,52,52,52	0
56	MG	BA	3515	1/1	0.96	0.24	46,46,46,46	0
56	MG	BA	3165	1/1	0.96	0.47	44,44,44,44	0
56	MG	BA	3395	1/1	0.96	0.41	56,56,56,56	0
56	MG	AA	3151	1/1	0.96	0.07	49,49,49,49	0
56	MG	BA	3398	1/1	0.96	0.13	36,36,36,36	0
56	MG	DA	3538	1/1	0.96	0.19	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	CA	3083	1/1	0.96	0.10	30,30,30,30	0
56	MG	BA	3525	1/1	0.96	0.16	31,31,31,31	0
56	MG	CA	3085	1/1	0.96	0.27	58,58,58,58	0
56	MG	CA	3086	1/1	0.96	0.13	70,70,70,70	0
56	MG	BN	3006	1/1	0.96	0.06	33,33,33,33	0
56	MG	BA	3658	1/1	0.96	0.25	62,62,62,62	0
56	MG	BA	3526	1/1	0.96	0.09	49,49,49,49	0
56	MG	BA	3529	1/1	0.96	0.22	22,22,22,22	0
56	MG	DA	3550	1/1	0.96	0.10	54,54,54,54	0
56	MG	CA	3093	1/1	0.96	0.09	65,65,65,65	0
56	MG	DA	3553	1/1	0.96	0.18	58,58,58,58	0
56	MG	DA	3277	1/1	0.96	0.07	46,46,46,46	0
56	MG	BA	3303	1/1	0.96	0.21	11,11,11,11	0
56	MG	DA	3280	1/1	0.96	0.25	46,46,46,46	0
56	MG	BQ	3001	1/1	0.96	0.32	38,38,38,38	0
56	MG	DA	3088	1/1	0.96	0.16	47,47,47,47	0
56	MG	DA	3562	1/1	0.96	0.21	41,41,41,41	0
56	MG	DA	3563	1/1	0.96	0.15	49,49,49,49	0
56	MG	BA	3663	1/1	0.96	0.21	73,73,73,73	0
56	MG	BA	3400	1/1	0.96	0.18	29,29,29,29	0
56	MG	BA	3306	1/1	0.96	0.16	19,19,19,19	0
56	MG	AA	3111	1/1	0.96	0.16	70,70,70,70	0
56	MG	BA	3671	1/1	0.96	0.10	44,44,44,44	0
56	MG	BU	202	1/1	0.96	0.71	41,41,41,41	0
56	MG	DA	3571	1/1	0.96	0.09	57,57,57,57	0
56	MG	DA	3095	1/1	0.96	0.24	53,53,53,53	0
56	MG	CA	3109	1/1	0.96	0.10	79,79,79,79	0
56	MG	BU	203	1/1	0.96	0.26	26,26,26,26	0
56	MG	DA	3576	1/1	0.96	0.18	57,57,57,57	0
56	MG	DA	3577	1/1	0.96	0.19	44,44,44,44	0
56	MG	BA	3127	1/1	0.96	0.36	42,42,42,42	0
56	MG	DA	3297	1/1	0.96	0.16	36,36,36,36	0
56	MG	CA	3113	1/1	0.96	0.26	84,84,84,84	0
56	MG	BA	3406	1/1	0.96	0.22	54,54,54,54	0
56	MG	DA	3300	1/1	0.96	0.16	47,47,47,47	0
56	MG	DA	3302	1/1	0.96	0.27	42,42,42,42	0
56	MG	DA	3303	1/1	0.96	0.17	37,37,37,37	0
56	MG	DA	3305	1/1	0.96	0.20	33,33,33,33	0
56	MG	AA	3034	1/1	0.96	0.20	46,46,46,46	0
56	MG	DA	3308	1/1	0.96	0.09	32,32,32,32	0
56	MG	DA	3310	1/1	0.96	0.27	30,30,30,30	0
56	MG	DA	3594	1/1	0.96	0.31	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
56	MG	BA	3214	1/1	0.96	0.22	37,37,37,37	0
56	MG	BA	3413	1/1	0.96	0.08	19,19,19,19	0
56	MG	DA	3597	1/1	0.96	0.14	66,66,66,66	0
56	MG	CA	3118	1/1	0.96	0.08	39,39,39,39	0
56	MG	BU	209	1/1	0.96	0.96	36,36,36,36	0
56	MG	BA	3314	1/1	0.96	0.14	22,22,22,22	0
56	MG	DA	3323	1/1	0.96	0.19	60,60,60,60	0
56	MG	BA	3548	1/1	0.96	0.28	40,40,40,40	0
56	MG	DA	3604	1/1	0.96	0.08	50,50,50,50	0
56	MG	DA	3605	1/1	0.96	0.07	58,58,58,58	0
56	MG	BA	3681	1/1	0.96	0.15	54,54,54,54	0
56	MG	DA	3329	1/1	0.96	0.13	40,40,40,40	0
56	MG	AA	3202	1/1	0.96	0.22	72,72,72,72	0
56	MG	DA	3610	1/1	0.96	0.11	49,49,49,49	0
56	MG	BA	3685	1/1	0.96	0.26	58,58,58,58	0
56	MG	DA	3334	1/1	0.96	0.16	37,37,37,37	0
56	MG	DA	3335	1/1	0.96	0.21	36,36,36,36	0
56	MG	BA	3420	1/1	0.96	0.18	13,13,13,13	0
56	MG	BA	3552	1/1	0.96	0.28	30,30,30,30	0
56	MG	DA	3343	1/1	0.96	0.12	37,37,37,37	0
56	MG	DA	3114	1/1	0.96	0.19	47,47,47,47	0
56	MG	BA	3555	1/1	0.96	0.25	31,31,31,31	0
56	MG	BA	3319	1/1	0.96	0.14	34,34,34,34	0
56	MG	AA	3021	1/1	0.96	0.16	76,76,76,76	0
56	MG	DA	3624	1/1	0.96	0.11	54,54,54,54	0
56	MG	B0	102	1/1	0.96	0.18	50,50,50,50	0
56	MG	DA	3120	1/1	0.96	0.62	50,50,50,50	0
56	MG	BA	3427	1/1	0.96	0.19	20,20,20,20	0
56	MG	BA	3036	1/1	0.96	0.17	25,25,25,25	0
56	MG	AA	3122	1/1	0.96	0.42	40,40,40,40	0
56	MG	B1	3001	1/1	0.96	0.79	63,63,63,63	0
56	MG	CA	3140	1/1	0.96	0.14	75,75,75,75	0
56	MG	DA	3126	1/1	0.96	0.12	61,61,61,61	0
56	MG	BA	3566	1/1	0.96	0.22	43,43,43,43	0
56	MG	AA	3036	1/1	0.96	0.22	69,69,69,69	0
56	MG	CA	3143	1/1	0.96	0.06	91,91,91,91	0
56	MG	DA	3376	1/1	0.96	0.16	42,42,42,42	0
56	MG	BA	3136	1/1	0.96	0.19	47,47,47,47	0
56	MG	BA	3700	1/1	0.96	0.25	26,26,26,26	0
56	MG	DA	3133	1/1	0.96	0.12	31,31,31,31	0
56	MG	AA	3066	1/1	0.96	0.20	41,41,41,41	0
56	MG	BA	3434	1/1	0.96	0.31	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	CA	3148	1/1	0.96	0.17	65,65,65,65	0
56	MG	BA	3013	1/1	0.96	0.45	36,36,36,36	0
56	MG	BA	3438	1/1	0.96	0.21	30,30,30,30	0
56	MG	DA	3657	1/1	0.96	0.35	55,55,55,55	0
56	MG	BA	3576	1/1	0.96	0.10	45,45,45,45	0
56	MG	BA	3439	1/1	0.96	0.09	35,35,35,35	0
56	MG	AA	3144	1/1	0.96	0.09	56,56,56,56	0
56	MG	BA	3335	1/1	0.96	0.15	51,51,51,51	0
56	MG	AA	3145	1/1	0.96	0.24	63,63,63,63	0
56	MG	AA	3172	1/1	0.96	0.07	36,36,36,36	0
56	MG	BA	3342	1/1	0.96	0.24	46,46,46,46	0
56	MG	DB	3007	1/1	0.96	0.29	45,45,45,45	0
56	MG	DA	3399	1/1	0.96	0.21	39,39,39,39	0
56	MG	BA	3715	1/1	0.96	0.34	44,44,44,44	0
56	MG	BA	3586	1/1	0.96	0.25	26,26,26,26	0
56	MG	BA	3451	1/1	0.96	0.10	31,31,31,31	0
56	MG	BA	3344	1/1	0.96	0.15	65,65,65,65	0
56	MG	CA	3169	1/1	0.96	0.19	52,52,52,52	0
56	MG	BA	3592	1/1	0.96	0.16	43,43,43,43	0
56	MG	BA	3231	1/1	0.96	0.26	50,50,50,50	0
56	MG	BA	3347	1/1	0.96	0.14	44,44,44,44	0
56	MG	BA	3273	1/1	0.96	0.61	35,35,35,35	0
56	MG	CE	3002	1/1	0.96	0.07	69,69,69,69	0
56	MG	BA	3458	1/1	0.96	0.21	46,46,46,46	0
56	MG	DE	303	1/1	0.96	0.15	36,36,36,36	0
56	MG	BA	3724	1/1	0.96	0.21	22,22,22,22	0
56	MG	BA	3459	1/1	0.96	0.13	51,51,51,51	0
56	MG	CX	102	1/1	0.96	0.07	60,60,60,60	0
56	MG	CA	3020	1/1	0.96	0.22	45,45,45,45	0
56	MG	BA	3274	1/1	0.96	0.14	54,54,54,54	0
56	MG	CA	3022	1/1	0.96	0.05	67,67,67,67	0
56	MG	BA	3728	1/1	0.96	0.24	56,56,56,56	0
56	MG	BA	3461	1/1	0.96	0.14	33,33,33,33	0
56	MG	DA	3433	1/1	0.96	0.23	39,39,39,39	0
56	MG	DA	3004	1/1	0.96	0.16	24,24,24,24	0
56	MG	DQ	3002	1/1	0.96	0.34	51,51,51,51	0
56	MG	DA	3435	1/1	0.96	0.16	56,56,56,56	0
56	MG	BA	3464	1/1	0.96	0.18	40,40,40,40	0
56	MG	DR	5001	1/1	0.96	0.19	39,39,39,39	0
56	MG	AA	3108	1/1	0.96	0.31	72,72,72,72	0
56	MG	DA	3438	1/1	0.96	0.30	50,50,50,50	0
56	MG	DA	3007	1/1	0.96	0.26	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\AA^2$)	Q<0.9
56	MG	BA	3233	1/1	0.96	0.19	49,49,49,49	0
56	MG	BA	3735	1/1	0.96	0.28	47,47,47,47	0
56	MG	DA	3442	1/1	0.96	0.30	58,58,58,58	0
56	MG	AA	3191	1/1	0.96	0.11	56,56,56,56	0
56	MG	DY	502	1/1	0.96	0.07	66,66,66,66	0
56	MG	BA	3608	1/1	0.96	0.15	51,51,51,51	0
56	MG	BA	3609	1/1	0.96	0.26	29,29,29,29	0
56	MG	BA	3050	1/1	0.96	0.17	33,33,33,33	0
56	MG	DA	3014	1/1	0.96	0.26	38,38,38,38	0
56	MG	BA	3470	1/1	0.96	0.05	44,44,44,44	0
56	MG	DA	3451	1/1	0.96	0.06	68,68,68,68	0
56	MG	AA	3174	1/1	0.96	0.18	49,49,49,49	0
56	MG	BA	3148	1/1	0.96	0.60	49,49,49,49	0
56	MG	BA	3364	1/1	0.96	0.21	30,30,30,30	0
56	MG	BA	3365	1/1	0.96	0.06	63,63,63,63	0
56	MG	DA	3021	1/1	0.96	0.09	43,43,43,43	0
56	MG	AA	3010	1/1	0.97	0.15	71,71,71,71	0
56	MG	DA	3459	1/1	0.97	0.12	43,43,43,43	0
56	MG	BA	3032	1/1	0.97	0.30	36,36,36,36	0
56	MG	BA	3508	1/1	0.97	0.17	46,46,46,46	0
56	MG	DA	3216	1/1	0.97	0.18	47,47,47,47	0
56	MG	DA	3218	1/1	0.97	0.11	31,31,31,31	0
56	MG	DA	3466	1/1	0.97	0.09	43,43,43,43	0
56	MG	BA	3308	1/1	0.97	0.18	33,33,33,33	0
56	MG	BA	3633	1/1	0.97	0.32	54,54,54,54	0
56	MG	AA	3152	1/1	0.97	0.12	29,29,29,29	0
56	MG	BA	3511	1/1	0.97	0.13	40,40,40,40	0
56	MG	DA	3224	1/1	0.97	0.10	53,53,53,53	0
56	MG	DA	3046	1/1	0.97	0.09	48,48,48,48	0
56	MG	DA	3047	1/1	0.97	0.09	36,36,36,36	0
56	MG	DA	3048	1/1	0.97	0.36	29,29,29,29	0
56	MG	BA	3396	1/1	0.97	0.20	41,41,41,41	0
56	MG	DA	3229	1/1	0.97	0.14	44,44,44,44	0
56	MG	DA	3477	1/1	0.97	0.53	35,35,35,35	0
56	MG	CA	3069	1/1	0.97	0.21	63,63,63,63	0
56	MG	DA	3481	1/1	0.97	0.08	59,59,59,59	0
56	MG	AA	3154	1/1	0.97	0.08	60,60,60,60	0
56	MG	BE	309	1/1	0.97	0.14	37,37,37,37	0
56	MG	BF	301	1/1	0.97	0.56	46,46,46,46	0
56	MG	AA	3155	1/1	0.97	0.19	54,54,54,54	0
56	MG	DA	3488	1/1	0.97	0.19	48,48,48,48	0
56	MG	BA	3220	1/1	0.97	0.27	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	DA	3238	1/1	0.97	0.13	37,37,37,37	0
56	MG	BA	3642	1/1	0.97	0.16	52,52,52,52	0
56	MG	BA	3516	1/1	0.97	0.20	64,64,64,64	0
56	MG	BA	3316	1/1	0.97	0.14	51,51,51,51	0
56	MG	DA	3242	1/1	0.97	0.23	31,31,31,31	0
56	MG	DA	3497	1/1	0.97	0.06	37,37,37,37	0
56	MG	DA	3498	1/1	0.97	0.12	75,75,75,75	0
56	MG	CA	3080	1/1	0.97	0.13	51,51,51,51	0
56	MG	CA	3081	1/1	0.97	0.09	72,72,72,72	0
56	MG	BA	3401	1/1	0.97	0.14	49,49,49,49	0
56	MG	DA	3063	1/1	0.97	0.10	55,55,55,55	0
56	MG	BA	3145	1/1	0.97	0.30	40,40,40,40	0
56	MG	BA	3520	1/1	0.97	0.08	69,69,69,69	0
56	MG	BA	3521	1/1	0.97	0.12	38,38,38,38	0
56	MG	DA	3251	1/1	0.97	0.29	50,50,50,50	0
56	MG	BA	3318	1/1	0.97	0.13	30,30,30,30	0
56	MG	DA	3512	1/1	0.97	0.07	37,37,37,37	0
56	MG	BA	3651	1/1	0.97	0.34	52,52,52,52	0
56	MG	DA	3069	1/1	0.97	0.20	49,49,49,49	0
56	MG	CA	3088	1/1	0.97	0.19	49,49,49,49	0
56	MG	DA	3258	1/1	0.97	0.28	39,39,39,39	0
56	MG	BA	3653	1/1	0.97	0.15	46,46,46,46	0
56	MG	DA	3519	1/1	0.97	0.10	39,39,39,39	0
56	MG	BO	201	1/1	0.97	0.10	63,63,63,63	0
56	MG	BA	3222	1/1	0.97	0.52	56,56,56,56	0
56	MG	CA	3092	1/1	0.97	0.08	56,56,56,56	0
56	MG	BA	3655	1/1	0.97	0.12	44,44,44,44	0
56	MG	CA	3096	1/1	0.97	0.10	54,54,54,54	0
56	MG	CA	3097	1/1	0.97	0.16	60,60,60,60	0
56	MG	CA	3098	1/1	0.97	0.17	37,37,37,37	0
56	MG	BA	3321	1/1	0.97	0.20	47,47,47,47	0
56	MG	BA	3527	1/1	0.97	0.22	45,45,45,45	0
56	MG	DA	3271	1/1	0.97	0.08	45,45,45,45	0
56	MG	BA	3322	1/1	0.97	0.14	46,46,46,46	0
56	MG	BA	3263	1/1	0.97	0.58	35,35,35,35	0
56	MG	CA	3104	1/1	0.97	0.14	60,60,60,60	0
56	MG	DA	3535	1/1	0.97	0.14	58,58,58,58	0
56	MG	AA	3188	1/1	0.97	0.25	52,52,52,52	0
56	MG	BR	201	1/1	0.97	0.38	44,44,44,44	0
56	MG	BA	3325	1/1	0.97	0.20	39,39,39,39	0
56	MG	BA	3535	1/1	0.97	0.18	42,42,42,42	0
56	MG	BA	3666	1/1	0.97	0.34	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	AA	3158	1/1	0.97	0.17	47,47,47,47	0
56	MG	BA	3537	1/1	0.97	0.16	45,45,45,45	0
56	MG	DA	3286	1/1	0.97	0.22	26,26,26,26	0
56	MG	CA	3112	1/1	0.97	0.26	69,69,69,69	0
56	MG	AA	3040	1/1	0.97	0.07	46,46,46,46	0
56	MG	BA	3422	1/1	0.97	0.14	23,23,23,23	0
56	MG	BA	3329	1/1	0.97	0.08	49,49,49,49	0
56	MG	DA	3551	1/1	0.97	0.10	43,43,43,43	0
56	MG	BA	3424	1/1	0.97	0.17	44,44,44,44	0
56	MG	DA	3294	1/1	0.97	0.20	30,30,30,30	0
56	MG	BA	3543	1/1	0.97	0.22	24,24,24,24	0
56	MG	BA	3544	1/1	0.97	0.22	35,35,35,35	0
56	MG	BA	3330	1/1	0.97	0.09	35,35,35,35	0
56	MG	DA	3558	1/1	0.97	0.17	77,77,77,77	0
56	MG	CA	3120	1/1	0.97	0.21	59,59,59,59	0
56	MG	BA	3678	1/1	0.97	0.10	47,47,47,47	0
56	MG	BA	3546	1/1	0.97	0.26	46,46,46,46	0
56	MG	BA	3426	1/1	0.97	0.08	34,34,34,34	0
56	MG	BA	3149	1/1	0.97	0.04	58,58,58,58	0
56	MG	BA	3227	1/1	0.97	0.16	67,67,67,67	0
56	MG	BA	3115	1/1	0.97	0.17	28,28,28,28	0
56	MG	BA	3551	1/1	0.97	0.17	31,31,31,31	0
56	MG	DA	3309	1/1	0.97	0.17	25,25,25,25	0
56	MG	BA	3229	1/1	0.97	0.35	50,50,50,50	0
56	MG	DA	3313	1/1	0.97	0.18	30,30,30,30	0
56	MG	BA	3554	1/1	0.97	0.21	25,25,25,25	0
56	MG	CA	3130	1/1	0.97	0.10	59,59,59,59	0
56	MG	DA	3317	1/1	0.97	0.19	34,34,34,34	0
56	MG	BA	3272	1/1	0.97	0.07	49,49,49,49	0
56	MG	BA	3557	1/1	0.97	0.28	35,35,35,35	0
56	MG	BA	3336	1/1	0.97	0.18	46,46,46,46	0
56	MG	DA	3580	1/1	0.97	0.17	35,35,35,35	0
56	MG	DA	3118	1/1	0.97	0.09	44,44,44,44	0
56	MG	DA	3324	1/1	0.97	0.17	24,24,24,24	0
56	MG	BA	3560	1/1	0.97	0.27	24,24,24,24	0
56	MG	DA	3326	1/1	0.97	0.08	61,61,61,61	0
56	MG	BA	3040	1/1	0.97	0.23	40,40,40,40	0
56	MG	B1	3002	1/1	0.97	0.14	29,29,29,29	0
56	MG	BA	3340	1/1	0.97	0.19	57,57,57,57	0
56	MG	DA	3331	1/1	0.97	0.17	27,27,27,27	0
56	MG	DA	3332	1/1	0.97	0.12	29,29,29,29	0
56	MG	DA	3592	1/1	0.97	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	BA	3152	1/1	0.97	0.08	52,52,52,52	0
56	MG	BA	3698	1/1	0.97	0.38	58,58,58,58	0
56	MG	BA	3276	1/1	0.97	0.27	9,9,9,9	0
56	MG	DA	3336	1/1	0.97	0.16	36,36,36,36	0
56	MG	DA	3337	1/1	0.97	0.15	50,50,50,50	0
56	MG	B7	103	1/1	0.97	0.40	46,46,46,46	0
56	MG	DA	3339	1/1	0.97	0.29	35,35,35,35	0
56	MG	DA	3600	1/1	0.97	0.17	73,73,73,73	0
56	MG	BA	3440	1/1	0.97	0.10	40,40,40,40	0
56	MG	DA	3341	1/1	0.97	0.07	40,40,40,40	0
56	MG	DA	3342	1/1	0.97	0.18	31,31,31,31	0
56	MG	BA	3701	1/1	0.97	0.15	69,69,69,69	0
56	MG	DA	3129	1/1	0.97	0.38	45,45,45,45	0
56	MG	BA	3343	1/1	0.97	0.19	37,37,37,37	0
56	MG	BA	3041	1/1	0.97	0.42	45,45,45,45	0
56	MG	BA	3091	1/1	0.97	0.34	55,55,55,55	0
56	MG	BA	3706	1/1	0.97	0.14	38,38,38,38	0
56	MG	BA	3065	1/1	0.97	0.30	31,31,31,31	0
56	MG	BA	3120	1/1	0.97	0.26	56,56,56,56	0
56	MG	DA	3136	1/1	0.97	0.08	39,39,39,39	0
56	MG	CA	3155	1/1	0.97	0.18	71,71,71,71	0
56	MG	DA	3615	1/1	0.97	0.08	57,57,57,57	0
56	MG	DA	3358	1/1	0.97	0.16	38,38,38,38	0
56	MG	AA	3141	1/1	0.97	0.23	51,51,51,51	0
56	MG	DA	3362	1/1	0.97	0.36	42,42,42,42	0
56	MG	BA	3574	1/1	0.97	0.08	52,52,52,52	0
56	MG	CA	3158	1/1	0.97	0.10	64,64,64,64	0
56	MG	DA	3366	1/1	0.97	0.09	43,43,43,43	0
56	MG	DA	3367	1/1	0.97	0.07	55,55,55,55	0
56	MG	DA	3368	1/1	0.97	0.17	34,34,34,34	0
56	MG	DA	3370	1/1	0.97	0.23	40,40,40,40	0
56	MG	BA	3352	1/1	0.97	0.16	58,58,58,58	0
56	MG	DA	3372	1/1	0.97	0.10	37,37,37,37	0
56	MG	BA	3282	1/1	0.97	0.15	34,34,34,34	0
56	MG	DA	3631	1/1	0.97	0.19	49,49,49,49	0
56	MG	DA	3632	1/1	0.97	0.18	60,60,60,60	0
56	MG	DA	3634	1/1	0.97	0.20	33,33,33,33	0
56	MG	BA	3579	1/1	0.97	0.30	21,21,21,21	0
56	MG	DA	3375	1/1	0.97	0.08	40,40,40,40	0
56	MG	BA	3002	1/1	0.97	0.14	38,38,38,38	0
56	MG	DA	3145	1/1	0.97	0.42	52,52,52,52	0
56	MG	CA	3011	1/1	0.97	0.26	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	BA	3095	1/1	0.97	0.70	55,55,55,55	0
56	MG	CA	3165	1/1	0.97	0.15	47,47,47,47	0
56	MG	CA	3166	1/1	0.97	0.08	71,71,71,71	0
56	MG	BA	3457	1/1	0.97	0.11	25,25,25,25	0
56	MG	DA	3152	1/1	0.97	0.26	43,43,43,43	0
56	MG	DA	3389	1/1	0.97	0.23	32,32,32,32	0
56	MG	BA	3287	1/1	0.97	0.14	11,11,11,11	0
56	MG	DA	3648	1/1	0.97	0.23	43,43,43,43	0
56	MG	BA	3584	1/1	0.97	0.10	43,43,43,43	0
56	MG	DA	3653	1/1	0.97	0.12	52,52,52,52	0
56	MG	AA	3193	1/1	0.97	0.13	65,65,65,65	0
56	MG	DA	3393	1/1	0.97	0.26	35,35,35,35	0
56	MG	DA	3656	1/1	0.97	0.07	62,62,62,62	0
56	MG	DA	3156	1/1	0.97	0.64	38,38,38,38	0
56	MG	BA	3360	1/1	0.97	0.18	39,39,39,39	0
56	MG	AA	3208	1/1	0.97	0.34	38,38,38,38	0
56	MG	BA	3462	1/1	0.97	0.23	30,30,30,30	0
56	MG	BA	3363	1/1	0.97	0.17	29,29,29,29	0
56	MG	BA	3197	1/1	0.97	0.44	39,39,39,39	0
56	MG	AA	3018	1/1	0.97	0.22	51,51,51,51	0
56	MG	BA	3243	1/1	0.97	0.09	43,43,43,43	0
56	MG	BA	3727	1/1	0.97	0.18	27,27,27,27	0
56	MG	BA	3200	1/1	0.97	0.28	32,32,32,32	0
56	MG	BA	3469	1/1	0.97	0.13	60,60,60,60	0
56	MG	DA	3169	1/1	0.97	0.25	58,58,58,58	0
56	MG	BA	3730	1/1	0.97	0.19	43,43,43,43	0
56	MG	DA	3410	1/1	0.97	0.09	40,40,40,40	0
56	MG	BA	3731	1/1	0.97	0.39	52,52,52,52	0
56	MG	DA	3413	1/1	0.97	0.18	44,44,44,44	0
56	MG	DA	3414	1/1	0.97	0.18	59,59,59,59	0
56	MG	BA	3598	1/1	0.97	0.23	32,32,32,32	0
56	MG	DA	3416	1/1	0.97	0.36	34,34,34,34	0
56	MG	AA	3008	1/1	0.97	0.27	61,61,61,61	0
56	MG	BA	3600	1/1	0.97	0.33	54,54,54,54	0
56	MG	DA	3419	1/1	0.97	0.11	53,53,53,53	0
56	MG	DE	304	1/1	0.97	0.18	30,30,30,30	0
56	MG	DA	3421	1/1	0.97	0.16	43,43,43,43	0
56	MG	BA	3369	1/1	0.97	0.12	49,49,49,49	0
56	MG	BA	3736	1/1	0.97	0.14	40,40,40,40	0
56	MG	BA	3370	1/1	0.97	0.07	39,39,39,39	0
56	MG	DF	303	1/1	0.97	0.28	42,42,42,42	0
56	MG	BA	3072	1/1	0.97	0.69	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	3474	1/1	0.97	0.27	43,43,43,43	0
56	MG	BA	3049	1/1	0.97	0.17	17,17,17,17	0
56	MG	DA	3429	1/1	0.97	0.09	30,30,30,30	0
56	MG	DP	201	1/1	0.97	0.31	52,52,52,52	0
56	MG	BA	3476	1/1	0.97	0.09	47,47,47,47	0
56	MG	BA	3205	1/1	0.97	0.29	38,38,38,38	0
56	MG	BA	3478	1/1	0.97	0.21	36,36,36,36	0
56	MG	BA	3102	1/1	0.97	0.08	45,45,45,45	0
56	MG	AA	3212	1/1	0.97	0.15	36,36,36,36	0
56	MG	BA	3209	1/1	0.97	0.43	39,39,39,39	0
56	MG	BA	3379	1/1	0.97	0.08	43,43,43,43	0
56	MG	BA	3382	1/1	0.97	0.20	21,21,21,21	0
56	MG	BA	3383	1/1	0.97	0.14	51,51,51,51	0
56	MG	BA	3489	1/1	0.97	0.12	50,50,50,50	0
56	MG	BA	3619	1/1	0.97	0.15	42,42,42,42	0
56	MG	CA	3050	1/1	0.97	0.18	54,54,54,54	0
56	MG	AA	3165	1/1	0.97	0.13	24,24,24,24	0
56	MG	CA	3052	1/1	0.97	0.15	47,47,47,47	0
56	MG	BA	3493	1/1	0.97	0.13	51,51,51,51	0
56	MG	DA	3446	1/1	0.97	0.16	46,46,46,46	0
56	MG	AA	3149	1/1	0.97	0.07	49,49,49,49	0
56	MG	D8	5001	1/1	0.97	0.23	53,53,53,53	0
58	ZN	AN	102	1/1	0.97	0.11	88,88,88,88	0
56	MG	DA	3031	1/1	0.97	0.18	60,60,60,60	0
56	MG	AA	3150	1/1	0.97	0.27	67,67,67,67	0
56	MG	DA	3207	1/1	0.97	0.11	41,41,41,41	0
56	MG	BA	3387	1/1	0.97	0.26	49,49,49,49	0
56	MG	BA	3503	1/1	0.97	0.14	56,56,56,56	0
56	MG	BA	3305	1/1	0.97	0.13	48,48,48,48	0
56	MG	BD	307	1/1	0.97	0.26	36,36,36,36	0
56	MG	BA	3389	1/1	0.97	0.14	52,52,52,52	0
56	MG	BA	3607	1/1	0.98	0.20	74,74,74,74	0
56	MG	AA	3104	1/1	0.98	0.16	35,35,35,35	0
56	MG	BA	3380	1/1	0.98	0.10	32,32,32,32	0
56	MG	BV	3002	1/1	0.98	0.55	42,42,42,42	0
56	MG	BA	3522	1/1	0.98	0.13	42,42,42,42	0
56	MG	AA	3159	1/1	0.98	0.32	57,57,57,57	0
56	MG	DA	3518	1/1	0.98	0.10	40,40,40,40	0
56	MG	BA	3450	1/1	0.98	0.14	40,40,40,40	0
56	MG	BA	3129	1/1	0.98	0.67	44,44,44,44	0
56	MG	BA	3452	1/1	0.98	0.11	16,16,16,16	0
56	MG	DA	3522	1/1	0.98	0.23	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	3130	1/1	0.98	0.40	51,51,51,51	0
56	MG	BA	3003	1/1	0.98	0.08	24,24,24,24	0
56	MG	CA	3094	1/1	0.98	0.22	37,37,37,37	0
56	MG	DA	3526	1/1	0.98	0.12	49,49,49,49	0
56	MG	CA	3095	1/1	0.98	0.15	35,35,35,35	0
56	MG	DA	3174	1/1	0.98	0.44	26,26,26,26	0
56	MG	BA	3531	1/1	0.98	0.18	28,28,28,28	0
56	MG	BA	3160	1/1	0.98	0.17	24,24,24,24	0
56	MG	AA	3168	1/1	0.98	0.27	80,80,80,80	0
56	MG	CA	3099	1/1	0.98	0.39	64,64,64,64	0
56	MG	DA	3045	1/1	0.98	0.25	49,49,49,49	0
56	MG	DA	3183	1/1	0.98	0.14	42,42,42,42	0
56	MG	BA	3534	1/1	0.98	0.22	36,36,36,36	0
56	MG	AA	3153	1/1	0.98	0.10	46,46,46,46	0
56	MG	B0	105	1/1	0.98	0.27	44,44,44,44	0
56	MG	DA	3347	1/1	0.98	0.20	39,39,39,39	0
56	MG	AA	3161	1/1	0.98	0.08	61,61,61,61	0
56	MG	DA	3349	1/1	0.98	0.09	27,27,27,27	0
56	MG	DA	3350	1/1	0.98	0.24	21,21,21,21	0
56	MG	BA	3339	1/1	0.98	0.14	47,47,47,47	0
56	MG	AA	3192	1/1	0.98	0.08	73,73,73,73	0
56	MG	DA	3544	1/1	0.98	0.36	42,42,42,42	0
56	MG	DA	3545	1/1	0.98	0.28	35,35,35,35	0
56	MG	DA	3546	1/1	0.98	0.22	38,38,38,38	0
56	MG	DA	3052	1/1	0.98	0.10	20,20,20,20	0
56	MG	AA	3091	1/1	0.98	0.26	75,75,75,75	0
56	MG	B3	3401	1/1	0.98	0.18	24,24,24,24	0
56	MG	DA	3357	1/1	0.98	0.12	50,50,50,50	0
56	MG	BA	3393	1/1	0.98	0.23	27,27,27,27	0
56	MG	DA	3359	1/1	0.98	0.21	21,21,21,21	0
56	MG	BA	3628	1/1	0.98	0.10	39,39,39,39	0
56	MG	DA	3196	1/1	0.98	0.09	54,54,54,54	0
56	MG	DA	3555	1/1	0.98	0.14	43,43,43,43	0
56	MG	B5	502	1/1	0.98	0.10	56,56,56,56	0
56	MG	BA	3463	1/1	0.98	0.10	32,32,32,32	0
56	MG	DA	3365	1/1	0.98	0.06	52,52,52,52	0
56	MG	DA	3559	1/1	0.98	0.12	47,47,47,47	0
56	MG	B7	102	1/1	0.98	0.28	29,29,29,29	0
56	MG	BA	3394	1/1	0.98	0.21	45,45,45,45	0
56	MG	AA	3046	1/1	0.98	0.15	60,60,60,60	0
56	MG	DA	3369	1/1	0.98	0.05	53,53,53,53	0
56	MG	DA	3564	1/1	0.98	0.11	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	AA	3220	1/1	0.98	0.09	42,42,42,42	0
56	MG	AA	3183	1/1	0.98	0.11	56,56,56,56	0
56	MG	DA	3204	1/1	0.98	0.36	44,44,44,44	0
56	MG	BA	3198	1/1	0.98	0.35	29,29,29,29	0
56	MG	AA	3156	1/1	0.98	0.13	31,31,31,31	0
56	MG	BA	3348	1/1	0.98	0.10	29,29,29,29	0
56	MG	BA	3637	1/1	0.98	0.79	52,52,52,52	0
56	MG	BA	3170	1/1	0.98	0.48	34,34,34,34	0
56	MG	DA	3378	1/1	0.98	0.09	38,38,38,38	0
56	MG	BA	3639	1/1	0.98	0.10	35,35,35,35	0
56	MG	BA	3268	1/1	0.98	0.19	29,29,29,29	0
56	MG	BA	3403	1/1	0.98	0.20	28,28,28,28	0
56	MG	BB	3001	1/1	0.98	0.15	56,56,56,56	0
56	MG	DA	3579	1/1	0.98	0.21	38,38,38,38	0
56	MG	BA	3553	1/1	0.98	0.17	46,46,46,46	0
56	MG	DA	3582	1/1	0.98	0.36	44,44,44,44	0
56	MG	BA	3351	1/1	0.98	0.25	21,21,21,21	0
56	MG	DA	3387	1/1	0.98	0.15	50,50,50,50	0
56	MG	DA	3388	1/1	0.98	0.11	25,25,25,25	0
56	MG	BA	3201	1/1	0.98	0.27	36,36,36,36	0
56	MG	DA	3217	1/1	0.98	0.27	33,33,33,33	0
56	MG	BA	3645	1/1	0.98	0.16	63,63,63,63	0
56	MG	BA	3556	1/1	0.98	0.18	25,25,25,25	0
56	MG	BA	3030	1/1	0.98	0.33	26,26,26,26	0
56	MG	CA	3132	1/1	0.98	0.08	66,66,66,66	0
56	MG	DA	3080	1/1	0.98	0.11	43,43,43,43	0
56	MG	DA	3223	1/1	0.98	0.09	41,41,41,41	0
56	MG	CA	3133	1/1	0.98	0.20	45,45,45,45	0
56	MG	DA	3082	1/1	0.98	0.08	7,7,7,7	0
56	MG	DA	3083	1/1	0.98	0.18	44,44,44,44	0
56	MG	DA	3400	1/1	0.98	0.18	42,42,42,42	0
56	MG	DA	3401	1/1	0.98	0.13	41,41,41,41	0
56	MG	BA	3309	1/1	0.98	0.13	43,43,43,43	0
56	MG	DA	3085	1/1	0.98	0.09	35,35,35,35	0
56	MG	BA	3559	1/1	0.98	0.40	29,29,29,29	0
56	MG	BA	3355	1/1	0.98	0.09	39,39,39,39	0
56	MG	CA	3137	1/1	0.98	0.12	59,59,59,59	0
56	MG	BB	3013	1/1	0.98	0.17	31,31,31,31	0
56	MG	DA	3408	1/1	0.98	0.18	35,35,35,35	0
56	MG	DA	3233	1/1	0.98	0.34	58,58,58,58	0
56	MG	BA	3410	1/1	0.98	0.18	21,21,21,21	0
56	MG	BA	3652	1/1	0.98	0.22	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DA	3609	1/1	0.98	0.23	49,49,49,49	0
56	MG	DA	3412	1/1	0.98	0.16	34,34,34,34	0
56	MG	BB	3016	1/1	0.98	0.15	24,24,24,24	0
56	MG	BA	3562	1/1	0.98	0.14	42,42,42,42	0
56	MG	BA	3411	1/1	0.98	0.19	21,21,21,21	0
56	MG	BA	3482	1/1	0.98	0.09	59,59,59,59	0
56	MG	BA	3356	1/1	0.98	0.13	33,33,33,33	0
56	MG	AA	3157	1/1	0.98	0.06	26,26,26,26	0
56	MG	BA	3311	1/1	0.98	0.27	52,52,52,52	0
56	MG	DA	3420	1/1	0.98	0.06	43,43,43,43	0
56	MG	BA	3659	1/1	0.98	0.10	42,42,42,42	0
56	MG	CA	3149	1/1	0.98	0.18	81,81,81,81	0
56	MG	DA	3622	1/1	0.98	0.17	40,40,40,40	0
56	MG	DA	3101	1/1	0.98	0.28	59,59,59,59	0
56	MG	DA	3247	1/1	0.98	0.32	34,34,34,34	0
56	MG	BD	306	1/1	0.98	0.47	47,47,47,47	0
56	MG	CA	3151	1/1	0.98	0.14	80,80,80,80	0
56	MG	BA	3014	1/1	0.98	0.37	48,48,48,48	0
56	MG	BD	308	1/1	0.98	0.34	21,21,21,21	0
56	MG	DA	3430	1/1	0.98	0.18	75,75,75,75	0
56	MG	BA	3488	1/1	0.98	0.29	43,43,43,43	0
56	MG	DA	3253	1/1	0.98	0.13	35,35,35,35	0
56	MG	DA	3633	1/1	0.98	0.26	25,25,25,25	0
56	MG	BA	3570	1/1	0.98	0.20	33,33,33,33	0
56	MG	BA	3421	1/1	0.98	0.15	28,28,28,28	0
56	MG	BA	3664	1/1	0.98	0.12	63,63,63,63	0
56	MG	DA	3257	1/1	0.98	0.20	25,25,25,25	0
56	MG	DA	3638	1/1	0.98	0.10	53,53,53,53	0
56	MG	BE	301	1/1	0.98	0.22	28,28,28,28	0
56	MG	BA	3490	1/1	0.98	0.11	40,40,40,40	0
56	MG	BE	303	1/1	0.98	0.10	39,39,39,39	0
56	MG	BA	3491	1/1	0.98	0.23	38,38,38,38	0
56	MG	AA	3210	1/1	0.98	0.07	48,48,48,48	0
56	MG	BA	3206	1/1	0.98	0.28	32,32,32,32	0
56	MG	DA	3265	1/1	0.98	0.29	44,44,44,44	0
56	MG	BA	3577	1/1	0.98	0.15	63,63,63,63	0
56	MG	BA	3494	1/1	0.98	0.27	28,28,28,28	0
56	MG	BA	3673	1/1	0.98	0.16	60,60,60,60	0
56	MG	DA	3649	1/1	0.98	0.08	39,39,39,39	0
56	MG	DA	3650	1/1	0.98	0.05	35,35,35,35	0
56	MG	CA	3045	1/1	0.98	0.09	60,60,60,60	0
56	MG	BA	3495	1/1	0.98	0.27	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\AA^2$)	Q<0.9
56	MG	BA	3497	1/1	0.98	0.42	28,28,28,28	0
56	MG	DA	3450	1/1	0.98	0.18	47,47,47,47	0
56	MG	DA	3273	1/1	0.98	0.23	32,32,32,32	0
56	MG	BF	303	1/1	0.98	0.12	42,42,42,42	0
56	MG	DA	3453	1/1	0.98	0.10	44,44,44,44	0
56	MG	DA	3275	1/1	0.98	0.26	34,34,34,34	0
56	MG	BA	3315	1/1	0.98	0.31	43,43,43,43	0
56	MG	AA	3186	1/1	0.98	0.14	51,51,51,51	0
56	MG	BA	3500	1/1	0.98	0.13	43,43,43,43	0
56	MG	DA	3279	1/1	0.98	0.29	32,32,32,32	0
56	MG	BG	3001	1/1	0.98	0.09	65,65,65,65	0
56	MG	BA	3501	1/1	0.98	0.18	35,35,35,35	0
56	MG	DA	3461	1/1	0.98	0.08	40,40,40,40	0
56	MG	BA	3176	1/1	0.98	0.21	50,50,50,50	0
56	MG	DA	3463	1/1	0.98	0.06	32,32,32,32	0
56	MG	BA	3035	1/1	0.98	0.15	32,32,32,32	0
56	MG	BA	3682	1/1	0.98	0.35	50,50,50,50	0
56	MG	BA	3587	1/1	0.98	0.22	23,23,23,23	0
56	MG	BA	3210	1/1	0.98	0.30	39,39,39,39	0
56	MG	BN	3004	1/1	0.98	0.47	69,69,69,69	0
56	MG	BA	3589	1/1	0.98	0.23	34,34,34,34	0
56	MG	BA	3320	1/1	0.98	0.21	41,41,41,41	0
56	MG	BA	3591	1/1	0.98	0.22	38,38,38,38	0
56	MG	AX	110	1/1	0.98	0.17	45,45,45,45	0
56	MG	BA	3057	1/1	0.98	0.40	36,36,36,36	0
56	MG	BA	3079	1/1	0.98	0.33	50,50,50,50	0
56	MG	BA	3124	1/1	0.98	0.20	46,46,46,46	0
56	MG	BA	3125	1/1	0.98	0.30	26,26,26,26	0
56	MG	BA	3695	1/1	0.98	0.25	34,34,34,34	0
56	MG	BQ	3003	1/1	0.98	0.19	15,15,15,15	0
56	MG	DA	3479	1/1	0.98	0.14	35,35,35,35	0
56	MG	DA	3480	1/1	0.98	0.17	42,42,42,42	0
56	MG	DF	305	1/1	0.98	0.43	55,55,55,55	0
56	MG	BA	3436	1/1	0.98	0.29	35,35,35,35	0
56	MG	DA	3301	1/1	0.98	0.28	30,30,30,30	0
56	MG	BA	3437	1/1	0.98	0.12	37,37,37,37	0
56	MG	BA	3374	1/1	0.98	0.28	26,26,26,26	0
56	MG	DA	3304	1/1	0.98	0.20	44,44,44,44	0
56	MG	DA	3486	1/1	0.98	0.08	52,52,52,52	0
56	MG	DA	3487	1/1	0.98	0.09	44,44,44,44	0
56	MG	BA	3286	1/1	0.98	0.23	42,42,42,42	0
56	MG	BA	3327	1/1	0.98	0.16	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DA	3490	1/1	0.98	0.14	46,46,46,46	0
56	MG	DA	3307	1/1	0.98	0.12	40,40,40,40	0
56	MG	DA	3149	1/1	0.98	0.07	47,47,47,47	0
56	MG	CA	3075	1/1	0.98	0.35	76,76,76,76	0
56	MG	BA	3080	1/1	0.98	0.09	12,12,12,12	0
56	MG	DA	3495	1/1	0.98	0.07	53,53,53,53	0
56	MG	DA	3311	1/1	0.98	0.32	33,33,33,33	0
56	MG	DA	3312	1/1	0.98	0.23	24,24,24,24	0
56	MG	DA	3020	1/1	0.98	0.32	45,45,45,45	0
56	MG	CA	3077	1/1	0.98	0.27	51,51,51,51	0
56	MG	DA	3315	1/1	0.98	0.12	39,39,39,39	0
56	MG	BA	3603	1/1	0.98	0.29	40,40,40,40	0
56	MG	BA	3703	1/1	0.98	0.14	44,44,44,44	0
56	MG	BA	3443	1/1	0.98	0.34	34,34,34,34	0
58	ZN	BY	501	1/1	0.98	0.09	67,67,67,67	0
56	MG	BA	3378	1/1	0.98	0.18	24,24,24,24	0
56	MG	DA	3505	1/1	0.98	0.14	24,24,24,24	0
56	MG	DA	3320	1/1	0.98	0.21	50,50,50,50	0
56	MG	DA	3321	1/1	0.98	0.12	31,31,31,31	0
58	ZN	D5	103	1/1	0.98	0.07	61,61,61,61	0
58	ZN	D6	501	1/1	0.98	0.11	65,65,65,65	0
58	ZN	D9	501	1/1	0.98	0.05	63,63,63,63	0
56	MG	DA	3508	1/1	0.98	0.06	30,30,30,30	0
56	MG	BA	3445	1/1	0.98	0.17	16,16,16,16	0
56	MG	DA	3510	1/1	0.98	0.13	67,67,67,67	0
56	MG	DA	3511	1/1	0.98	0.10	47,47,47,47	0
56	MG	DA	3158	1/1	0.99	0.40	47,47,47,47	0
56	MG	DA	3293	1/1	0.99	0.10	34,34,34,34	0
56	MG	DA	3159	1/1	0.99	0.13	50,50,50,50	0
56	MG	BA	3337	1/1	0.99	0.10	48,48,48,48	0
56	MG	BA	3496	1/1	0.99	0.45	21,21,21,21	0
56	MG	BA	3523	1/1	0.99	0.16	32,32,32,32	0
56	MG	BA	3448	1/1	0.99	0.22	23,23,23,23	0
56	MG	AA	3013	1/1	0.99	0.25	75,75,75,75	0
56	MG	BA	3407	1/1	0.99	0.22	35,35,35,35	0
56	MG	BA	3218	1/1	0.99	0.12	58,58,58,58	0
56	MG	DA	3616	1/1	0.99	0.18	41,41,41,41	0
56	MG	BA	3617	1/1	0.99	0.35	30,30,30,30	0
56	MG	BA	3528	1/1	0.99	0.22	44,44,44,44	0
56	MG	BX	101	1/1	0.99	0.09	38,38,38,38	0
56	MG	BA	3683	1/1	0.99	0.29	37,37,37,37	0
56	MG	BA	3140	1/1	0.99	0.31	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\AA^2$)	Q<0.9
56	MG	DA	3355	1/1	0.99	0.38	39,39,39,39	0
56	MG	DA	3260	1/1	0.99	0.07	32,32,32,32	0
56	MG	BA	3430	1/1	0.99	0.12	47,47,47,47	0
56	MG	DA	3625	1/1	0.99	0.16	48,48,48,48	0
56	MG	BA	3381	1/1	0.99	0.07	25,25,25,25	0
56	MG	AA	3024	1/1	0.99	0.11	49,49,49,49	0
56	MG	DA	3360	1/1	0.99	0.10	36,36,36,36	0
56	MG	BA	3412	1/1	0.99	0.27	29,29,29,29	0
56	MG	DA	3573	1/1	0.99	0.17	32,32,32,32	0
56	MG	DA	3176	1/1	0.99	0.09	52,52,52,52	0
56	MG	BA	3480	1/1	0.99	0.12	22,22,22,22	0
56	MG	BA	3285	1/1	0.99	0.17	44,44,44,44	0
56	MG	DA	3179	1/1	0.99	0.41	36,36,36,36	0
56	MG	BA	3691	1/1	0.99	0.10	40,40,40,40	0
56	MG	CA	3168	1/1	0.99	0.46	79,79,79,79	0
56	MG	DA	3182	1/1	0.99	0.20	29,29,29,29	0
56	MG	DA	3581	1/1	0.99	0.24	41,41,41,41	0
56	MG	DA	3272	1/1	0.99	0.14	36,36,36,36	0
56	MG	DA	3422	1/1	0.99	0.23	45,45,45,45	0
56	MG	DA	3026	1/1	0.99	0.22	36,36,36,36	0
56	MG	BA	3414	1/1	0.99	0.22	51,51,51,51	0
56	MG	BA	3483	1/1	0.99	0.21	18,18,18,18	0
56	MG	BA	3275	1/1	0.99	0.18	28,28,28,28	0
56	MG	BA	3045	1/1	0.99	0.16	27,27,27,27	0
56	MG	BA	3417	1/1	0.99	0.19	21,21,21,21	0
56	MG	BA	3541	1/1	0.99	0.14	37,37,37,37	0
56	MG	DA	3327	1/1	0.99	0.12	45,45,45,45	0
56	MG	BA	3418	1/1	0.99	0.26	20,20,20,20	0
56	MG	BA	3419	1/1	0.99	0.31	36,36,36,36	0
57	SF4	AD	501	8/8	0.99	0.13	62,75,82,88	0
57	SF4	CD	501	8/8	0.99	0.11	63,76,87,96	0
56	MG	BA	3665	1/1	0.99	0.18	39,39,39,39	0
56	MG	DA	3652	1/1	0.99	0.26	26,26,26,26	0
56	MG	BA	3441	1/1	0.99	0.23	29,29,29,29	0
58	ZN	B5	501	1/1	0.99	0.10	49,49,49,49	0
58	ZN	B6	501	1/1	0.99	0.12	51,51,51,51	0
56	MG	DA	3382	1/1	0.99	0.06	44,44,44,44	0
56	MG	DA	3383	1/1	0.99	0.18	27,27,27,27	0
56	MG	BA	3345	1/1	0.99	0.05	37,37,37,37	0
56	MG	BA	3575	1/1	0.99	0.13	26,26,26,26	0
56	MG	AA	3169	1/1	0.99	0.26	62,62,62,62	0
56	MG	BA	3670	1/1	0.99	0.10	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	BA	3077	1/1	0.99	0.18	20,20,20,20	0
56	MG	BA	3159	1/1	0.99	0.29	47,47,47,47	0
56	MG	AA	3103	1/1	0.99	0.12	43,43,43,43	0
56	MG	DA	3291	1/1	0.99	0.18	42,42,42,42	0
56	MG	DA	3191	1/1	1.00	0.16	31,31,31,31	0
56	MG	BB	3010	1/1	1.00	0.20	44,44,44,44	0
56	MG	BA	3362	1/1	1.00	0.17	23,23,23,23	0
56	MG	BB	3012	1/1	1.00	0.16	42,42,42,42	0
58	ZN	B9	501	1/1	1.00	0.12	49,49,49,49	0

6.5 Other polymers ⓘ

There are no such residues in this entry.