wwPDB X-ray Structure Validation Summary Report (i)

Aug 4, 2026 – 10:13 AM EDT

PDB ID	:	1VY6 / pdb_00001vy6
Title	:	Crystal structure of the Thermus thermophilus 70S ribosome in the pre-attack state of peptide bond formation containing short substrate-mimic Cytidine-Puromycin in the A site and acylated tRNA in the P site.
Authors	:	Polikanov, Y.S.; Steitz, T.A.; Innis, C.A.
Deposited on	:	2014-05-13
Resolution	:	2.90 Å(reported)

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

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

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

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

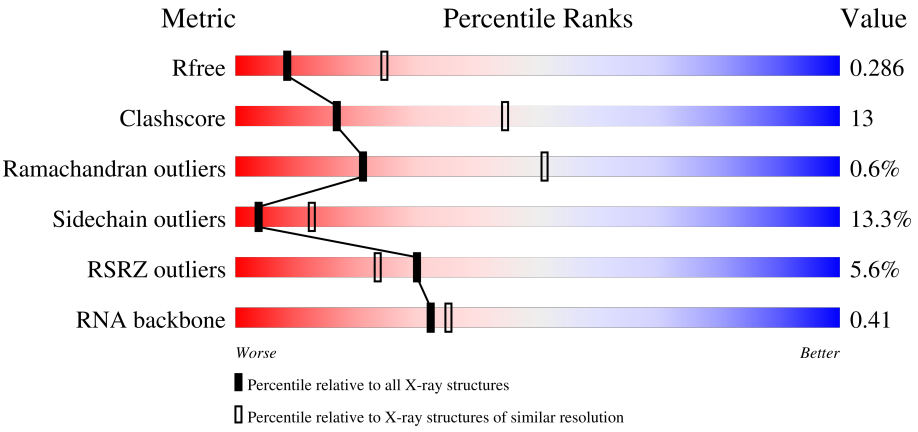
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)
RNA backbone	3983	1120 (3.10-2.70)

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	1521	3% 42% 42% 14% •
1	CA	1521	6% 40% 45% 14% •
2	AB	256	11% 39% 39% 10% • 10%
2	CB	256	20% 35% 45% 10% • 10%

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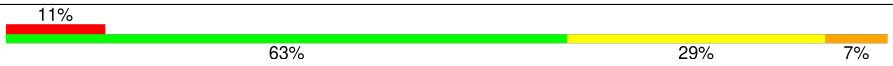
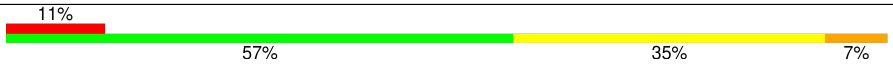
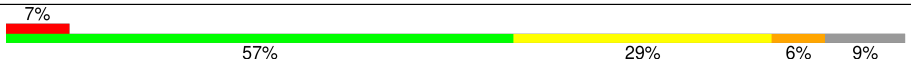
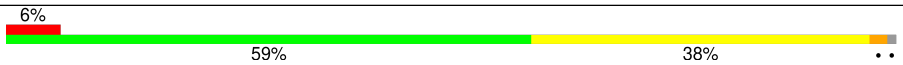
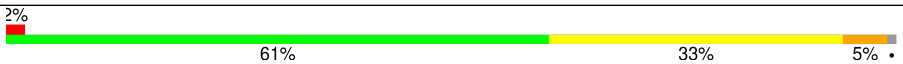
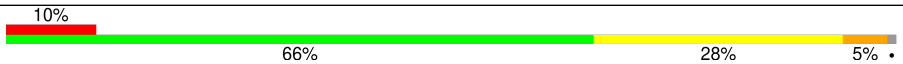
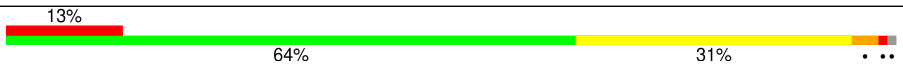
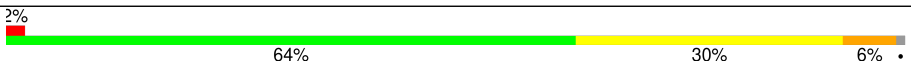
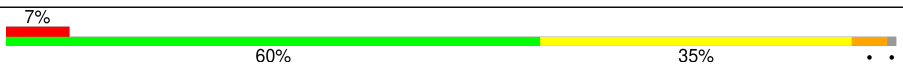
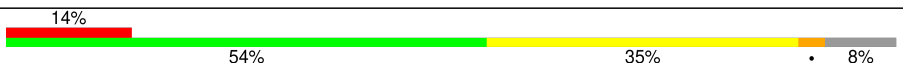
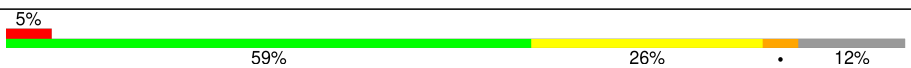
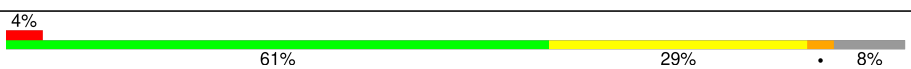
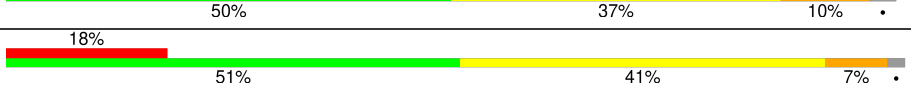
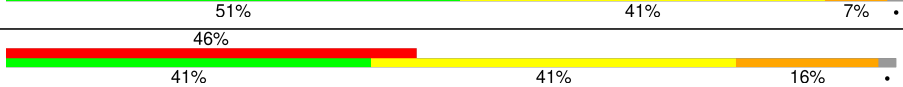
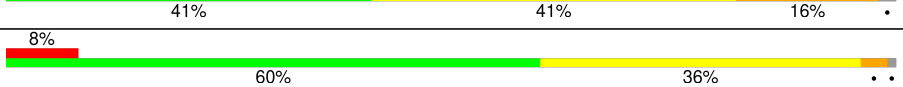
Mol	Chain	Length	Quality of chain
3	AC	239	
3	CC	239	
4	AD	209	
4	CD	209	
5	AE	162	
5	CE	162	
6	AF	101	
6	CF	101	
7	AG	156	
7	CG	156	
8	AH	138	
8	CH	138	
9	AI	128	
9	CI	128	
10	AJ	105	
10	CJ	105	
11	AK	129	
11	CK	129	
12	AL	132	
12	CL	132	
13	AM	126	
13	CM	126	
14	AN	61	
14	CN	61	
15	AO	89	

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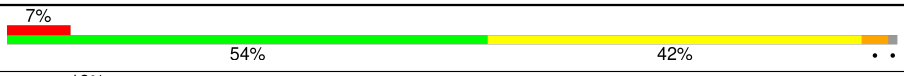
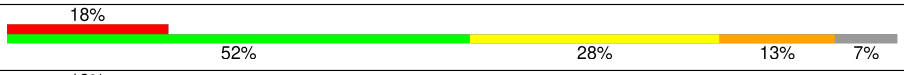
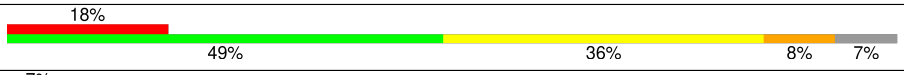
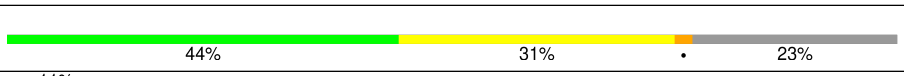
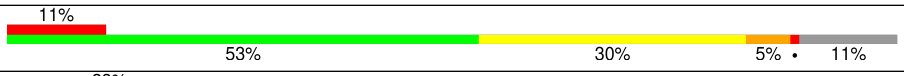
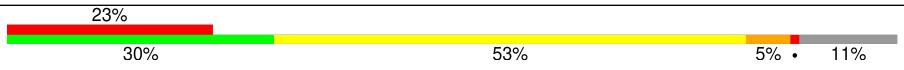
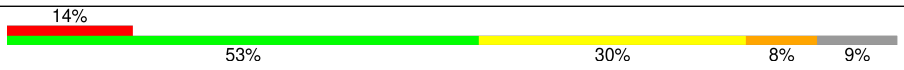
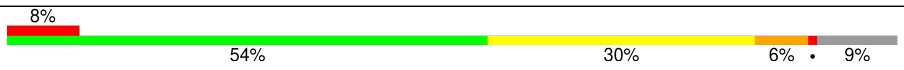
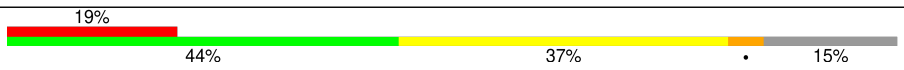
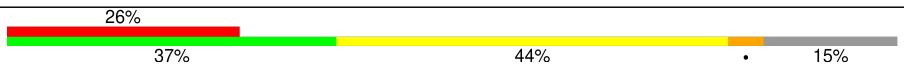
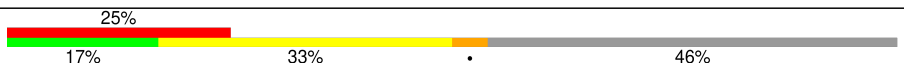
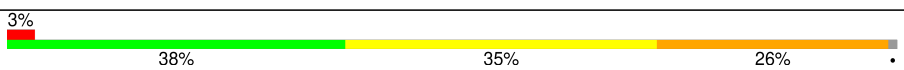
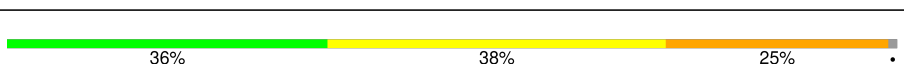
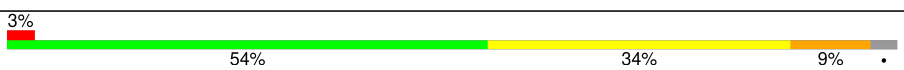
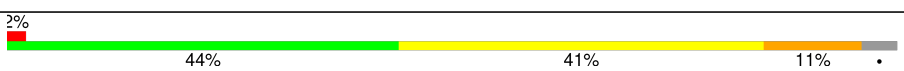
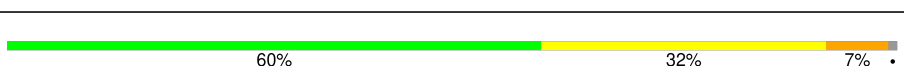
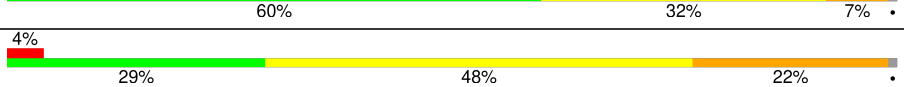
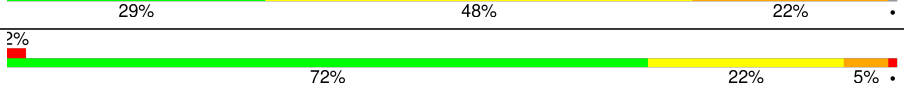
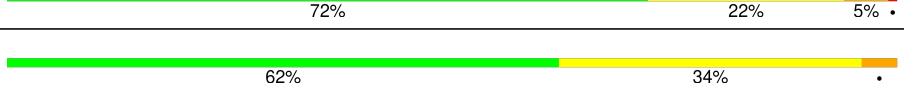
Mol	Chain	Length	Quality of chain
15	CO	89	
16	AP	88	
16	CP	88	
17	AQ	105	
17	CQ	105	
18	AR	88	
18	CR	88	
19	AS	93	
19	CS	93	
20	AT	106	
20	CT	106	
21	AU	27	
21	CU	27	
22	AV	24	
22	CV	24	
23	AW	2	
23	CW	2	
24	AX	77	
24	CX	77	
25	BA	2915	
25	DA	2915	
26	BB	121	
26	DB	121	
27	BD	276	
27	DD	276	

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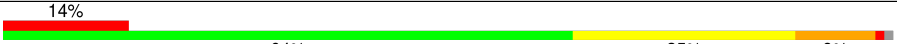
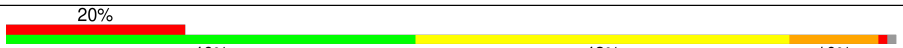
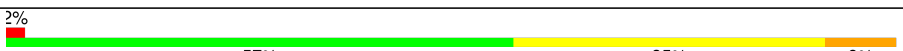
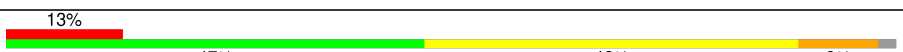
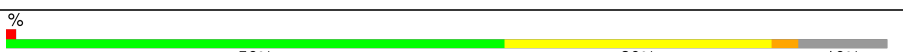
Mol	Chain	Length	Quality of chain
28	BE	206	
28	DE	206	
29	BF	210	
29	DF	210	
30	BG	182	
30	DG	182	
31	BH	180	
31	DH	180	
32	BI	148	
32	DI	148	
33	BN	140	
33	DN	140	
34	BO	122	
34	DO	122	
35	BP	150	
35	DP	150	
36	BQ	141	
36	DQ	141	
37	BR	118	
37	DR	118	
38	BS	112	
38	DS	112	
39	BT	146	
39	DT	146	
40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

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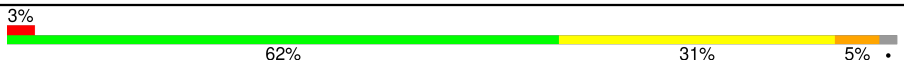
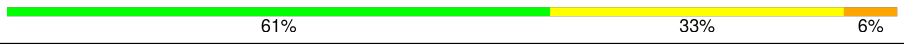
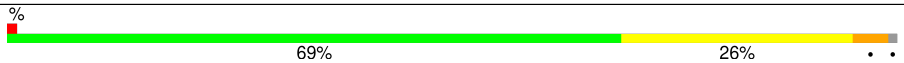
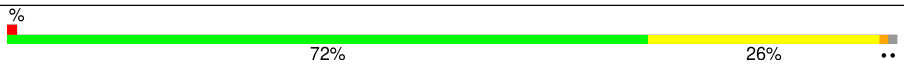
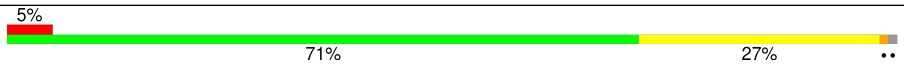
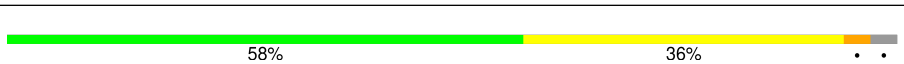
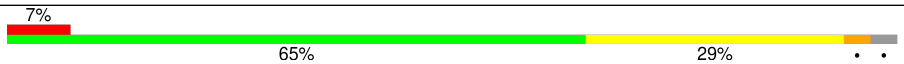
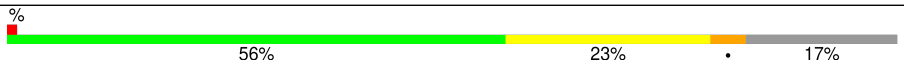
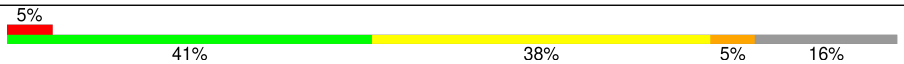
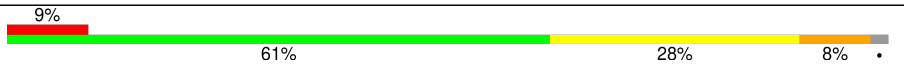
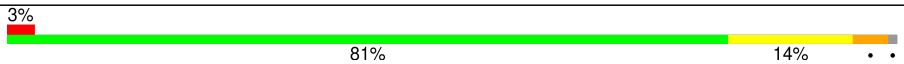
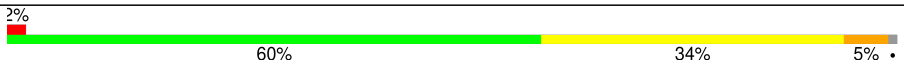
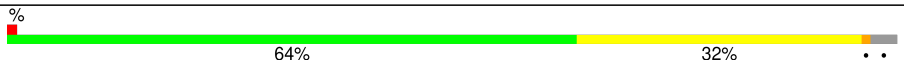
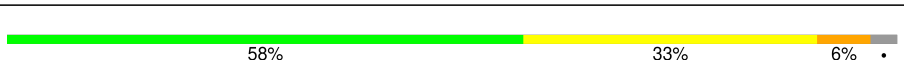
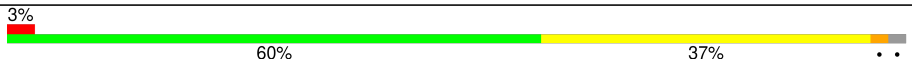
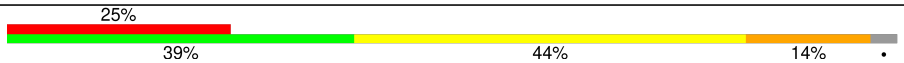
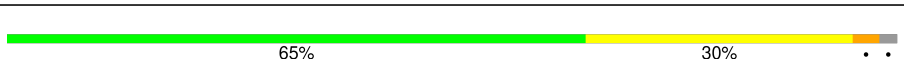
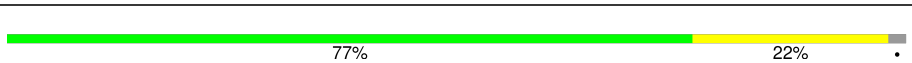
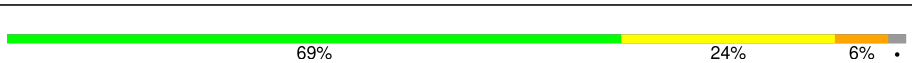
Mol	Chain	Length	Quality of chain
40	DU	118	
41	BV	101	
41	DV	101	
42	BW	113	
42	DW	113	
43	BX	96	
43	DX	96	
44	BY	110	
44	DY	110	
45	BZ	206	
45	DZ	206	
46	B0	85	
46	D0	85	
47	B1	98	
47	D1	98	
48	B2	72	
48	D2	72	
49	B3	60	
49	D3	60	
50	B4	71	
50	D4	71	
51	B5	60	
51	D5	60	
52	B6	54	
52	D6	54	

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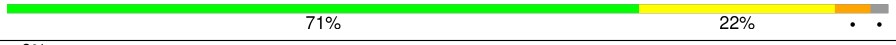
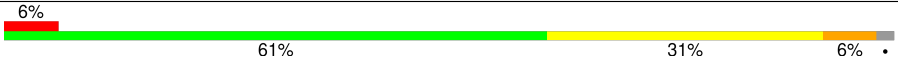
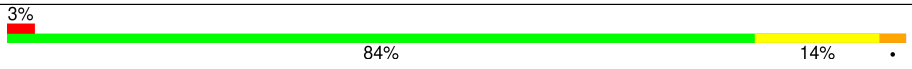
Mol	Chain	Length	Quality of chain
53	B7	49	
53	D7	49	
54	B8	65	
54	D8	65	
55	B9	37	
55	D9	37	

2 Entry composition (i)

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1498	Total	C	N	O	P	0	0	0
			32205	14333	5970	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
			1670	1047	332	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	0	0	0
			1129	714	213	198	4			
5	CE	148	Total	C	N	O	S	0	0	0
			1133	716	214	199	4			

- 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	0	0	0
			806	511	143	149	3			
6	CF	100	Total	C	N	O	S	0	0	0
			816	516	146	151	3			

- 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	0	0	0
			1231	766	243	216	6			
7	CG	155	Total	C	N	O	S	0	0	0
			1235	769	244	216	6			

- 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	0	0	0
			1088	689	206	191	2			
8	CH	137	Total	C	N	O	S	0	0	0
			1088	689	206	191	2			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 22 is a RNA chain called mRNA.

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

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

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

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

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

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

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

- 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	0	0	0
			2573	1146	476	832	119			

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

- 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	0	0	0
			2136	1349	423	361	3			
27	DD	275	Total	C	N	O	S	0	0	0
			2136	1349	423	361	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	BE	204	Total	C	N	O	S	0	0	0
			1559	985	298	270	6			
28	DE	204	Total	C	N	O	S	0	0	0
			1559	985	298	270	6			

- 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	0	0	1
			1584	1009	298	275	2			
29	DF	203	Total	C	N	O	S	0	0	1
			1580	1007	297	274	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	BG	181	Total	C	N	O	S	0	0	0
			1425	914	256	251	4			
30	DG	181	Total	C	N	O	S	0	0	0
			1424	911	258	251	4			

- 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	0	0	0
			1330	845	248	236	1			
31	DH	174	Total	C	N	O	S	0	0	0
			1330	845	248	236	1			

- 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	0	0	0
			1085	693	189	202	1			
32	DI	146	Total	C	N	O	S	0	0	0
			1061	680	186	194	1			

- 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	0	0	0
			1117	719	207	187	4			
33	DN	140	Total	C	N	O	S	0	0	0
			1117	719	207	187	4			

- 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	0	0	0
			933	588	171	170	4			
34	DO	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

- 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	0	0	0
			1135	706	230	196	3			
35	DP	149	Total	C	N	O	S	0	0	0
			1135	706	230	196	3			

- 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	0	0	0
			1122	715	212	188	7			
36	DQ	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- 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	0	0	0
			552	349	99	99	5			
50	D4	69	Total	C	N	O	S	0	0	0
			532	339	97	91	5			

- 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	0	0	0
			455	285	89	76	5			
51	D5	59	Total	C	N	O	S	0	0	0
			455	285	89	76	5			

- 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	0	0	0
			453	281	91	77	4			
52	D6	53	Total	C	N	O	S	0	0	0
			449	279	91	75	4			

- 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	0	0	0
			418	257	104	55	2			
53	D7	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			

- 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	0	0	0
			511	328	99	82	2			
54	D8	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			

- 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	0	0	0
			307	188	68	47	4			
55	D9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			

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

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

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

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

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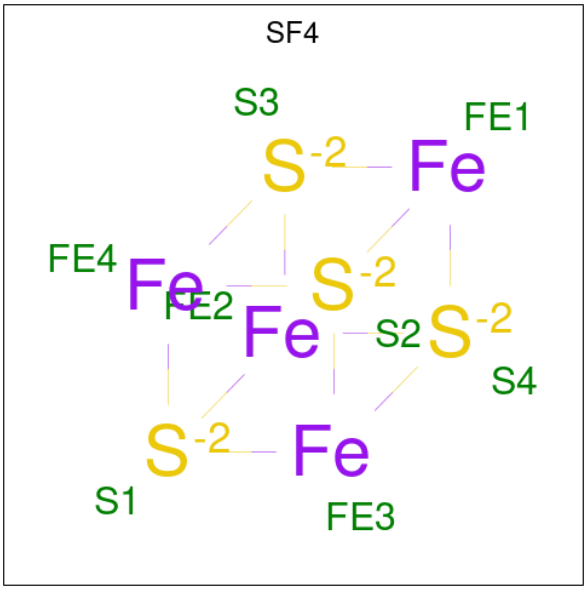
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	DT	1	Total Mg 1 1	0	0
56	DU	1	Total Mg 1 1	0	0
56	DV	2	Total Mg 2 2	0	0
56	DW	2	Total Mg 2 2	0	0
56	DY	1	Total Mg 1 1	0	0
56	D0	1	Total Mg 1 1	0	0
56	D3	1	Total Mg 1 1	0	0
56	D5	1	Total Mg 1 1	0	0
56	D7	1	Total Mg 1 1	0	0
56	D8	2	Total Mg 2 2	0	0

- Molecule 57 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



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

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

- Molecule 58 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 59 is POTASSIUM ION (CCD ID: K) (formula: K).

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

- Molecule 60 is water.

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

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

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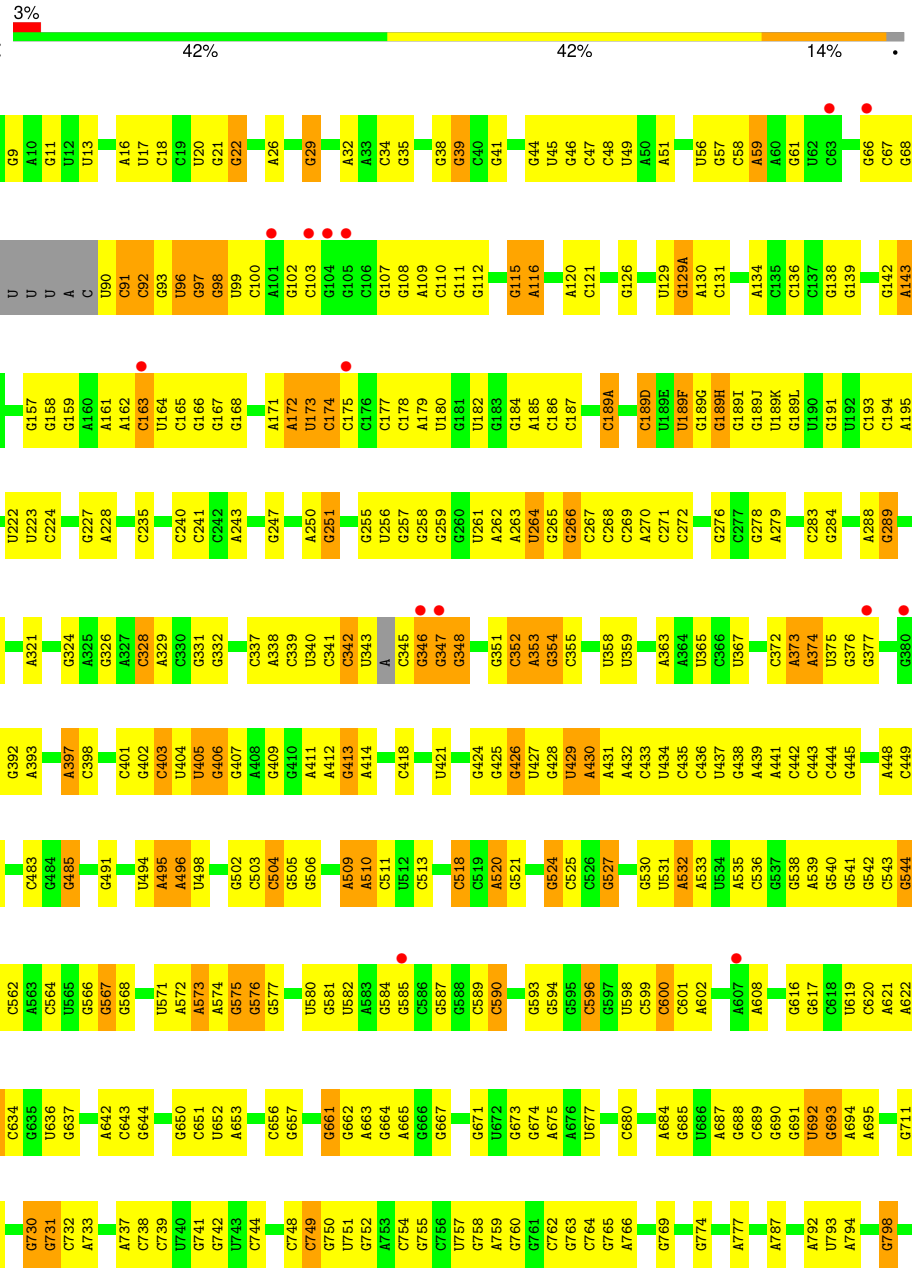
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	DF	6	Total O 6 6	0	0
60	DO	1	Total O 1 1	0	0
60	DP	6	Total O 6 6	0	0
60	DU	3	Total O 3 3	0	0
60	DV	1	Total O 1 1	0	0
60	DW	1	Total O 1 1	0	0
60	DX	3	Total O 3 3	0	0
60	D0	5	Total O 5 5	0	0
60	D1	1	Total O 1 1	0	0
60	D3	1	Total O 1 1	0	0
60	D8	3	Total O 3 3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

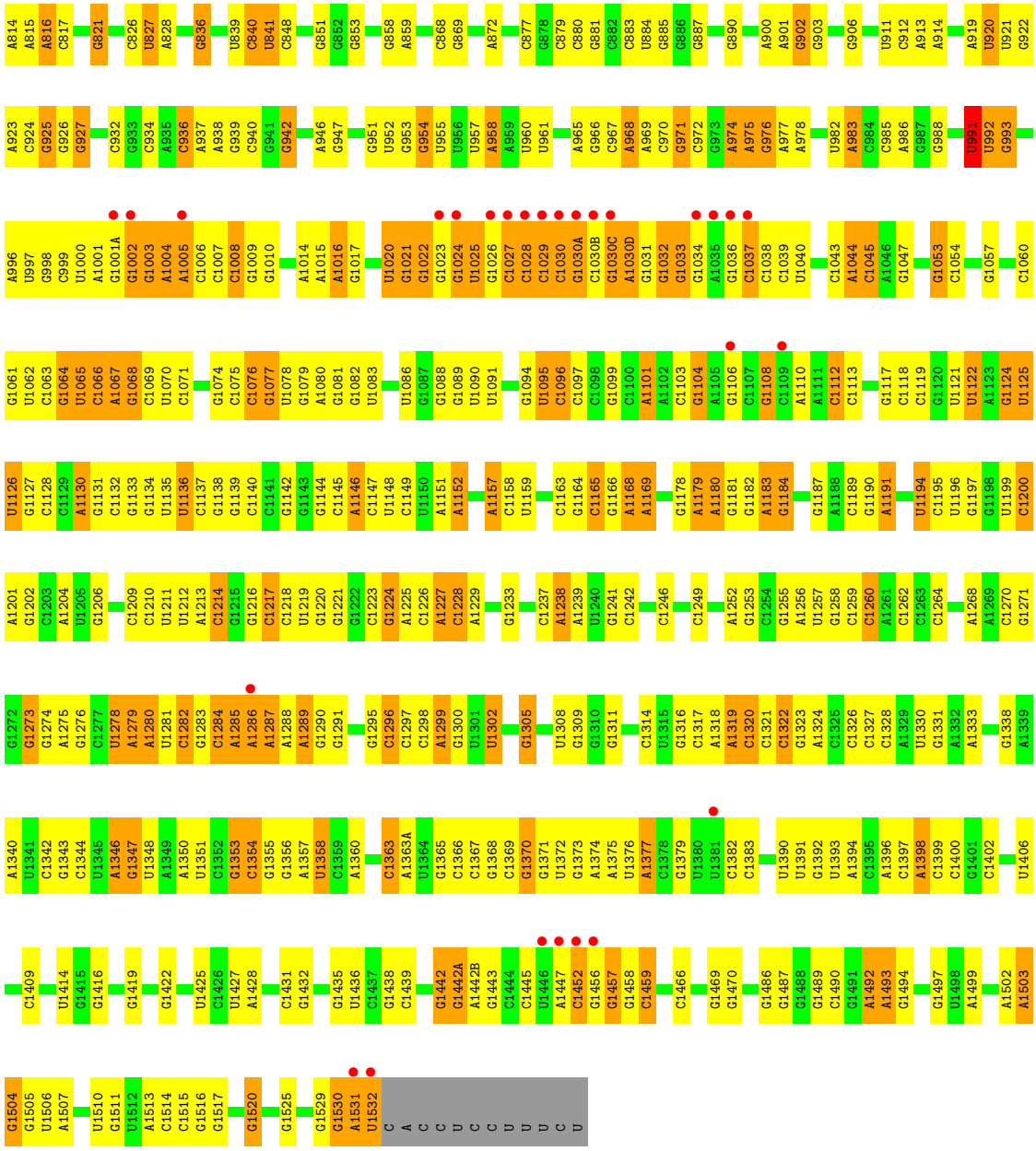
3 Residue-property plots (i)

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

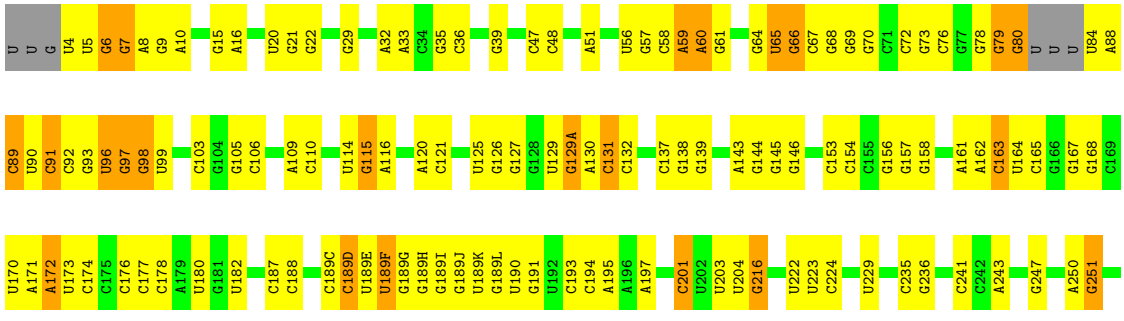
Chain AA:

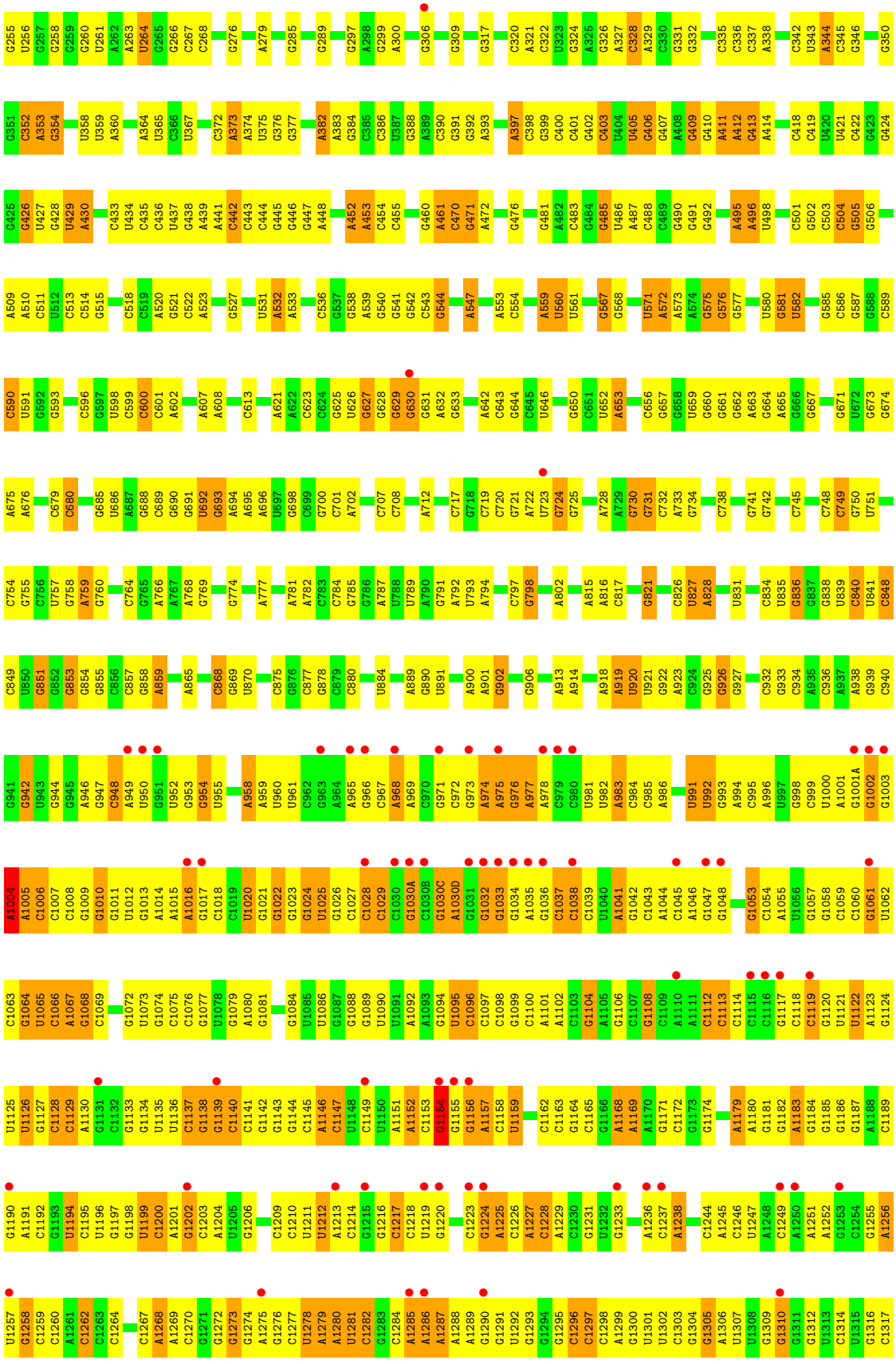


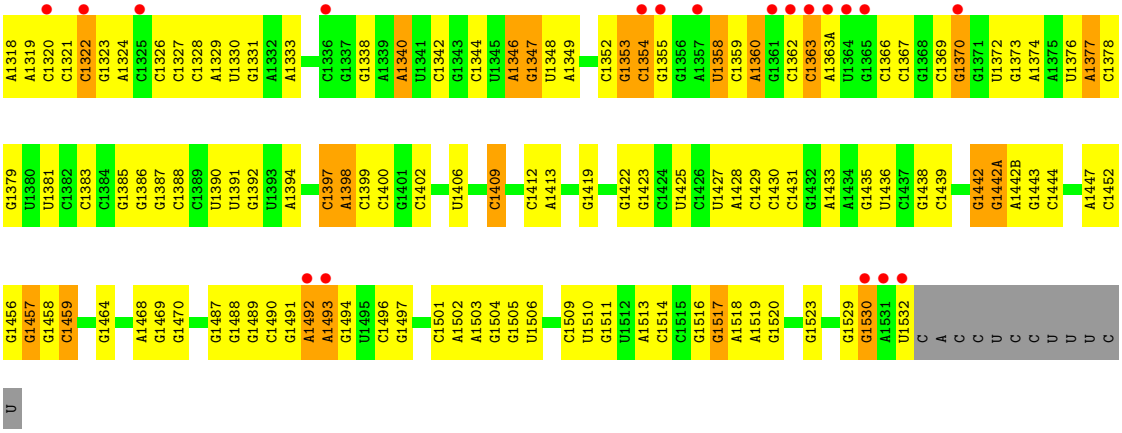


• Molecule 1: 16S Ribosomal RNA

Chain CA:

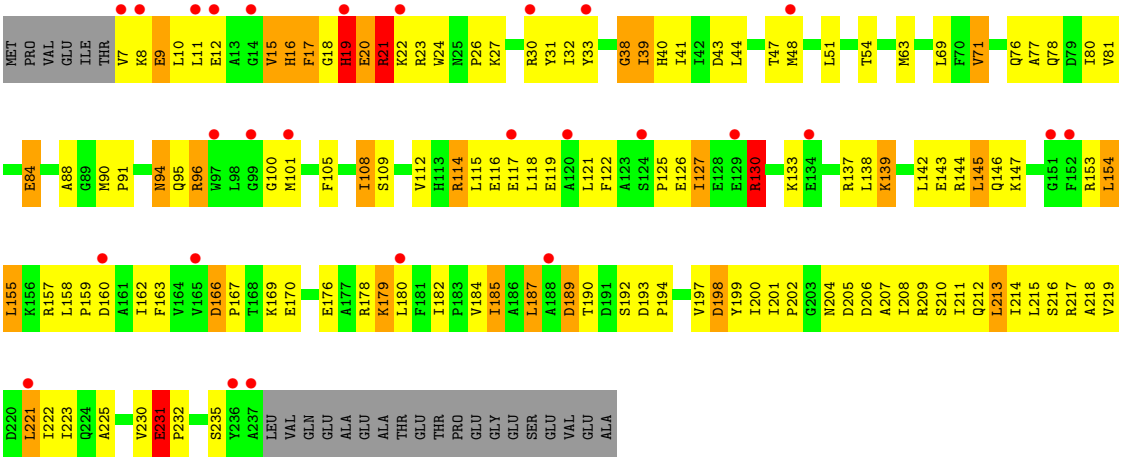






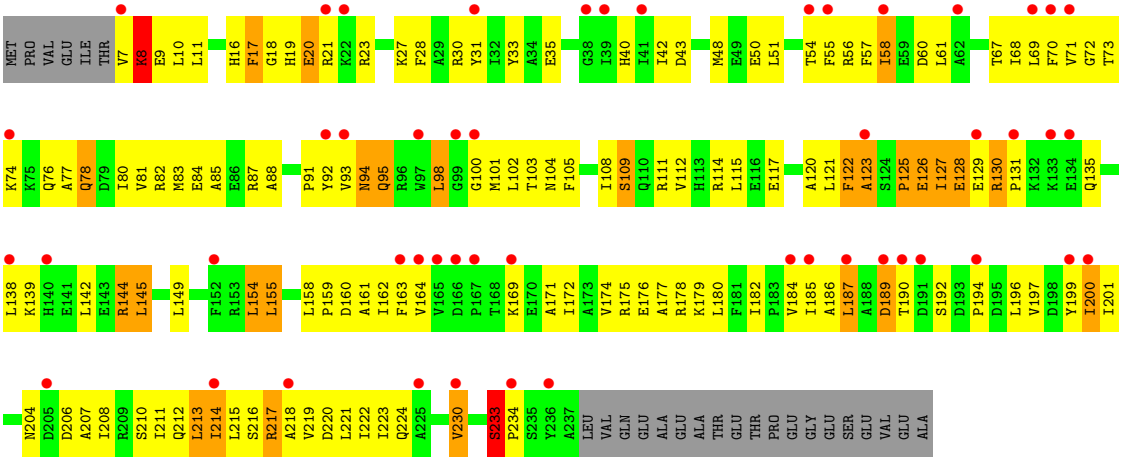
• Molecule 2: 30S ribosomal protein S2

Chain AB:



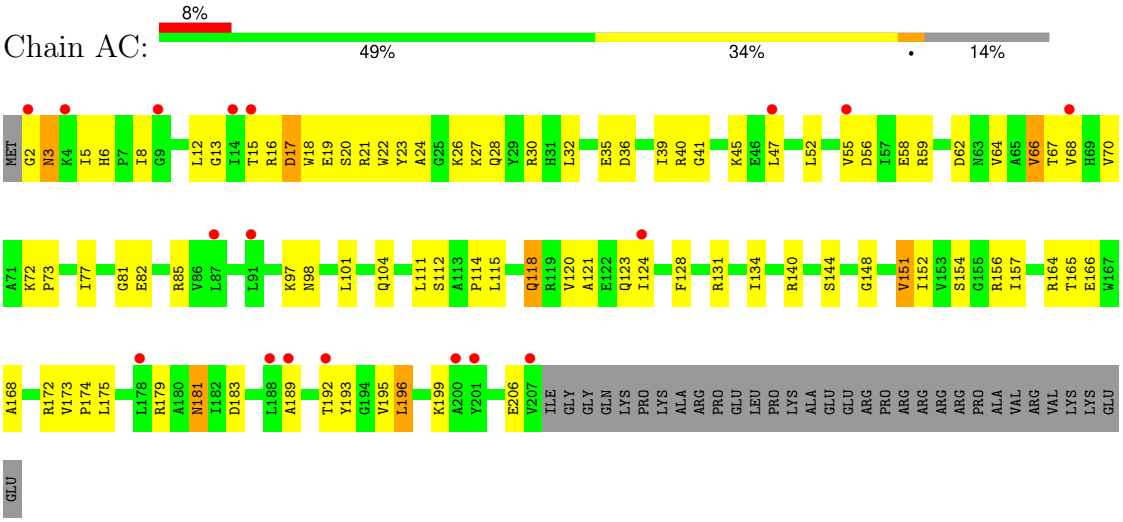
• Molecule 2: 30S ribosomal protein S2

Chain CB:



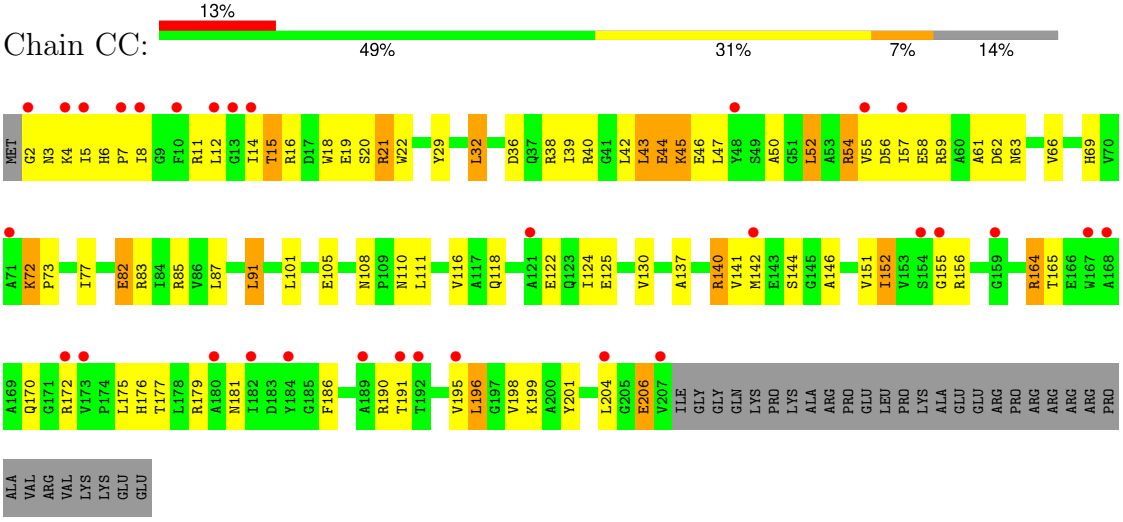
• Molecule 3: 30S ribosomal protein S3

Chain AC:



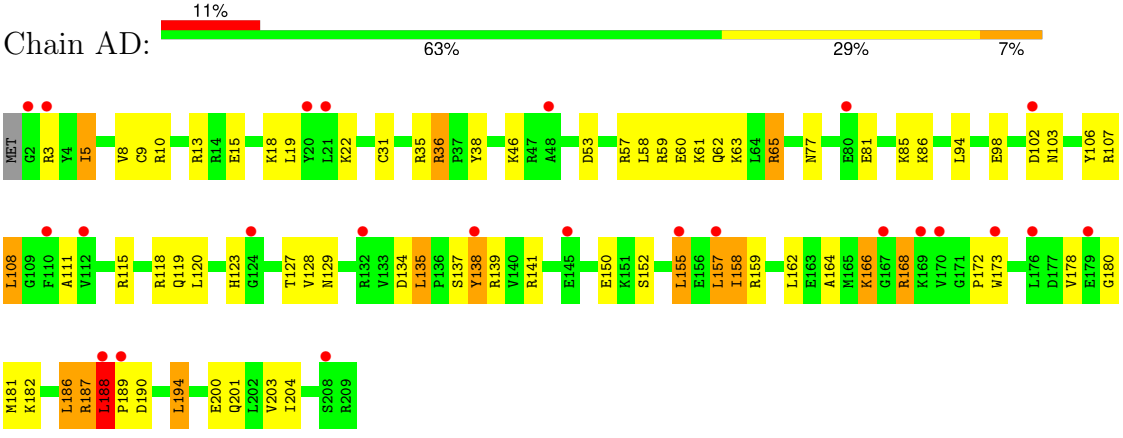
• Molecule 3: 30S ribosomal protein S3

Chain CC:



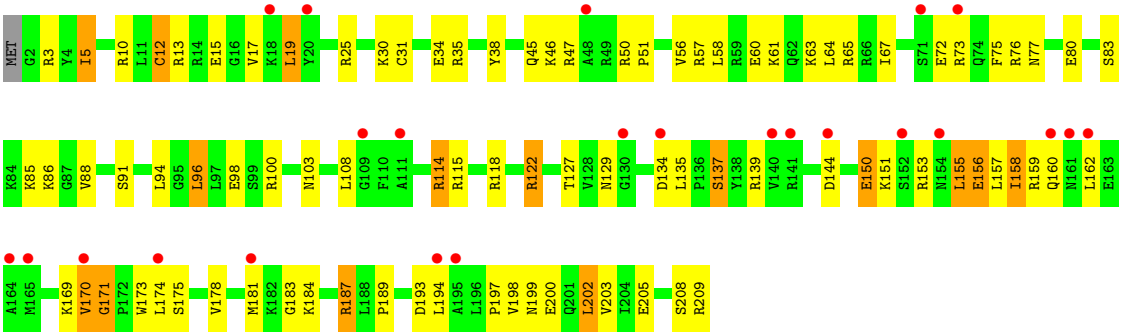
• Molecule 4: 30S ribosomal protein S4

Chain AD:

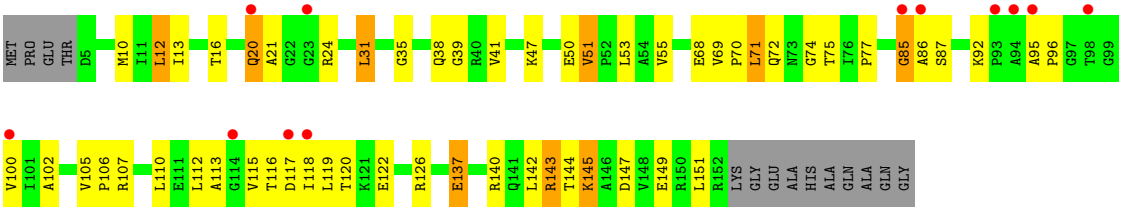


• Molecule 4: 30S ribosomal protein S4

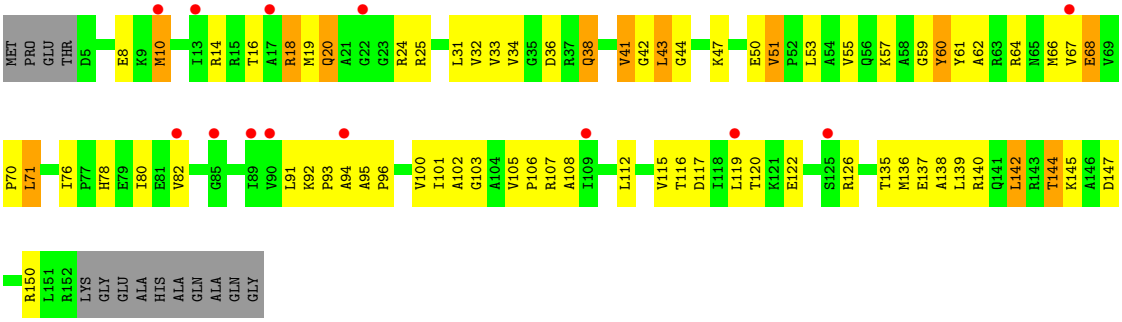
Chain CD:



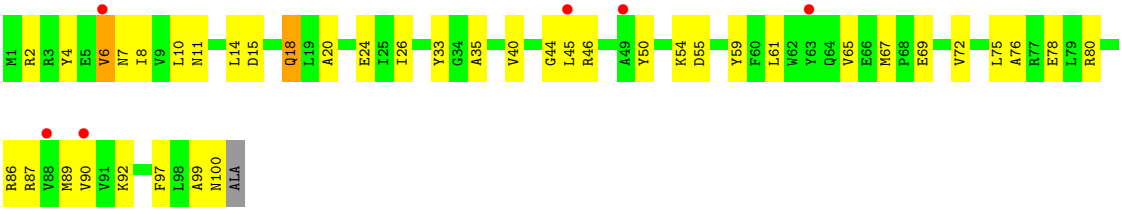
• Molecule 5: 30S ribosomal protein S5



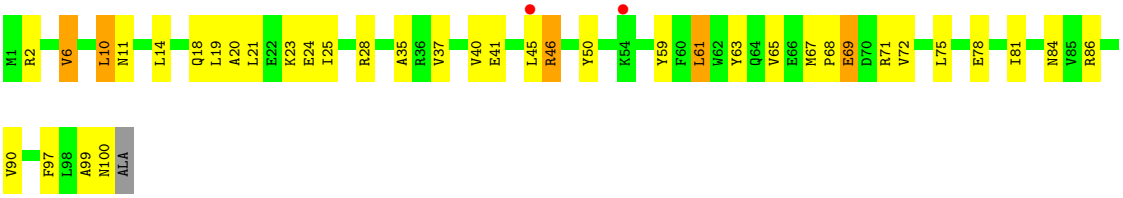
• Molecule 5: 30S ribosomal protein S5



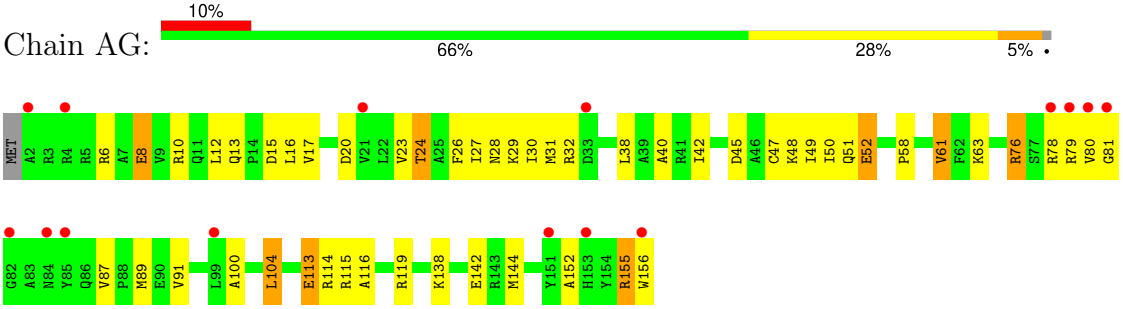
• Molecule 6: 30S ribosomal protein S6



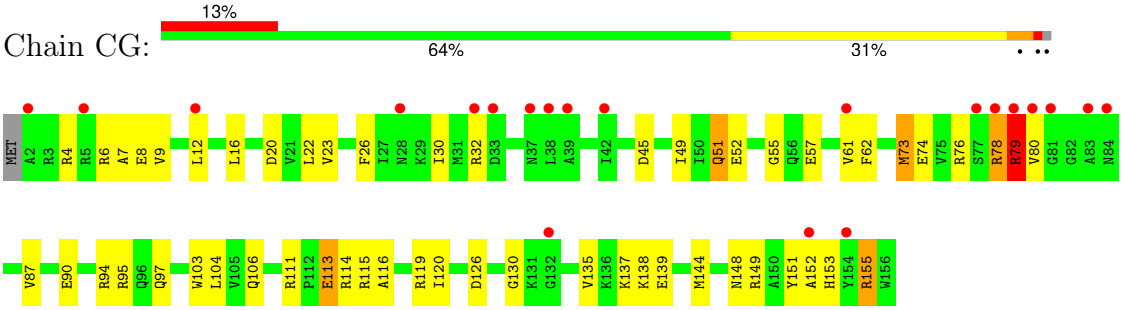
• Molecule 6: 30S ribosomal protein S6



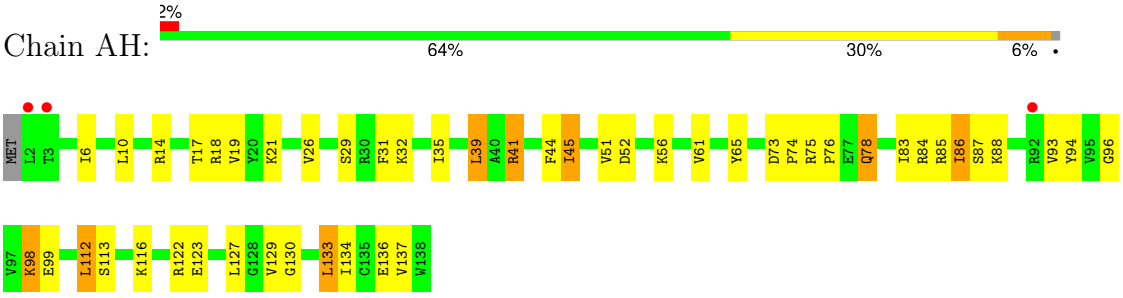
• Molecule 7: 30S ribosomal protein S7



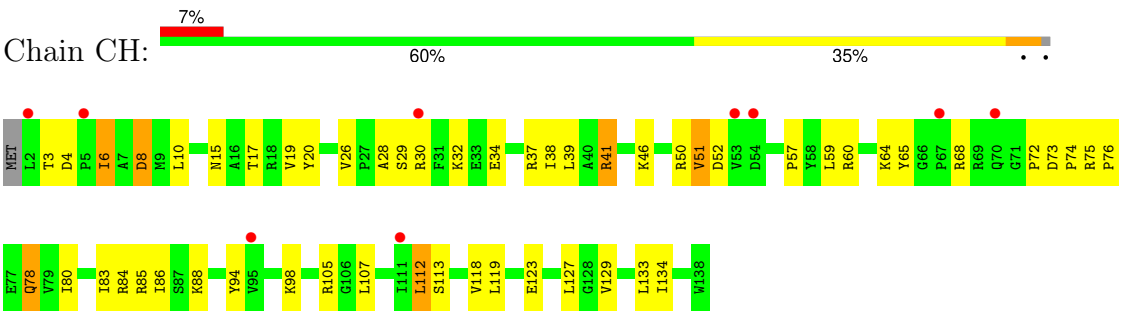
• Molecule 7: 30S ribosomal protein S7



• Molecule 8: 30S ribosomal protein S8

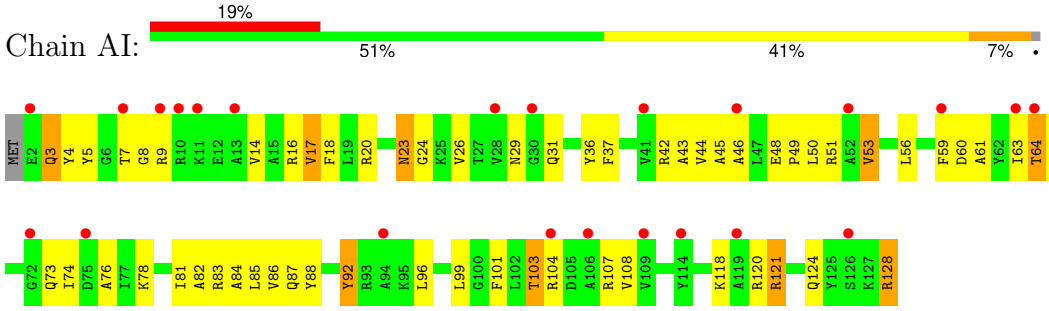


• Molecule 8: 30S ribosomal protein S8



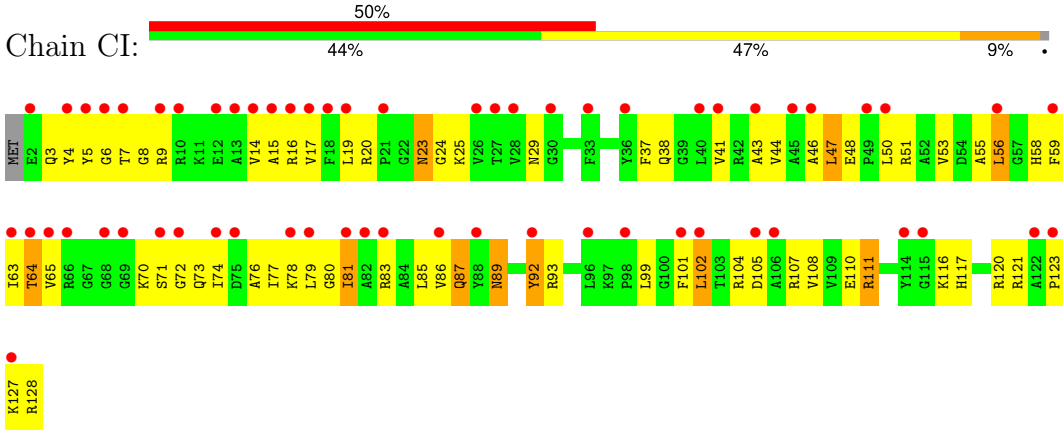
• Molecule 9: 30S ribosomal protein S9

Chain AI:



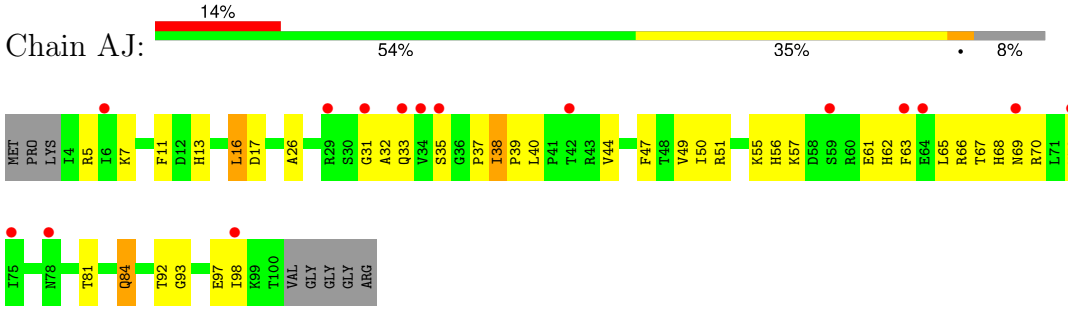
• Molecule 9: 30S ribosomal protein S9

Chain CI:



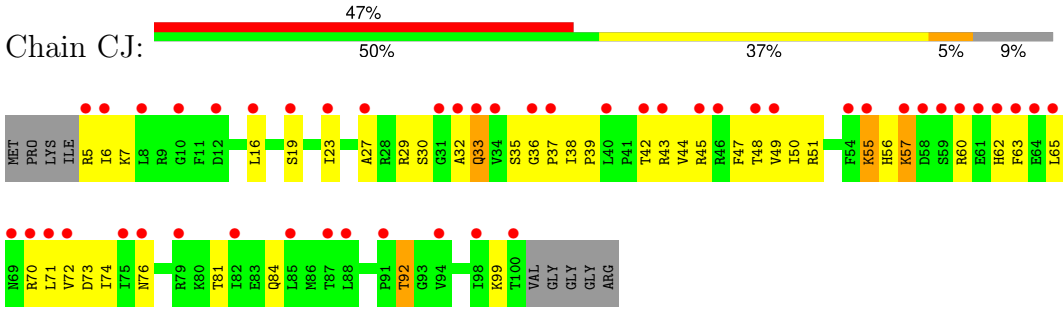
• Molecule 10: 30S ribosomal protein S10

Chain AJ:



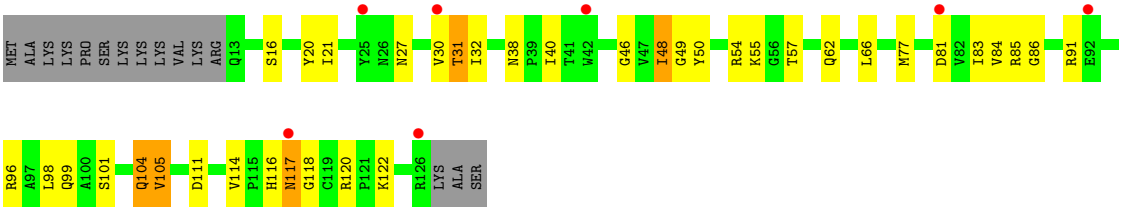
• Molecule 10: 30S ribosomal protein S10

Chain CJ:



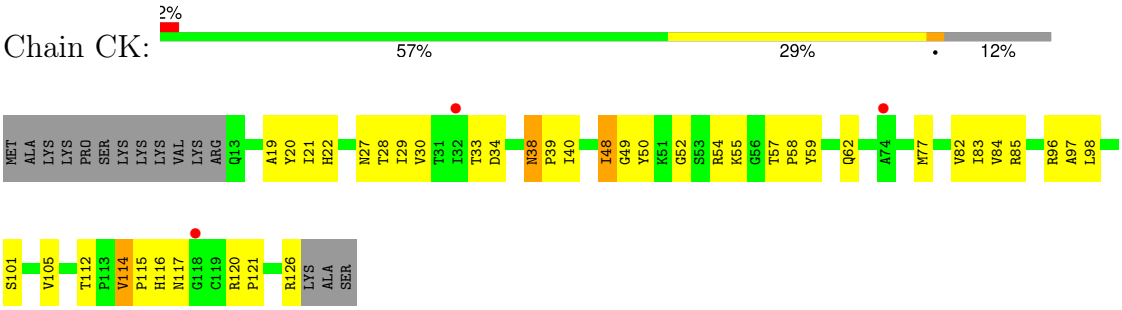
• Molecule 11: 30S ribosomal protein S11

Chain AK:



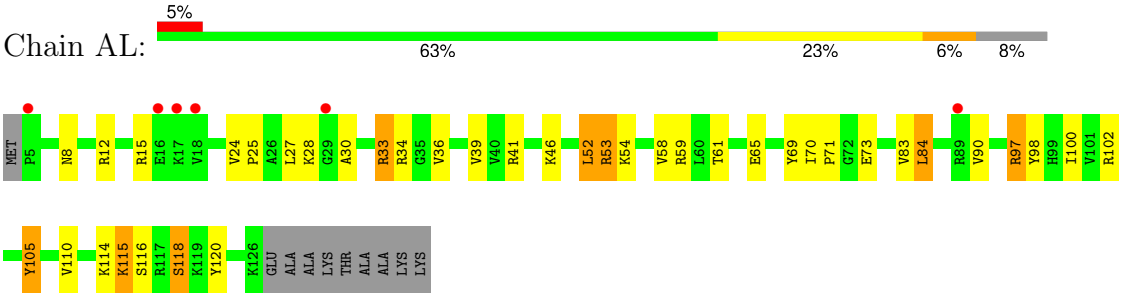
• Molecule 11: 30S ribosomal protein S11

Chain CK:



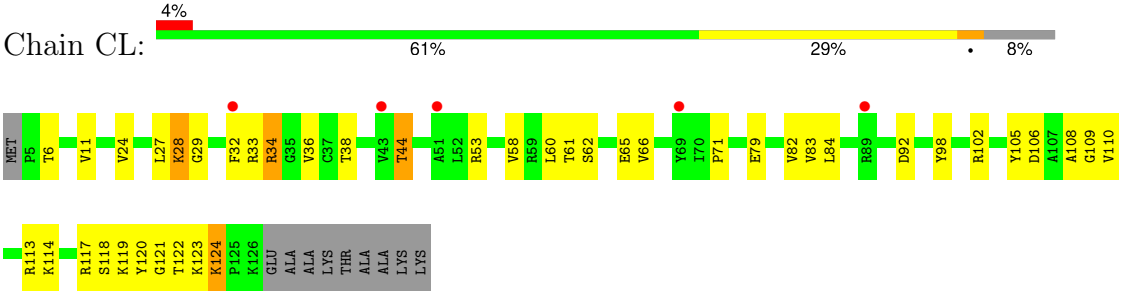
• Molecule 12: 30S ribosomal protein S12

Chain AL:



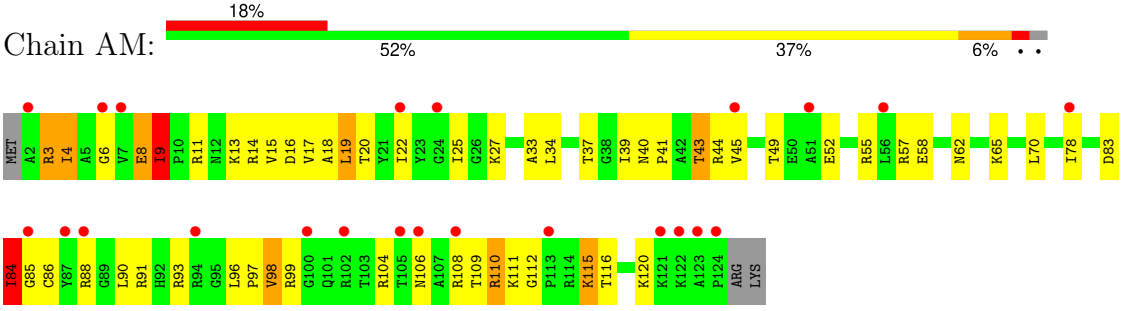
• Molecule 12: 30S ribosomal protein S12

Chain CL:



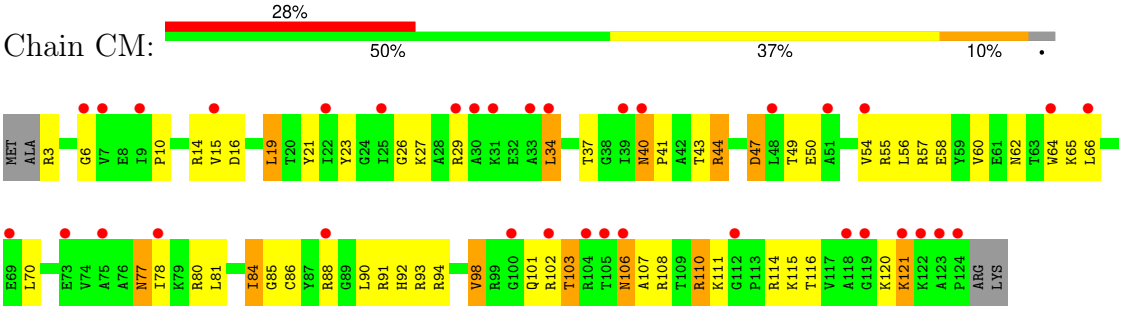
• Molecule 13: 30S ribosomal protein S13

Chain AM:



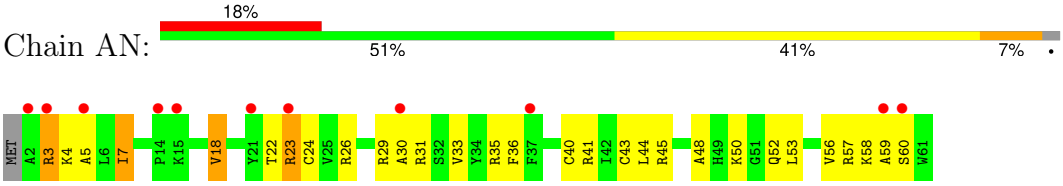
• Molecule 13: 30S ribosomal protein S13

Chain CM:



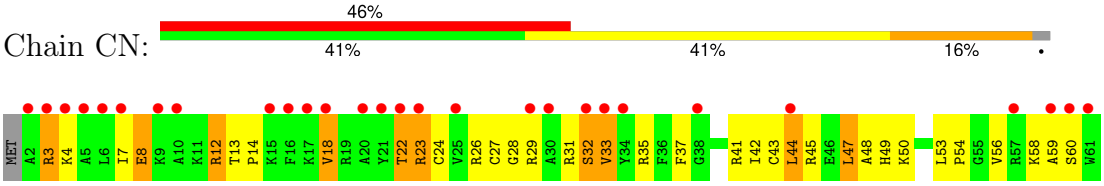
• Molecule 14: 30S ribosomal protein S14 type Z

Chain AN:



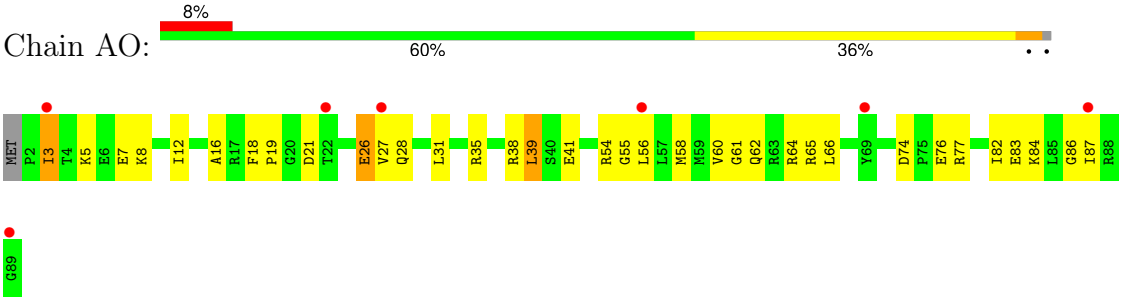
• Molecule 14: 30S ribosomal protein S14 type Z

Chain CN:



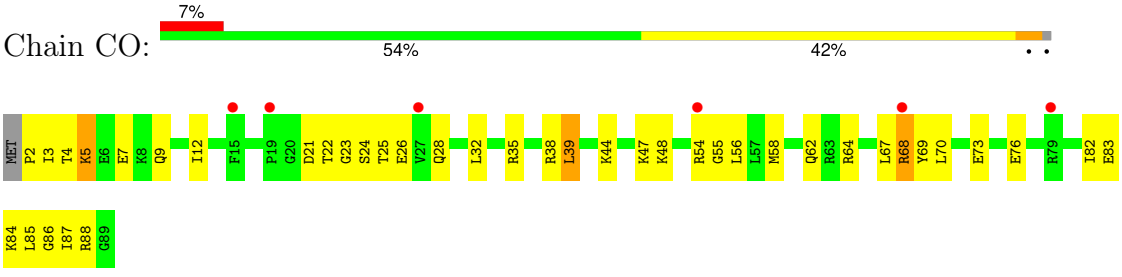
• Molecule 15: 30S ribosomal protein S15

Chain AO:



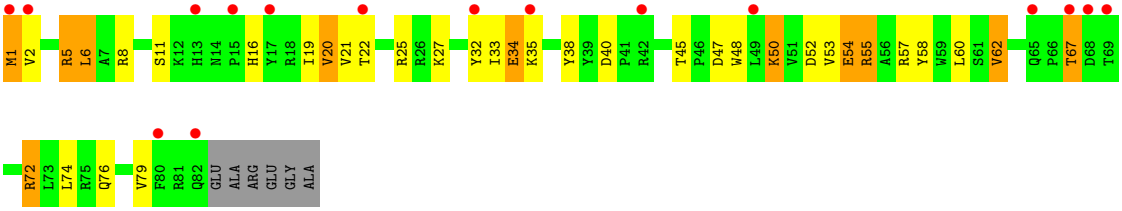
• Molecule 15: 30S ribosomal protein S15

Chain CO:



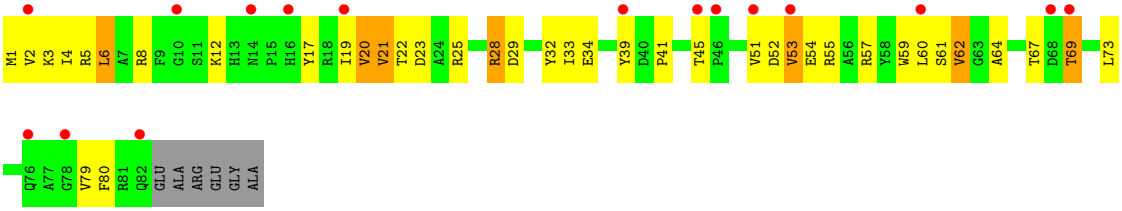
• Molecule 16: 30S ribosomal protein S16

Chain AP:



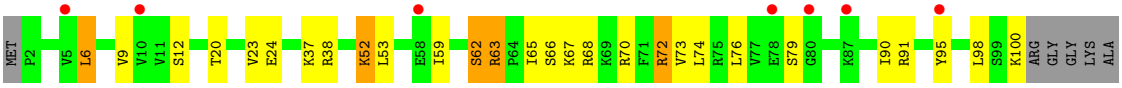
• Molecule 16: 30S ribosomal protein S16

Chain CP:



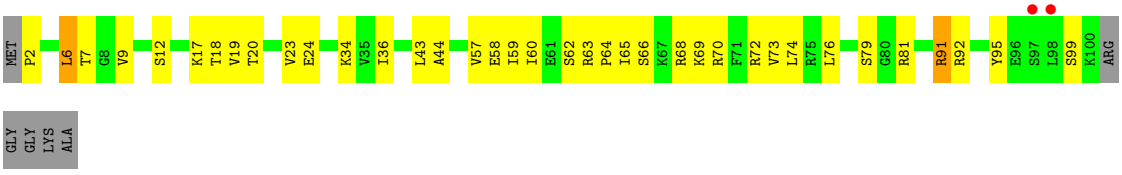
• Molecule 17: 30S ribosomal protein S17

Chain AQ:



• Molecule 17: 30S ribosomal protein S17

Chain CQ:



• Molecule 18: 30S ribosomal protein S18

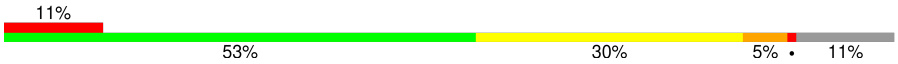
Chain AR:

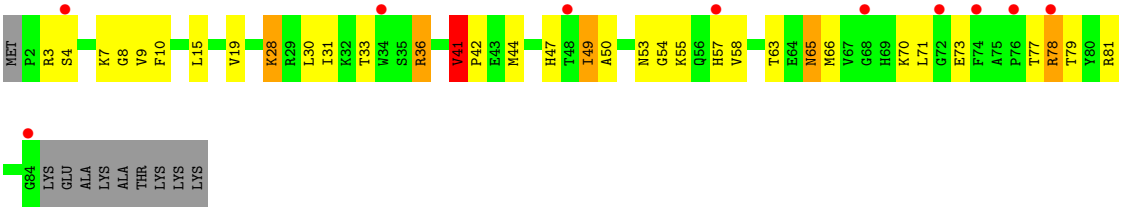
• Molecule 18: 30S ribosomal protein S18

Chain CR:

• Molecule 19: 30S ribosomal protein S19

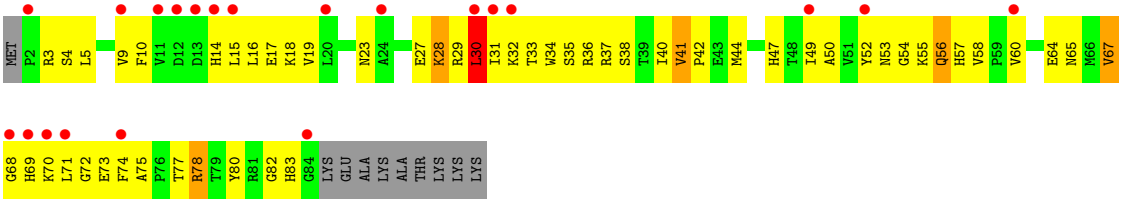
Chain AS:





• Molecule 19: 30S ribosomal protein S19

Chain CS:

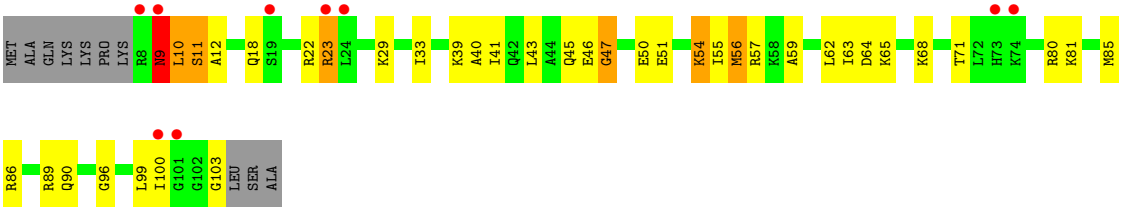


• Molecule 20: 30S ribosomal protein S20

Chain AT:

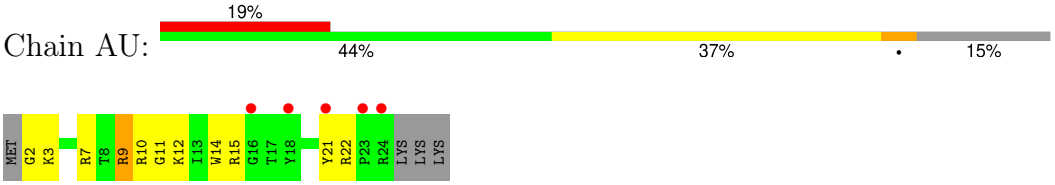
• Molecule 20: 30S ribosomal protein S20

Chain CT:



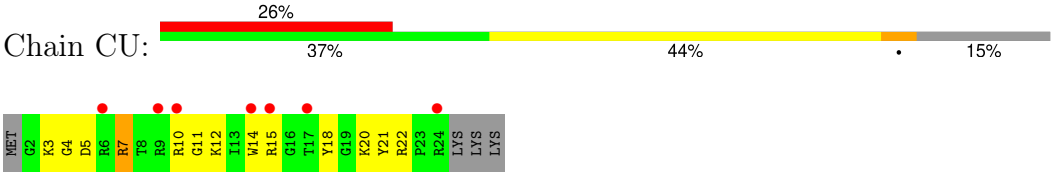
• Molecule 21: 30S ribosomal protein Thx

Chain AU:



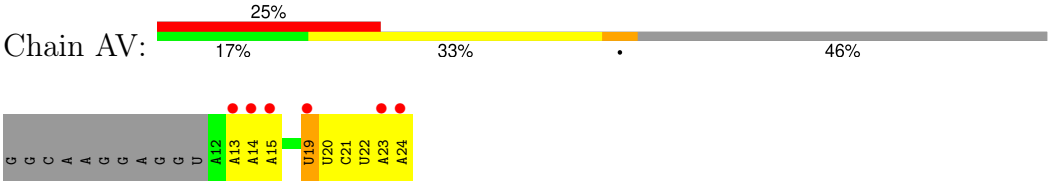
• Molecule 21: 30S ribosomal protein Thx

Chain CU:



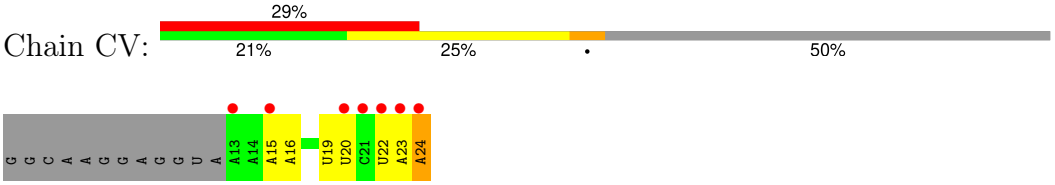
• Molecule 22: mRNA

Chain AV:



• Molecule 22: mRNA

Chain CV:



• Molecule 23: Cytidine-Puromycin

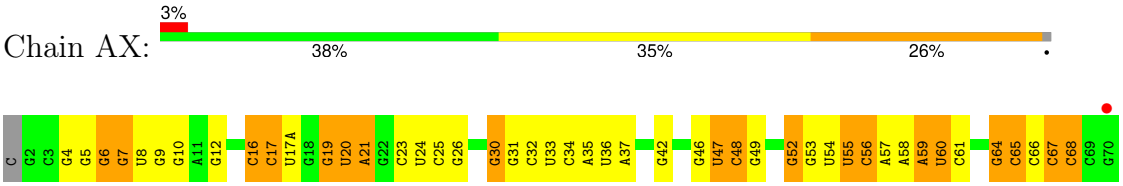
Chain AW:

• Molecule 23: Cytidine-Puromycin

Chain CW:

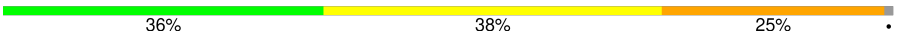
• Molecule 24: P-site tRNA

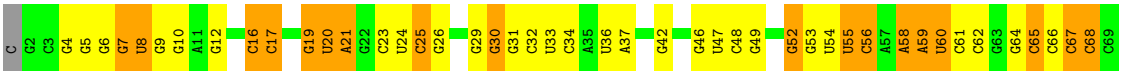
Chain AX:



• Molecule 24: P-site tRNA

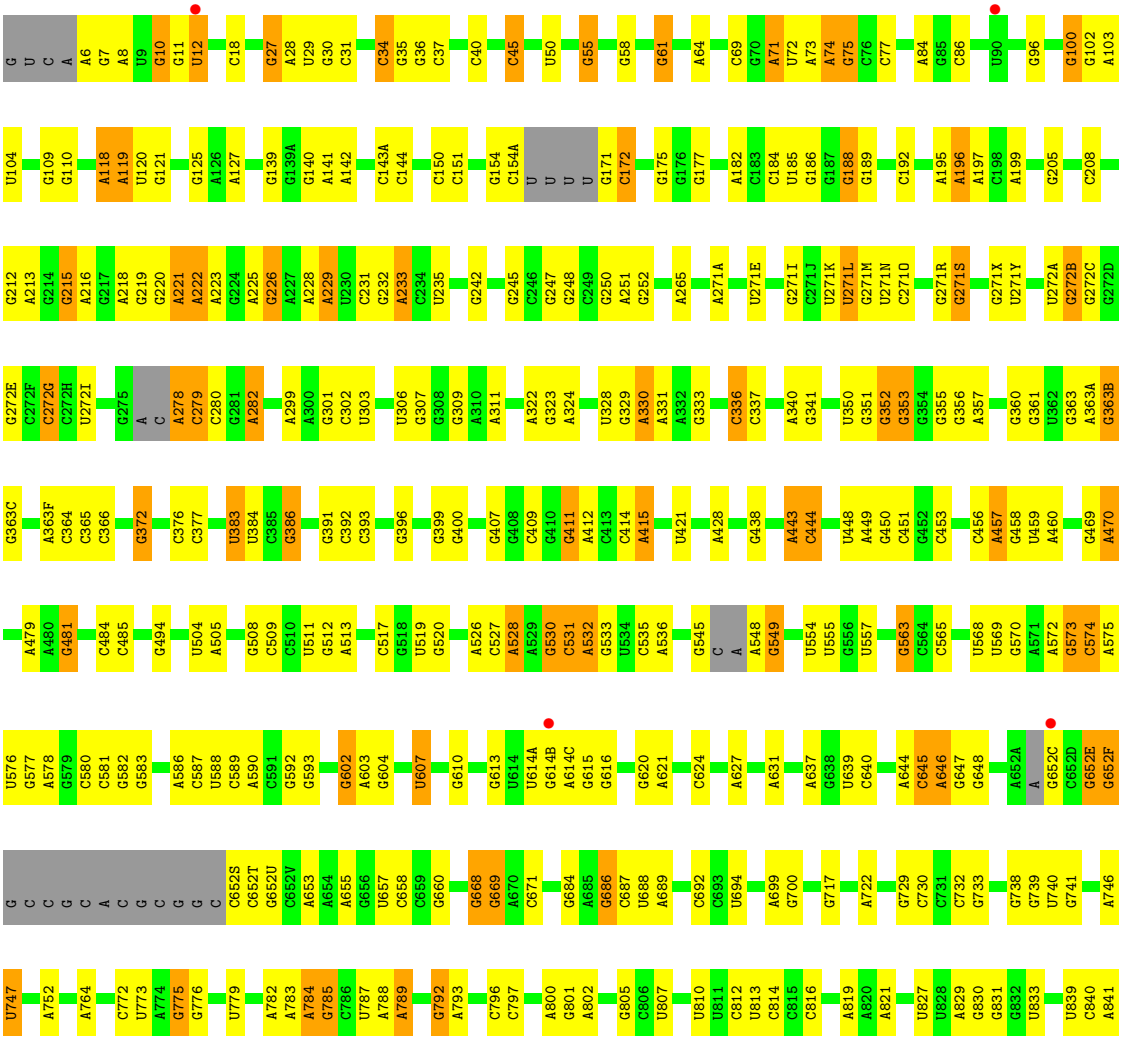
Chain CX:

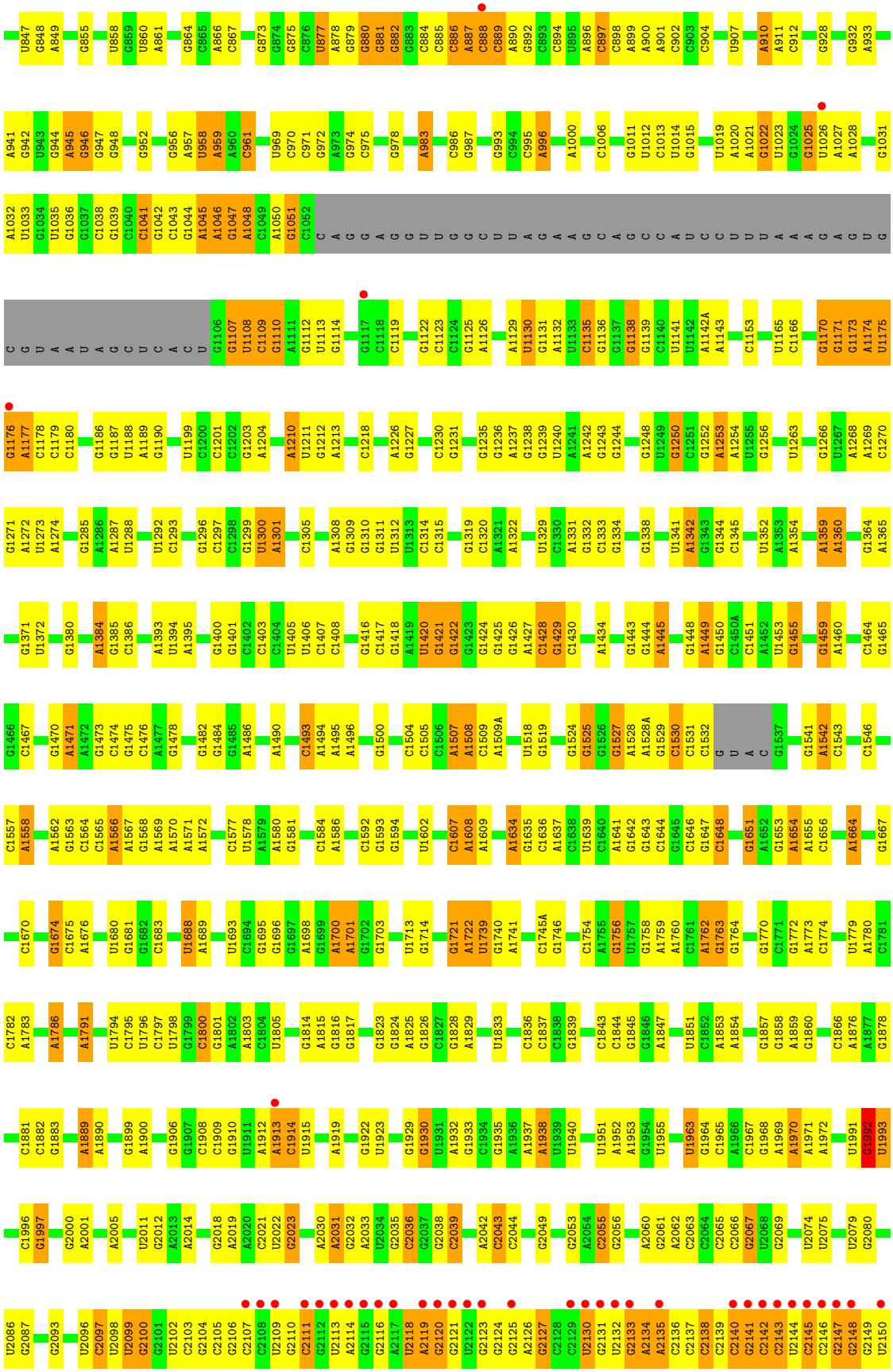


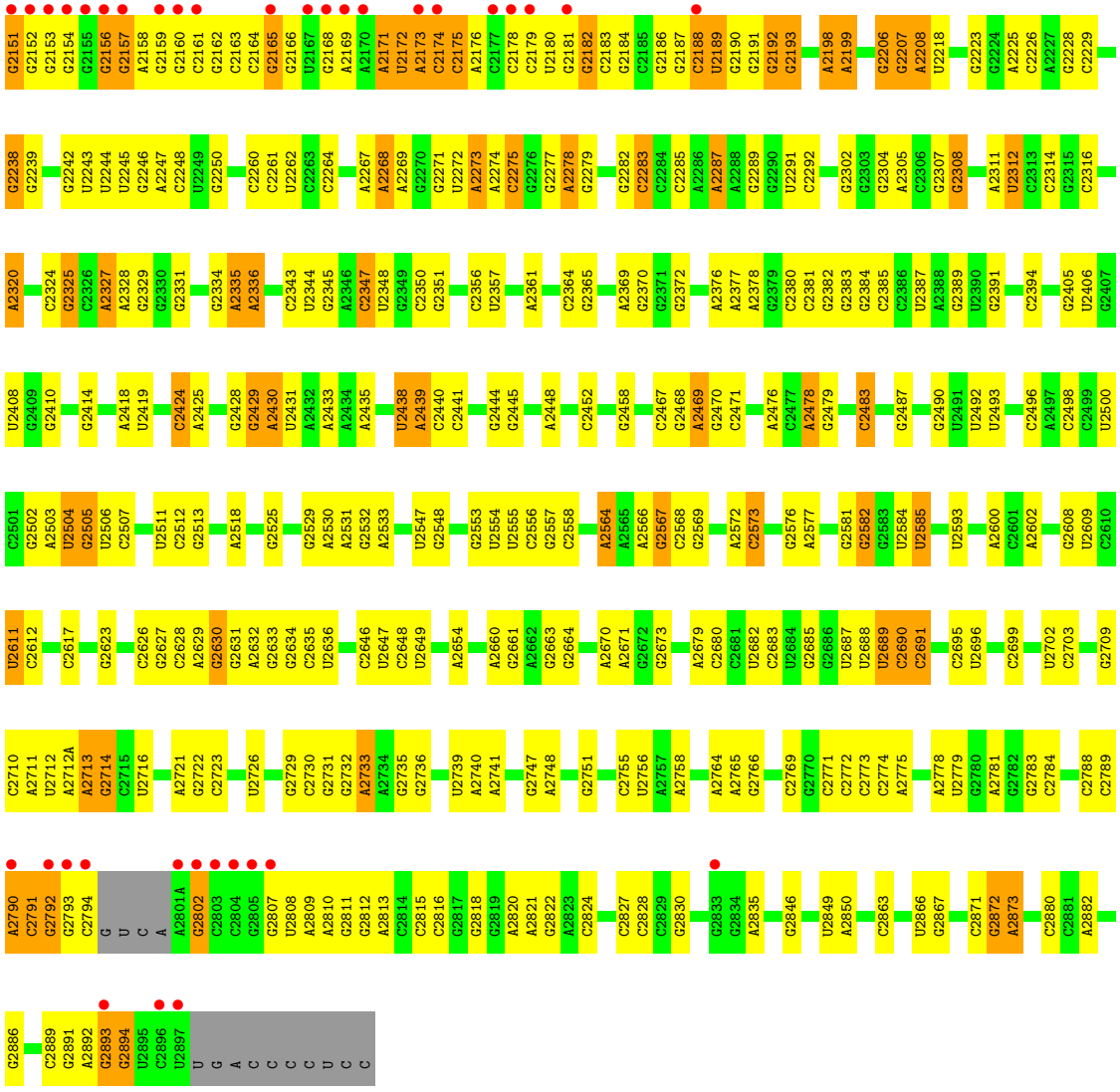


• Molecule 25: 23S Ribosomal RNA

Chain BA:

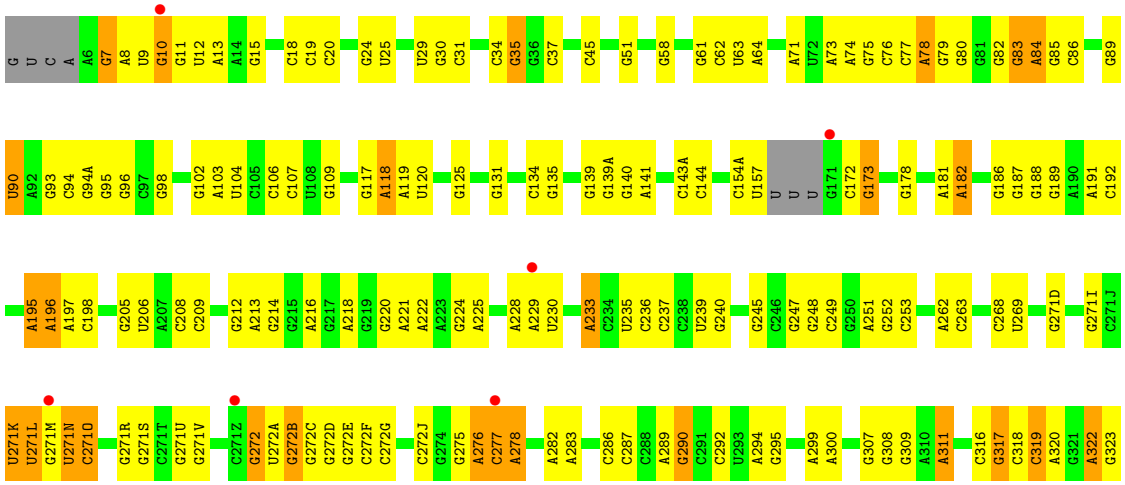


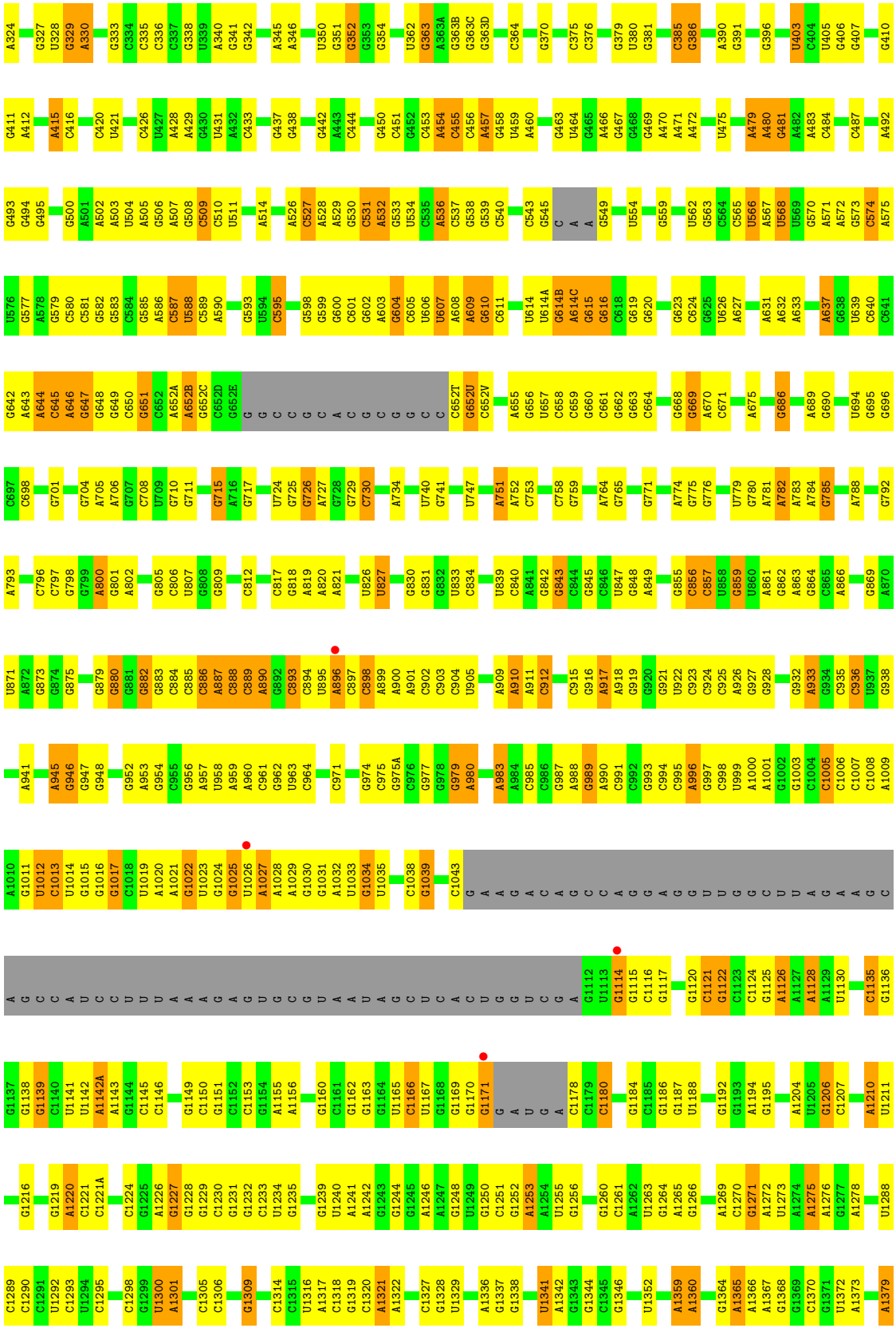




• Molecule 25: 23S Ribosomal RNA

Chain DA:

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G411 A412 A415 C416 C420 U421 C426 U427 A428 A429 G430 U431 A432 C433 G437 G438 G442 A443 C444 G450 C451 G452 C453 A454 C455 C456 A457 G458 U459 A460 G463 U464 G465 A466 G467 G468 G469 A470 A471 A472 U475 A479 A480 G481 A482 A483 C484 C487 A492
G493 G494 G495 G500 A501 A502 A503 U504 A505 G506 A507 G508 C509 C510 U511 A514 A526 C527 A528 A529 G530 C531 A532 G533 U534 C535 A536 C537 G538 G539 C540 C543 G545 C A A G549 U554 G559 U562 G563 C564 C565 U566 A567 U568 U569 G570 A571 A572 G573 C574 A575
U576 G577 A578 G579 C580 C581 G582 G583 C584 G585 A586 C587 U588 C589 A590 G593 U594 C595 G598 G599 G600 C601 G602 A603 G604 C605 U606 U607 A608 A609 G610 C611 U614 U614A G614B A614C G615 G616 C618 G619 G620 G623 C624 G625 U626 A627 A631 A632 A633 A637 G638 U639 C640 C641
G642 A643 A644 C645 A646 G647 G648 G649 C650 G651 C652 A652A A652B G652C C652D G652E G C C C G C A C G C G C C652T G652U C652V A655 G656 U657 C658 C659 G660 C661 G662 G663 C664 G668 G669 A670 C671 A675 G686 A689 G690 U694 G695 G696
C697 C698 G701 G704 A705 A706 G707 C708 U709 G710 G711 G715 A716 G717 U724 G725 G726 A727 G728 G729 C730 A734 U740 G741 U747 A751 A752 C753 C758 G759 A764 G765 G771 A774 G775 G776 U779 G780 A781 A782 A783 A784 G785 A788 G792
A793 C796 C797 G798 G799 A800 G801 A802 G805 C806 U807 G808 G809 C812 C817 G818 A819 A820 A821 U826 U827 G830 G831 G832 U833 C834 U839 C840 A841 G842 G843 C844 G845 C846 U847 G848 A849 G855 C856 C857 U858 G859 U860 A861 G862 A863 G864 C865 A866 G869 A870
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A941 A945 G946 G947 G948 G952 A953 G954 C955 G956 A957 U958 A959 A960 C961 G962 U963 C964 C971 G974 C975 G975A C976 G977 G978 G979 A980 A983 A984 C985 C986 G987 A988 G989 A990 C991 C992 G993 C994 C995 A996 G997 C998 U999 A1000 A1001 G1002 G1003 C1004 C1005 C1006 C1007 C1008 A1009
A1010 G1011 U1012 C1013 U1014 G1015 G1016 G1017 C1018 U1019 A1020 A1021 G1022 U1023 G1024 G1025 U1026 A1027 A1028 A1029 G1030 G1031 A1032 U1033 G1034 U1035 C1038 G1039 C1043 G A A G A C A G C C C G A
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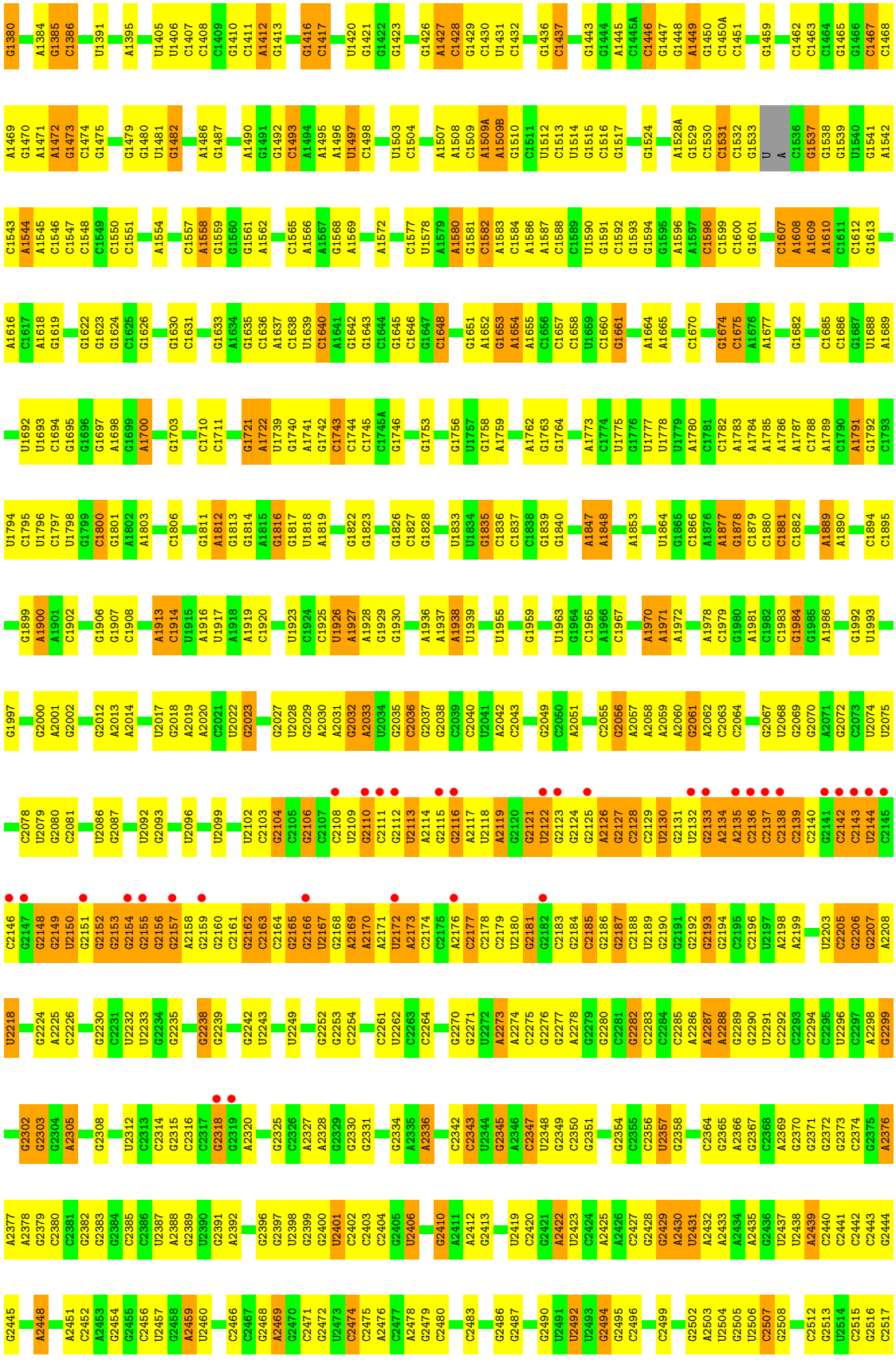
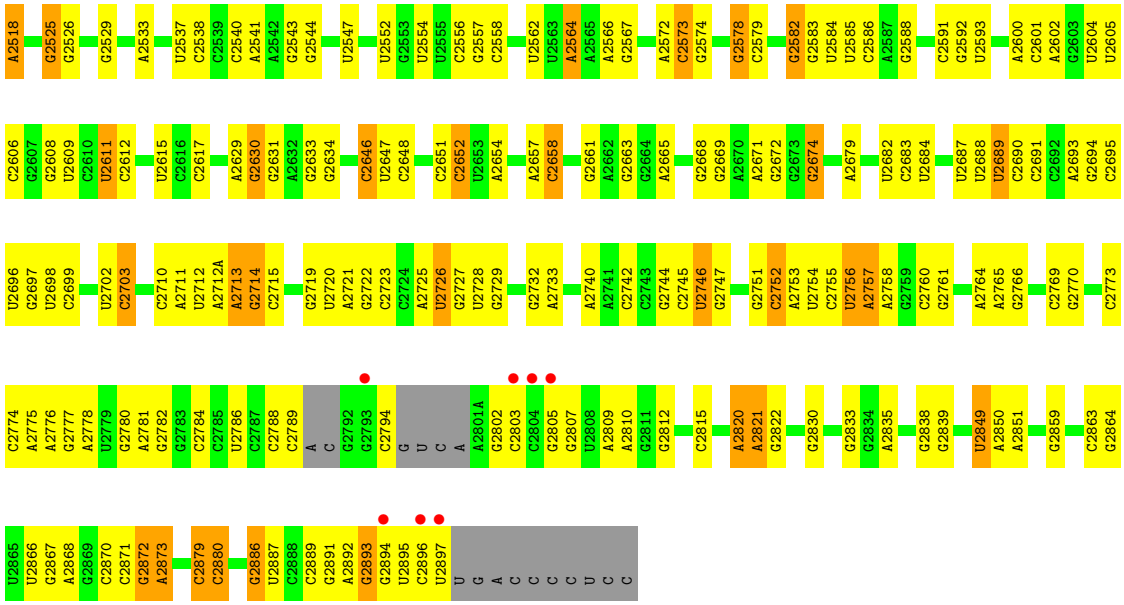


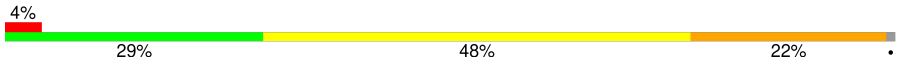


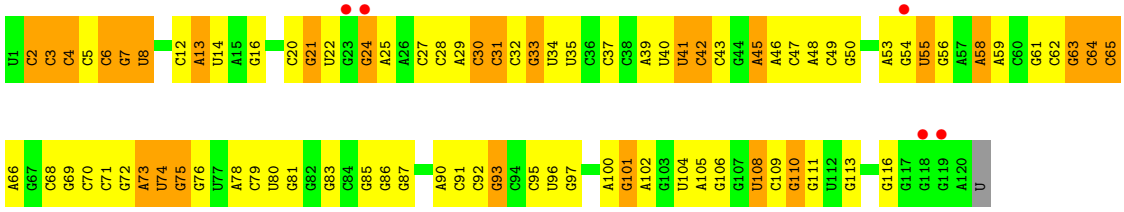
• Molecule 26: 5S Ribosomal RNA

Chain BB:

• Molecule 26: 5S Ribosomal RNA

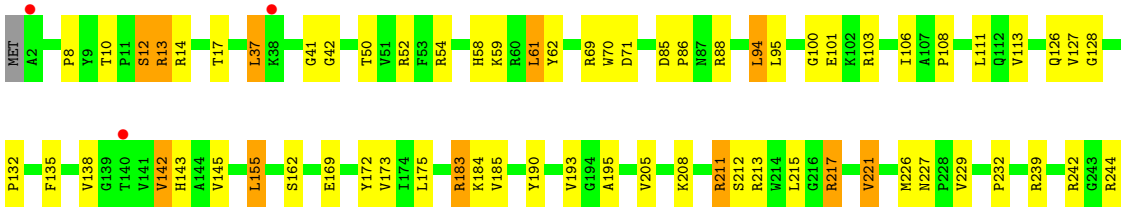
Chain DB:

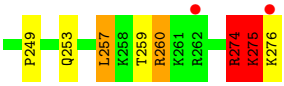




• Molecule 27: 50S ribosomal protein L2

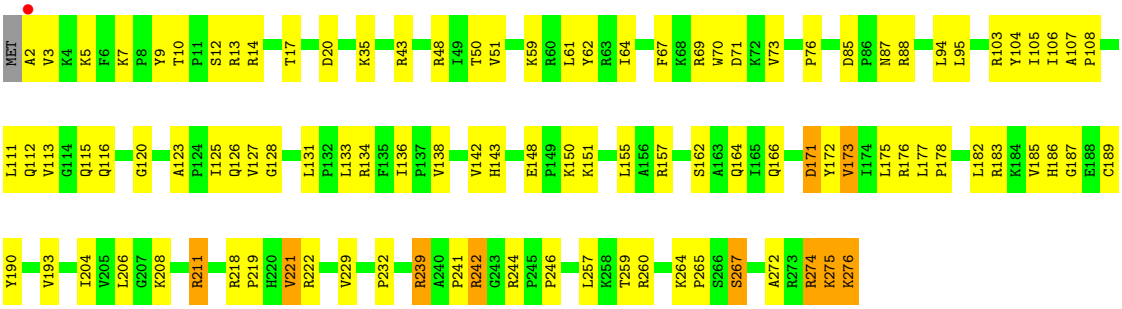
Chain BD:





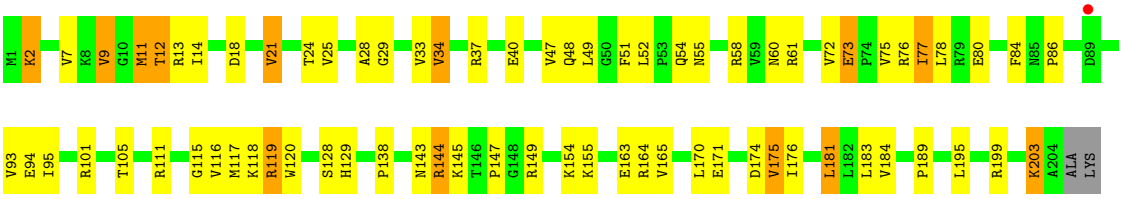
• Molecule 27: 50S ribosomal protein L2

Chain DD:



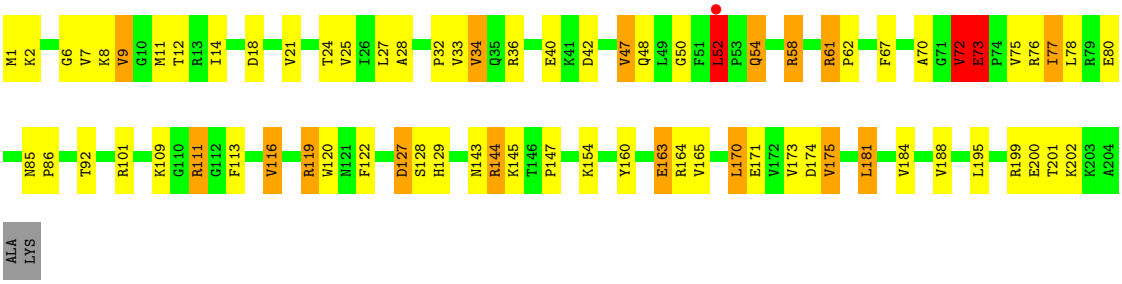
• Molecule 28: 50S ribosomal protein L3

Chain BE:



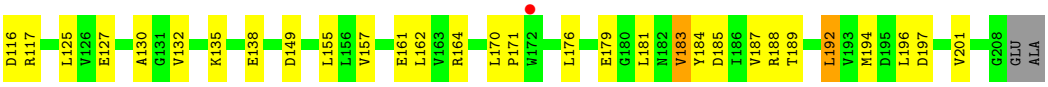
• Molecule 28: 50S ribosomal protein L3

Chain DE:



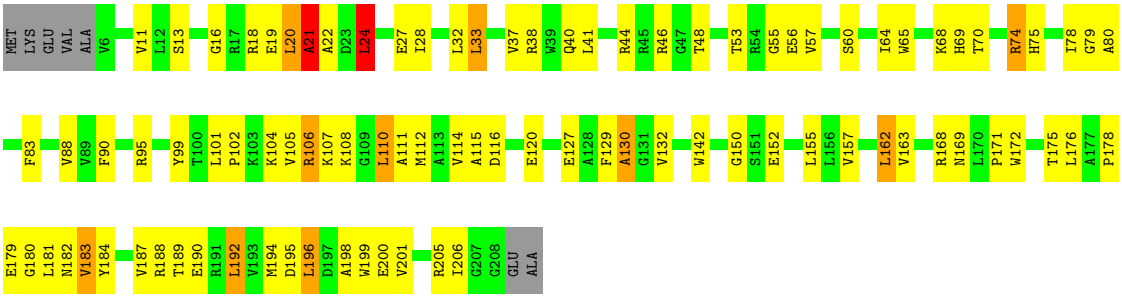
• Molecule 29: 50S ribosomal protein L4

Chain BF:



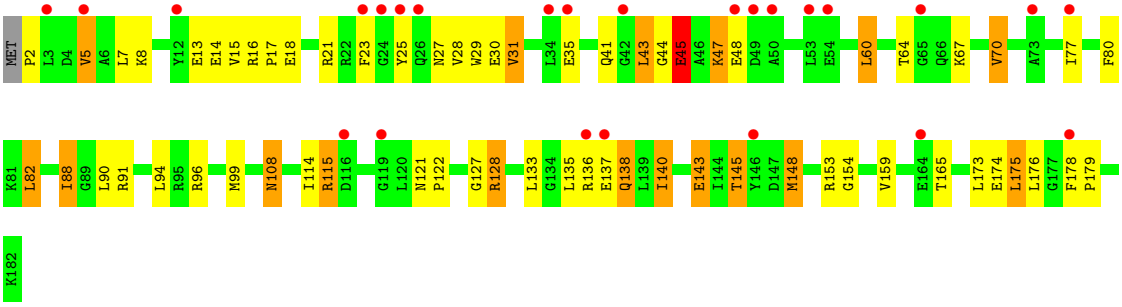
• Molecule 29: 50S ribosomal protein L4

Chain DF:



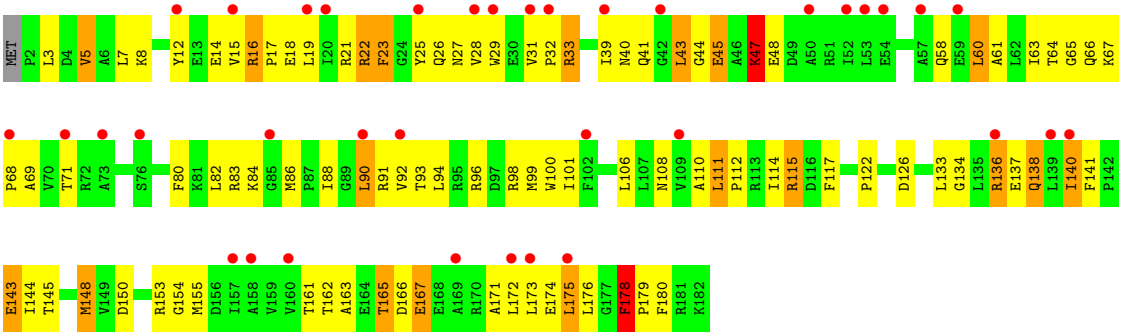
• Molecule 30: 50S ribosomal protein L5

Chain BG:



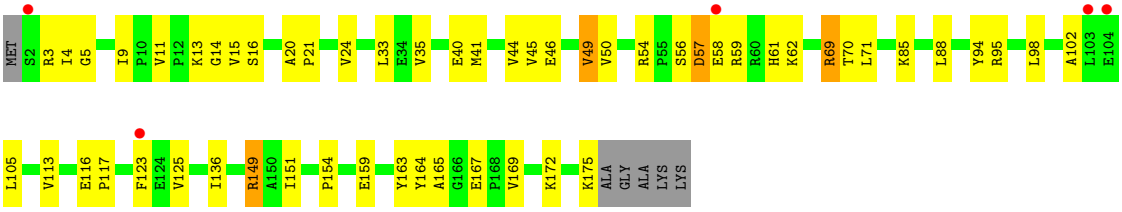
• Molecule 30: 50S ribosomal protein L5

Chain DG:

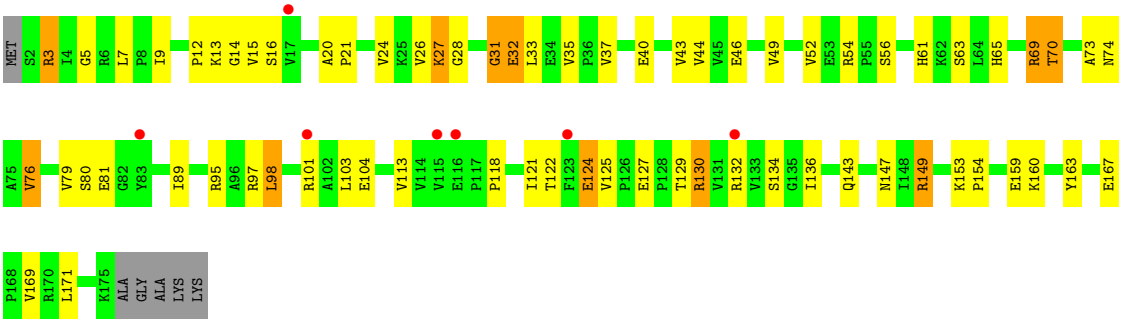


• Molecule 31: 50S ribosomal protein L6

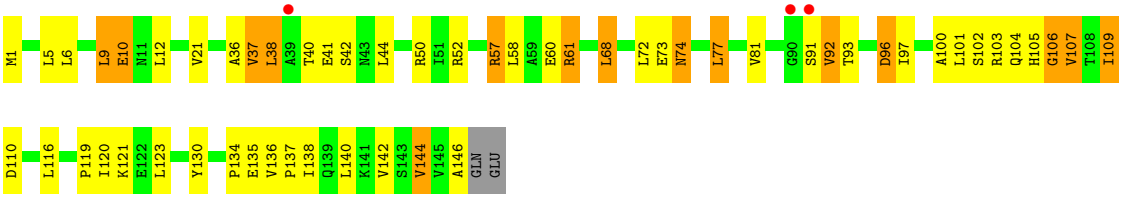
Chain BH:



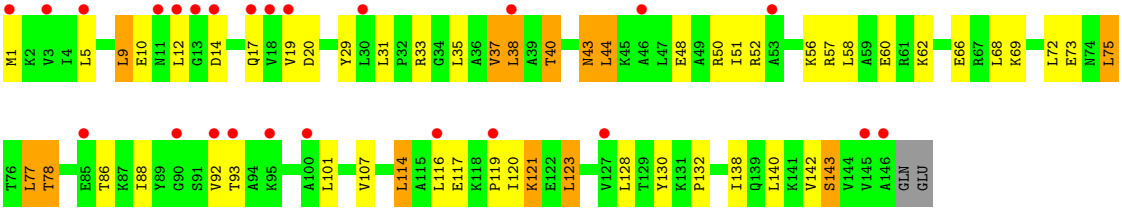
• Molecule 31: 50S ribosomal protein L6



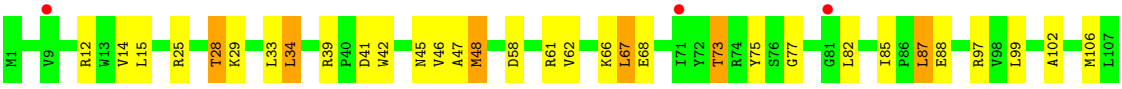
• Molecule 32: 50S ribosomal protein L9



• Molecule 32: 50S ribosomal protein L9

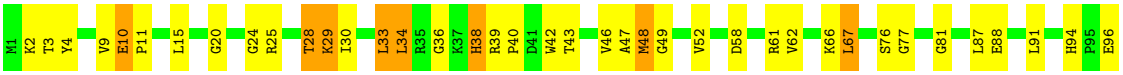


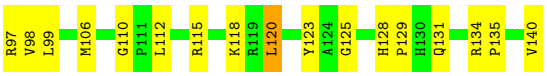
• Molecule 33: 50S ribosomal protein L13



• Molecule 33: 50S ribosomal protein L13

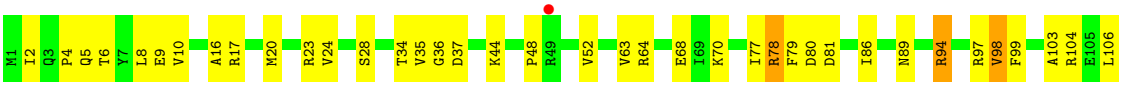
Chain DN:

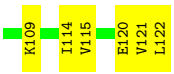




• Molecule 34: 50S ribosomal protein L14

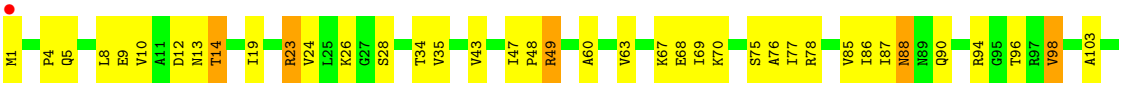
Chain BO:





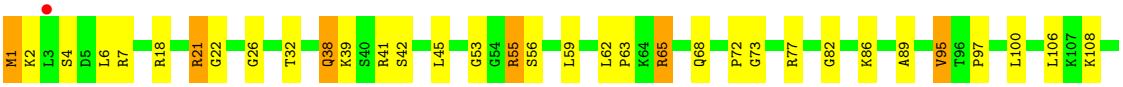
• Molecule 34: 50S ribosomal protein L14

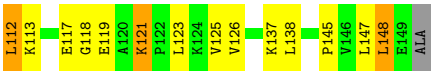
Chain DO:



• Molecule 35: 50S ribosomal protein L15

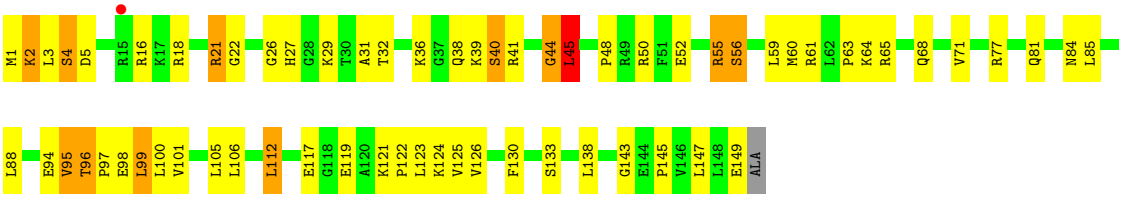
Chain BP:





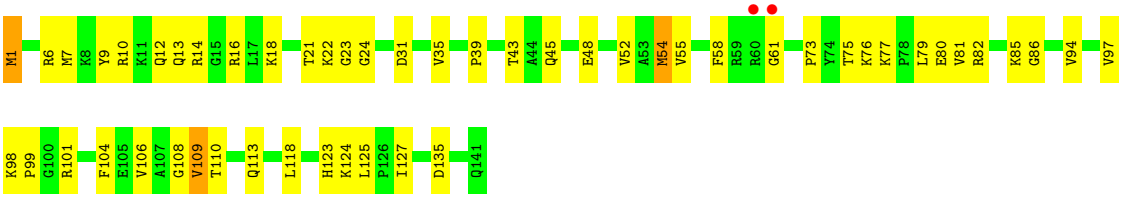
• Molecule 35: 50S ribosomal protein L15

Chain DP:



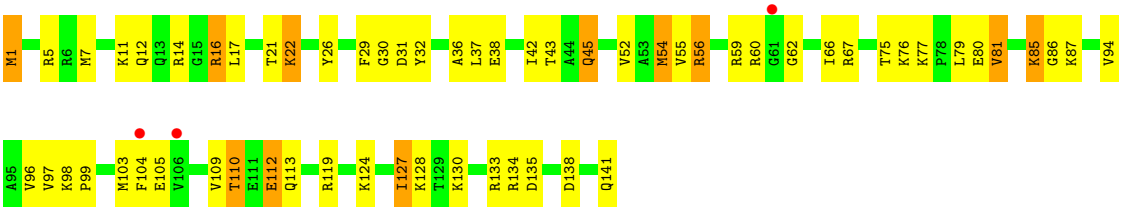
• Molecule 36: 50S ribosomal protein L16

Chain BQ:



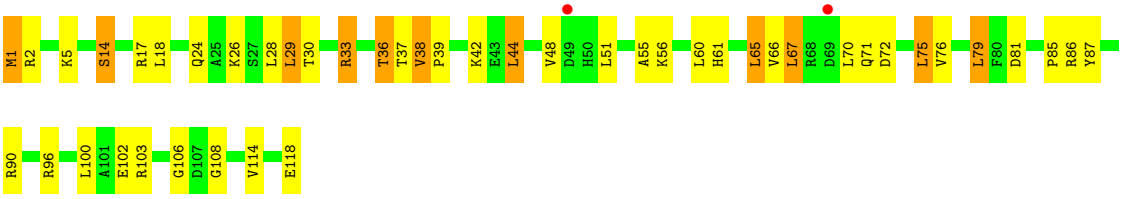
• Molecule 36: 50S ribosomal protein L16

Chain DQ:



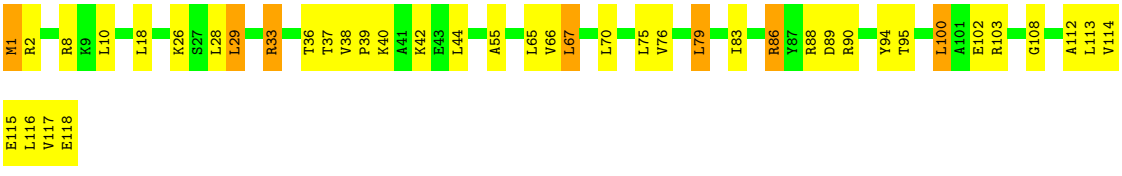
• Molecule 37: 50S ribosomal protein L17

Chain BR:



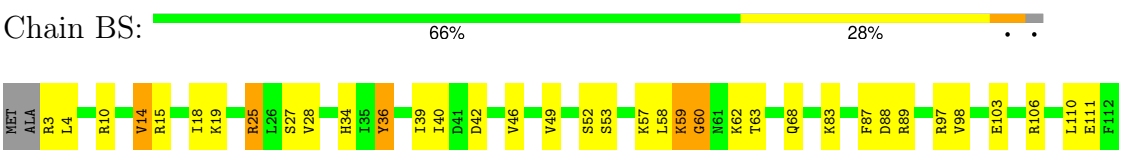
• Molecule 37: 50S ribosomal protein L17

Chain DR:



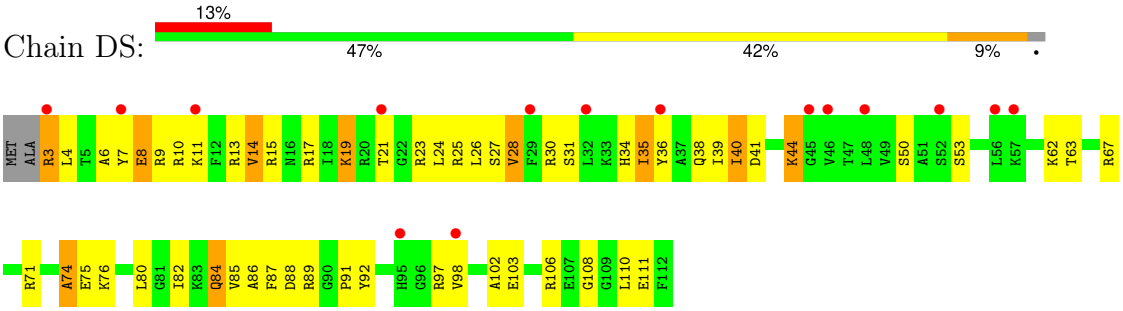
• Molecule 38: 50S ribosomal protein L18

Chain BS:



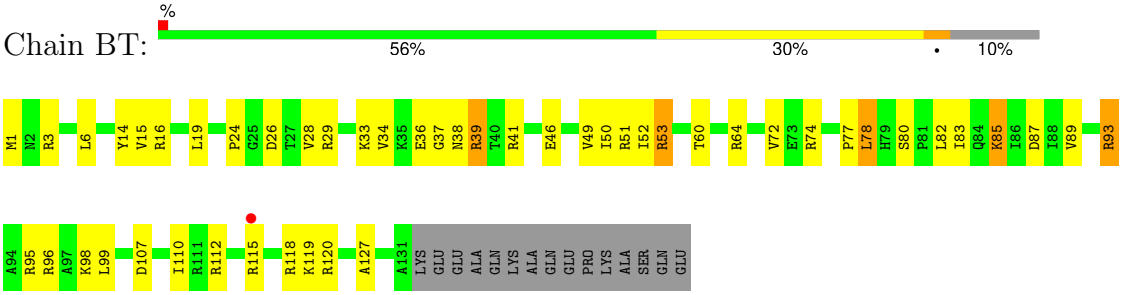
• Molecule 38: 50S ribosomal protein L18

Chain DS:



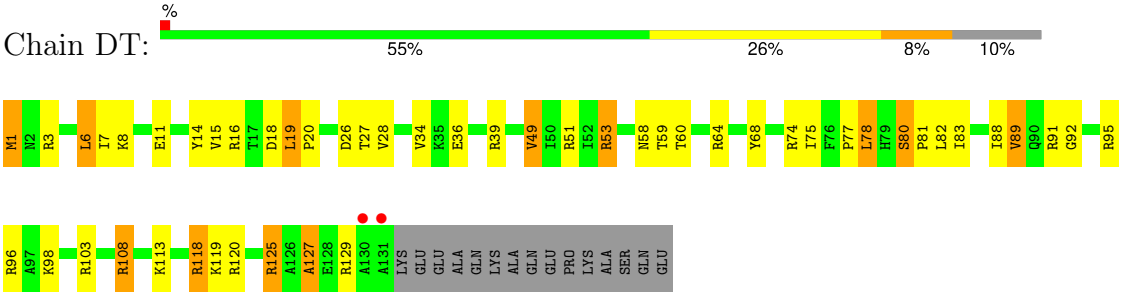
• Molecule 39: 50S ribosomal protein L19

Chain BT:



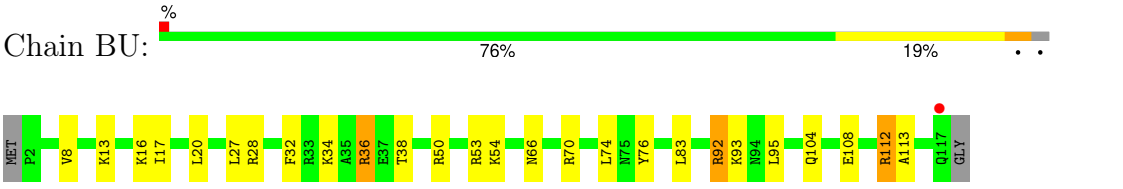
• Molecule 39: 50S ribosomal protein L19

Chain DT:



• Molecule 40: 50S ribosomal protein L20

Chain BU:



• Molecule 40: 50S ribosomal protein L20

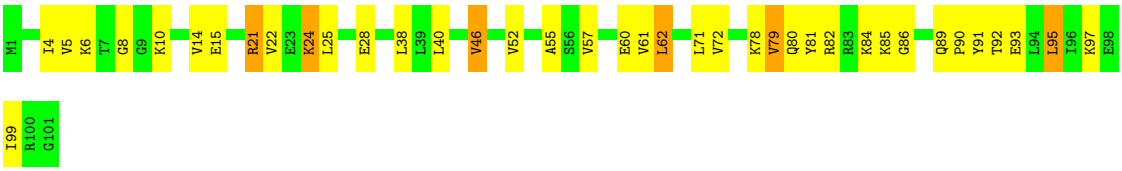
Chain DU:

• Molecule 41: 50S ribosomal protein L21

Chain BV:

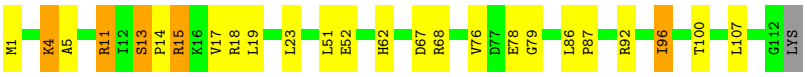
• Molecule 41: 50S ribosomal protein L21

Chain DV:



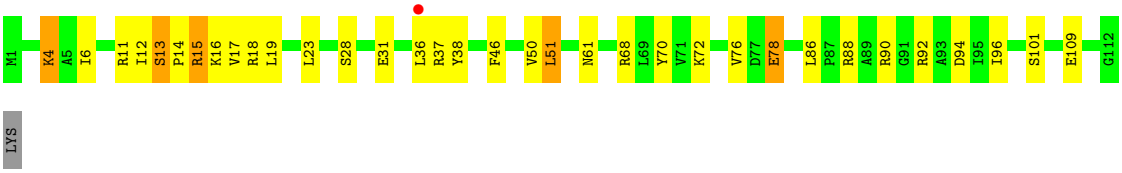
• Molecule 42: 50S ribosomal protein L22

Chain BW:



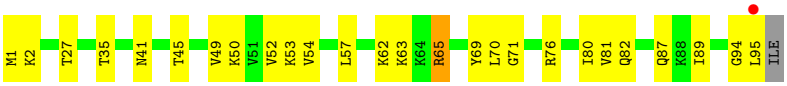
• Molecule 42: 50S ribosomal protein L22

Chain DW:



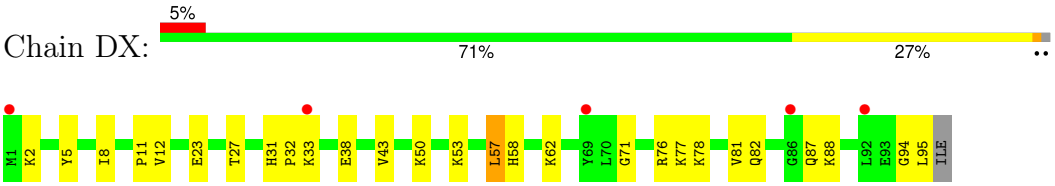
• Molecule 43: 50S ribosomal protein L23

Chain BX:



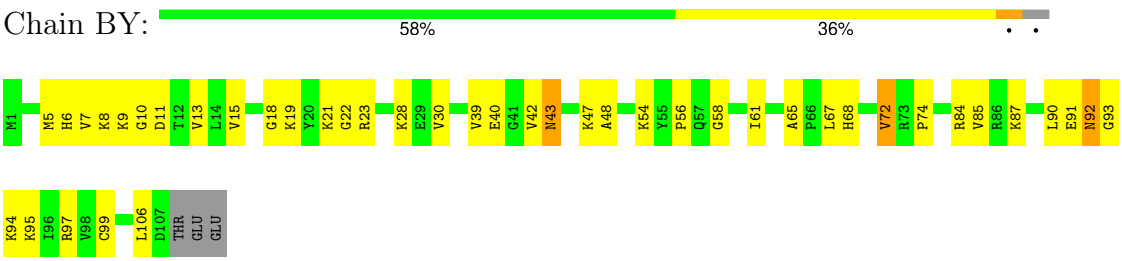
• Molecule 43: 50S ribosomal protein L23

Chain DX:



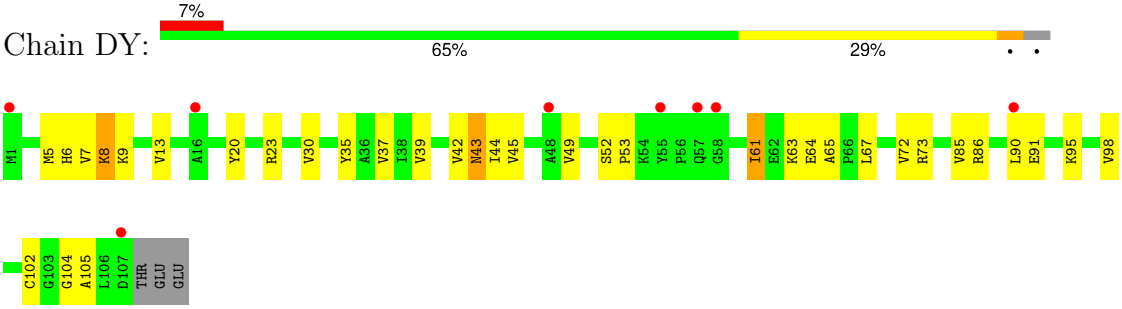
• Molecule 44: 50S ribosomal protein L24

Chain BY:



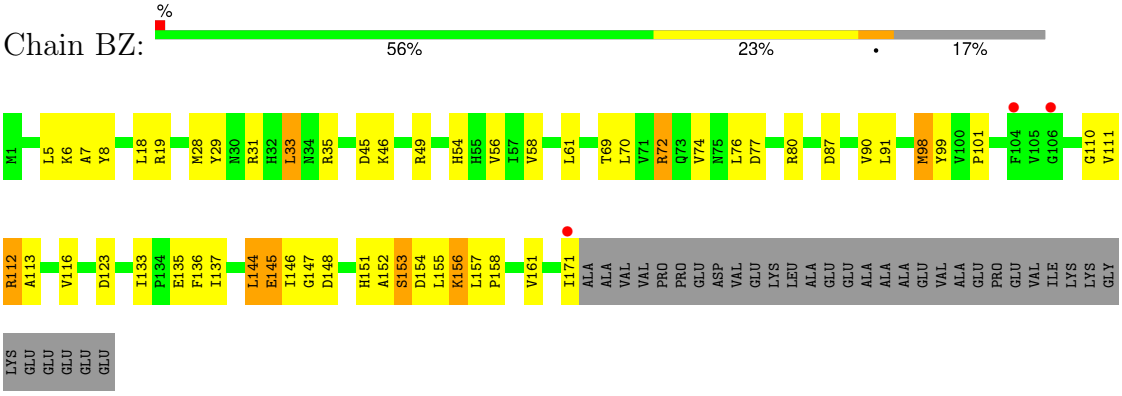
• Molecule 44: 50S ribosomal protein L24

Chain DY:



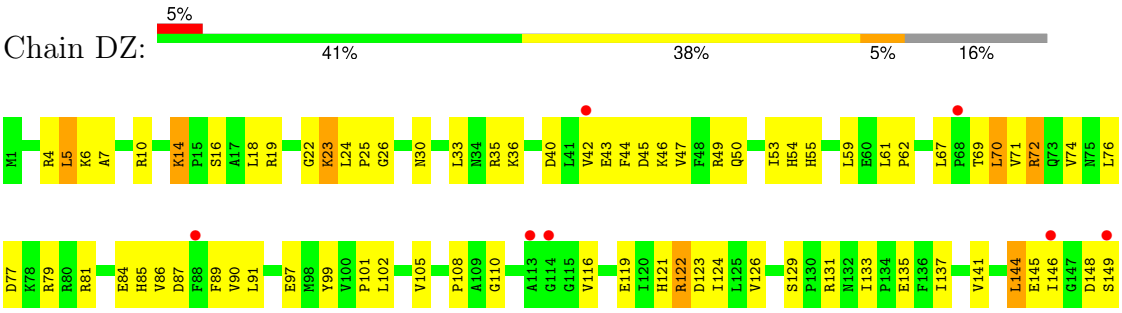
• Molecule 45: 50S ribosomal protein L25

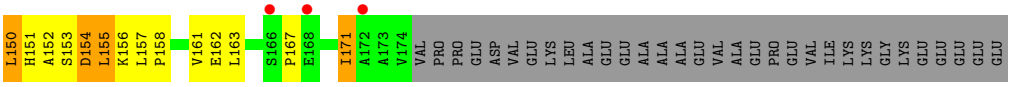
Chain BZ:



• Molecule 45: 50S ribosomal protein L25

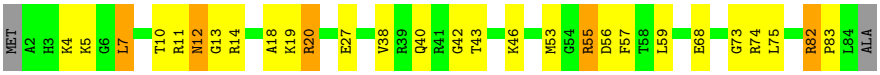
Chain DZ:





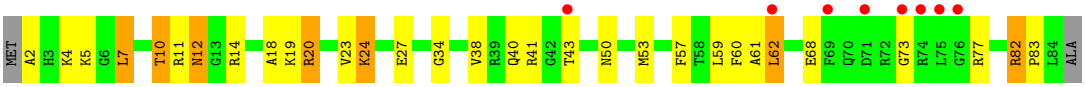
• Molecule 46: 50S ribosomal protein L27

Chain B0:



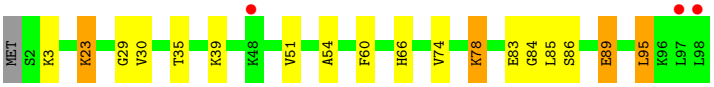
• Molecule 46: 50S ribosomal protein L27

Chain D0:



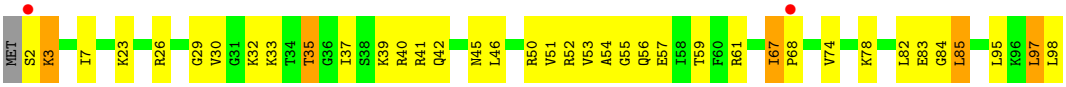
• Molecule 47: 50S ribosomal protein L28

Chain B1:



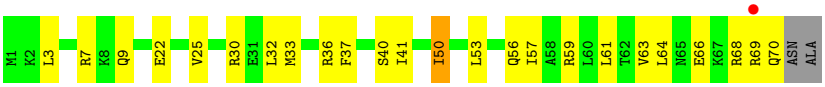
• Molecule 47: 50S ribosomal protein L28

Chain D1:



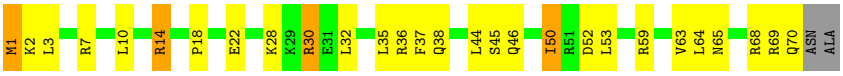
• Molecule 48: 50S ribosomal protein L29

Chain B2:



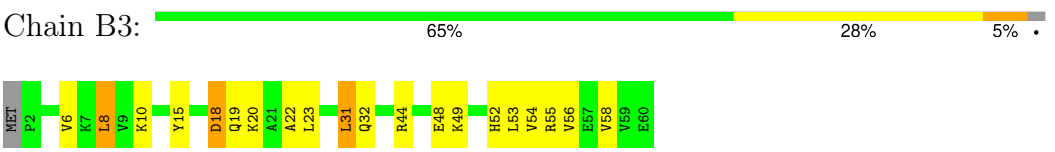
• Molecule 48: 50S ribosomal protein L29

Chain D2:



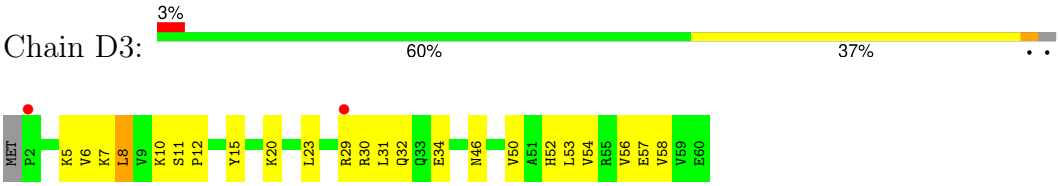
• Molecule 49: 50S ribosomal protein L30

Chain B3:



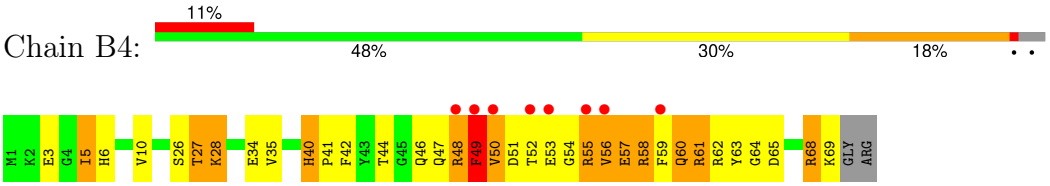
• Molecule 49: 50S ribosomal protein L30

Chain D3:



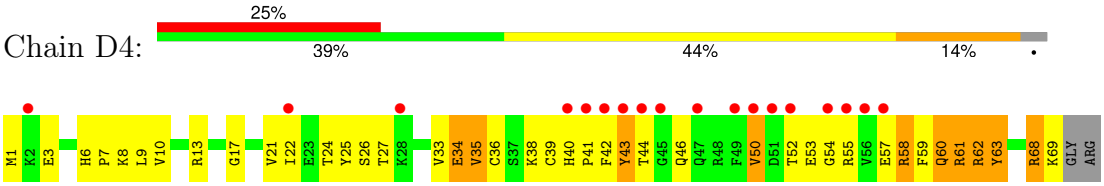
• Molecule 50: 50S ribosomal protein L31

Chain B4:



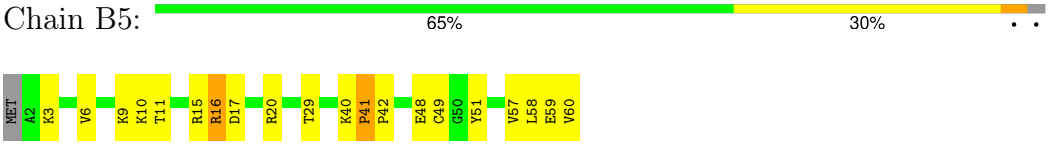
• Molecule 50: 50S ribosomal protein L31

Chain D4:



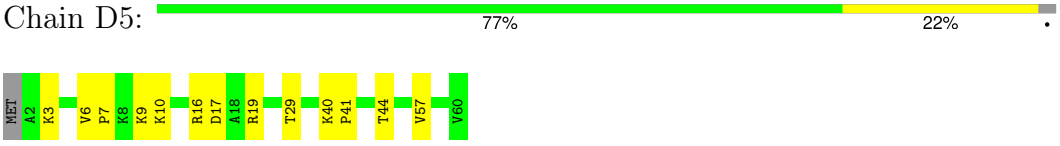
• Molecule 51: 50S ribosomal protein L32

Chain B5:



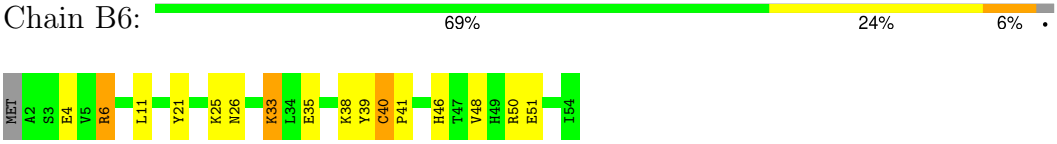
• Molecule 51: 50S ribosomal protein L32

Chain D5:



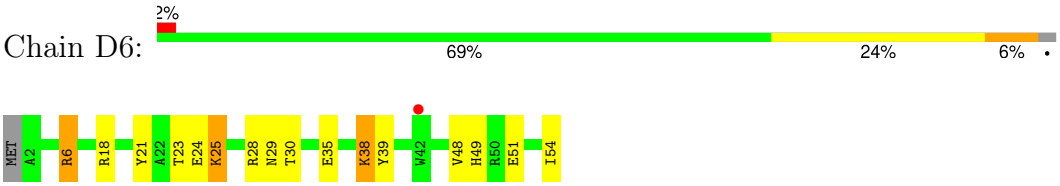
• Molecule 52: 50S ribosomal protein L33

Chain B6:



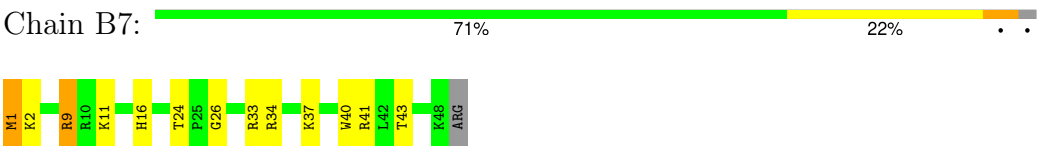
• Molecule 52: 50S ribosomal protein L33

Chain D6:



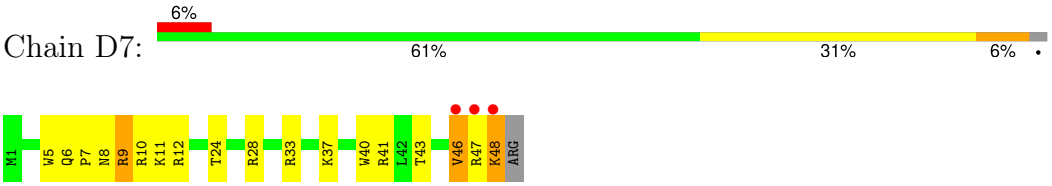
• Molecule 53: 50S ribosomal protein L34

Chain B7:



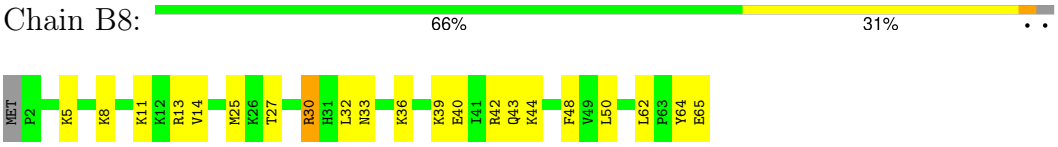
• Molecule 53: 50S ribosomal protein L34

Chain D7:



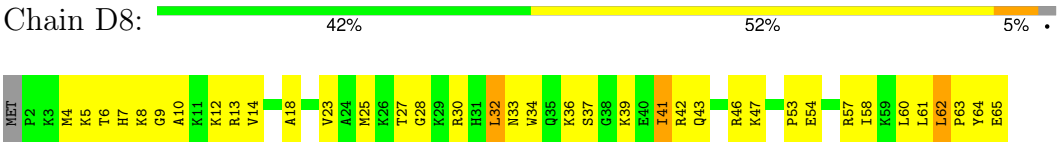
• Molecule 54: 50S ribosomal protein L35

Chain B8:



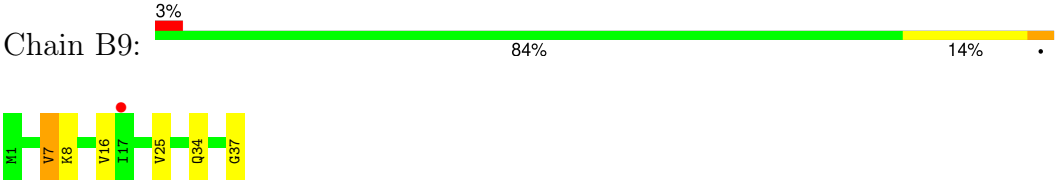
• Molecule 54: 50S ribosomal protein L35

Chain D8:



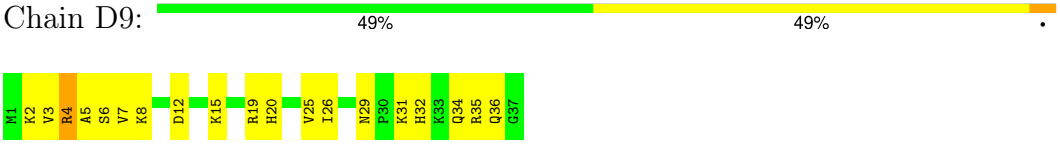
• Molecule 55: 50S ribosomal protein L36

Chain B9:



• Molecule 55: 50S ribosomal protein L36

Chain D9:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	209.25Å 448.46Å 618.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	362.98 – 2.90 362.98 – 2.90	Depositor EDS
% Data completeness (in resolution range)	96.9 (362.98-2.90) 96.9 (362.98-2.90)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.31 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.231 , 0.286 0.232 , 0.286	Depositor DCC
R_{free} test set	61606 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å^2)	54.8	Xtriage
Anisotropy	0.140	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 74.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.37$, $< L^2 > = 0.19$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	289646	wwPDB-VP
Average B, all atoms (Å^2)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.87% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	AA	0.22	0/36049	0.44	2/56261 (0.0%)
1	CA	0.23	0/36170	0.46	5/56452 (0.0%)
2	AB	0.43	0/1881	1.04	14/2542 (0.6%)
2	CB	0.44	0/1860	1.04	12/2518 (0.5%)
3	AC	0.42	0/1576	0.85	0/2130
3	CC	0.42	0/1566	0.96	2/2119 (0.1%)
4	AD	0.41	0/1689	0.96	4/2267 (0.2%)
4	CD	0.40	0/1700	0.91	2/2280 (0.1%)
5	AE	0.41	0/1145	0.88	0/1543
5	CE	0.41	0/1149	0.97	5/1548 (0.3%)
6	AF	0.41	0/819	0.84	0/1111
6	CF	0.37	0/829	0.75	0/1123
7	AG	0.37	0/1250	0.88	2/1679 (0.1%)
7	CG	0.40	0/1254	0.99	6/1683 (0.4%)
8	AH	0.37	0/1108	0.90	2/1494 (0.1%)
8	CH	0.36	0/1108	0.88	1/1494 (0.1%)
9	AI	0.41	0/1002	0.96	2/1346 (0.1%)
9	CI	0.44	0/997	0.95	2/1343 (0.1%)
10	AJ	0.39	0/722	0.91	2/982 (0.2%)
10	CJ	0.45	0/727	0.96	0/988
11	AK	0.38	0/844	0.88	2/1145 (0.2%)
11	CK	0.39	0/848	0.89	2/1149 (0.2%)
12	AL	0.39	0/946	0.82	1/1274 (0.1%)
12	CL	0.39	0/946	0.94	5/1274 (0.4%)
13	AM	0.40	0/969	1.04	3/1302 (0.2%)
13	CM	0.45	0/961	0.96	3/1291 (0.2%)
14	AN	0.39	0/501	0.83	0/664
14	CN	0.40	0/501	0.90	0/664
15	AO	0.39	0/739	0.89	1/985 (0.1%)
15	CO	0.38	0/739	0.84	0/985
16	AP	0.39	0/697	0.86	0/939
16	CP	0.37	0/693	0.87	2/935 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	AQ	0.37	0/836	0.80	0/1117
17	CQ	0.34	0/836	0.84	0/1117
18	AR	0.36	0/560	0.85	0/746
18	CR	0.39	0/560	0.86	0/746
19	AS	0.37	0/667	0.94	3/900 (0.3%)
19	CS	0.46	0/661	1.09	5/893 (0.6%)
20	AT	0.40	0/730	0.96	0/965
20	CT	0.42	0/729	0.98	1/965 (0.1%)
21	AU	0.36	0/203	0.87	0/266
21	CU	0.38	0/203	0.92	0/266
22	AV	0.24	0/310	0.39	0/480
22	CV	0.25	0/282	0.43	0/437
23	AW	0.20	0/18	0.39	0/26
23	CW	0.15	0/18	0.34	0/26
24	AX	0.29	0/1700	0.48	0/2650
24	CX	0.30	0/1700	0.49	0/2650
25	BA	0.26	0/68013	0.44	1/106165 (0.0%)
25	DA	0.23	0/67542	0.44	0/105428
26	BB	0.24	0/2878	0.48	0/4490
26	DB	0.24	0/2878	0.44	0/4490
27	BD	0.48	0/2186	0.90	4/2944 (0.1%)
27	DD	0.43	0/2186	0.93	5/2944 (0.2%)
28	BE	0.44	0/1592	0.89	2/2149 (0.1%)
28	DE	0.44	0/1592	0.94	5/2149 (0.2%)
29	BF	0.47	0/1619	0.85	0/2193
29	DF	0.41	0/1615	0.94	5/2188 (0.2%)
30	BG	0.40	0/1450	0.96	5/1959 (0.3%)
30	DG	0.45	0/1449	1.10	11/1958 (0.6%)
31	BH	0.44	0/1356	0.91	1/1834 (0.1%)
31	DH	0.39	0/1356	0.96	3/1834 (0.2%)
32	BI	0.40	0/1100	0.93	2/1501 (0.1%)
32	DI	0.39	0/1076	0.91	0/1471
33	BN	0.44	0/1144	0.89	6/1543 (0.4%)
33	DN	0.42	0/1144	1.01	9/1543 (0.6%)
34	BO	0.47	0/943	0.85	0/1269
34	DO	0.44	0/943	0.85	0/1269
35	BP	0.44	0/1152	0.89	3/1533 (0.2%)
35	DP	0.39	0/1152	0.94	6/1533 (0.4%)
36	BQ	0.47	0/1143	0.82	1/1527 (0.1%)
36	DQ	0.42	0/1143	0.89	0/1527
37	BR	0.45	0/982	0.82	1/1312 (0.1%)
37	DR	0.41	0/982	0.78	0/1312
38	BS	0.43	0/887	0.87	1/1180 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
38	DS	0.40	0/880	0.96	2/1172 (0.2%)
39	BT	0.41	0/1105	0.85	0/1477
39	DT	0.38	0/1097	0.84	2/1468 (0.1%)
40	BU	0.47	0/977	0.84	0/1301
40	DU	0.42	0/977	0.84	0/1301
41	BV	0.45	0/782	0.83	0/1049
41	DV	0.40	0/782	0.90	1/1049 (0.1%)
42	BW	0.49	0/897	0.86	2/1205 (0.2%)
42	DW	0.43	0/897	0.85	2/1205 (0.2%)
43	BX	0.48	0/764	0.84	1/1025 (0.1%)
43	DX	0.41	0/764	0.85	0/1025
44	BY	0.46	0/819	0.91	1/1095 (0.1%)
44	DY	0.40	0/819	0.94	1/1095 (0.1%)
45	BZ	0.43	0/1379	0.98	7/1873 (0.4%)
45	DZ	0.39	0/1390	1.00	8/1890 (0.4%)
46	B0	0.42	0/662	0.90	2/881 (0.2%)
46	D0	0.38	0/662	0.91	3/881 (0.3%)
47	B1	0.44	0/762	0.88	1/1014 (0.1%)
47	D1	0.40	0/762	0.85	1/1014 (0.1%)
48	B2	0.44	0/590	0.88	1/781 (0.1%)
48	D2	0.39	0/590	0.82	0/781
49	B3	0.45	0/474	0.90	0/635
49	D3	0.37	0/469	0.88	0/630
50	B4	0.50	0/565	1.23	10/761 (1.3%)
50	D4	0.49	0/545	1.13	2/737 (0.3%)
51	B5	0.48	0/469	0.80	1/635 (0.2%)
51	D5	0.44	0/469	0.81	0/635
52	B6	0.46	0/460	0.82	2/613 (0.3%)
52	D6	0.37	0/456	0.81	0/608
53	B7	0.48	0/426	0.80	0/561
53	D7	0.46	0/426	0.83	2/561 (0.4%)
54	B8	0.49	0/519	0.88	0/684
54	D8	0.38	0/525	0.89	2/691 (0.3%)
55	B9	0.42	0/310	0.78	0/407
55	D9	0.38	0/310	0.84	0/407
All	All	0.31	0/310281	0.61	216/464152 (0.0%)

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

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

There are no bond length outliers.

The worst 5 of 216 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	AM	84	ILE	N-CA-C	10.82	122.79	111.00
30	DG	178	PHE	CA-C-N	9.77	130.16	119.90
30	DG	178	PHE	C-N-CA	9.77	130.16	119.90
7	CG	79	ARG	N-CA-C	9.07	122.09	108.31
33	DN	10	GLU	CA-C-N	8.92	129.00	119.90

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

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

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32205	0	16254	643	0
1	CA	32312	0	16307	730	0
2	AB	1846	0	1867	87	0
2	CB	1825	0	1828	99	0
3	AC	1552	0	1546	69	0
3	CC	1542	0	1517	72	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	AD	1659	0	1676	66	0
4	CD	1670	0	1703	68	0
5	AE	1129	0	1185	31	0
5	CE	1133	0	1191	55	0
6	AF	806	0	793	32	0
6	CF	816	0	808	25	0
7	AG	1231	0	1238	30	0
7	CG	1235	0	1249	31	0
8	AH	1088	0	1126	26	0
8	CH	1088	0	1126	38	0
9	AI	983	0	986	52	0
9	CI	978	0	966	56	0
10	AJ	709	0	650	35	0
10	CJ	714	0	672	35	0
11	AK	829	0	825	18	0
11	CK	833	0	836	24	0
12	AL	930	0	979	32	0
12	CL	930	0	980	34	0
13	AM	958	0	1002	40	0
13	CM	950	0	988	56	0
14	AN	492	0	529	25	0
14	CN	492	0	529	36	0
15	AO	728	0	760	22	0
15	CO	728	0	760	31	0
16	AP	681	0	697	30	0
16	CP	677	0	686	28	0
17	AQ	823	0	891	23	0
17	CQ	823	0	891	22	0
18	AR	555	0	618	16	0
18	CR	555	0	618	22	0
19	AS	652	0	662	28	0
19	CS	646	0	644	53	0
20	AT	728	0	798	29	0
20	CT	727	0	796	29	0
21	AU	199	0	208	8	0
21	CU	199	0	208	12	0
22	AV	277	0	140	6	0
22	CV	252	0	130	8	0
23	AW	54	0	40	5	0
23	CW	54	0	40	7	0
24	AX	1635	0	838	33	0
24	CX	1635	0	838	39	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	BA	60729	0	30621	828	0
25	DA	60311	0	30408	1074	0
26	BB	2573	0	1306	30	0
26	DB	2573	0	1306	90	0
27	BD	2136	0	2218	60	0
27	DD	2136	0	2217	68	0
28	BE	1559	0	1618	55	0
28	DE	1559	0	1618	59	0
29	BF	1584	0	1625	39	0
29	DF	1580	0	1619	71	0
30	BG	1425	0	1443	45	0
30	DG	1424	0	1434	79	0
31	BH	1330	0	1407	29	0
31	DH	1330	0	1407	43	0
32	BI	1085	0	1114	40	0
32	DI	1061	0	1080	34	0
33	BN	1117	0	1184	26	0
33	DN	1117	0	1184	35	0
34	BO	933	0	996	27	0
34	DO	933	0	996	36	0
35	BP	1135	0	1212	36	0
35	DP	1135	0	1211	54	0
36	BQ	1122	0	1179	35	0
36	DQ	1122	0	1179	48	0
37	BR	968	0	1033	28	0
37	DR	968	0	1033	30	0
38	BS	877	0	938	23	0
38	DS	870	0	923	52	0
39	BT	1091	0	1151	32	0
39	DT	1083	0	1136	39	0
40	BU	959	0	1019	19	0
40	DU	959	0	1019	32	0
41	BV	771	0	830	16	0
41	DV	771	0	830	24	0
42	BW	886	0	940	11	0
42	DW	886	0	940	18	0
43	BX	750	0	814	14	0
43	DX	750	0	814	17	0
44	BY	806	0	881	31	0
44	DY	806	0	881	25	0
45	BZ	1349	0	1355	33	0
45	DZ	1360	0	1363	64	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
46	B0	653	0	674	29	0
46	D0	653	0	674	25	0
47	B1	755	0	826	12	0
47	D1	755	0	826	26	0
48	B2	588	0	643	13	0
48	D2	588	0	643	18	0
49	B3	469	0	518	9	0
49	D3	464	0	514	16	0
50	B4	552	0	533	27	0
50	D4	532	0	503	31	0
51	B5	455	0	465	12	0
51	D5	455	0	465	13	0
52	B6	453	0	473	9	0
52	D6	449	0	469	14	0
53	B7	418	0	467	13	0
53	D7	418	0	467	13	0
54	B8	511	0	571	18	0
54	D8	517	0	582	34	0
55	B9	307	0	335	4	0
55	D9	307	0	335	13	0
56	AA	187	0	0	0	0
56	AD	1	0	0	0	0
56	AE	2	0	0	0	0
56	AF	1	0	0	0	0
56	AK	1	0	0	0	0
56	AL	1	0	0	0	0
56	AM	1	0	0	0	0
56	AN	1	0	0	0	0
56	AX	7	0	0	0	0
56	B0	5	0	0	0	0
56	B3	2	0	0	0	0
56	B4	1	0	0	0	0
56	B5	2	0	0	0	0
56	B7	4	0	0	0	0
56	B8	1	0	0	0	0
56	B9	1	0	0	0	0
56	BA	675	0	0	0	0
56	BB	18	0	0	0	0
56	BD	8	0	0	0	0
56	BE	6	0	0	0	0
56	BF	5	0	0	0	0
56	BG	3	0	0	0	0

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	B4	1	0	0	0	0
58	B5	1	0	0	0	0
58	B6	1	0	0	0	0
58	B9	1	0	0	0	0
58	BY	1	0	0	0	0
58	CN	1	0	0	0	0
58	D4	1	0	0	0	0
58	D5	1	0	0	0	0
58	D6	1	0	0	0	0
58	D9	1	0	0	0	0
58	DY	1	0	0	0	0
59	AX	1	0	0	0	0
59	DA	1	0	0	0	0
60	AA	165	0	0	12	0
60	AJ	1	0	0	0	0
60	AL	3	0	0	2	0
60	AP	1	0	0	0	0
60	AU	1	0	0	0	0
60	AV	2	0	0	0	0
60	AW	3	0	0	0	0
60	B0	4	0	0	0	0
60	B1	2	0	0	0	0
60	B2	1	0	0	0	0
60	B3	1	0	0	0	0
60	B5	2	0	0	0	0
60	B7	2	0	0	1	0
60	B8	8	0	0	2	0
60	BA	924	0	0	62	0
60	BB	27	0	0	0	0
60	BD	6	0	0	2	0
60	BE	8	0	0	0	0
60	BF	6	0	0	1	0
60	BG	1	0	0	0	0
60	BH	1	0	0	1	0
60	BN	3	0	0	0	0
60	BO	1	0	0	0	0
60	BP	14	0	0	2	0
60	BQ	2	0	0	0	0
60	BS	1	0	0	0	0
60	BT	4	0	0	1	0
60	BU	2	0	0	0	0
60	BV	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	BW	1	0	0	0	0
60	BX	2	0	0	0	0
60	BZ	1	0	0	0	0
60	CA	113	0	0	5	0
60	CE	2	0	0	0	0
60	CJ	2	0	0	1	0
60	CL	1	0	0	1	0
60	CO	1	0	0	0	0
60	CW	1	0	0	1	0
60	CX	1	0	0	1	0
60	D0	5	0	0	0	0
60	D1	1	0	0	0	0
60	D3	1	0	0	2	0
60	D8	3	0	0	0	0
60	DA	689	0	0	58	0
60	DB	9	0	0	0	0
60	DD	11	0	0	2	0
60	DE	5	0	0	1	0
60	DF	6	0	0	0	0
60	DO	1	0	0	0	0
60	DP	6	0	0	0	0
60	DU	3	0	0	0	0
60	DV	1	0	0	0	0
60	DW	1	0	0	0	0
60	DX	3	0	0	0	0
All	All	289646	0	193084	5817	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

The worst 5 of 5817 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:DA:2121:G:H1	25:DA:2177:C:N4	1.35	1.23
19:CS:42:PRO:HG3	50:D4:61:ARG:HG2	1.39	1.04
1:AA:1028:C:N4	1:AA:1033:G:H1	1.56	1.01
25:DA:2128:C:H42	25:DA:2160:G:H1	1.08	1.00
25:DA:2137:C:H42	25:DA:2154:G:H1	1.05	0.99

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	AB	229/256 (90%)	208 (91%)	18 (8%)	3 (1%)	9 32
2	CB	229/256 (90%)	206 (90%)	17 (7%)	6 (3%)	4 17
3	AC	204/239 (85%)	193 (95%)	10 (5%)	1 (0%)	24 54
3	CC	204/239 (85%)	187 (92%)	15 (7%)	2 (1%)	12 39
4	AD	206/209 (99%)	195 (95%)	9 (4%)	2 (1%)	12 39
4	CD	206/209 (99%)	194 (94%)	11 (5%)	1 (0%)	24 54
5	AE	146/162 (90%)	140 (96%)	4 (3%)	2 (1%)	9 30
5	CE	146/162 (90%)	142 (97%)	4 (3%)	0	100 100
6	AF	98/101 (97%)	96 (98%)	2 (2%)	0	100 100
6	CF	98/101 (97%)	96 (98%)	2 (2%)	0	100 100
7	AG	153/156 (98%)	148 (97%)	2 (1%)	3 (2%)	6 22
7	CG	153/156 (98%)	151 (99%)	1 (1%)	1 (1%)	18 48
8	AH	135/138 (98%)	133 (98%)	2 (2%)	0	100 100
8	CH	135/138 (98%)	132 (98%)	3 (2%)	0	100 100
9	AI	125/128 (98%)	118 (94%)	7 (6%)	0	100 100
9	CI	125/128 (98%)	120 (96%)	5 (4%)	0	100 100
10	AJ	95/105 (90%)	87 (92%)	7 (7%)	1 (1%)	11 36
10	CJ	94/105 (90%)	87 (93%)	5 (5%)	2 (2%)	5 21
11	AK	112/129 (87%)	104 (93%)	5 (4%)	3 (3%)	4 16
11	CK	112/129 (87%)	103 (92%)	7 (6%)	2 (2%)	6 25
12	AL	120/132 (91%)	115 (96%)	5 (4%)	0	100 100
12	CL	120/132 (91%)	113 (94%)	7 (6%)	0	100 100
13	AM	121/126 (96%)	113 (93%)	8 (7%)	0	100 100
13	CM	120/126 (95%)	114 (95%)	5 (4%)	1 (1%)	16 44
14	AN	58/61 (95%)	55 (95%)	3 (5%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	CN	58/61 (95%)	55 (95%)	3 (5%)	0	100	100
15	AO	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
15	CO	86/89 (97%)	81 (94%)	5 (6%)	0	100	100
16	AP	80/88 (91%)	77 (96%)	3 (4%)	0	100	100
16	CP	80/88 (91%)	77 (96%)	2 (2%)	1 (1%)	9	32
17	AQ	97/105 (92%)	92 (95%)	4 (4%)	1 (1%)	12	39
17	CQ	97/105 (92%)	94 (97%)	3 (3%)	0	100	100
18	AR	66/88 (75%)	65 (98%)	1 (2%)	0	100	100
18	CR	66/88 (75%)	65 (98%)	1 (2%)	0	100	100
19	AS	81/93 (87%)	76 (94%)	5 (6%)	0	100	100
19	CS	81/93 (87%)	75 (93%)	6 (7%)	0	100	100
20	AT	94/106 (89%)	87 (93%)	6 (6%)	1 (1%)	11	36
20	CT	94/106 (89%)	86 (92%)	5 (5%)	3 (3%)	3	13
21	AU	21/27 (78%)	21 (100%)	0	0	100	100
21	CU	21/27 (78%)	21 (100%)	0	0	100	100
27	BD	273/276 (99%)	263 (96%)	9 (3%)	1 (0%)	30	59
27	DD	273/276 (99%)	262 (96%)	9 (3%)	2 (1%)	18	48
28	BE	202/206 (98%)	195 (96%)	6 (3%)	1 (0%)	24	54
28	DE	202/206 (98%)	193 (96%)	7 (4%)	2 (1%)	12	39
29	BF	201/210 (96%)	197 (98%)	3 (2%)	1 (0%)	24	54
29	DF	201/210 (96%)	197 (98%)	2 (1%)	2 (1%)	12	39
30	BG	179/182 (98%)	171 (96%)	7 (4%)	1 (1%)	21	51
30	DG	179/182 (98%)	167 (93%)	11 (6%)	1 (1%)	21	51
31	BH	172/180 (96%)	169 (98%)	3 (2%)	0	100	100
31	DH	172/180 (96%)	168 (98%)	4 (2%)	0	100	100
32	BI	144/148 (97%)	130 (90%)	10 (7%)	4 (3%)	4	15
32	DI	144/148 (97%)	137 (95%)	6 (4%)	1 (1%)	18	48
33	BN	138/140 (99%)	137 (99%)	1 (1%)	0	100	100
33	DN	138/140 (99%)	135 (98%)	2 (1%)	1 (1%)	18	48
34	BO	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
34	DO	120/122 (98%)	113 (94%)	7 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
35	BP	147/150 (98%)	141 (96%)	6 (4%)	0	100 100
35	DP	147/150 (98%)	140 (95%)	5 (3%)	2 (1%)	9 30
36	BQ	139/141 (99%)	134 (96%)	5 (4%)	0	100 100
36	DQ	139/141 (99%)	133 (96%)	6 (4%)	0	100 100
37	BR	116/118 (98%)	112 (97%)	4 (3%)	0	100 100
37	DR	116/118 (98%)	111 (96%)	5 (4%)	0	100 100
38	BS	108/112 (96%)	103 (95%)	4 (4%)	1 (1%)	14 41
38	DS	108/112 (96%)	105 (97%)	2 (2%)	1 (1%)	14 41
39	BT	129/146 (88%)	123 (95%)	4 (3%)	2 (2%)	7 27
39	DT	129/146 (88%)	125 (97%)	3 (2%)	1 (1%)	16 44
40	BU	114/118 (97%)	114 (100%)	0	0	100 100
40	DU	114/118 (97%)	114 (100%)	0	0	100 100
41	BV	99/101 (98%)	93 (94%)	6 (6%)	0	100 100
41	DV	99/101 (98%)	95 (96%)	4 (4%)	0	100 100
42	BW	110/113 (97%)	110 (100%)	0	0	100 100
42	DW	110/113 (97%)	110 (100%)	0	0	100 100
43	BX	93/96 (97%)	89 (96%)	4 (4%)	0	100 100
43	DX	93/96 (97%)	90 (97%)	3 (3%)	0	100 100
44	BY	105/110 (96%)	99 (94%)	6 (6%)	0	100 100
44	DY	105/110 (96%)	102 (97%)	3 (3%)	0	100 100
45	BZ	169/206 (82%)	152 (90%)	16 (10%)	1 (1%)	21 51
45	DZ	172/206 (84%)	158 (92%)	14 (8%)	0	100 100
46	B0	81/85 (95%)	81 (100%)	0	0	100 100
46	D0	81/85 (95%)	79 (98%)	1 (1%)	1 (1%)	10 34
47	B1	95/98 (97%)	94 (99%)	1 (1%)	0	100 100
47	D1	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	11 36
48	B2	68/72 (94%)	67 (98%)	1 (2%)	0	100 100
48	D2	68/72 (94%)	67 (98%)	1 (2%)	0	100 100
49	B3	57/60 (95%)	57 (100%)	0	0	100 100
49	D3	57/60 (95%)	56 (98%)	1 (2%)	0	100 100
50	B4	67/71 (94%)	56 (84%)	9 (13%)	2 (3%)	3 14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
50	D4	67/71 (94%)	54 (81%)	8 (12%)	5 (8%)	1 2
51	B5	57/60 (95%)	57 (100%)	0	0	100 100
51	D5	57/60 (95%)	56 (98%)	1 (2%)	0	100 100
52	B6	51/54 (94%)	50 (98%)	1 (2%)	0	100 100
52	D6	51/54 (94%)	49 (96%)	2 (4%)	0	100 100
53	B7	46/49 (94%)	46 (100%)	0	0	100 100
53	D7	46/49 (94%)	45 (98%)	0	1 (2%)	5 20
54	B8	62/65 (95%)	62 (100%)	0	0	100 100
54	D8	62/65 (95%)	62 (100%)	0	0	100 100
55	B9	35/37 (95%)	35 (100%)	0	0	100 100
55	D9	35/37 (95%)	35 (100%)	0	0	100 100
All	All	11409/12128 (94%)	10906 (96%)	432 (4%)	71 (1%)	21 51

5 of 71 Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	AB	192/220 (87%)	150 (78%)	42 (22%)	1 3
2	CB	187/220 (85%)	153 (82%)	34 (18%)	2 6
3	AC	143/188 (76%)	126 (88%)	17 (12%)	5 16
3	CC	140/188 (74%)	119 (85%)	21 (15%)	3 10
4	AD	170/181 (94%)	144 (85%)	26 (15%)	3 9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	CD	172/181 (95%)	144 (84%)	28 (16%)	2 8
5	AE	113/123 (92%)	98 (87%)	15 (13%)	4 12
5	CE	114/123 (93%)	96 (84%)	18 (16%)	2 8
6	AF	83/90 (92%)	77 (93%)	6 (7%)	13 39
6	CF	85/90 (94%)	76 (89%)	9 (11%)	6 22
7	AG	119/127 (94%)	104 (87%)	15 (13%)	4 14
7	CG	120/127 (94%)	107 (89%)	13 (11%)	6 21
8	AH	114/119 (96%)	100 (88%)	14 (12%)	4 15
8	CH	114/119 (96%)	101 (89%)	13 (11%)	5 18
9	AI	90/99 (91%)	75 (83%)	15 (17%)	2 7
9	CI	89/99 (90%)	70 (79%)	19 (21%)	1 4
10	AJ	66/92 (72%)	63 (96%)	3 (4%)	24 58
10	CJ	69/92 (75%)	62 (90%)	7 (10%)	7 24
11	AK	82/99 (83%)	71 (87%)	11 (13%)	4 12
11	CK	83/99 (84%)	76 (92%)	7 (8%)	10 31
12	AL	97/109 (89%)	86 (89%)	11 (11%)	5 19
12	CL	97/109 (89%)	88 (91%)	9 (9%)	8 27
13	AM	93/101 (92%)	74 (80%)	19 (20%)	1 4
13	CM	92/101 (91%)	75 (82%)	17 (18%)	1 5
14	AN	49/50 (98%)	42 (86%)	7 (14%)	3 11
14	CN	49/50 (98%)	39 (80%)	10 (20%)	1 4
15	AO	78/80 (98%)	68 (87%)	10 (13%)	4 14
15	CO	78/80 (98%)	69 (88%)	9 (12%)	5 18
16	AP	69/74 (93%)	52 (75%)	17 (25%)	1 2
16	CP	68/74 (92%)	56 (82%)	12 (18%)	2 6
17	AQ	94/97 (97%)	83 (88%)	11 (12%)	5 17
17	CQ	94/97 (97%)	84 (89%)	10 (11%)	6 22
18	AR	59/77 (77%)	51 (86%)	8 (14%)	3 12
18	CR	59/77 (77%)	51 (86%)	8 (14%)	3 12
19	AS	69/80 (86%)	60 (87%)	9 (13%)	4 13
19	CS	67/80 (84%)	57 (85%)	10 (15%)	3 10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
20	AT	70/82 (85%)	60 (86%)	10 (14%)	3 11
20	CT	70/82 (85%)	58 (83%)	12 (17%)	2 7
21	AU	18/22 (82%)	15 (83%)	3 (17%)	2 7
21	CU	18/22 (82%)	16 (89%)	2 (11%)	6 20
27	BD	215/218 (99%)	194 (90%)	21 (10%)	7 25
27	DD	215/218 (99%)	191 (89%)	24 (11%)	6 19
28	BE	164/166 (99%)	138 (84%)	26 (16%)	2 8
28	DE	164/166 (99%)	138 (84%)	26 (16%)	2 8
29	BF	160/166 (96%)	141 (88%)	19 (12%)	5 16
29	DF	159/166 (96%)	140 (88%)	19 (12%)	5 16
30	BG	143/156 (92%)	117 (82%)	26 (18%)	2 6
30	DG	142/156 (91%)	116 (82%)	26 (18%)	2 6
31	BH	144/148 (97%)	131 (91%)	13 (9%)	9 28
31	DH	144/148 (97%)	127 (88%)	17 (12%)	5 17
32	BI	110/124 (89%)	90 (82%)	20 (18%)	2 6
32	DI	104/124 (84%)	83 (80%)	21 (20%)	1 4
33	BN	118/119 (99%)	103 (87%)	15 (13%)	4 14
33	DN	118/119 (99%)	103 (87%)	15 (13%)	4 14
34	BO	100/100 (100%)	90 (90%)	10 (10%)	7 24
34	DO	100/100 (100%)	88 (88%)	12 (12%)	5 16
35	BP	115/116 (99%)	99 (86%)	16 (14%)	3 11
35	DP	115/116 (99%)	99 (86%)	16 (14%)	3 11
36	BQ	111/111 (100%)	99 (89%)	12 (11%)	6 21
36	DQ	111/111 (100%)	94 (85%)	17 (15%)	3 9
37	BR	101/101 (100%)	83 (82%)	18 (18%)	2 6
37	DR	101/101 (100%)	87 (86%)	14 (14%)	3 11
38	BS	87/88 (99%)	79 (91%)	8 (9%)	8 27
38	DS	85/88 (97%)	74 (87%)	11 (13%)	4 13
39	BT	115/127 (91%)	103 (90%)	12 (10%)	7 23
39	DT	113/127 (89%)	97 (86%)	16 (14%)	3 11
40	BU	93/94 (99%)	84 (90%)	9 (10%)	8 25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
40	DU	93/94 (99%)	84 (90%)	9 (10%)	8 25
41	BV	80/82 (98%)	66 (82%)	14 (18%)	2 6
41	DV	80/82 (98%)	66 (82%)	14 (18%)	2 6
42	BW	90/92 (98%)	77 (86%)	13 (14%)	3 11
42	DW	90/92 (98%)	82 (91%)	8 (9%)	9 28
43	BX	77/78 (99%)	71 (92%)	6 (8%)	11 35
43	DX	77/78 (99%)	73 (95%)	4 (5%)	21 52
44	BY	85/91 (93%)	77 (91%)	8 (9%)	8 26
44	DY	85/91 (93%)	78 (92%)	7 (8%)	10 32
45	BZ	145/179 (81%)	125 (86%)	20 (14%)	3 12
45	DZ	145/179 (81%)	125 (86%)	20 (14%)	3 12
46	B0	65/67 (97%)	60 (92%)	5 (8%)	12 35
46	D0	65/67 (97%)	60 (92%)	5 (8%)	12 35
47	B1	80/83 (96%)	75 (94%)	5 (6%)	16 45
47	D1	80/83 (96%)	70 (88%)	10 (12%)	4 15
48	B2	65/67 (97%)	60 (92%)	5 (8%)	12 35
48	D2	65/67 (97%)	55 (85%)	10 (15%)	2 9
49	B3	51/52 (98%)	44 (86%)	7 (14%)	3 12
49	D3	50/52 (96%)	45 (90%)	5 (10%)	7 24
50	B4	59/63 (94%)	44 (75%)	15 (25%)	0 2
50	D4	53/63 (84%)	38 (72%)	15 (28%)	0 1
51	B5	50/52 (96%)	44 (88%)	6 (12%)	5 16
51	D5	50/52 (96%)	48 (96%)	2 (4%)	28 62
52	B6	51/52 (98%)	46 (90%)	5 (10%)	7 25
52	D6	50/52 (96%)	45 (90%)	5 (10%)	7 24
53	B7	41/42 (98%)	38 (93%)	3 (7%)	13 38
53	D7	41/42 (98%)	36 (88%)	5 (12%)	5 16
54	B8	53/55 (96%)	49 (92%)	4 (8%)	12 37
54	D8	54/55 (98%)	48 (89%)	6 (11%)	6 20
55	B9	34/34 (100%)	33 (97%)	1 (3%)	37 71
55	D9	34/34 (100%)	30 (88%)	4 (12%)	5 17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	9318/10066 (93%)	8076 (87%)	1242 (13%)	4 12

5 of 1242 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
28	DE	175	VAL
43	DX	76	ARG
30	DG	40	ASN
28	DE	170	LEU
35	DP	4	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 155 such sidechains are listed below:

Mol	Chain	Res	Type
12	CL	78	GLN
38	DS	68	GLN
19	CS	56	GLN
29	DF	75	HIS
45	DZ	75	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1495/1521 (98%)	388 (25%)	22 (1%)
1	CA	1501/1521 (98%)	392 (26%)	24 (1%)
22	AV	12/24 (50%)	4 (33%)	0
22	CV	11/24 (45%)	4 (36%)	0
23	AW	0/2	-	-
23	CW	0/2	-	-
24	AX	74/77 (96%)	25 (33%)	1 (1%)
24	CX	74/77 (96%)	26 (35%)	1 (1%)
25	BA	2811/2915 (96%)	539 (19%)	24 (0%)
25	DA	2791/2915 (95%)	623 (22%)	29 (1%)
26	BB	120/121 (99%)	19 (15%)	3 (2%)
26	DB	119/121 (98%)	36 (30%)	0
All	All	9008/9320 (96%)	2056 (22%)	104 (1%)

5 of 2056 RNA backbone outliers are listed below:

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

5 of 104 RNA pucker outliers are listed below:

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

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
24	5MC	AX	32	24	19,22,23	1.68	3 (15%)	26,32,35	1.31	3 (11%)
24	5MU	AX	54	56,24	19,22,23	1.37	5 (26%)	27,32,35	2.08	6 (22%)
24	5MC	CX	32	24	19,22,23	1.60	3 (15%)	26,32,35	1.12	2 (7%)
24	PSU	CX	55	24	18,21,22	1.36	2 (11%)	21,30,33	1.98	4 (19%)
24	PSU	AX	55	24	18,21,22	1.38	3 (16%)	21,30,33	2.06	3 (14%)
24	31H	AX	76	56,24	31,34,35	1.24	3 (9%)	35,47,50	2.24	13 (37%)
24	31H	CX	76	24	31,34,35	1.29	3 (9%)	35,47,50	2.31	12 (34%)
23	PPU	AW	76	25,23	37,40,41	1.35	5 (13%)	47,57,60	2.24	15 (31%)
24	5MU	CX	54	24	19,22,23	1.28	5 (26%)	27,32,35	2.17	6 (22%)
24	4SU	CX	8	24	18,21,22	2.12	6 (33%)	25,30,33	1.56	5 (20%)
23	PPU	CW	76	23	37,40,41	1.30	5 (13%)	47,57,60	2.15	14 (29%)
24	4SU	AX	8	24	18,21,22	2.27	5 (27%)	25,30,33	1.65	5 (20%)

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	5MC	AX	32	24	-	0/7/25/26	0/2/2/2
24	5MU	AX	54	56,24	-	0/7/25/26	0/2/2/2
24	5MC	CX	32	24	-	0/7/25/26	0/2/2/2
24	PSU	CX	55	24	-	1/7/25/26	0/2/2/2
24	PSU	AX	55	24	-	1/7/25/26	0/2/2/2
24	31H	AX	76	56,24	-	5/22/40/41	0/3/3/3
24	31H	CX	76	24	-	10/22/40/41	0/3/3/3
23	PPU	AW	76	25,23	-	5/25/43/44	0/4/4/4
24	5MU	CX	54	24	-	0/7/25/26	0/2/2/2
24	4SU	CX	8	24	-	0/7/25/26	0/2/2/2
23	PPU	CW	76	23	-	5/25/43/44	0/4/4/4
24	4SU	AX	8	24	-	0/7/25/26	0/2/2/2

The worst 5 of 48 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AX	32	5MC	C5-C4	6.11	1.48	1.44
24	CX	32	5MC	C5-C4	5.76	1.48	1.44
24	AX	8	4SU	C4-N3	-5.30	1.32	1.37
23	CW	76	PPU	C5-C4	5.03	1.48	1.39
23	AW	76	PPU	C5-C4	4.98	1.48	1.39

The worst 5 of 88 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	AX	55	PSU	N1-C2-N3	6.30	121.81	115.17
24	CX	55	PSU	N1-C2-N3	6.22	121.73	115.17
23	AW	76	PPU	C5-C4-N3	-6.18	118.21	126.72
23	CW	76	PPU	C5-C4-N3	-5.95	118.52	126.72
24	AX	76	31H	N1-C2-N3	-5.94	119.59	128.58

There are no chirality outliers.

5 of 27 torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
24	CX	76	31H	C-CA-CB-CG
24	CX	76	31H	OCN-CN-N-CA
24	CX	76	31H	CA-CB-CG-SD

There are no ring outliers.

7 monomers are involved in 19 short contacts:

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

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

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

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

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

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	AA	1498/1521 (98%)	0.51	48 (3%) 50 41	39, 74, 94, 105	0
1	CA	1503/1521 (98%)	0.61	86 (5%) 29 23	41, 75, 94, 105	0
2	AB	231/256 (90%)	1.05	27 (11%) 9 8	65, 82, 90, 96	0
2	CB	231/256 (90%)	1.45	50 (21%) 2 2	67, 83, 92, 96	0
3	AC	206/239 (86%)	0.94	18 (8%) 16 13	67, 78, 86, 94	0
3	CC	206/239 (86%)	1.31	31 (15%) 5 4	69, 80, 87, 92	0
4	AD	208/209 (99%)	1.02	24 (11%) 9 8	57, 72, 82, 86	0
4	CD	208/209 (99%)	1.14	24 (11%) 9 8	57, 73, 82, 87	0
5	AE	148/162 (91%)	0.80	12 (8%) 18 15	55, 71, 81, 86	0
5	CE	148/162 (91%)	1.01	13 (8%) 15 13	58, 73, 82, 89	0
6	AF	100/101 (99%)	0.74	6 (6%) 27 21	55, 71, 80, 82	0
6	CF	100/101 (99%)	0.57	2 (2%) 65 56	58, 73, 80, 82	0
7	AG	155/156 (99%)	0.81	15 (9%) 13 11	67, 76, 85, 94	0
7	CG	155/156 (99%)	1.08	21 (13%) 7 5	68, 78, 86, 96	0
8	AH	137/138 (99%)	0.56	3 (2%) 62 53	62, 72, 78, 86	0
8	CH	137/138 (99%)	0.94	9 (6%) 24 19	62, 73, 80, 88	0
9	AI	127/128 (99%)	1.39	24 (18%) 3 3	64, 82, 87, 90	0
9	CI	127/128 (99%)	2.16	64 (50%) 0 0	67, 83, 89, 91	0
10	AJ	97/105 (92%)	1.21	15 (15%) 5 4	63, 80, 89, 95	0
10	CJ	96/105 (91%)	2.01	49 (51%) 0 0	70, 86, 93, 100	0
11	AK	114/129 (88%)	0.87	7 (6%) 27 21	54, 72, 81, 83	0
11	CK	114/129 (88%)	0.67	3 (2%) 57 48	56, 72, 80, 83	0
12	AL	122/132 (92%)	0.74	6 (4%) 35 27	55, 65, 75, 78	0
12	CL	122/132 (92%)	0.83	5 (4%) 41 33	57, 67, 75, 80	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	AM	123/126 (97%)	1.37	23 (18%) 3 3	64, 78, 86, 91	0
13	CM	122/126 (96%)	1.70	35 (28%) 1 1	68, 80, 88, 93	0
14	AN	60/61 (98%)	1.32	11 (18%) 3 3	65, 76, 83, 86	0
14	CN	60/61 (98%)	2.07	28 (46%) 0 0	69, 79, 84, 88	0
15	AO	88/89 (98%)	0.90	7 (7%) 18 15	56, 69, 80, 90	0
15	CO	88/89 (98%)	0.71	6 (6%) 23 18	56, 70, 80, 90	0
16	AP	82/88 (93%)	1.49	16 (19%) 3 2	58, 73, 83, 85	0
16	CP	82/88 (93%)	1.30	16 (19%) 3 2	58, 72, 82, 85	0
17	AQ	99/105 (94%)	1.11	7 (7%) 22 17	60, 70, 81, 85	0
17	CQ	99/105 (94%)	0.75	2 (2%) 65 56	57, 70, 80, 84	0
18	AR	68/88 (77%)	0.59	4 (5%) 28 22	60, 70, 81, 85	0
18	CR	68/88 (77%)	0.59	0 100 100	61, 72, 82, 86	0
19	AS	83/93 (89%)	1.22	10 (12%) 9 7	67, 81, 88, 96	0
19	CS	83/93 (89%)	1.52	21 (25%) 1 1	71, 83, 91, 97	0
20	AT	96/106 (90%)	1.10	15 (15%) 5 4	58, 72, 82, 89	0
20	CT	96/106 (90%)	0.95	9 (9%) 14 12	59, 72, 82, 88	0
21	AU	23/27 (85%)	1.46	5 (21%) 2 2	65, 75, 80, 86	0
21	CU	23/27 (85%)	1.78	7 (30%) 1 1	66, 76, 83, 87	0
22	AV	13/24 (54%)	1.97	6 (46%) 0 0	60, 92, 100, 100	0
22	CV	12/24 (50%)	1.91	7 (58%) 0 0	63, 93, 99, 99	0
23	AW	1/2 (50%)	-0.24	0 100 100	42, 42, 42, 42	0
23	CW	1/2 (50%)	0.94	0 100 100	59, 59, 59, 59	0
24	AX	71/77 (92%)	0.42	2 (2%) 55 46	37, 72, 84, 92	0
24	CX	71/77 (92%)	0.24	0 100 100	39, 73, 86, 92	0
25	BA	2819/2915 (96%)	-0.18	77 (2%) 56 47	23, 46, 89, 107	0
25	DA	2800/2915 (96%)	-0.14	50 (1%) 67 59	26, 50, 90, 107	0
26	BB	120/121 (99%)	0.10	0 100 100	40, 65, 76, 91	0
26	DB	120/121 (99%)	0.67	5 (4%) 40 32	44, 70, 81, 93	0
27	BD	275/276 (99%)	0.33	5 (1%) 67 59	24, 45, 61, 77	0
27	DD	275/276 (99%)	0.18	1 (0%) 88 85	27, 47, 63, 78	0
28	BE	204/206 (99%)	-0.07	1 (0%) 87 83	18, 44, 66, 80	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
28	DE	204/206 (99%)	0.12	1 (0%) 87 83	32, 57, 72, 86	0
29	BF	203/210 (96%)	0.30	1 (0%) 87 83	26, 55, 74, 84	0
29	DF	203/210 (96%)	0.28	0 100 100	26, 58, 75, 85	0
30	BG	181/182 (99%)	1.02	25 (13%) 6 5	56, 70, 82, 91	0
30	DG	181/182 (99%)	1.37	36 (19%) 3 2	61, 73, 85, 91	0
31	BH	174/180 (96%)	0.47	5 (2%) 53 45	51, 66, 76, 82	0
31	DH	174/180 (96%)	0.82	7 (4%) 42 34	55, 69, 80, 85	0
32	BI	146/148 (98%)	0.75	3 (2%) 63 54	46, 74, 85, 87	0
32	DI	146/148 (98%)	1.25	25 (17%) 4 3	50, 75, 84, 87	0
33	BN	140/140 (100%)	0.26	4 (2%) 53 45	33, 53, 72, 80	0
33	DN	140/140 (100%)	0.26	0 100 100	36, 56, 72, 81	0
34	BO	122/122 (100%)	-0.19	1 (0%) 82 77	25, 43, 60, 76	0
34	DO	122/122 (100%)	0.30	1 (0%) 82 77	42, 59, 73, 77	0
35	BP	149/150 (99%)	0.37	1 (0%) 84 79	27, 57, 73, 87	0
35	DP	149/150 (99%)	0.33	1 (0%) 84 79	29, 59, 76, 86	0
36	BQ	141/141 (100%)	0.36	2 (1%) 73 65	35, 53, 64, 71	0
36	DQ	141/141 (100%)	0.52	3 (2%) 63 54	38, 56, 68, 76	0
37	BR	118/118 (100%)	-0.21	2 (1%) 69 61	25, 37, 56, 66	0
37	DR	118/118 (100%)	0.24	0 100 100	40, 54, 66, 76	0
38	BS	110/112 (98%)	0.00	0 100 100	40, 52, 63, 68	0
38	DS	110/112 (98%)	1.15	15 (13%) 7 5	57, 76, 86, 92	0
39	BT	131/146 (89%)	0.00	1 (0%) 82 77	32, 50, 74, 86	0
39	DT	131/146 (89%)	0.47	2 (1%) 72 64	44, 60, 75, 85	0
40	BU	116/118 (98%)	-0.30	1 (0%) 81 75	23, 35, 55, 76	0
40	DU	116/118 (98%)	0.39	4 (3%) 48 39	41, 61, 77, 87	0
41	BV	101/101 (100%)	-0.30	0 100 100	19, 43, 64, 76	0
41	DV	101/101 (100%)	0.35	0 100 100	44, 71, 80, 88	0
42	BW	112/113 (99%)	-0.33	0 100 100	21, 38, 53, 75	0
42	DW	112/113 (99%)	0.12	1 (0%) 81 75	31, 51, 69, 85	0
43	BX	95/96 (98%)	-0.03	1 (1%) 78 71	25, 43, 64, 82	0
43	DX	95/96 (98%)	0.59	5 (5%) 32 25	43, 62, 78, 91	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
44	BY	107/110 (97%)	0.10	0 100 100	36, 51, 69, 80	0
44	DY	107/110 (97%)	0.90	8 (7%) 20 16	55, 72, 81, 89	0
45	BZ	171/206 (83%)	0.30	3 (1%) 67 59	42, 63, 77, 92	0
45	DZ	174/206 (84%)	0.89	10 (5%) 29 23	61, 80, 90, 100	0
46	B0	83/85 (97%)	-0.07	0 100 100	16, 43, 56, 66	0
46	D0	83/85 (97%)	0.85	8 (9%) 13 11	44, 65, 74, 80	0
47	B1	97/98 (98%)	0.10	3 (3%) 51 42	27, 49, 70, 77	0
47	D1	97/98 (98%)	0.57	2 (2%) 63 54	38, 59, 75, 78	0
48	B2	70/72 (97%)	0.07	1 (1%) 73 65	37, 50, 66, 72	0
48	D2	70/72 (97%)	0.53	0 100 100	58, 70, 79, 85	0
49	B3	59/60 (98%)	-0.27	0 100 100	26, 41, 61, 72	0
49	D3	59/60 (98%)	0.29	2 (3%) 48 39	44, 64, 77, 80	0
50	B4	69/71 (97%)	1.01	8 (11%) 9 8	57, 76, 91, 94	0
50	D4	69/71 (97%)	1.55	18 (26%) 1 1	77, 87, 97, 104	0
51	B5	59/60 (98%)	-0.39	0 100 100	19, 38, 57, 78	0
51	D5	59/60 (98%)	0.04	0 100 100	31, 52, 69, 76	0
52	B6	53/54 (98%)	-0.19	0 100 100	29, 43, 60, 71	0
52	D6	53/54 (98%)	0.71	1 (1%) 66 58	50, 63, 75, 83	0
53	B7	48/49 (97%)	-0.15	0 100 100	20, 30, 53, 72	0
53	D7	48/49 (97%)	0.26	3 (6%) 26 20	35, 46, 71, 76	0
54	B8	64/65 (98%)	-0.10	0 100 100	27, 36, 47, 55	0
54	D8	64/65 (98%)	0.57	0 100 100	44, 58, 67, 75	0
55	B9	37/37 (100%)	0.18	1 (2%) 56 47	31, 52, 64, 69	0
55	D9	37/37 (100%)	0.56	0 100 100	44, 58, 67, 73	0
All	All	20634/21448 (96%)	0.42	1154 (5%) 30 23	16, 64, 87, 107	0

The worst 5 of 1154 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
9	CI	126	SER	7.5
13	CM	124	PRO	7.3
13	CM	123	ALA	6.9
5	CE	94	ALA	6.6
25	BA	2804	C	6.4

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
24	4SU	CX	8	20/21	0.85	0.11	65,84,90,94	0
24	5MU	CX	54	21/22	0.86	0.12	66,78,87,98	0
24	PSU	CX	55	20/21	0.86	0.11	59,68,84,85	0
24	PSU	AX	55	20/21	0.92	0.10	57,66,78,79	0
24	5MC	CX	32	21/22	0.92	0.12	52,69,78,83	0
24	4SU	AX	8	20/21	0.93	0.10	50,63,78,79	0
24	31H	CX	76	32/33	0.93	0.12	33,54,78,89	0
24	5MC	AX	32	21/22	0.94	0.11	46,61,70,75	0
24	5MU	AX	54	21/22	0.94	0.09	55,69,75,82	0
23	PPU	CW	76	37/38	0.96	0.11	31,50,63,70	0
24	31H	AX	76	32/33	0.96	0.12	27,44,76,98	0
23	PPU	AW	76	37/38	0.97	0.09	25,33,43,45	0

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DG	3001	1/1	0.55	0.21	81,81,81,81	0
56	MG	DA	3574	1/1	0.66	0.33	56,56,56,56	0
56	MG	CA	3138	1/1	0.69	0.17	58,58,58,58	0
56	MG	DA	3504	1/1	0.71	0.17	49,49,49,49	0
56	MG	DA	3247	1/1	0.73	0.15	49,49,49,49	0
56	MG	AA	3184	1/1	0.75	0.23	74,74,74,74	0
56	MG	AA	3056	1/1	0.75	0.29	69,69,69,69	0
56	MG	AA	3180	1/1	0.75	0.15	56,56,56,56	0
56	MG	CA	3105	1/1	0.76	0.25	84,84,84,84	0
56	MG	AA	3167	1/1	0.76	0.25	73,73,73,73	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	0.76	0.13	62,62,62,62	0
56	MG	DA	3478	1/1	0.77	0.25	53,53,53,53	0
56	MG	CA	3126	1/1	0.77	0.15	73,73,73,73	0
56	MG	BA	3639	1/1	0.77	0.19	64,64,64,64	0
56	MG	CA	3119	1/1	0.77	0.12	48,48,48,48	0
56	MG	DA	3326	1/1	0.78	0.13	41,41,41,41	0
56	MG	DA	3354	1/1	0.78	0.16	51,51,51,51	0
56	MG	CA	3149	1/1	0.78	0.38	66,66,66,66	0
56	MG	DA	3271	1/1	0.79	0.17	55,55,55,55	0
56	MG	AA	3055	1/1	0.79	0.20	72,72,72,72	0
56	MG	CA	3068	1/1	0.79	0.20	74,74,74,74	0
56	MG	DA	3446	1/1	0.79	0.12	46,46,46,46	0
56	MG	AF	3001	1/1	0.80	0.18	52,52,52,52	0
56	MG	CA	3140	1/1	0.80	0.23	61,61,61,61	0
56	MG	DA	3475	1/1	0.80	0.14	41,41,41,41	0
56	MG	BA	3634	1/1	0.80	0.23	41,41,41,41	0
56	MG	CA	3108	1/1	0.80	0.20	59,59,59,59	0
56	MG	BA	3569	1/1	0.80	0.17	55,55,55,55	0
56	MG	BB	3009	1/1	0.80	0.18	67,67,67,67	0
56	MG	CA	3125	1/1	0.81	0.24	71,71,71,71	0
56	MG	BA	3631	1/1	0.81	0.13	41,41,41,41	0
56	MG	DA	3103	1/1	0.81	0.08	56,56,56,56	0
56	MG	DA	3443	1/1	0.81	0.12	49,49,49,49	0
56	MG	AA	3106	1/1	0.81	0.15	50,50,50,50	0
56	MG	DA	3366	1/1	0.82	0.12	43,43,43,43	0
56	MG	DA	3416	1/1	0.82	0.13	44,44,44,44	0
56	MG	BA	3536	1/1	0.82	0.21	53,53,53,53	0
56	MG	BA	3497	1/1	0.82	0.14	34,34,34,34	0
56	MG	BA	3633	1/1	0.82	0.15	57,57,57,57	0
56	MG	BZ	3001	1/1	0.82	0.12	58,58,58,58	0
56	MG	CA	3016	1/1	0.82	0.16	68,68,68,68	0
56	MG	DA	3507	1/1	0.82	0.13	54,54,54,54	0
56	MG	DA	3566	1/1	0.82	0.15	61,61,61,61	0
56	MG	CA	3035	1/1	0.82	0.13	66,66,66,66	0
56	MG	DB	3006	1/1	0.82	0.13	55,55,55,55	0
56	MG	CA	3065	1/1	0.82	0.14	55,55,55,55	0
56	MG	DW	3002	1/1	0.82	0.11	60,60,60,60	0
56	MG	CA	3145	1/1	0.83	0.18	59,59,59,59	0
56	MG	DA	3518	1/1	0.83	0.19	53,53,53,53	0
56	MG	DA	3301	1/1	0.83	0.13	56,56,56,56	0
56	MG	DA	3302	1/1	0.83	0.10	43,43,43,43	0
56	MG	BA	3062	1/1	0.83	0.18	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	CA	3104	1/1	0.83	0.29	74,74,74,74	0
56	MG	AA	3024	1/1	0.83	0.38	60,60,60,60	0
56	MG	DY	502	1/1	0.83	0.14	51,51,51,51	0
56	MG	BA	3466	1/1	0.84	0.26	49,49,49,49	0
56	MG	AA	3049	1/1	0.84	0.14	47,47,47,47	0
56	MG	CA	3151	1/1	0.84	0.20	50,50,50,50	0
56	MG	DA	3020	1/1	0.84	0.22	50,50,50,50	0
56	MG	DA	3474	1/1	0.84	0.11	62,62,62,62	0
56	MG	DA	3090	1/1	0.84	0.10	54,54,54,54	0
56	MG	BA	3505	1/1	0.84	0.23	46,46,46,46	0
56	MG	DA	3479	1/1	0.84	0.18	63,63,63,63	0
56	MG	DA	3150	1/1	0.84	0.35	55,55,55,55	0
56	MG	AA	3181	1/1	0.84	0.17	53,53,53,53	0
56	MG	AA	3109	1/1	0.84	0.22	44,44,44,44	0
56	MG	DA	3538	1/1	0.84	0.10	39,39,39,39	0
56	MG	DA	3300	1/1	0.84	0.18	58,58,58,58	0
56	MG	AA	3160	1/1	0.84	0.12	71,71,71,71	0
56	MG	AA	3086	1/1	0.84	0.37	61,61,61,61	0
56	MG	DB	3009	1/1	0.84	0.14	60,60,60,60	0
56	MG	CA	3139	1/1	0.84	0.15	67,67,67,67	0
56	MG	DA	3343	1/1	0.84	0.23	56,56,56,56	0
56	MG	BA	3331	1/1	0.84	0.12	59,59,59,59	0
56	MG	CA	3103	1/1	0.85	0.16	52,52,52,52	0
56	MG	CA	3129	1/1	0.85	0.11	55,55,55,55	0
56	MG	CA	3011	1/1	0.85	0.17	66,66,66,66	0
56	MG	DA	3539	1/1	0.85	0.16	52,52,52,52	0
56	MG	BA	3617	1/1	0.85	0.25	66,66,66,66	0
56	MG	AA	3088	1/1	0.85	0.20	62,62,62,62	0
56	MG	BA	3632	1/1	0.85	0.25	54,54,54,54	0
56	MG	BA	3611	1/1	0.85	0.20	59,59,59,59	0
56	MG	DA	3485	1/1	0.85	0.18	60,60,60,60	0
56	MG	DA	3501	1/1	0.85	0.11	55,55,55,55	0
56	MG	DA	3381	1/1	0.85	0.20	56,56,56,56	0
56	MG	AA	3149	1/1	0.86	0.17	68,68,68,68	0
56	MG	AA	3027	1/1	0.86	0.21	71,71,71,71	0
56	MG	DA	3359	1/1	0.86	0.17	43,43,43,43	0
56	MG	BA	3043	1/1	0.86	0.20	36,36,36,36	0
56	MG	CA	3132	1/1	0.86	0.25	73,73,73,73	0
56	MG	DA	3398	1/1	0.86	0.14	51,51,51,51	0
56	MG	BA	3545	1/1	0.86	0.11	54,54,54,54	0
56	MG	BA	3557	1/1	0.86	0.18	42,42,42,42	0
56	MG	AA	3092	1/1	0.86	0.23	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	BA	3244	1/1	0.86	0.21	46,46,46,46	0
56	MG	BA	3582	1/1	0.86	0.14	31,31,31,31	0
56	MG	CA	3036	1/1	0.86	0.14	56,56,56,56	0
56	MG	BA	3583	1/1	0.86	0.12	37,37,37,37	0
56	MG	DA	3058	1/1	0.86	0.20	45,45,45,45	0
56	MG	BA	3584	1/1	0.86	0.14	44,44,44,44	0
56	MG	CA	3083	1/1	0.86	0.22	66,66,66,66	0
56	MG	DA	3135	1/1	0.86	0.12	47,47,47,47	0
56	MG	CA	3084	1/1	0.86	0.13	72,72,72,72	0
56	MG	BA	3601	1/1	0.86	0.15	50,50,50,50	0
56	MG	DA	3251	1/1	0.86	0.22	62,62,62,62	0
56	MG	DA	3557	1/1	0.86	0.13	62,62,62,62	0
56	MG	DA	3561	1/1	0.86	0.14	63,63,63,63	0
56	MG	AA	3013	1/1	0.86	0.25	58,58,58,58	0
56	MG	DA	3568	1/1	0.86	0.11	60,60,60,60	0
56	MG	DA	3274	1/1	0.86	0.13	56,56,56,56	0
56	MG	DA	3580	1/1	0.86	0.10	58,58,58,58	0
56	MG	DB	3005	1/1	0.86	0.11	56,56,56,56	0
56	MG	AA	3054	1/1	0.86	0.17	65,65,65,65	0
56	MG	BA	3483	1/1	0.86	0.14	47,47,47,47	0
56	MG	BA	3496	1/1	0.86	0.16	31,31,31,31	0
56	MG	DQ	3003	1/1	0.86	0.13	50,50,50,50	0
56	MG	DA	3309	1/1	0.86	0.13	60,60,60,60	0
56	MG	CA	3121	1/1	0.86	0.15	61,61,61,61	0
56	MG	BA	3307	1/1	0.87	0.08	63,63,63,63	0
56	MG	BA	3585	1/1	0.87	0.25	50,50,50,50	0
56	MG	BA	3510	1/1	0.87	0.19	25,25,25,25	0
56	MG	CA	3019	1/1	0.87	0.34	71,71,71,71	0
56	MG	CA	3034	1/1	0.87	0.24	67,67,67,67	0
56	MG	AA	3061	1/1	0.87	0.22	62,62,62,62	0
56	MG	BA	3395	1/1	0.87	0.10	54,54,54,54	0
56	MG	CA	3049	1/1	0.87	0.18	51,51,51,51	0
56	MG	DA	3325	1/1	0.87	0.12	54,54,54,54	0
56	MG	BA	3412	1/1	0.87	0.11	48,48,48,48	0
56	MG	CA	3067	1/1	0.87	0.19	63,63,63,63	0
56	MG	AA	3171	1/1	0.87	0.10	62,62,62,62	0
56	MG	CA	3078	1/1	0.87	0.18	66,66,66,66	0
56	MG	BA	3574	1/1	0.87	0.19	55,55,55,55	0
56	MG	DA	3022	1/1	0.87	0.19	39,39,39,39	0
56	MG	BA	3211	1/1	0.87	0.22	29,29,29,29	0
56	MG	BA	3229	1/1	0.87	0.20	54,54,54,54	0
56	MG	DA	3425	1/1	0.87	0.10	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DA	3428	1/1	0.87	0.15	33,33,33,33	0
56	MG	DF	303	1/1	0.87	0.17	57,57,57,57	0
56	MG	DA	3437	1/1	0.87	0.15	48,48,48,48	0
56	MG	AA	3102	1/1	0.87	0.23	60,60,60,60	0
56	MG	BB	3010	1/1	0.87	0.09	77,77,77,77	0
56	MG	BB	3015	1/1	0.87	0.10	48,48,48,48	0
56	MG	DA	3467	1/1	0.88	0.14	47,47,47,47	0
56	MG	DA	3470	1/1	0.88	0.30	52,52,52,52	0
56	MG	DA	3252	1/1	0.88	0.12	53,53,53,53	0
56	MG	AA	3121	1/1	0.88	0.14	40,40,40,40	0
56	MG	AA	3003	1/1	0.88	0.12	57,57,57,57	0
56	MG	DA	3275	1/1	0.88	0.12	45,45,45,45	0
56	MG	CA	3041	1/1	0.88	0.18	67,67,67,67	0
56	MG	DA	3496	1/1	0.88	0.10	46,46,46,46	0
56	MG	CA	3133	1/1	0.88	0.19	68,68,68,68	0
56	MG	CA	3048	1/1	0.88	0.39	52,52,52,52	0
56	MG	AA	3057	1/1	0.88	0.29	67,67,67,67	0
56	MG	BB	3003	1/1	0.88	0.09	61,61,61,61	0
56	MG	DA	3526	1/1	0.88	0.14	64,64,64,64	0
56	MG	AA	3058	1/1	0.88	0.19	62,62,62,62	0
56	MG	AA	3023	1/1	0.88	0.30	71,71,71,71	0
56	MG	DA	3347	1/1	0.88	0.09	41,41,41,41	0
56	MG	BA	3553	1/1	0.88	0.49	48,48,48,48	0
56	MG	BG	3003	1/1	0.88	0.09	41,41,41,41	0
56	MG	DA	3567	1/1	0.88	0.11	41,41,41,41	0
56	MG	BA	3094	1/1	0.88	0.14	45,45,45,45	0
56	MG	DA	3373	1/1	0.88	0.09	42,42,42,42	0
56	MG	CA	3003	1/1	0.88	0.21	65,65,65,65	0
56	MG	DA	3585	1/1	0.88	0.09	37,37,37,37	0
56	MG	CA	3009	1/1	0.88	0.17	55,55,55,55	0
56	MG	BA	3612	1/1	0.88	0.18	51,51,51,51	0
56	MG	DA	3420	1/1	0.88	0.09	46,46,46,46	0
56	MG	AA	3176	1/1	0.88	0.14	60,60,60,60	0
56	MG	DA	3147	1/1	0.88	0.20	47,47,47,47	0
56	MG	DN	5001	1/1	0.88	0.12	65,65,65,65	0
56	MG	AA	3045	1/1	0.88	0.25	60,60,60,60	0
56	MG	CA	3021	1/1	0.88	0.14	52,52,52,52	0
56	MG	BA	3576	1/1	0.88	0.13	48,48,48,48	0
56	MG	AA	3042	1/1	0.89	0.20	54,54,54,54	0
56	MG	AA	3164	1/1	0.89	0.14	61,61,61,61	0
56	MG	BA	3306	1/1	0.89	0.17	54,54,54,54	0
56	MG	DA	3412	1/1	0.89	0.19	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	3004	1/1	0.89	0.11	51,51,51,51	0
56	MG	AA	3016	1/1	0.89	0.16	49,49,49,49	0
56	MG	BA	3323	1/1	0.89	0.11	61,61,61,61	0
56	MG	BA	3578	1/1	0.89	0.12	59,59,59,59	0
56	MG	BA	3579	1/1	0.89	0.10	46,46,46,46	0
56	MG	BA	3036	1/1	0.89	0.13	56,56,56,56	0
56	MG	CA	3025	1/1	0.89	0.11	48,48,48,48	0
56	MG	CA	3033	1/1	0.89	0.28	52,52,52,52	0
56	MG	BA	3357	1/1	0.89	0.10	30,30,30,30	0
56	MG	DA	3066	1/1	0.89	0.13	49,49,49,49	0
56	MG	DA	3083	1/1	0.89	0.09	48,48,48,48	0
56	MG	BA	3367	1/1	0.89	0.12	49,49,49,49	0
56	MG	DA	3100	1/1	0.89	0.09	34,34,34,34	0
56	MG	BA	3387	1/1	0.89	0.21	49,49,49,49	0
56	MG	DA	3109	1/1	0.89	0.08	50,50,50,50	0
56	MG	AA	3169	1/1	0.89	0.15	71,71,71,71	0
56	MG	BA	3593	1/1	0.89	0.23	39,39,39,39	0
56	MG	BA	3401	1/1	0.89	0.14	32,32,32,32	0
56	MG	DA	3173	1/1	0.89	0.15	54,54,54,54	0
56	MG	DA	3191	1/1	0.89	0.14	53,53,53,53	0
56	MG	CA	3055	1/1	0.89	0.11	62,62,62,62	0
56	MG	BA	3605	1/1	0.89	0.08	46,46,46,46	0
56	MG	DA	3545	1/1	0.89	0.16	58,58,58,58	0
56	MG	BA	3056	1/1	0.89	0.13	46,46,46,46	0
56	MG	AA	3002	1/1	0.89	0.23	43,43,43,43	0
56	MG	BA	3469	1/1	0.89	0.09	28,28,28,28	0
56	MG	CA	3082	1/1	0.89	0.32	62,62,62,62	0
56	MG	BA	3619	1/1	0.89	0.12	30,30,30,30	0
56	MG	BA	3075	1/1	0.89	0.31	58,58,58,58	0
56	MG	BA	3495	1/1	0.89	0.23	48,48,48,48	0
56	MG	DA	3307	1/1	0.89	0.09	53,53,53,53	0
56	MG	BA	3090	1/1	0.89	0.16	44,44,44,44	0
56	MG	AA	3142	1/1	0.89	0.17	60,60,60,60	0
56	MG	DB	3007	1/1	0.89	0.09	38,38,38,38	0
56	MG	BA	3111	1/1	0.89	0.08	27,27,27,27	0
56	MG	DA	3337	1/1	0.89	0.07	42,42,42,42	0
56	MG	CA	3118	1/1	0.89	0.15	78,78,78,78	0
56	MG	BA	3192	1/1	0.89	0.26	58,58,58,58	0
56	MG	BA	3523	1/1	0.89	0.10	50,50,50,50	0
56	MG	AA	3073	1/1	0.89	0.24	50,50,50,50	0
56	MG	BA	3213	1/1	0.89	0.20	21,21,21,21	0
56	MG	BA	3609	1/1	0.90	0.10	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DA	3399	1/1	0.90	0.08	40,40,40,40	0
56	MG	DA	3402	1/1	0.90	0.11	63,63,63,63	0
56	MG	BA	3488	1/1	0.90	0.22	36,36,36,36	0
56	MG	BA	3237	1/1	0.90	0.21	57,57,57,57	0
56	MG	DA	3067	1/1	0.90	0.24	53,53,53,53	0
56	MG	AA	3093	1/1	0.90	0.14	45,45,45,45	0
56	MG	BA	3246	1/1	0.90	0.20	56,56,56,56	0
56	MG	DA	3098	1/1	0.90	0.09	46,46,46,46	0
56	MG	BA	3503	1/1	0.90	0.13	30,30,30,30	0
56	MG	BA	3293	1/1	0.90	0.11	17,17,17,17	0
56	MG	DA	3108	1/1	0.90	0.10	46,46,46,46	0
56	MG	CA	3072	1/1	0.90	0.22	57,57,57,57	0
56	MG	BA	3044	1/1	0.90	0.15	30,30,30,30	0
56	MG	AA	3038	1/1	0.90	0.23	53,53,53,53	0
56	MG	AA	3062	1/1	0.90	0.30	58,58,58,58	0
56	MG	DA	3163	1/1	0.90	0.26	31,31,31,31	0
56	MG	DA	3166	1/1	0.90	0.16	35,35,35,35	0
56	MG	DA	3487	1/1	0.90	0.09	50,50,50,50	0
56	MG	AA	3041	1/1	0.90	0.20	52,52,52,52	0
56	MG	DA	3500	1/1	0.90	0.17	46,46,46,46	0
56	MG	BB	3005	1/1	0.90	0.18	30,30,30,30	0
56	MG	DA	3211	1/1	0.90	0.17	35,35,35,35	0
56	MG	BA	3549	1/1	0.90	0.16	57,57,57,57	0
56	MG	DA	3515	1/1	0.90	0.09	64,64,64,64	0
56	MG	BA	3350	1/1	0.90	0.14	59,59,59,59	0
56	MG	AA	3113	1/1	0.90	0.21	53,53,53,53	0
56	MG	DA	3530	1/1	0.90	0.14	60,60,60,60	0
56	MG	DA	3531	1/1	0.90	0.11	69,69,69,69	0
56	MG	BA	3567	1/1	0.90	0.09	53,53,53,53	0
56	MG	BA	3359	1/1	0.90	0.10	54,54,54,54	0
56	MG	DA	3541	1/1	0.90	0.11	57,57,57,57	0
56	MG	DA	3544	1/1	0.90	0.12	51,51,51,51	0
56	MG	AA	3085	1/1	0.90	0.23	63,63,63,63	0
56	MG	CA	3123	1/1	0.90	0.17	66,66,66,66	0
56	MG	BA	3373	1/1	0.90	0.13	41,41,41,41	0
56	MG	BA	3381	1/1	0.90	0.18	31,31,31,31	0
56	MG	AA	3010	1/1	0.90	0.20	60,60,60,60	0
56	MG	CA	3013	1/1	0.90	0.16	53,53,53,53	0
56	MG	AA	3015	1/1	0.90	0.12	56,56,56,56	0
56	MG	CA	3137	1/1	0.90	0.14	66,66,66,66	0
56	MG	DA	3584	1/1	0.90	0.13	61,61,61,61	0
56	MG	BA	3206	1/1	0.90	0.21	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	BA	3403	1/1	0.90	0.13	18,18,18,18	0
56	MG	AA	3185	1/1	0.90	0.08	64,64,64,64	0
56	MG	DA	3351	1/1	0.90	0.09	46,46,46,46	0
56	MG	BA	3415	1/1	0.90	0.15	54,54,54,54	0
56	MG	AA	3151	1/1	0.90	0.18	45,45,45,45	0
56	MG	AA	3035	1/1	0.90	0.23	65,65,65,65	0
56	MG	DA	3371	1/1	0.90	0.07	46,46,46,46	0
56	MG	DA	3017	1/1	0.90	0.25	46,46,46,46	0
56	MG	DA	3375	1/1	0.90	0.12	49,49,49,49	0
56	MG	BA	3230	1/1	0.90	0.07	40,40,40,40	0
56	MG	DA	3340	1/1	0.91	0.11	47,47,47,47	0
56	MG	CA	3120	1/1	0.91	0.17	51,51,51,51	0
56	MG	AA	3110	1/1	0.91	0.12	60,60,60,60	0
56	MG	AA	3012	1/1	0.91	0.10	64,64,64,64	0
56	MG	AA	3119	1/1	0.91	0.16	57,57,57,57	0
56	MG	BA	3235	1/1	0.91	0.09	51,51,51,51	0
56	MG	BH	3001	1/1	0.91	0.19	56,56,56,56	0
56	MG	BO	5001	1/1	0.91	0.18	62,62,62,62	0
56	MG	AA	3076	1/1	0.91	0.14	52,52,52,52	0
56	MG	BA	3404	1/1	0.91	0.16	38,38,38,38	0
56	MG	BA	3405	1/1	0.91	0.11	26,26,26,26	0
56	MG	CA	3007	1/1	0.91	0.07	50,50,50,50	0
56	MG	AA	3126	1/1	0.91	0.29	54,54,54,54	0
56	MG	AA	3006	1/1	0.91	0.11	67,67,67,67	0
56	MG	DA	3406	1/1	0.91	0.09	50,50,50,50	0
56	MG	CA	3148	1/1	0.91	0.11	57,57,57,57	0
56	MG	CA	3012	1/1	0.91	0.18	52,52,52,52	0
56	MG	BA	3423	1/1	0.91	0.11	47,47,47,47	0
56	MG	DA	3424	1/1	0.91	0.14	30,30,30,30	0
56	MG	CA	3152	1/1	0.91	0.13	75,75,75,75	0
56	MG	BA	3428	1/1	0.91	0.08	58,58,58,58	0
56	MG	CA	3018	1/1	0.91	0.10	43,43,43,43	0
56	MG	BA	3443	1/1	0.91	0.09	44,44,44,44	0
56	MG	DA	3445	1/1	0.91	0.13	48,48,48,48	0
56	MG	DA	3028	1/1	0.91	0.10	47,47,47,47	0
56	MG	BA	3278	1/1	0.91	0.08	50,50,50,50	0
56	MG	AA	3018	1/1	0.91	0.16	50,50,50,50	0
56	MG	DA	3473	1/1	0.91	0.10	50,50,50,50	0
56	MG	BA	3476	1/1	0.91	0.07	51,51,51,51	0
56	MG	DA	3070	1/1	0.91	0.30	49,49,49,49	0
56	MG	DA	3477	1/1	0.91	0.09	42,42,42,42	0
56	MG	DA	3076	1/1	0.91	0.07	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	BA	3596	1/1	0.91	0.15	56,56,56,56	0
56	MG	DA	3483	1/1	0.91	0.10	54,54,54,54	0
56	MG	DA	3484	1/1	0.91	0.12	34,34,34,34	0
56	MG	DA	3088	1/1	0.91	0.06	39,39,39,39	0
56	MG	BA	3600	1/1	0.91	0.20	68,68,68,68	0
56	MG	BA	3480	1/1	0.91	0.17	43,43,43,43	0
56	MG	BA	3604	1/1	0.91	0.07	28,28,28,28	0
56	MG	BA	3297	1/1	0.91	0.08	39,39,39,39	0
56	MG	BA	3300	1/1	0.91	0.15	39,39,39,39	0
56	MG	DA	3506	1/1	0.91	0.11	65,65,65,65	0
56	MG	CA	3050	1/1	0.91	0.21	67,67,67,67	0
56	MG	AA	3019	1/1	0.91	0.27	62,62,62,62	0
56	MG	DA	3516	1/1	0.91	0.08	61,61,61,61	0
56	MG	AA	3153	1/1	0.91	0.17	50,50,50,50	0
56	MG	CA	3066	1/1	0.91	0.21	43,43,43,43	0
56	MG	BA	3112	1/1	0.91	0.14	40,40,40,40	0
56	MG	BA	3125	1/1	0.91	0.14	51,51,51,51	0
56	MG	BA	3626	1/1	0.91	0.15	50,50,50,50	0
56	MG	CA	3077	1/1	0.91	0.18	44,44,44,44	0
56	MG	DA	3192	1/1	0.91	0.12	51,51,51,51	0
56	MG	DA	3206	1/1	0.91	0.08	50,50,50,50	0
56	MG	BA	3627	1/1	0.91	0.13	54,54,54,54	0
56	MG	DA	3552	1/1	0.91	0.17	49,49,49,49	0
56	MG	DA	3213	1/1	0.91	0.12	34,34,34,34	0
56	MG	BA	3629	1/1	0.91	0.17	60,60,60,60	0
56	MG	BA	3140	1/1	0.91	0.17	33,33,33,33	0
56	MG	BA	3507	1/1	0.91	0.11	53,53,53,53	0
56	MG	DA	3257	1/1	0.91	0.11	55,55,55,55	0
56	MG	CA	3085	1/1	0.91	0.13	52,52,52,52	0
56	MG	DA	3578	1/1	0.91	0.10	47,47,47,47	0
56	MG	DA	3272	1/1	0.91	0.10	57,57,57,57	0
56	MG	CA	3090	1/1	0.91	0.17	66,66,66,66	0
56	MG	CA	3091	1/1	0.91	0.19	66,66,66,66	0
56	MG	DB	3004	1/1	0.91	0.11	36,36,36,36	0
56	MG	BA	3171	1/1	0.91	0.09	44,44,44,44	0
56	MG	BA	3513	1/1	0.91	0.08	60,60,60,60	0
56	MG	AA	3156	1/1	0.91	0.10	61,61,61,61	0
56	MG	BA	3642	1/1	0.91	0.20	47,47,47,47	0
56	MG	DB	3012	1/1	0.91	0.13	53,53,53,53	0
56	MG	CA	3113	1/1	0.91	0.14	57,57,57,57	0
56	MG	CA	3114	1/1	0.91	0.14	80,80,80,80	0
56	MG	AA	3187	1/1	0.91	0.13	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	DA	3327	1/1	0.91	0.14	34,34,34,34	0
56	MG	DA	3328	1/1	0.91	0.13	48,48,48,48	0
56	MG	AA	3158	1/1	0.91	0.11	54,54,54,54	0
56	MG	D8	5002	1/1	0.91	0.17	64,64,64,64	0
56	MG	BD	302	1/1	0.92	0.09	45,45,45,45	0
56	MG	BA	3347	1/1	0.92	0.14	53,53,53,53	0
56	MG	BA	3130	1/1	0.92	0.09	40,40,40,40	0
56	MG	BA	3550	1/1	0.92	0.17	44,44,44,44	0
56	MG	BW	3002	1/1	0.92	0.13	57,57,57,57	0
56	MG	CA	3131	1/1	0.92	0.10	65,65,65,65	0
56	MG	DA	3346	1/1	0.92	0.10	33,33,33,33	0
56	MG	BY	502	1/1	0.92	0.08	35,35,35,35	0
56	MG	BY	503	1/1	0.92	0.07	42,42,42,42	0
56	MG	DA	3352	1/1	0.92	0.07	45,45,45,45	0
56	MG	CA	3136	1/1	0.92	0.08	53,53,53,53	0
56	MG	BA	3013	1/1	0.92	0.08	35,35,35,35	0
56	MG	DA	3360	1/1	0.92	0.09	39,39,39,39	0
56	MG	DA	3361	1/1	0.92	0.15	38,38,38,38	0
56	MG	BA	3141	1/1	0.92	0.10	45,45,45,45	0
56	MG	BA	3019	1/1	0.92	0.23	49,49,49,49	0
56	MG	BA	3023	1/1	0.92	0.10	40,40,40,40	0
56	MG	BA	3571	1/1	0.92	0.16	50,50,50,50	0
56	MG	AA	3154	1/1	0.92	0.19	51,51,51,51	0
56	MG	DA	3386	1/1	0.92	0.17	48,48,48,48	0
56	MG	BA	3575	1/1	0.92	0.08	55,55,55,55	0
56	MG	AA	3125	1/1	0.92	0.21	41,41,41,41	0
56	MG	AA	3179	1/1	0.92	0.21	63,63,63,63	0
56	MG	DA	3004	1/1	0.92	0.18	51,51,51,51	0
56	MG	DA	3409	1/1	0.92	0.22	53,53,53,53	0
56	MG	DA	3009	1/1	0.92	0.08	42,42,42,42	0
56	MG	BA	3046	1/1	0.92	0.13	29,29,29,29	0
56	MG	DA	3418	1/1	0.92	0.10	29,29,29,29	0
56	MG	AA	3112	1/1	0.92	0.19	94,94,94,94	0
56	MG	DA	3021	1/1	0.92	0.11	55,55,55,55	0
56	MG	AA	3159	1/1	0.92	0.07	56,56,56,56	0
56	MG	BA	3074	1/1	0.92	0.11	45,45,45,45	0
56	MG	DA	3432	1/1	0.92	0.18	33,33,33,33	0
56	MG	DA	3032	1/1	0.92	0.17	42,42,42,42	0
56	MG	DA	3438	1/1	0.92	0.15	38,38,38,38	0
56	MG	DA	3050	1/1	0.92	0.10	41,41,41,41	0
56	MG	DA	3052	1/1	0.92	0.08	49,49,49,49	0
56	MG	BA	3408	1/1	0.92	0.09	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	3454	1/1	0.92	0.11	64,64,64,64	0
56	MG	DA	3465	1/1	0.92	0.13	38,38,38,38	0
56	MG	BA	3241	1/1	0.92	0.29	26,26,26,26	0
56	MG	AA	3004	1/1	0.92	0.15	67,67,67,67	0
56	MG	BA	3594	1/1	0.92	0.13	37,37,37,37	0
56	MG	DA	3075	1/1	0.92	0.13	41,41,41,41	0
56	MG	BA	3077	1/1	0.92	0.22	37,37,37,37	0
56	MG	BA	3254	1/1	0.92	0.12	45,45,45,45	0
56	MG	BA	3437	1/1	0.92	0.26	58,58,58,58	0
56	MG	BA	3602	1/1	0.92	0.10	31,31,31,31	0
56	MG	DA	3092	1/1	0.92	0.21	45,45,45,45	0
56	MG	BA	3265	1/1	0.92	0.27	47,47,47,47	0
56	MG	CA	3059	1/1	0.92	0.20	58,58,58,58	0
56	MG	CA	3062	1/1	0.92	0.13	57,57,57,57	0
56	MG	DA	3494	1/1	0.92	0.13	49,49,49,49	0
56	MG	BA	3449	1/1	0.92	0.08	47,47,47,47	0
56	MG	BA	3084	1/1	0.92	0.13	34,34,34,34	0
56	MG	DA	3113	1/1	0.92	0.12	41,41,41,41	0
56	MG	DA	3503	1/1	0.92	0.07	38,38,38,38	0
56	MG	DA	3118	1/1	0.92	0.17	49,49,49,49	0
56	MG	DA	3121	1/1	0.92	0.11	50,50,50,50	0
56	MG	DA	3125	1/1	0.92	0.10	47,47,47,47	0
56	MG	DA	3508	1/1	0.92	0.07	38,38,38,38	0
56	MG	DA	3510	1/1	0.92	0.14	53,53,53,53	0
56	MG	DA	3127	1/1	0.92	0.10	41,41,41,41	0
56	MG	AA	3079	1/1	0.92	0.33	49,49,49,49	0
56	MG	AA	3105	1/1	0.92	0.15	44,44,44,44	0
56	MG	CA	3071	1/1	0.92	0.30	51,51,51,51	0
56	MG	DA	3162	1/1	0.92	0.19	57,57,57,57	0
56	MG	BA	3098	1/1	0.92	0.23	56,56,56,56	0
56	MG	AA	3124	1/1	0.92	0.13	30,30,30,30	0
56	MG	BA	3624	1/1	0.92	0.13	49,49,49,49	0
56	MG	DA	3178	1/1	0.92	0.18	46,46,46,46	0
56	MG	CA	3081	1/1	0.92	0.12	56,56,56,56	0
56	MG	BA	3001	1/1	0.92	0.15	35,35,35,35	0
56	MG	DA	3201	1/1	0.92	0.13	51,51,51,51	0
56	MG	DA	3553	1/1	0.92	0.15	46,46,46,46	0
56	MG	BA	3309	1/1	0.92	0.09	32,32,32,32	0
56	MG	BA	3316	1/1	0.92	0.09	61,61,61,61	0
56	MG	DA	3563	1/1	0.92	0.11	60,60,60,60	0
56	MG	BA	3124	1/1	0.92	0.15	58,58,58,58	0
56	MG	DA	3236	1/1	0.92	0.14	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	3239	1/1	0.92	0.15	56,56,56,56	0
56	MG	DA	3242	1/1	0.92	0.17	60,60,60,60	0
56	MG	CA	3086	1/1	0.92	0.17	68,68,68,68	0
56	MG	BA	3498	1/1	0.92	0.16	37,37,37,37	0
56	MG	BA	3324	1/1	0.92	0.10	53,53,53,53	0
56	MG	CA	3096	1/1	0.92	0.13	61,61,61,61	0
56	MG	DA	3592	1/1	0.92	0.30	52,52,52,52	0
56	MG	DA	3263	1/1	0.92	0.07	39,39,39,39	0
56	MG	DA	3269	1/1	0.92	0.14	43,43,43,43	0
56	MG	BA	3328	1/1	0.92	0.10	39,39,39,39	0
56	MG	BA	3329	1/1	0.92	0.09	30,30,30,30	0
56	MG	BA	3002	1/1	0.92	0.11	39,39,39,39	0
56	MG	CA	3107	1/1	0.92	0.23	56,56,56,56	0
56	MG	DE	3001	1/1	0.92	0.07	43,43,43,43	0
56	MG	BA	3675	1/1	0.92	0.25	33,33,33,33	0
56	MG	BA	3339	1/1	0.92	0.11	34,34,34,34	0
56	MG	BA	3515	1/1	0.92	0.10	25,25,25,25	0
56	MG	BA	3340	1/1	0.92	0.08	42,42,42,42	0
56	MG	BA	3524	1/1	0.92	0.08	57,57,57,57	0
56	MG	DA	3323	1/1	0.92	0.07	35,35,35,35	0
56	MG	D7	101	1/1	0.92	0.40	51,51,51,51	0
56	MG	BA	3345	1/1	0.92	0.15	41,41,41,41	0
56	MG	BU	205	1/1	0.93	0.11	53,53,53,53	0
56	MG	BV	201	1/1	0.93	0.25	36,36,36,36	0
56	MG	BA	3561	1/1	0.93	0.09	55,55,55,55	0
56	MG	BA	3565	1/1	0.93	0.12	51,51,51,51	0
56	MG	BA	3566	1/1	0.93	0.11	46,46,46,46	0
56	MG	DA	3329	1/1	0.93	0.07	48,48,48,48	0
56	MG	BA	3398	1/1	0.93	0.12	41,41,41,41	0
56	MG	B0	104	1/1	0.93	0.21	48,48,48,48	0
56	MG	BA	3064	1/1	0.93	0.15	30,30,30,30	0
56	MG	BA	3073	1/1	0.93	0.10	14,14,14,14	0
56	MG	AA	3065	1/1	0.93	0.20	48,48,48,48	0
56	MG	AA	3107	1/1	0.93	0.22	36,36,36,36	0
56	MG	CE	202	1/1	0.93	0.10	68,68,68,68	0
56	MG	CF	3001	1/1	0.93	0.11	45,45,45,45	0
56	MG	CJ	5001	1/1	0.93	0.07	60,60,60,60	0
56	MG	CK	3001	1/1	0.93	0.14	50,50,50,50	0
56	MG	CX	101	1/1	0.93	0.18	48,48,48,48	0
56	MG	DA	3365	1/1	0.93	0.07	29,29,29,29	0
56	MG	AA	3066	1/1	0.93	0.22	46,46,46,46	0
56	MG	AE	3001	1/1	0.93	0.06	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	BA	3261	1/1	0.93	0.15	53,53,53,53	0
56	MG	CA	3015	1/1	0.93	0.10	43,43,43,43	0
56	MG	BA	3416	1/1	0.93	0.12	64,64,64,64	0
56	MG	DA	3384	1/1	0.93	0.16	52,52,52,52	0
56	MG	BA	3088	1/1	0.93	0.09	42,42,42,42	0
56	MG	DA	3392	1/1	0.93	0.09	54,54,54,54	0
56	MG	DA	3025	1/1	0.93	0.09	41,41,41,41	0
56	MG	BA	3425	1/1	0.93	0.16	53,53,53,53	0
56	MG	AA	3039	1/1	0.93	0.07	45,45,45,45	0
56	MG	DA	3033	1/1	0.93	0.15	37,37,37,37	0
56	MG	DA	3408	1/1	0.93	0.11	28,28,28,28	0
56	MG	DA	3039	1/1	0.93	0.24	51,51,51,51	0
56	MG	DA	3044	1/1	0.93	0.05	47,47,47,47	0
56	MG	DA	3414	1/1	0.93	0.07	42,42,42,42	0
56	MG	DA	3047	1/1	0.93	0.17	41,41,41,41	0
56	MG	BA	3288	1/1	0.93	0.11	48,48,48,48	0
56	MG	CA	3028	1/1	0.93	0.07	52,52,52,52	0
56	MG	DA	3423	1/1	0.93	0.09	40,40,40,40	0
56	MG	CA	3029	1/1	0.93	0.18	48,48,48,48	0
56	MG	DA	3065	1/1	0.93	0.22	49,49,49,49	0
56	MG	CA	3032	1/1	0.93	0.12	68,68,68,68	0
56	MG	BA	3586	1/1	0.93	0.23	45,45,45,45	0
56	MG	BA	3588	1/1	0.93	0.12	51,51,51,51	0
56	MG	BA	3441	1/1	0.93	0.08	44,44,44,44	0
56	MG	DA	3441	1/1	0.93	0.21	45,45,45,45	0
56	MG	BA	3093	1/1	0.93	0.08	40,40,40,40	0
56	MG	DA	3444	1/1	0.93	0.20	53,53,53,53	0
56	MG	BA	3595	1/1	0.93	0.09	47,47,47,47	0
56	MG	CA	3043	1/1	0.93	0.16	60,60,60,60	0
56	MG	DA	3450	1/1	0.93	0.10	37,37,37,37	0
56	MG	DA	3089	1/1	0.93	0.20	33,33,33,33	0
56	MG	DA	3459	1/1	0.93	0.18	38,38,38,38	0
56	MG	CA	3044	1/1	0.93	0.13	56,56,56,56	0
56	MG	DA	3091	1/1	0.93	0.12	45,45,45,45	0
56	MG	DA	3469	1/1	0.93	0.16	33,33,33,33	0
56	MG	BA	3447	1/1	0.93	0.15	55,55,55,55	0
56	MG	DA	3472	1/1	0.93	0.08	53,53,53,53	0
56	MG	DA	3096	1/1	0.93	0.06	29,29,29,29	0
56	MG	DA	3097	1/1	0.93	0.07	46,46,46,46	0
56	MG	BA	3597	1/1	0.93	0.11	43,43,43,43	0
56	MG	AK	3001	1/1	0.93	0.15	43,43,43,43	0
56	MG	BA	3298	1/1	0.93	0.07	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DA	3106	1/1	0.93	0.06	43,43,43,43	0
56	MG	DA	3481	1/1	0.93	0.07	41,41,41,41	0
56	MG	CA	3057	1/1	0.93	0.12	41,41,41,41	0
56	MG	AX	3002	1/1	0.93	0.12	56,56,56,56	0
56	MG	BA	3472	1/1	0.93	0.13	34,34,34,34	0
56	MG	BA	3106	1/1	0.93	0.11	40,40,40,40	0
56	MG	DA	3488	1/1	0.93	0.08	41,41,41,41	0
56	MG	AX	3007	1/1	0.93	0.18	60,60,60,60	0
56	MG	AA	3128	1/1	0.93	0.15	57,57,57,57	0
56	MG	AA	3131	1/1	0.93	0.10	55,55,55,55	0
56	MG	DA	3132	1/1	0.93	0.05	35,35,35,35	0
56	MG	BA	3615	1/1	0.93	0.10	42,42,42,42	0
56	MG	DA	3145	1/1	0.93	0.04	31,31,31,31	0
56	MG	BA	3616	1/1	0.93	0.10	34,34,34,34	0
56	MG	AA	3136	1/1	0.93	0.13	56,56,56,56	0
56	MG	DA	3155	1/1	0.93	0.24	45,45,45,45	0
56	MG	DA	3158	1/1	0.93	0.15	36,36,36,36	0
56	MG	BA	3016	1/1	0.93	0.24	50,50,50,50	0
56	MG	AA	3111	1/1	0.93	0.20	45,45,45,45	0
56	MG	AA	3170	1/1	0.93	0.12	54,54,54,54	0
56	MG	BA	3165	1/1	0.93	0.25	43,43,43,43	0
56	MG	BA	3334	1/1	0.93	0.10	32,32,32,32	0
56	MG	DA	3187	1/1	0.93	0.08	46,46,46,46	0
56	MG	DA	3534	1/1	0.93	0.12	54,54,54,54	0
56	MG	DA	3535	1/1	0.93	0.10	22,22,22,22	0
56	MG	BA	3028	1/1	0.93	0.08	41,41,41,41	0
56	MG	BA	3172	1/1	0.93	0.17	54,54,54,54	0
56	MG	DA	3195	1/1	0.93	0.10	38,38,38,38	0
56	MG	BA	3191	1/1	0.93	0.11	33,33,33,33	0
56	MG	AA	3147	1/1	0.93	0.09	67,67,67,67	0
56	MG	BA	3638	1/1	0.93	0.10	32,32,32,32	0
56	MG	BA	3517	1/1	0.93	0.12	40,40,40,40	0
56	MG	DA	3223	1/1	0.93	0.17	47,47,47,47	0
56	MG	DA	3559	1/1	0.93	0.10	55,55,55,55	0
56	MG	DA	3230	1/1	0.93	0.14	41,41,41,41	0
56	MG	DA	3232	1/1	0.93	0.08	38,38,38,38	0
56	MG	BA	3199	1/1	0.93	0.12	32,32,32,32	0
56	MG	BA	3673	1/1	0.93	0.10	37,37,37,37	0
56	MG	AA	3148	1/1	0.93	0.07	56,56,56,56	0
56	MG	DA	3569	1/1	0.93	0.10	55,55,55,55	0
56	MG	DA	3245	1/1	0.93	0.19	46,46,46,46	0
56	MG	BA	3532	1/1	0.93	0.08	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	DA	3249	1/1	0.93	0.11	34,34,34,34	0
56	MG	DA	3582	1/1	0.93	0.14	38,38,38,38	0
56	MG	CA	3110	1/1	0.93	0.13	64,64,64,64	0
56	MG	BB	3004	1/1	0.93	0.11	49,49,49,49	0
56	MG	DA	3587	1/1	0.93	0.17	53,53,53,53	0
56	MG	AA	3059	1/1	0.93	0.19	54,54,54,54	0
56	MG	DA	3593	1/1	0.93	0.13	51,51,51,51	0
56	MG	DA	3259	1/1	0.93	0.17	42,42,42,42	0
56	MG	DA	3260	1/1	0.93	0.16	36,36,36,36	0
56	MG	DA	3261	1/1	0.93	0.15	49,49,49,49	0
56	MG	BB	3006	1/1	0.93	0.09	49,49,49,49	0
56	MG	AA	3051	1/1	0.93	0.17	49,49,49,49	0
56	MG	DB	3010	1/1	0.93	0.23	60,60,60,60	0
56	MG	BA	3220	1/1	0.93	0.11	31,31,31,31	0
56	MG	AA	3020	1/1	0.93	0.07	49,49,49,49	0
56	MG	DA	3273	1/1	0.93	0.11	31,31,31,31	0
56	MG	CA	3122	1/1	0.93	0.19	54,54,54,54	0
56	MG	AA	3183	1/1	0.93	0.20	55,55,55,55	0
56	MG	BE	305	1/1	0.93	0.11	51,51,51,51	0
56	MG	DT	5001	1/1	0.93	0.08	42,42,42,42	0
56	MG	BF	303	1/1	0.93	0.11	20,20,20,20	0
56	MG	BA	3554	1/1	0.93	0.14	47,47,47,47	0
56	MG	BA	3234	1/1	0.93	0.20	57,57,57,57	0
56	MG	BA	3559	1/1	0.93	0.16	52,52,52,52	0
56	MG	CA	3109	1/1	0.94	0.13	50,50,50,50	0
56	MG	BA	3087	1/1	0.94	0.06	36,36,36,36	0
56	MG	CA	3112	1/1	0.94	0.17	55,55,55,55	0
56	MG	BA	3260	1/1	0.94	0.15	49,49,49,49	0
56	MG	BA	3471	1/1	0.94	0.14	35,35,35,35	0
56	MG	DA	3281	1/1	0.94	0.08	56,56,56,56	0
56	MG	DA	3288	1/1	0.94	0.12	64,64,64,64	0
56	MG	CA	3116	1/1	0.94	0.14	59,59,59,59	0
56	MG	CA	3117	1/1	0.94	0.18	42,42,42,42	0
56	MG	AX	3006	1/1	0.94	0.10	54,54,54,54	0
56	MG	DA	3306	1/1	0.94	0.06	38,38,38,38	0
56	MG	AA	3166	1/1	0.94	0.11	53,53,53,53	0
56	MG	BA	3635	1/1	0.94	0.13	63,63,63,63	0
56	MG	DA	3310	1/1	0.94	0.07	41,41,41,41	0
56	MG	DA	3316	1/1	0.94	0.17	57,57,57,57	0
56	MG	DA	3320	1/1	0.94	0.08	46,46,46,46	0
56	MG	BA	3478	1/1	0.94	0.08	47,47,47,47	0
56	MG	BA	3266	1/1	0.94	0.15	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	BA	3092	1/1	0.94	0.15	44,44,44,44	0
56	MG	BA	3645	1/1	0.94	0.07	66,66,66,66	0
56	MG	BA	3649	1/1	0.94	0.10	50,50,50,50	0
56	MG	BA	3652	1/1	0.94	0.17	49,49,49,49	0
56	MG	DA	3330	1/1	0.94	0.10	42,42,42,42	0
56	MG	BA	3654	1/1	0.94	0.21	64,64,64,64	0
56	MG	DA	3338	1/1	0.94	0.10	36,36,36,36	0
56	MG	BA	3667	1/1	0.94	0.34	38,38,38,38	0
56	MG	BA	3484	1/1	0.94	0.10	46,46,46,46	0
56	MG	BA	3283	1/1	0.94	0.16	57,57,57,57	0
56	MG	BA	3491	1/1	0.94	0.11	39,39,39,39	0
56	MG	BA	3493	1/1	0.94	0.09	40,40,40,40	0
56	MG	BA	3494	1/1	0.94	0.15	34,34,34,34	0
56	MG	BA	3285	1/1	0.94	0.12	48,48,48,48	0
56	MG	AA	3047	1/1	0.94	0.14	45,45,45,45	0
56	MG	AA	3074	1/1	0.94	0.17	38,38,38,38	0
56	MG	AA	3026	1/1	0.94	0.13	40,40,40,40	0
56	MG	BB	3017	1/1	0.94	0.09	40,40,40,40	0
56	MG	BA	3500	1/1	0.94	0.09	35,35,35,35	0
56	MG	BA	3101	1/1	0.94	0.07	30,30,30,30	0
56	MG	BE	306	1/1	0.94	0.07	32,32,32,32	0
56	MG	AA	3017	1/1	0.94	0.13	63,63,63,63	0
56	MG	BF	304	1/1	0.94	0.10	37,37,37,37	0
56	MG	BF	305	1/1	0.94	0.17	61,61,61,61	0
56	MG	DA	3003	1/1	0.94	0.24	47,47,47,47	0
56	MG	BG	3002	1/1	0.94	0.07	27,27,27,27	0
56	MG	DA	3393	1/1	0.94	0.06	48,48,48,48	0
56	MG	DA	3396	1/1	0.94	0.07	45,45,45,45	0
56	MG	AA	3081	1/1	0.94	0.13	44,44,44,44	0
56	MG	AA	3178	1/1	0.94	0.12	62,62,62,62	0
56	MG	BA	3308	1/1	0.94	0.12	52,52,52,52	0
56	MG	BP	201	1/1	0.94	0.18	36,36,36,36	0
56	MG	BP	203	1/1	0.94	0.13	47,47,47,47	0
56	MG	BA	3116	1/1	0.94	0.07	50,50,50,50	0
56	MG	DA	3410	1/1	0.94	0.21	64,64,64,64	0
56	MG	BA	3311	1/1	0.94	0.09	39,39,39,39	0
56	MG	DA	3030	1/1	0.94	0.12	30,30,30,30	0
56	MG	BA	3117	1/1	0.94	0.22	40,40,40,40	0
56	MG	BX	102	1/1	0.94	0.09	38,38,38,38	0
56	MG	DA	3419	1/1	0.94	0.15	59,59,59,59	0
56	MG	AA	3053	1/1	0.94	0.16	50,50,50,50	0
56	MG	DA	3421	1/1	0.94	0.10	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	BA	3527	1/1	0.94	0.09	40,40,40,40	0
56	MG	AA	3043	1/1	0.94	0.08	53,53,53,53	0
56	MG	B0	101	1/1	0.94	0.12	71,71,71,71	0
56	MG	B0	102	1/1	0.94	0.11	42,42,42,42	0
56	MG	DA	3431	1/1	0.94	0.13	61,61,61,61	0
56	MG	DA	3056	1/1	0.94	0.06	36,36,36,36	0
56	MG	DA	3434	1/1	0.94	0.15	41,41,41,41	0
56	MG	DA	3435	1/1	0.94	0.14	33,33,33,33	0
56	MG	BA	3126	1/1	0.94	0.13	45,45,45,45	0
56	MG	DA	3064	1/1	0.94	0.12	48,48,48,48	0
56	MG	BA	3543	1/1	0.94	0.12	47,47,47,47	0
56	MG	BA	3040	1/1	0.94	0.10	43,43,43,43	0
56	MG	BA	3136	1/1	0.94	0.07	44,44,44,44	0
56	MG	AA	3087	1/1	0.94	0.07	62,62,62,62	0
56	MG	DA	3071	1/1	0.94	0.08	36,36,36,36	0
56	MG	BA	3338	1/1	0.94	0.06	48,48,48,48	0
56	MG	DA	3452	1/1	0.94	0.14	56,56,56,56	0
56	MG	AA	3044	1/1	0.94	0.25	50,50,50,50	0
56	MG	DA	3458	1/1	0.94	0.15	34,34,34,34	0
56	MG	DA	3082	1/1	0.94	0.33	58,58,58,58	0
56	MG	DA	3460	1/1	0.94	0.08	50,50,50,50	0
56	MG	BA	3145	1/1	0.94	0.09	30,30,30,30	0
56	MG	DA	3466	1/1	0.94	0.07	38,38,38,38	0
56	MG	BA	3558	1/1	0.94	0.12	59,59,59,59	0
56	MG	BA	3344	1/1	0.94	0.09	35,35,35,35	0
56	MG	BA	3153	1/1	0.94	0.14	39,39,39,39	0
56	MG	BA	3164	1/1	0.94	0.08	37,37,37,37	0
56	MG	BA	3348	1/1	0.94	0.07	31,31,31,31	0
56	MG	DA	3093	1/1	0.94	0.11	46,46,46,46	0
56	MG	AA	3034	1/1	0.94	0.30	54,54,54,54	0
56	MG	CA	3026	1/1	0.94	0.19	44,44,44,44	0
56	MG	BA	3048	1/1	0.94	0.13	47,47,47,47	0
56	MG	BA	3050	1/1	0.94	0.15	44,44,44,44	0
56	MG	BA	3177	1/1	0.94	0.08	44,44,44,44	0
56	MG	DA	3105	1/1	0.94	0.05	36,36,36,36	0
56	MG	BA	3183	1/1	0.94	0.16	35,35,35,35	0
56	MG	BA	3186	1/1	0.94	0.12	39,39,39,39	0
56	MG	DA	3486	1/1	0.94	0.16	37,37,37,37	0
56	MG	BA	3188	1/1	0.94	0.13	39,39,39,39	0
56	MG	BA	3393	1/1	0.94	0.09	49,49,49,49	0
56	MG	DA	3492	1/1	0.94	0.09	44,44,44,44	0
56	MG	CA	3039	1/1	0.94	0.19	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	BA	3394	1/1	0.94	0.15	35,35,35,35	0
56	MG	AA	3069	1/1	0.94	0.15	50,50,50,50	0
56	MG	BA	3396	1/1	0.94	0.12	38,38,38,38	0
56	MG	DA	3131	1/1	0.94	0.10	46,46,46,46	0
56	MG	BA	3058	1/1	0.94	0.11	43,43,43,43	0
56	MG	BA	3400	1/1	0.94	0.18	45,45,45,45	0
56	MG	DA	3137	1/1	0.94	0.06	37,37,37,37	0
56	MG	AA	3157	1/1	0.94	0.08	55,55,55,55	0
56	MG	CA	3053	1/1	0.94	0.14	44,44,44,44	0
56	MG	DA	3514	1/1	0.94	0.07	40,40,40,40	0
56	MG	BA	3587	1/1	0.94	0.07	42,42,42,42	0
56	MG	DA	3152	1/1	0.94	0.11	34,34,34,34	0
56	MG	AD	502	1/1	0.94	0.27	55,55,55,55	0
56	MG	DA	3524	1/1	0.94	0.11	51,51,51,51	0
56	MG	DA	3525	1/1	0.94	0.06	44,44,44,44	0
56	MG	BA	3590	1/1	0.94	0.16	55,55,55,55	0
56	MG	DA	3529	1/1	0.94	0.13	41,41,41,41	0
56	MG	CA	3060	1/1	0.94	0.23	50,50,50,50	0
56	MG	BA	3210	1/1	0.94	0.24	24,24,24,24	0
56	MG	DA	3164	1/1	0.94	0.12	36,36,36,36	0
56	MG	DA	3165	1/1	0.94	0.14	34,34,34,34	0
56	MG	CA	3063	1/1	0.94	0.35	53,53,53,53	0
56	MG	DA	3171	1/1	0.94	0.13	51,51,51,51	0
56	MG	DA	3172	1/1	0.94	0.07	35,35,35,35	0
56	MG	DA	3543	1/1	0.94	0.11	63,63,63,63	0
56	MG	CA	3064	1/1	0.94	0.10	60,60,60,60	0
56	MG	BA	3066	1/1	0.94	0.12	48,48,48,48	0
56	MG	DA	3548	1/1	0.94	0.16	40,40,40,40	0
56	MG	DA	3549	1/1	0.94	0.07	41,41,41,41	0
56	MG	DA	3183	1/1	0.94	0.07	37,37,37,37	0
56	MG	BA	3070	1/1	0.94	0.09	30,30,30,30	0
56	MG	DA	3554	1/1	0.94	0.07	68,68,68,68	0
56	MG	BA	3217	1/1	0.94	0.19	29,29,29,29	0
56	MG	AA	3122	1/1	0.94	0.09	58,58,58,58	0
56	MG	DA	3560	1/1	0.94	0.11	51,51,51,51	0
56	MG	BA	3599	1/1	0.94	0.06	46,46,46,46	0
56	MG	DA	3198	1/1	0.94	0.11	54,54,54,54	0
56	MG	DA	3565	1/1	0.94	0.10	51,51,51,51	0
56	MG	DA	3199	1/1	0.94	0.07	52,52,52,52	0
56	MG	AA	3096	1/1	0.94	0.15	53,53,53,53	0
56	MG	BA	3422	1/1	0.94	0.10	46,46,46,46	0
56	MG	AA	3097	1/1	0.94	0.13	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	3098	1/1	0.94	0.21	48,48,48,48	0
56	MG	DA	3576	1/1	0.94	0.10	36,36,36,36	0
56	MG	DA	3217	1/1	0.94	0.06	39,39,39,39	0
56	MG	DA	3218	1/1	0.94	0.07	33,33,33,33	0
56	MG	DA	3581	1/1	0.94	0.10	53,53,53,53	0
56	MG	BA	3426	1/1	0.94	0.07	43,43,43,43	0
56	MG	DA	3226	1/1	0.94	0.07	27,27,27,27	0
56	MG	BA	3607	1/1	0.94	0.19	51,51,51,51	0
56	MG	BA	3079	1/1	0.94	0.05	46,46,46,46	0
56	MG	DA	3233	1/1	0.94	0.21	36,36,36,36	0
56	MG	DA	3234	1/1	0.94	0.10	45,45,45,45	0
56	MG	DA	3594	1/1	0.94	0.18	48,48,48,48	0
56	MG	DB	3002	1/1	0.94	0.12	50,50,50,50	0
56	MG	DA	3235	1/1	0.94	0.14	42,42,42,42	0
56	MG	BA	3429	1/1	0.94	0.13	41,41,41,41	0
56	MG	BA	3430	1/1	0.94	0.09	29,29,29,29	0
56	MG	DA	3240	1/1	0.94	0.12	54,54,54,54	0
56	MG	CA	3089	1/1	0.94	0.12	40,40,40,40	0
56	MG	BA	3081	1/1	0.94	0.14	42,42,42,42	0
56	MG	BA	3239	1/1	0.94	0.21	52,52,52,52	0
56	MG	CA	3093	1/1	0.94	0.21	72,72,72,72	0
56	MG	DE	3002	1/1	0.94	0.10	35,35,35,35	0
56	MG	CA	3094	1/1	0.94	0.16	67,67,67,67	0
56	MG	BA	3082	1/1	0.94	0.10	47,47,47,47	0
56	MG	CA	3097	1/1	0.94	0.13	67,67,67,67	0
56	MG	DQ	3001	1/1	0.94	0.06	48,48,48,48	0
56	MG	BA	3446	1/1	0.94	0.12	61,61,61,61	0
56	MG	BA	3621	1/1	0.94	0.08	30,30,30,30	0
56	MG	DV	3002	1/1	0.94	0.06	43,43,43,43	0
56	MG	AX	3003	1/1	0.94	0.19	50,50,50,50	0
56	MG	BA	3086	1/1	0.94	0.15	39,39,39,39	0
56	MG	DA	3264	1/1	0.94	0.15	47,47,47,47	0
56	MG	BA	3463	1/1	0.94	0.06	43,43,43,43	0
56	MG	BB	3014	1/1	0.95	0.08	35,35,35,35	0
56	MG	BA	3327	1/1	0.95	0.06	44,44,44,44	0
56	MG	BA	3166	1/1	0.95	0.06	35,35,35,35	0
56	MG	DA	3305	1/1	0.95	0.09	30,30,30,30	0
56	MG	AA	3134	1/1	0.95	0.22	52,52,52,52	0
56	MG	BE	303	1/1	0.95	0.15	41,41,41,41	0
56	MG	CA	3142	1/1	0.95	0.12	42,42,42,42	0
56	MG	CA	3143	1/1	0.95	0.13	42,42,42,42	0
56	MG	CA	3144	1/1	0.95	0.12	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	3330	1/1	0.95	0.16	44,44,44,44	0
56	MG	BA	3518	1/1	0.95	0.19	41,41,41,41	0
56	MG	AA	3021	1/1	0.95	0.13	41,41,41,41	0
56	MG	BA	3332	1/1	0.95	0.09	61,61,61,61	0
56	MG	BA	3526	1/1	0.95	0.13	25,25,25,25	0
56	MG	CE	201	1/1	0.95	0.14	52,52,52,52	0
56	MG	BA	3173	1/1	0.95	0.17	45,45,45,45	0
56	MG	BA	3174	1/1	0.95	0.04	29,29,29,29	0
56	MG	DA	3333	1/1	0.95	0.07	38,38,38,38	0
56	MG	BA	3533	1/1	0.95	0.08	45,45,45,45	0
56	MG	BA	3176	1/1	0.95	0.08	47,47,47,47	0
56	MG	BA	3537	1/1	0.95	0.21	58,58,58,58	0
56	MG	BA	3539	1/1	0.95	0.12	58,58,58,58	0
56	MG	BA	3540	1/1	0.95	0.13	46,46,46,46	0
56	MG	AA	3009	1/1	0.95	0.09	54,54,54,54	0
56	MG	DA	3349	1/1	0.95	0.13	46,46,46,46	0
56	MG	BV	202	1/1	0.95	0.08	36,36,36,36	0
56	MG	DA	3018	1/1	0.95	0.10	39,39,39,39	0
56	MG	DA	3353	1/1	0.95	0.06	32,32,32,32	0
56	MG	BA	3180	1/1	0.95	0.09	33,33,33,33	0
56	MG	DA	3356	1/1	0.95	0.06	31,31,31,31	0
56	MG	DA	3357	1/1	0.95	0.07	33,33,33,33	0
56	MG	BW	3004	1/1	0.95	0.13	30,30,30,30	0
56	MG	BA	3078	1/1	0.95	0.13	53,53,53,53	0
56	MG	BA	3010	1/1	0.95	0.07	33,33,33,33	0
56	MG	BA	3187	1/1	0.95	0.12	37,37,37,37	0
56	MG	BA	3012	1/1	0.95	0.09	39,39,39,39	0
56	MG	DA	3368	1/1	0.95	0.05	25,25,25,25	0
56	MG	DA	3369	1/1	0.95	0.11	45,45,45,45	0
56	MG	BA	3556	1/1	0.95	0.09	41,41,41,41	0
56	MG	BA	3352	1/1	0.95	0.07	32,32,32,32	0
56	MG	BA	3356	1/1	0.95	0.10	46,46,46,46	0
56	MG	DA	3041	1/1	0.95	0.06	35,35,35,35	0
56	MG	DA	3382	1/1	0.95	0.14	50,50,50,50	0
56	MG	DA	3043	1/1	0.95	0.08	30,30,30,30	0
56	MG	B5	503	1/1	0.95	0.20	47,47,47,47	0
56	MG	CA	3001	1/1	0.95	0.08	72,72,72,72	0
56	MG	BA	3189	1/1	0.95	0.18	26,26,26,26	0
56	MG	DA	3394	1/1	0.95	0.07	41,41,41,41	0
56	MG	AA	3174	1/1	0.95	0.12	55,55,55,55	0
56	MG	BA	3563	1/1	0.95	0.14	47,47,47,47	0
56	MG	BA	3362	1/1	0.95	0.08	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DA	3059	1/1	0.95	0.07	33,33,33,33	0
56	MG	DA	3405	1/1	0.95	0.16	45,45,45,45	0
56	MG	DA	3062	1/1	0.95	0.19	42,42,42,42	0
56	MG	BA	3365	1/1	0.95	0.12	41,41,41,41	0
56	MG	AA	3080	1/1	0.95	0.20	39,39,39,39	0
56	MG	BA	3018	1/1	0.95	0.15	47,47,47,47	0
56	MG	BA	3374	1/1	0.95	0.07	29,29,29,29	0
56	MG	DA	3069	1/1	0.95	0.06	35,35,35,35	0
56	MG	DA	3415	1/1	0.95	0.10	40,40,40,40	0
56	MG	BA	3572	1/1	0.95	0.07	59,59,59,59	0
56	MG	DA	3417	1/1	0.95	0.10	40,40,40,40	0
56	MG	BA	3376	1/1	0.95	0.09	39,39,39,39	0
56	MG	DA	3073	1/1	0.95	0.16	51,51,51,51	0
56	MG	AA	3068	1/1	0.95	0.11	31,31,31,31	0
56	MG	BA	3384	1/1	0.95	0.07	28,28,28,28	0
56	MG	DA	3078	1/1	0.95	0.15	46,46,46,46	0
56	MG	CA	3024	1/1	0.95	0.10	64,64,64,64	0
56	MG	BA	3021	1/1	0.95	0.09	37,37,37,37	0
56	MG	BA	3390	1/1	0.95	0.10	47,47,47,47	0
56	MG	DA	3430	1/1	0.95	0.15	30,30,30,30	0
56	MG	CA	3027	1/1	0.95	0.24	64,64,64,64	0
56	MG	AA	3114	1/1	0.95	0.15	56,56,56,56	0
56	MG	BA	3581	1/1	0.95	0.05	34,34,34,34	0
56	MG	BA	3026	1/1	0.95	0.24	46,46,46,46	0
56	MG	AA	3150	1/1	0.95	0.20	51,51,51,51	0
56	MG	BA	3218	1/1	0.95	0.19	38,38,38,38	0
56	MG	AA	3116	1/1	0.95	0.13	51,51,51,51	0
56	MG	BA	3222	1/1	0.95	0.12	45,45,45,45	0
56	MG	BA	3223	1/1	0.95	0.19	51,51,51,51	0
56	MG	CA	3040	1/1	0.95	0.24	52,52,52,52	0
56	MG	BA	3224	1/1	0.95	0.12	45,45,45,45	0
56	MG	AA	3182	1/1	0.95	0.19	57,57,57,57	0
56	MG	BA	3591	1/1	0.95	0.08	36,36,36,36	0
56	MG	CA	3045	1/1	0.95	0.14	52,52,52,52	0
56	MG	DA	3456	1/1	0.95	0.08	34,34,34,34	0
56	MG	DA	3111	1/1	0.95	0.21	39,39,39,39	0
56	MG	CA	3046	1/1	0.95	0.07	41,41,41,41	0
56	MG	DA	3114	1/1	0.95	0.05	37,37,37,37	0
56	MG	CA	3047	1/1	0.95	0.21	51,51,51,51	0
56	MG	DA	3120	1/1	0.95	0.15	33,33,33,33	0
56	MG	BA	3592	1/1	0.95	0.08	52,52,52,52	0
56	MG	DA	3468	1/1	0.95	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	DA	3123	1/1	0.95	0.07	51,51,51,51	0
56	MG	BA	3042	1/1	0.95	0.08	33,33,33,33	0
56	MG	DA	3471	1/1	0.95	0.07	50,50,50,50	0
56	MG	DA	3126	1/1	0.95	0.16	42,42,42,42	0
56	MG	BA	3232	1/1	0.95	0.06	41,41,41,41	0
56	MG	DA	3128	1/1	0.95	0.07	42,42,42,42	0
56	MG	DA	3129	1/1	0.95	0.18	54,54,54,54	0
56	MG	BA	3102	1/1	0.95	0.08	49,49,49,49	0
56	MG	AA	3083	1/1	0.95	0.12	59,59,59,59	0
56	MG	BA	3107	1/1	0.95	0.05	21,21,21,21	0
56	MG	DA	3480	1/1	0.95	0.06	32,32,32,32	0
56	MG	CA	3058	1/1	0.95	0.17	56,56,56,56	0
56	MG	DA	3141	1/1	0.95	0.05	42,42,42,42	0
56	MG	DA	3144	1/1	0.95	0.06	38,38,38,38	0
56	MG	BA	3108	1/1	0.95	0.08	38,38,38,38	0
56	MG	DA	3146	1/1	0.95	0.08	34,34,34,34	0
56	MG	BA	3110	1/1	0.95	0.11	31,31,31,31	0
56	MG	BA	3242	1/1	0.95	0.23	46,46,46,46	0
56	MG	DA	3491	1/1	0.95	0.06	40,40,40,40	0
56	MG	DA	3151	1/1	0.95	0.07	34,34,34,34	0
56	MG	AA	3120	1/1	0.95	0.08	47,47,47,47	0
56	MG	AA	3100	1/1	0.95	0.14	35,35,35,35	0
56	MG	DA	3156	1/1	0.95	0.07	38,38,38,38	0
56	MG	BA	3047	1/1	0.95	0.18	41,41,41,41	0
56	MG	BA	3256	1/1	0.95	0.24	41,41,41,41	0
56	MG	BA	3435	1/1	0.95	0.11	36,36,36,36	0
56	MG	AA	3001	1/1	0.95	0.11	57,57,57,57	0
56	MG	CA	3069	1/1	0.95	0.10	34,34,34,34	0
56	MG	AA	3123	1/1	0.95	0.15	38,38,38,38	0
56	MG	DA	3509	1/1	0.95	0.06	36,36,36,36	0
56	MG	DA	3170	1/1	0.95	0.19	38,38,38,38	0
56	MG	DA	3512	1/1	0.95	0.10	36,36,36,36	0
56	MG	BA	3051	1/1	0.95	0.14	41,41,41,41	0
56	MG	CA	3073	1/1	0.95	0.18	57,57,57,57	0
56	MG	CA	3074	1/1	0.95	0.26	48,48,48,48	0
56	MG	DA	3517	1/1	0.95	0.18	47,47,47,47	0
56	MG	CA	3076	1/1	0.95	0.22	48,48,48,48	0
56	MG	DA	3520	1/1	0.95	0.08	34,34,34,34	0
56	MG	DA	3179	1/1	0.95	0.14	20,20,20,20	0
56	MG	AA	3071	1/1	0.95	0.04	36,36,36,36	0
56	MG	DA	3185	1/1	0.95	0.06	32,32,32,32	0
56	MG	BA	3268	1/1	0.95	0.30	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	CA	3079	1/1	0.95	0.30	55,55,55,55	0
56	MG	BA	3448	1/1	0.95	0.09	42,42,42,42	0
56	MG	DA	3533	1/1	0.95	0.07	60,60,60,60	0
56	MG	DA	3193	1/1	0.95	0.17	49,49,49,49	0
56	MG	DA	3194	1/1	0.95	0.10	47,47,47,47	0
56	MG	BA	3620	1/1	0.95	0.12	41,41,41,41	0
56	MG	DA	3197	1/1	0.95	0.13	38,38,38,38	0
56	MG	DA	3540	1/1	0.95	0.15	46,46,46,46	0
56	MG	AE	3002	1/1	0.95	0.10	38,38,38,38	0
56	MG	BA	3623	1/1	0.95	0.06	48,48,48,48	0
56	MG	BA	3061	1/1	0.95	0.20	44,44,44,44	0
56	MG	DA	3204	1/1	0.95	0.06	37,37,37,37	0
56	MG	BA	3137	1/1	0.95	0.12	30,30,30,30	0
56	MG	DA	3207	1/1	0.95	0.14	39,39,39,39	0
56	MG	DA	3551	1/1	0.95	0.08	52,52,52,52	0
56	MG	BA	3286	1/1	0.95	0.10	32,32,32,32	0
56	MG	DA	3212	1/1	0.95	0.17	39,39,39,39	0
56	MG	BA	3287	1/1	0.95	0.09	46,46,46,46	0
56	MG	AA	3048	1/1	0.95	0.22	42,42,42,42	0
56	MG	CA	3092	1/1	0.95	0.15	54,54,54,54	0
56	MG	DA	3222	1/1	0.95	0.06	36,36,36,36	0
56	MG	BA	3474	1/1	0.95	0.12	53,53,53,53	0
56	MG	DA	3225	1/1	0.95	0.06	33,33,33,33	0
56	MG	AA	3014	1/1	0.95	0.16	49,49,49,49	0
56	MG	BA	3296	1/1	0.95	0.06	25,25,25,25	0
56	MG	AA	3165	1/1	0.95	0.07	43,43,43,43	0
56	MG	CA	3099	1/1	0.95	0.20	57,57,57,57	0
56	MG	CA	3101	1/1	0.95	0.14	53,53,53,53	0
56	MG	DA	3571	1/1	0.95	0.14	48,48,48,48	0
56	MG	BA	3146	1/1	0.95	0.08	31,31,31,31	0
56	MG	BA	3149	1/1	0.95	0.10	50,50,50,50	0
56	MG	DA	3577	1/1	0.95	0.12	35,35,35,35	0
56	MG	DA	3237	1/1	0.95	0.09	39,39,39,39	0
56	MG	DA	3238	1/1	0.95	0.11	42,42,42,42	0
56	MG	BA	3641	1/1	0.95	0.15	33,33,33,33	0
56	MG	BA	3486	1/1	0.95	0.14	21,21,21,21	0
56	MG	BA	3643	1/1	0.95	0.07	42,42,42,42	0
56	MG	DA	3243	1/1	0.95	0.06	50,50,50,50	0
56	MG	DA	3244	1/1	0.95	0.07	48,48,48,48	0
56	MG	BA	3644	1/1	0.95	0.07	41,41,41,41	0
56	MG	BA	3301	1/1	0.95	0.09	46,46,46,46	0
56	MG	BA	3646	1/1	0.95	0.10	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DB	3001	1/1	0.95	0.13	40,40,40,40	0
56	MG	BA	3150	1/1	0.95	0.11	32,32,32,32	0
56	MG	BA	3151	1/1	0.95	0.05	34,34,34,34	0
56	MG	DA	3256	1/1	0.95	0.06	45,45,45,45	0
56	MG	BA	3069	1/1	0.95	0.06	47,47,47,47	0
56	MG	BA	3662	1/1	0.95	0.11	36,36,36,36	0
56	MG	BA	3154	1/1	0.95	0.17	40,40,40,40	0
56	MG	BA	3671	1/1	0.95	0.12	48,48,48,48	0
56	MG	BA	3156	1/1	0.95	0.12	48,48,48,48	0
56	MG	BA	3314	1/1	0.95	0.12	36,36,36,36	0
56	MG	BA	3162	1/1	0.95	0.13	39,39,39,39	0
56	MG	DE	3003	1/1	0.95	0.11	40,40,40,40	0
56	MG	DF	301	1/1	0.95	0.20	44,44,44,44	0
56	MG	BA	3318	1/1	0.95	0.07	44,44,44,44	0
56	MG	AA	3108	1/1	0.95	0.19	54,54,54,54	0
56	MG	AA	3089	1/1	0.95	0.11	36,36,36,36	0
56	MG	DP	3001	1/1	0.95	0.11	44,44,44,44	0
56	MG	BB	3007	1/1	0.95	0.09	35,35,35,35	0
56	MG	BA	3325	1/1	0.95	0.09	42,42,42,42	0
56	MG	DA	3277	1/1	0.95	0.09	48,48,48,48	0
56	MG	BA	3509	1/1	0.95	0.12	23,23,23,23	0
56	MG	DA	3286	1/1	0.95	0.07	35,35,35,35	0
56	MG	DA	3287	1/1	0.95	0.12	38,38,38,38	0
56	MG	BB	3013	1/1	0.95	0.15	57,57,57,57	0
56	MG	D8	5001	1/1	0.95	0.14	50,50,50,50	0
56	MG	DA	3292	1/1	0.95	0.12	45,45,45,45	0
56	MG	DA	3255	1/1	0.96	0.22	32,32,32,32	0
56	MG	BA	3637	1/1	0.96	0.13	24,24,24,24	0
56	MG	AA	3104	1/1	0.96	0.09	56,56,56,56	0
56	MG	CA	3115	1/1	0.96	0.06	62,62,62,62	0
56	MG	BA	3267	1/1	0.96	0.07	40,40,40,40	0
56	MG	BA	3142	1/1	0.96	0.05	40,40,40,40	0
56	MG	BA	3450	1/1	0.96	0.06	45,45,45,45	0
56	MG	BA	3451	1/1	0.96	0.06	48,48,48,48	0
56	MG	DA	3265	1/1	0.96	0.26	51,51,51,51	0
56	MG	DA	3266	1/1	0.96	0.07	46,46,46,46	0
56	MG	DA	3268	1/1	0.96	0.08	38,38,38,38	0
56	MG	BA	3458	1/1	0.96	0.07	60,60,60,60	0
56	MG	BA	3459	1/1	0.96	0.13	42,42,42,42	0
56	MG	BA	3460	1/1	0.96	0.06	57,57,57,57	0
56	MG	BA	3270	1/1	0.96	0.12	21,21,21,21	0
56	MG	BA	3271	1/1	0.96	0.12	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	3653	1/1	0.96	0.08	33,33,33,33	0
56	MG	BA	3277	1/1	0.96	0.12	32,32,32,32	0
56	MG	DA	3278	1/1	0.96	0.10	50,50,50,50	0
56	MG	CA	3130	1/1	0.96	0.15	57,57,57,57	0
56	MG	DA	3282	1/1	0.96	0.05	30,30,30,30	0
56	MG	DA	3285	1/1	0.96	0.12	52,52,52,52	0
56	MG	BA	3655	1/1	0.96	0.09	18,18,18,18	0
56	MG	BA	3659	1/1	0.96	0.10	28,28,28,28	0
56	MG	BA	3660	1/1	0.96	0.09	49,49,49,49	0
56	MG	DA	3291	1/1	0.96	0.07	38,38,38,38	0
56	MG	CA	3134	1/1	0.96	0.12	53,53,53,53	0
56	MG	DA	3295	1/1	0.96	0.07	61,61,61,61	0
56	MG	DA	3298	1/1	0.96	0.05	32,32,32,32	0
56	MG	CA	3135	1/1	0.96	0.23	62,62,62,62	0
56	MG	BA	3470	1/1	0.96	0.09	48,48,48,48	0
56	MG	BA	3057	1/1	0.96	0.06	38,38,38,38	0
56	MG	BA	3668	1/1	0.96	0.13	26,26,26,26	0
56	MG	BA	3280	1/1	0.96	0.12	48,48,48,48	0
56	MG	BA	3473	1/1	0.96	0.10	37,37,37,37	0
56	MG	DA	3308	1/1	0.96	0.08	29,29,29,29	0
56	MG	AA	3031	1/1	0.96	0.07	60,60,60,60	0
56	MG	BA	3284	1/1	0.96	0.12	41,41,41,41	0
56	MG	BA	3147	1/1	0.96	0.10	35,35,35,35	0
56	MG	BA	3148	1/1	0.96	0.06	25,25,25,25	0
56	MG	DA	3321	1/1	0.96	0.08	45,45,45,45	0
56	MG	DA	3322	1/1	0.96	0.07	23,23,23,23	0
56	MG	AL	201	1/1	0.96	0.05	63,63,63,63	0
56	MG	AM	3001	1/1	0.96	0.07	54,54,54,54	0
56	MG	BB	3008	1/1	0.96	0.10	21,21,21,21	0
56	MG	BA	3485	1/1	0.96	0.14	64,64,64,64	0
56	MG	CA	3153	1/1	0.96	0.11	37,37,37,37	0
56	MG	CA	3154	1/1	0.96	0.18	62,62,62,62	0
56	MG	BA	3292	1/1	0.96	0.11	43,43,43,43	0
56	MG	DA	3331	1/1	0.96	0.06	41,41,41,41	0
56	MG	DA	3332	1/1	0.96	0.06	43,43,43,43	0
56	MG	AA	3033	1/1	0.96	0.25	48,48,48,48	0
56	MG	BA	3295	1/1	0.96	0.08	61,61,61,61	0
56	MG	BA	3492	1/1	0.96	0.09	42,42,42,42	0
56	MG	BB	3016	1/1	0.96	0.05	24,24,24,24	0
56	MG	CT	3001	1/1	0.96	0.12	50,50,50,50	0
56	MG	DA	3344	1/1	0.96	0.14	31,31,31,31	0
56	MG	BA	3152	1/1	0.96	0.06	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	AA	3072	1/1	0.96	0.13	39,39,39,39	0
56	MG	BD	304	1/1	0.96	0.20	28,28,28,28	0
56	MG	AX	3005	1/1	0.96	0.25	42,42,42,42	0
56	MG	DA	3011	1/1	0.96	0.08	38,38,38,38	0
56	MG	DA	3015	1/1	0.96	0.09	41,41,41,41	0
56	MG	AA	3005	1/1	0.96	0.07	37,37,37,37	0
56	MG	BA	3157	1/1	0.96	0.13	34,34,34,34	0
56	MG	BF	301	1/1	0.96	0.10	56,56,56,56	0
56	MG	BA	3158	1/1	0.96	0.12	33,33,33,33	0
56	MG	AA	3129	1/1	0.96	0.06	35,35,35,35	0
56	MG	DA	3023	1/1	0.96	0.06	37,37,37,37	0
56	MG	DA	3024	1/1	0.96	0.12	36,36,36,36	0
56	MG	BA	3163	1/1	0.96	0.07	31,31,31,31	0
56	MG	DA	3367	1/1	0.96	0.10	47,47,47,47	0
56	MG	DA	3026	1/1	0.96	0.12	34,34,34,34	0
56	MG	DA	3027	1/1	0.96	0.07	30,30,30,30	0
56	MG	DA	3370	1/1	0.96	0.13	44,44,44,44	0
56	MG	BA	3504	1/1	0.96	0.10	39,39,39,39	0
56	MG	DA	3029	1/1	0.96	0.10	40,40,40,40	0
56	MG	AA	3130	1/1	0.96	0.10	50,50,50,50	0
56	MG	DA	3377	1/1	0.96	0.11	37,37,37,37	0
56	MG	AA	3091	1/1	0.96	0.06	36,36,36,36	0
56	MG	BA	3076	1/1	0.96	0.04	29,29,29,29	0
56	MG	DA	3034	1/1	0.96	0.21	46,46,46,46	0
56	MG	DA	3038	1/1	0.96	0.05	30,30,30,30	0
56	MG	BA	3169	1/1	0.96	0.09	39,39,39,39	0
56	MG	BA	3512	1/1	0.96	0.10	45,45,45,45	0
56	MG	BQ	201	1/1	0.96	0.14	52,52,52,52	0
56	MG	BQ	203	1/1	0.96	0.19	33,33,33,33	0
56	MG	DA	3045	1/1	0.96	0.17	48,48,48,48	0
56	MG	BU	202	1/1	0.96	0.07	40,40,40,40	0
56	MG	BU	203	1/1	0.96	0.15	32,32,32,32	0
56	MG	DA	3404	1/1	0.96	0.05	46,46,46,46	0
56	MG	DA	3051	1/1	0.96	0.07	50,50,50,50	0
56	MG	BA	3317	1/1	0.96	0.08	35,35,35,35	0
56	MG	DA	3054	1/1	0.96	0.21	45,45,45,45	0
56	MG	DA	3055	1/1	0.96	0.07	34,34,34,34	0
56	MG	BA	3514	1/1	0.96	0.10	32,32,32,32	0
56	MG	BA	3003	1/1	0.96	0.05	49,49,49,49	0
56	MG	BA	3516	1/1	0.96	0.08	43,43,43,43	0
56	MG	DA	3060	1/1	0.96	0.06	45,45,45,45	0
56	MG	BA	3319	1/1	0.96	0.12	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DA	3063	1/1	0.96	0.05	31,31,31,31	0
56	MG	BX	101	1/1	0.96	0.10	46,46,46,46	0
56	MG	BA	3005	1/1	0.96	0.06	29,29,29,29	0
56	MG	BA	3521	1/1	0.96	0.07	54,54,54,54	0
56	MG	BA	3009	1/1	0.96	0.06	34,34,34,34	0
56	MG	BA	3080	1/1	0.96	0.09	29,29,29,29	0
56	MG	BA	3525	1/1	0.96	0.07	46,46,46,46	0
56	MG	AA	3132	1/1	0.96	0.11	50,50,50,50	0
56	MG	DA	3072	1/1	0.96	0.08	33,33,33,33	0
56	MG	DA	3429	1/1	0.96	0.08	35,35,35,35	0
56	MG	AA	3133	1/1	0.96	0.06	38,38,38,38	0
56	MG	B0	105	1/1	0.96	0.08	43,43,43,43	0
56	MG	B4	502	1/1	0.96	0.05	61,61,61,61	0
56	MG	DA	3077	1/1	0.96	0.07	34,34,34,34	0
56	MG	B5	502	1/1	0.96	0.11	34,34,34,34	0
56	MG	DA	3436	1/1	0.96	0.06	27,27,27,27	0
56	MG	AA	3060	1/1	0.96	0.14	55,55,55,55	0
56	MG	BA	3182	1/1	0.96	0.13	30,30,30,30	0
56	MG	DA	3439	1/1	0.96	0.09	28,28,28,28	0
56	MG	DA	3440	1/1	0.96	0.12	52,52,52,52	0
56	MG	DA	3087	1/1	0.96	0.15	35,35,35,35	0
56	MG	AA	3135	1/1	0.96	0.07	46,46,46,46	0
56	MG	BA	3184	1/1	0.96	0.05	37,37,37,37	0
56	MG	CA	3005	1/1	0.96	0.08	42,42,42,42	0
56	MG	BA	3185	1/1	0.96	0.08	43,43,43,43	0
56	MG	DA	3447	1/1	0.96	0.07	33,33,33,33	0
56	MG	DA	3449	1/1	0.96	0.09	29,29,29,29	0
56	MG	BA	3335	1/1	0.96	0.10	40,40,40,40	0
56	MG	BA	3017	1/1	0.96	0.11	40,40,40,40	0
56	MG	DA	3094	1/1	0.96	0.09	35,35,35,35	0
56	MG	DA	3095	1/1	0.96	0.09	47,47,47,47	0
56	MG	DA	3457	1/1	0.96	0.10	38,38,38,38	0
56	MG	AA	3052	1/1	0.96	0.21	60,60,60,60	0
56	MG	AA	3175	1/1	0.96	0.19	53,53,53,53	0
56	MG	BA	3343	1/1	0.96	0.12	27,27,27,27	0
56	MG	DA	3099	1/1	0.96	0.12	37,37,37,37	0
56	MG	AA	3137	1/1	0.96	0.07	79,79,79,79	0
56	MG	DA	3101	1/1	0.96	0.08	46,46,46,46	0
56	MG	DA	3102	1/1	0.96	0.20	51,51,51,51	0
56	MG	CA	3017	1/1	0.96	0.09	41,41,41,41	0
56	MG	BA	3190	1/1	0.96	0.24	31,31,31,31	0
56	MG	BA	3555	1/1	0.96	0.08	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	BA	3346	1/1	0.96	0.09	43,43,43,43	0
56	MG	CA	3022	1/1	0.96	0.12	34,34,34,34	0
56	MG	AA	3177	1/1	0.96	0.15	32,32,32,32	0
56	MG	DA	3112	1/1	0.96	0.08	24,24,24,24	0
56	MG	AA	3138	1/1	0.96	0.08	50,50,50,50	0
56	MG	BA	3349	1/1	0.96	0.10	46,46,46,46	0
56	MG	DA	3115	1/1	0.96	0.08	36,36,36,36	0
56	MG	DA	3117	1/1	0.96	0.16	43,43,43,43	0
56	MG	BA	3560	1/1	0.96	0.13	55,55,55,55	0
56	MG	BA	3195	1/1	0.96	0.14	47,47,47,47	0
56	MG	BA	3562	1/1	0.96	0.05	46,46,46,46	0
56	MG	DA	3122	1/1	0.96	0.14	45,45,45,45	0
56	MG	BA	3095	1/1	0.96	0.04	33,33,33,33	0
56	MG	BA	3564	1/1	0.96	0.10	29,29,29,29	0
56	MG	BA	3202	1/1	0.96	0.06	30,30,30,30	0
56	MG	BA	3205	1/1	0.96	0.14	40,40,40,40	0
56	MG	BA	3358	1/1	0.96	0.10	39,39,39,39	0
56	MG	DA	3493	1/1	0.96	0.12	45,45,45,45	0
56	MG	CA	3038	1/1	0.96	0.14	44,44,44,44	0
56	MG	DA	3495	1/1	0.96	0.12	45,45,45,45	0
56	MG	BA	3096	1/1	0.96	0.15	44,44,44,44	0
56	MG	DA	3498	1/1	0.96	0.07	48,48,48,48	0
56	MG	DA	3499	1/1	0.96	0.07	45,45,45,45	0
56	MG	BA	3361	1/1	0.96	0.09	45,45,45,45	0
56	MG	BA	3027	1/1	0.96	0.07	28,28,28,28	0
56	MG	DA	3136	1/1	0.96	0.13	36,36,36,36	0
56	MG	CA	3042	1/1	0.96	0.16	56,56,56,56	0
56	MG	DA	3505	1/1	0.96	0.05	44,44,44,44	0
56	MG	DA	3139	1/1	0.96	0.20	39,39,39,39	0
56	MG	BA	3573	1/1	0.96	0.14	44,44,44,44	0
56	MG	AA	3141	1/1	0.96	0.09	47,47,47,47	0
56	MG	BA	3031	1/1	0.96	0.24	46,46,46,46	0
56	MG	BA	3105	1/1	0.96	0.07	32,32,32,32	0
56	MG	BA	3577	1/1	0.96	0.13	57,57,57,57	0
56	MG	BA	3034	1/1	0.96	0.16	24,24,24,24	0
56	MG	BA	3375	1/1	0.96	0.21	51,51,51,51	0
56	MG	BA	3219	1/1	0.96	0.05	20,20,20,20	0
56	MG	AA	3094	1/1	0.96	0.19	49,49,49,49	0
56	MG	CA	3054	1/1	0.96	0.13	44,44,44,44	0
56	MG	BA	3383	1/1	0.96	0.06	33,33,33,33	0
56	MG	DA	3521	1/1	0.96	0.22	51,51,51,51	0
56	MG	DA	3523	1/1	0.96	0.08	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	3159	1/1	0.96	0.12	31,31,31,31	0
56	MG	DA	3161	1/1	0.96	0.07	24,24,24,24	0
56	MG	CA	3056	1/1	0.96	0.19	40,40,40,40	0
56	MG	DA	3527	1/1	0.96	0.13	43,43,43,43	0
56	MG	BA	3221	1/1	0.96	0.18	41,41,41,41	0
56	MG	AA	3144	1/1	0.96	0.15	42,42,42,42	0
56	MG	BA	3388	1/1	0.96	0.04	54,54,54,54	0
56	MG	BA	3389	1/1	0.96	0.17	35,35,35,35	0
56	MG	DA	3167	1/1	0.96	0.06	51,51,51,51	0
56	MG	BA	3041	1/1	0.96	0.10	42,42,42,42	0
56	MG	DA	3536	1/1	0.96	0.06	56,56,56,56	0
56	MG	DA	3537	1/1	0.96	0.12	47,47,47,47	0
56	MG	BA	3392	1/1	0.96	0.10	41,41,41,41	0
56	MG	AA	3146	1/1	0.96	0.11	41,41,41,41	0
56	MG	BA	3226	1/1	0.96	0.25	32,32,32,32	0
56	MG	DA	3174	1/1	0.96	0.09	44,44,44,44	0
56	MG	DA	3175	1/1	0.96	0.08	47,47,47,47	0
56	MG	AA	3025	1/1	0.96	0.11	37,37,37,37	0
56	MG	AA	3036	1/1	0.96	0.12	41,41,41,41	0
56	MG	BA	3231	1/1	0.96	0.18	41,41,41,41	0
56	MG	BA	3045	1/1	0.96	0.11	34,34,34,34	0
56	MG	DA	3550	1/1	0.96	0.10	46,46,46,46	0
56	MG	DA	3186	1/1	0.96	0.06	41,41,41,41	0
56	MG	CA	3070	1/1	0.96	0.08	39,39,39,39	0
56	MG	DA	3189	1/1	0.96	0.20	31,31,31,31	0
56	MG	DA	3190	1/1	0.96	0.10	34,34,34,34	0
56	MG	DA	3555	1/1	0.96	0.10	51,51,51,51	0
56	MG	DA	3556	1/1	0.96	0.12	36,36,36,36	0
56	MG	BA	3120	1/1	0.96	0.08	44,44,44,44	0
56	MG	BA	3402	1/1	0.96	0.14	28,28,28,28	0
56	MG	BA	3598	1/1	0.96	0.12	48,48,48,48	0
56	MG	BA	3121	1/1	0.96	0.25	43,43,43,43	0
56	MG	CA	3075	1/1	0.96	0.15	53,53,53,53	0
56	MG	BA	3236	1/1	0.96	0.07	42,42,42,42	0
56	MG	AA	3037	1/1	0.96	0.06	51,51,51,51	0
56	MG	BA	3406	1/1	0.96	0.14	39,39,39,39	0
56	MG	BA	3603	1/1	0.96	0.07	49,49,49,49	0
56	MG	DA	3203	1/1	0.96	0.09	21,21,21,21	0
56	MG	DA	3570	1/1	0.96	0.06	52,52,52,52	0
56	MG	CA	3080	1/1	0.96	0.09	41,41,41,41	0
56	MG	DA	3572	1/1	0.96	0.10	51,51,51,51	0
56	MG	DA	3573	1/1	0.96	0.16	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	3407	1/1	0.96	0.10	43,43,43,43	0
56	MG	DA	3575	1/1	0.96	0.16	49,49,49,49	0
56	MG	BA	3238	1/1	0.96	0.21	47,47,47,47	0
56	MG	DA	3208	1/1	0.96	0.11	43,43,43,43	0
56	MG	DA	3210	1/1	0.96	0.06	37,37,37,37	0
56	MG	DA	3579	1/1	0.96	0.11	54,54,54,54	0
56	MG	BA	3410	1/1	0.96	0.09	43,43,43,43	0
56	MG	AA	3067	1/1	0.96	0.30	42,42,42,42	0
56	MG	BA	3240	1/1	0.96	0.18	43,43,43,43	0
56	MG	DA	3583	1/1	0.96	0.05	43,43,43,43	0
56	MG	DA	3214	1/1	0.96	0.14	30,30,30,30	0
56	MG	DA	3215	1/1	0.96	0.07	31,31,31,31	0
56	MG	AA	3101	1/1	0.96	0.29	53,53,53,53	0
56	MG	DA	3590	1/1	0.96	0.18	38,38,38,38	0
56	MG	CA	3087	1/1	0.96	0.06	33,33,33,33	0
56	MG	DA	3219	1/1	0.96	0.11	33,33,33,33	0
56	MG	DA	3220	1/1	0.96	0.08	43,43,43,43	0
56	MG	DA	3221	1/1	0.96	0.06	33,33,33,33	0
56	MG	CA	3088	1/1	0.96	0.14	41,41,41,41	0
56	MG	DB	3003	1/1	0.96	0.06	29,29,29,29	0
56	MG	BA	3127	1/1	0.96	0.06	45,45,45,45	0
56	MG	BA	3128	1/1	0.96	0.17	29,29,29,29	0
56	MG	BA	3245	1/1	0.96	0.12	27,27,27,27	0
56	MG	BA	3618	1/1	0.96	0.20	54,54,54,54	0
56	MG	BA	3129	1/1	0.96	0.10	42,42,42,42	0
56	MG	BA	3427	1/1	0.96	0.10	49,49,49,49	0
56	MG	BA	3252	1/1	0.96	0.10	51,51,51,51	0
56	MG	DD	301	1/1	0.96	0.11	43,43,43,43	0
56	MG	AA	3028	1/1	0.96	0.12	39,39,39,39	0
56	MG	CA	3098	1/1	0.96	0.14	42,42,42,42	0
56	MG	BA	3255	1/1	0.96	0.23	32,32,32,32	0
56	MG	CA	3100	1/1	0.96	0.15	56,56,56,56	0
56	MG	BA	3434	1/1	0.96	0.08	43,43,43,43	0
56	MG	CA	3102	1/1	0.96	0.16	30,30,30,30	0
56	MG	DA	3241	1/1	0.96	0.16	36,36,36,36	0
56	MG	BA	3135	1/1	0.96	0.10	36,36,36,36	0
56	MG	AA	3103	1/1	0.96	0.10	51,51,51,51	0
56	MG	BA	3630	1/1	0.96	0.08	47,47,47,47	0
56	MG	DR	202	1/1	0.96	0.06	32,32,32,32	0
56	MG	BA	3439	1/1	0.96	0.13	30,30,30,30	0
56	MG	DU	201	1/1	0.96	0.12	41,41,41,41	0
56	MG	DV	3001	1/1	0.96	0.13	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	3052	1/1	0.96	0.05	27,27,27,27	0
56	MG	BA	3263	1/1	0.96	0.22	64,64,64,64	0
56	MG	BA	3444	1/1	0.96	0.08	34,34,34,34	0
56	MG	D0	5001	1/1	0.96	0.06	39,39,39,39	0
56	MG	D3	3001	1/1	0.96	0.19	70,70,70,70	0
56	MG	BA	3053	1/1	0.96	0.10	31,31,31,31	0
56	MG	DA	3253	1/1	0.96	0.05	26,26,26,26	0
56	MG	DA	3254	1/1	0.96	0.11	46,46,46,46	0
59	K	AX	3001	1/1	0.96	0.06	48,48,48,48	0
59	K	DA	3001	1/1	0.96	0.05	48,48,48,48	0
56	MG	DA	3363	1/1	0.97	0.04	36,36,36,36	0
56	MG	DA	3364	1/1	0.97	0.07	37,37,37,37	0
56	MG	BB	3018	1/1	0.97	0.05	30,30,30,30	0
56	MG	BA	3322	1/1	0.97	0.10	40,40,40,40	0
56	MG	DA	3119	1/1	0.97	0.16	37,37,37,37	0
56	MG	BD	303	1/1	0.97	0.21	37,37,37,37	0
56	MG	BA	3118	1/1	0.97	0.09	45,45,45,45	0
56	MG	BD	305	1/1	0.97	0.09	38,38,38,38	0
56	MG	BD	307	1/1	0.97	0.05	27,27,27,27	0
56	MG	BD	308	1/1	0.97	0.07	35,35,35,35	0
56	MG	DA	3374	1/1	0.97	0.07	35,35,35,35	0
56	MG	BE	301	1/1	0.97	0.11	45,45,45,45	0
56	MG	DA	3376	1/1	0.97	0.06	38,38,38,38	0
56	MG	BE	302	1/1	0.97	0.28	36,36,36,36	0
56	MG	BA	3233	1/1	0.97	0.17	41,41,41,41	0
56	MG	BA	3431	1/1	0.97	0.06	44,44,44,44	0
56	MG	DA	3130	1/1	0.97	0.24	47,47,47,47	0
56	MG	BA	3432	1/1	0.97	0.06	37,37,37,37	0
56	MG	DA	3387	1/1	0.97	0.05	53,53,53,53	0
56	MG	BA	3167	1/1	0.97	0.08	46,46,46,46	0
56	MG	DA	3133	1/1	0.97	0.06	53,53,53,53	0
56	MG	DA	3134	1/1	0.97	0.19	33,33,33,33	0
56	MG	DA	3395	1/1	0.97	0.04	41,41,41,41	0
56	MG	BA	3568	1/1	0.97	0.07	42,42,42,42	0
56	MG	DA	3397	1/1	0.97	0.05	18,18,18,18	0
56	MG	BA	3168	1/1	0.97	0.09	47,47,47,47	0
56	MG	BA	3570	1/1	0.97	0.07	36,36,36,36	0
56	MG	DA	3138	1/1	0.97	0.11	33,33,33,33	0
56	MG	BG	3001	1/1	0.97	0.10	71,71,71,71	0
56	MG	AA	3077	1/1	0.97	0.08	39,39,39,39	0
56	MG	BA	3170	1/1	0.97	0.12	34,34,34,34	0
56	MG	DA	3407	1/1	0.97	0.06	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	AA	3099	1/1	0.97	0.17	33,33,33,33	0
56	MG	BN	3001	1/1	0.97	0.06	57,57,57,57	0
56	MG	BA	3123	1/1	0.97	0.06	36,36,36,36	0
56	MG	DA	3411	1/1	0.97	0.04	36,36,36,36	0
56	MG	DA	3149	1/1	0.97	0.14	41,41,41,41	0
56	MG	BA	3011	1/1	0.97	0.03	30,30,30,30	0
56	MG	BP	202	1/1	0.97	0.32	31,31,31,31	0
56	MG	BA	3333	1/1	0.97	0.09	35,35,35,35	0
56	MG	DA	3153	1/1	0.97	0.09	42,42,42,42	0
56	MG	AA	3152	1/1	0.97	0.11	57,57,57,57	0
56	MG	AA	3172	1/1	0.97	0.10	69,69,69,69	0
56	MG	BR	3003	1/1	0.97	0.11	39,39,39,39	0
56	MG	BA	3337	1/1	0.97	0.05	37,37,37,37	0
56	MG	DA	3422	1/1	0.97	0.05	63,63,63,63	0
56	MG	DA	3160	1/1	0.97	0.13	44,44,44,44	0
56	MG	BA	3243	1/1	0.97	0.09	45,45,45,45	0
56	MG	CA	3124	1/1	0.97	0.13	52,52,52,52	0
56	MG	BA	3014	1/1	0.97	0.14	35,35,35,35	0
56	MG	BA	3179	1/1	0.97	0.04	27,27,27,27	0
56	MG	CA	3127	1/1	0.97	0.13	49,49,49,49	0
56	MG	BA	3342	1/1	0.97	0.05	35,35,35,35	0
56	MG	AA	3078	1/1	0.97	0.08	34,34,34,34	0
56	MG	BA	3461	1/1	0.97	0.16	52,52,52,52	0
56	MG	BA	3249	1/1	0.97	0.07	48,48,48,48	0
56	MG	BA	3464	1/1	0.97	0.06	41,41,41,41	0
56	MG	BX	103	1/1	0.97	0.08	25,25,25,25	0
56	MG	BA	3251	1/1	0.97	0.08	37,37,37,37	0
56	MG	BA	3467	1/1	0.97	0.10	20,20,20,20	0
56	MG	DA	3176	1/1	0.97	0.12	29,29,29,29	0
56	MG	BA	3468	1/1	0.97	0.06	32,32,32,32	0
56	MG	DA	3442	1/1	0.97	0.18	42,42,42,42	0
56	MG	BA	3181	1/1	0.97	0.04	37,37,37,37	0
56	MG	BA	3253	1/1	0.97	0.18	47,47,47,47	0
56	MG	DA	3184	1/1	0.97	0.13	30,30,30,30	0
56	MG	AA	3063	1/1	0.97	0.19	39,39,39,39	0
56	MG	CA	3141	1/1	0.97	0.11	54,54,54,54	0
56	MG	AA	3155	1/1	0.97	0.10	61,61,61,61	0
56	MG	DA	3188	1/1	0.97	0.04	25,25,25,25	0
56	MG	BA	3131	1/1	0.97	0.06	36,36,36,36	0
56	MG	DA	3453	1/1	0.97	0.08	31,31,31,31	0
56	MG	BA	3257	1/1	0.97	0.04	29,29,29,29	0
56	MG	DA	3455	1/1	0.97	0.14	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	3258	1/1	0.97	0.14	30,30,30,30	0
56	MG	CA	3146	1/1	0.97	0.05	42,42,42,42	0
56	MG	B7	3001	1/1	0.97	0.06	45,45,45,45	0
56	MG	B7	3004	1/1	0.97	0.05	34,34,34,34	0
56	MG	CA	3150	1/1	0.97	0.07	62,62,62,62	0
56	MG	DA	3461	1/1	0.97	0.10	33,33,33,33	0
56	MG	DA	3463	1/1	0.97	0.07	28,28,28,28	0
56	MG	DA	3464	1/1	0.97	0.12	46,46,46,46	0
56	MG	B8	5001	1/1	0.97	0.09	36,36,36,36	0
56	MG	B9	502	1/1	0.97	0.07	41,41,41,41	0
56	MG	BA	3259	1/1	0.97	0.12	35,35,35,35	0
56	MG	CA	3002	1/1	0.97	0.08	43,43,43,43	0
56	MG	BA	3132	1/1	0.97	0.10	25,25,25,25	0
56	MG	BA	3133	1/1	0.97	0.04	33,33,33,33	0
56	MG	BA	3360	1/1	0.97	0.07	21,21,21,21	0
56	MG	CA	3006	1/1	0.97	0.24	37,37,37,37	0
56	MG	AA	3139	1/1	0.97	0.06	36,36,36,36	0
56	MG	DA	3209	1/1	0.97	0.06	38,38,38,38	0
56	MG	CA	3008	1/1	0.97	0.22	31,31,31,31	0
56	MG	BA	3020	1/1	0.97	0.10	33,33,33,33	0
56	MG	DA	3002	1/1	0.97	0.10	33,33,33,33	0
56	MG	CA	3010	1/1	0.97	0.06	53,53,53,53	0
56	MG	BA	3487	1/1	0.97	0.10	17,17,17,17	0
56	MG	DA	3006	1/1	0.97	0.06	33,33,33,33	0
56	MG	DA	3216	1/1	0.97	0.08	37,37,37,37	0
56	MG	DA	3007	1/1	0.97	0.05	39,39,39,39	0
56	MG	BA	3606	1/1	0.97	0.09	32,32,32,32	0
56	MG	DA	3010	1/1	0.97	0.08	36,36,36,36	0
56	MG	BA	3363	1/1	0.97	0.10	29,29,29,29	0
56	MG	DA	3014	1/1	0.97	0.07	33,33,33,33	0
56	MG	DA	3489	1/1	0.97	0.13	49,49,49,49	0
56	MG	CA	3014	1/1	0.97	0.09	39,39,39,39	0
56	MG	BA	3608	1/1	0.97	0.16	45,45,45,45	0
56	MG	BA	3089	1/1	0.97	0.07	37,37,37,37	0
56	MG	DA	3019	1/1	0.97	0.06	40,40,40,40	0
56	MG	DA	3227	1/1	0.97	0.21	49,49,49,49	0
56	MG	DA	3228	1/1	0.97	0.08	51,51,51,51	0
56	MG	BA	3610	1/1	0.97	0.08	47,47,47,47	0
56	MG	BA	3366	1/1	0.97	0.06	34,34,34,34	0
56	MG	BA	3138	1/1	0.97	0.10	35,35,35,35	0
56	MG	CA	3020	1/1	0.97	0.28	46,46,46,46	0
56	MG	DA	3502	1/1	0.97	0.10	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	BA	3613	1/1	0.97	0.08	45,45,45,45	0
56	MG	BA	3614	1/1	0.97	0.05	55,55,55,55	0
56	MG	CA	3023	1/1	0.97	0.08	38,38,38,38	0
56	MG	BA	3368	1/1	0.97	0.07	42,42,42,42	0
56	MG	BA	3370	1/1	0.97	0.09	29,29,29,29	0
56	MG	AA	3064	1/1	0.97	0.18	45,45,45,45	0
56	MG	BA	3269	1/1	0.97	0.05	34,34,34,34	0
56	MG	DA	3031	1/1	0.97	0.04	21,21,21,21	0
56	MG	DA	3511	1/1	0.97	0.14	53,53,53,53	0
56	MG	BA	3054	1/1	0.97	0.14	42,42,42,42	0
56	MG	BA	3499	1/1	0.97	0.09	35,35,35,35	0
56	MG	CA	3030	1/1	0.97	0.09	41,41,41,41	0
56	MG	DA	3246	1/1	0.97	0.17	38,38,38,38	0
56	MG	DA	3035	1/1	0.97	0.12	46,46,46,46	0
56	MG	DA	3248	1/1	0.97	0.20	52,52,52,52	0
56	MG	DA	3037	1/1	0.97	0.10	40,40,40,40	0
56	MG	CA	3031	1/1	0.97	0.08	52,52,52,52	0
56	MG	BA	3193	1/1	0.97	0.19	48,48,48,48	0
56	MG	DA	3040	1/1	0.97	0.14	34,34,34,34	0
56	MG	BA	3622	1/1	0.97	0.11	45,45,45,45	0
56	MG	BA	3501	1/1	0.97	0.09	44,44,44,44	0
56	MG	BA	3502	1/1	0.97	0.10	33,33,33,33	0
56	MG	BA	3276	1/1	0.97	0.06	42,42,42,42	0
56	MG	DA	3258	1/1	0.97	0.19	49,49,49,49	0
56	MG	DA	3046	1/1	0.97	0.17	34,34,34,34	0
56	MG	DA	3532	1/1	0.97	0.06	51,51,51,51	0
56	MG	CA	3037	1/1	0.97	0.06	45,45,45,45	0
56	MG	DA	3048	1/1	0.97	0.07	41,41,41,41	0
56	MG	DA	3262	1/1	0.97	0.06	39,39,39,39	0
56	MG	DA	3049	1/1	0.97	0.04	40,40,40,40	0
56	MG	BA	3194	1/1	0.97	0.03	23,23,23,23	0
56	MG	BA	3055	1/1	0.97	0.07	13,13,13,13	0
56	MG	BA	3385	1/1	0.97	0.06	20,20,20,20	0
56	MG	DA	3267	1/1	0.97	0.15	47,47,47,47	0
56	MG	DA	3053	1/1	0.97	0.12	41,41,41,41	0
56	MG	BA	3386	1/1	0.97	0.14	32,32,32,32	0
56	MG	DA	3270	1/1	0.97	0.06	37,37,37,37	0
56	MG	BA	3197	1/1	0.97	0.10	19,19,19,19	0
56	MG	DA	3547	1/1	0.97	0.09	41,41,41,41	0
56	MG	BA	3282	1/1	0.97	0.15	31,31,31,31	0
56	MG	DA	3057	1/1	0.97	0.04	30,30,30,30	0
56	MG	BA	3144	1/1	0.97	0.12	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	BA	3201	1/1	0.97	0.07	41,41,41,41	0
56	MG	BA	3636	1/1	0.97	0.04	32,32,32,32	0
56	MG	DA	3061	1/1	0.97	0.05	35,35,35,35	0
56	MG	DA	3279	1/1	0.97	0.05	27,27,27,27	0
56	MG	BA	3391	1/1	0.97	0.08	37,37,37,37	0
56	MG	AA	3046	1/1	0.97	0.10	42,42,42,42	0
56	MG	BA	3024	1/1	0.97	0.17	32,32,32,32	0
56	MG	DA	3558	1/1	0.97	0.05	39,39,39,39	0
56	MG	BA	3025	1/1	0.97	0.10	37,37,37,37	0
56	MG	CA	3051	1/1	0.97	0.09	66,66,66,66	0
56	MG	CA	3052	1/1	0.97	0.06	39,39,39,39	0
56	MG	DA	3290	1/1	0.97	0.06	36,36,36,36	0
56	MG	DA	3564	1/1	0.97	0.05	36,36,36,36	0
56	MG	DA	3068	1/1	0.97	0.08	35,35,35,35	0
56	MG	BA	3060	1/1	0.97	0.10	42,42,42,42	0
56	MG	AA	3082	1/1	0.97	0.20	57,57,57,57	0
56	MG	DA	3296	1/1	0.97	0.05	28,28,28,28	0
56	MG	BA	3212	1/1	0.97	0.14	28,28,28,28	0
56	MG	DA	3299	1/1	0.97	0.06	50,50,50,50	0
56	MG	AA	3145	1/1	0.97	0.07	35,35,35,35	0
56	MG	BA	3214	1/1	0.97	0.14	28,28,28,28	0
56	MG	DA	3074	1/1	0.97	0.04	29,29,29,29	0
56	MG	DA	3303	1/1	0.97	0.06	43,43,43,43	0
56	MG	BA	3103	1/1	0.97	0.10	42,42,42,42	0
56	MG	BA	3651	1/1	0.97	0.05	42,42,42,42	0
56	MG	BA	3529	1/1	0.97	0.10	33,33,33,33	0
56	MG	BA	3531	1/1	0.97	0.05	41,41,41,41	0
56	MG	AA	3029	1/1	0.97	0.12	52,52,52,52	0
56	MG	BA	3030	1/1	0.97	0.45	43,43,43,43	0
56	MG	DA	3313	1/1	0.97	0.07	40,40,40,40	0
56	MG	DA	3314	1/1	0.97	0.17	54,54,54,54	0
56	MG	DA	3084	1/1	0.97	0.07	39,39,39,39	0
56	MG	DA	3317	1/1	0.97	0.09	53,53,53,53	0
56	MG	DA	3318	1/1	0.97	0.12	43,43,43,43	0
56	MG	DA	3586	1/1	0.97	0.10	47,47,47,47	0
56	MG	DA	3319	1/1	0.97	0.18	38,38,38,38	0
56	MG	DA	3588	1/1	0.97	0.10	21,21,21,21	0
56	MG	DA	3589	1/1	0.97	0.06	33,33,33,33	0
56	MG	BA	3067	1/1	0.97	0.09	34,34,34,34	0
56	MG	DA	3591	1/1	0.97	0.09	42,42,42,42	0
56	MG	BA	3302	1/1	0.97	0.10	55,55,55,55	0
56	MG	BA	3661	1/1	0.97	0.06	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	BA	3155	1/1	0.97	0.20	27,27,27,27	0
56	MG	DA	3324	1/1	0.97	0.08	52,52,52,52	0
56	MG	BA	3666	1/1	0.97	0.16	35,35,35,35	0
56	MG	AA	3095	1/1	0.97	0.13	55,55,55,55	0
56	MG	BA	3409	1/1	0.97	0.07	28,28,28,28	0
56	MG	BA	3670	1/1	0.97	0.14	34,34,34,34	0
56	MG	BA	3544	1/1	0.97	0.12	25,25,25,25	0
56	MG	BA	3033	1/1	0.97	0.08	33,33,33,33	0
56	MG	DB	3008	1/1	0.97	0.08	35,35,35,35	0
56	MG	BA	3546	1/1	0.97	0.06	57,57,57,57	0
56	MG	BB	3001	1/1	0.97	0.08	36,36,36,36	0
56	MG	DB	3011	1/1	0.97	0.06	29,29,29,29	0
56	MG	BA	3547	1/1	0.97	0.05	60,60,60,60	0
56	MG	DA	3335	1/1	0.97	0.12	36,36,36,36	0
56	MG	DD	302	1/1	0.97	0.11	39,39,39,39	0
56	MG	BA	3548	1/1	0.97	0.07	30,30,30,30	0
56	MG	BA	3072	1/1	0.97	0.10	24,24,24,24	0
56	MG	DA	3339	1/1	0.97	0.09	32,32,32,32	0
56	MG	DE	3004	1/1	0.97	0.09	48,48,48,48	0
56	MG	BA	3413	1/1	0.97	0.10	26,26,26,26	0
56	MG	DA	3341	1/1	0.97	0.07	25,25,25,25	0
56	MG	DA	3342	1/1	0.97	0.14	37,37,37,37	0
56	MG	AA	3008	1/1	0.97	0.24	55,55,55,55	0
56	MG	DA	3104	1/1	0.97	0.17	35,35,35,35	0
56	MG	BA	3227	1/1	0.97	0.06	32,32,32,32	0
56	MG	DQ	3002	1/1	0.97	0.18	38,38,38,38	0
56	MG	BA	3418	1/1	0.97	0.06	46,46,46,46	0
56	MG	DA	3348	1/1	0.97	0.07	25,25,25,25	0
56	MG	DA	3107	1/1	0.97	0.19	46,46,46,46	0
56	MG	BA	3419	1/1	0.97	0.07	20,20,20,20	0
56	MG	BB	3012	1/1	0.97	0.10	44,44,44,44	0
56	MG	DA	3110	1/1	0.97	0.12	42,42,42,42	0
56	MG	BA	3315	1/1	0.97	0.15	31,31,31,31	0
56	MG	DA	3355	1/1	0.97	0.04	36,36,36,36	0
56	MG	BA	3228	1/1	0.97	0.08	40,40,40,40	0
56	MG	BA	3113	1/1	0.97	0.18	41,41,41,41	0
56	MG	DA	3358	1/1	0.97	0.10	45,45,45,45	0
56	MG	AA	3032	1/1	0.97	0.11	42,42,42,42	0
56	MG	AA	3186	1/1	0.97	0.12	55,55,55,55	0
58	ZN	B4	501	1/1	0.97	0.06	106,106,106,106	0
58	ZN	D4	501	1/1	0.97	0.08	141,141,141,141	0
56	MG	DA	3116	1/1	0.97	0.10	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	3362	1/1	0.97	0.07	43,43,43,43	0
56	MG	BA	3004	1/1	0.98	0.06	23,23,23,23	0
56	MG	BA	3203	1/1	0.98	0.13	35,35,35,35	0
56	MG	B0	103	1/1	0.98	0.07	33,33,33,33	0
56	MG	DA	3448	1/1	0.98	0.14	29,29,29,29	0
56	MG	BA	3204	1/1	0.98	0.12	35,35,35,35	0
56	MG	AA	3070	1/1	0.98	0.16	33,33,33,33	0
56	MG	DA	3451	1/1	0.98	0.05	30,30,30,30	0
56	MG	B3	101	1/1	0.98	0.12	35,35,35,35	0
56	MG	B3	102	1/1	0.98	0.15	22,22,22,22	0
56	MG	BA	3326	1/1	0.98	0.05	28,28,28,28	0
56	MG	BA	3068	1/1	0.98	0.04	39,39,39,39	0
56	MG	BA	3519	1/1	0.98	0.07	53,53,53,53	0
56	MG	BA	3520	1/1	0.98	0.06	24,24,24,24	0
56	MG	B7	3002	1/1	0.98	0.05	35,35,35,35	0
56	MG	B7	3003	1/1	0.98	0.06	28,28,28,28	0
56	MG	BA	3208	1/1	0.98	0.16	25,25,25,25	0
56	MG	BA	3522	1/1	0.98	0.06	52,52,52,52	0
56	MG	DA	3462	1/1	0.98	0.06	35,35,35,35	0
56	MG	BA	3628	1/1	0.98	0.07	38,38,38,38	0
56	MG	BA	3209	1/1	0.98	0.18	26,26,26,26	0
56	MG	BA	3022	1/1	0.98	0.04	26,26,26,26	0
56	MG	BA	3414	1/1	0.98	0.06	31,31,31,31	0
56	MG	BA	3006	1/1	0.98	0.12	36,36,36,36	0
56	MG	DA	3276	1/1	0.98	0.18	50,50,50,50	0
56	MG	BA	3099	1/1	0.98	0.20	32,32,32,32	0
56	MG	BA	3528	1/1	0.98	0.05	38,38,38,38	0
56	MG	BA	3262	1/1	0.98	0.09	24,24,24,24	0
56	MG	DA	3280	1/1	0.98	0.07	50,50,50,50	0
56	MG	BA	3007	1/1	0.98	0.03	32,32,32,32	0
56	MG	BA	3420	1/1	0.98	0.05	24,24,24,24	0
56	MG	DA	3283	1/1	0.98	0.04	38,38,38,38	0
56	MG	DA	3476	1/1	0.98	0.03	32,32,32,32	0
56	MG	DA	3284	1/1	0.98	0.04	23,23,23,23	0
56	MG	BA	3421	1/1	0.98	0.07	36,36,36,36	0
56	MG	BA	3535	1/1	0.98	0.05	47,47,47,47	0
56	MG	BA	3640	1/1	0.98	0.06	33,33,33,33	0
56	MG	BA	3264	1/1	0.98	0.15	35,35,35,35	0
56	MG	DA	3482	1/1	0.98	0.05	46,46,46,46	0
56	MG	DA	3124	1/1	0.98	0.09	29,29,29,29	0
56	MG	BA	3336	1/1	0.98	0.06	43,43,43,43	0
56	MG	BA	3538	1/1	0.98	0.14	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	DA	3294	1/1	0.98	0.04	37,37,37,37	0
56	MG	BA	3134	1/1	0.98	0.10	40,40,40,40	0
56	MG	BA	3215	1/1	0.98	0.10	32,32,32,32	0
56	MG	DA	3297	1/1	0.98	0.08	38,38,38,38	0
56	MG	DA	3490	1/1	0.98	0.06	34,34,34,34	0
56	MG	CA	3147	1/1	0.98	0.08	52,52,52,52	0
56	MG	BA	3542	1/1	0.98	0.07	51,51,51,51	0
56	MG	BA	3216	1/1	0.98	0.23	33,33,33,33	0
56	MG	BA	3650	1/1	0.98	0.04	31,31,31,31	0
56	MG	AN	502	1/1	0.98	0.18	53,53,53,53	0
56	MG	BA	3341	1/1	0.98	0.05	32,32,32,32	0
56	MG	DA	3497	1/1	0.98	0.11	45,45,45,45	0
56	MG	DA	3304	1/1	0.98	0.10	32,32,32,32	0
56	MG	AA	3168	1/1	0.98	0.14	56,56,56,56	0
56	MG	BA	3104	1/1	0.98	0.04	42,42,42,42	0
56	MG	BA	3049	1/1	0.98	0.09	43,43,43,43	0
56	MG	BA	3657	1/1	0.98	0.07	24,24,24,24	0
56	MG	BA	3658	1/1	0.98	0.06	27,27,27,27	0
56	MG	BA	3272	1/1	0.98	0.07	37,37,37,37	0
56	MG	DA	3311	1/1	0.98	0.08	43,43,43,43	0
56	MG	DA	3142	1/1	0.98	0.10	37,37,37,37	0
56	MG	DA	3143	1/1	0.98	0.05	27,27,27,27	0
56	MG	DA	3315	1/1	0.98	0.10	43,43,43,43	0
56	MG	BA	3273	1/1	0.98	0.05	29,29,29,29	0
56	MG	BA	3551	1/1	0.98	0.05	48,48,48,48	0
56	MG	BA	3274	1/1	0.98	0.08	47,47,47,47	0
56	MG	BA	3665	1/1	0.98	0.05	30,30,30,30	0
56	MG	DA	3513	1/1	0.98	0.06	32,32,32,32	0
56	MG	DA	3148	1/1	0.98	0.04	47,47,47,47	0
56	MG	BA	3175	1/1	0.98	0.10	33,33,33,33	0
56	MG	AA	3075	1/1	0.98	0.12	39,39,39,39	0
56	MG	DA	3005	1/1	0.98	0.06	26,26,26,26	0
56	MG	AX	3004	1/1	0.98	0.11	39,39,39,39	0
56	MG	DA	3519	1/1	0.98	0.05	42,42,42,42	0
56	MG	BA	3351	1/1	0.98	0.04	33,33,33,33	0
56	MG	DA	3008	1/1	0.98	0.03	38,38,38,38	0
56	MG	DA	3522	1/1	0.98	0.09	44,44,44,44	0
56	MG	BA	3279	1/1	0.98	0.07	38,38,38,38	0
56	MG	BA	3353	1/1	0.98	0.06	39,39,39,39	0
56	MG	BA	3674	1/1	0.98	0.05	54,54,54,54	0
56	MG	DA	3012	1/1	0.98	0.11	30,30,30,30	0
56	MG	DA	3013	1/1	0.98	0.06	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DA	3528	1/1	0.98	0.04	37,37,37,37	0
56	MG	BA	3354	1/1	0.98	0.05	42,42,42,42	0
56	MG	BA	3355	1/1	0.98	0.04	31,31,31,31	0
56	MG	DA	3016	1/1	0.98	0.15	31,31,31,31	0
56	MG	DA	3336	1/1	0.98	0.08	22,22,22,22	0
56	MG	BB	3002	1/1	0.98	0.12	41,41,41,41	0
56	MG	BA	3178	1/1	0.98	0.17	26,26,26,26	0
56	MG	BA	3281	1/1	0.98	0.12	51,51,51,51	0
56	MG	DA	3168	1/1	0.98	0.11	39,39,39,39	0
56	MG	DA	3169	1/1	0.98	0.04	38,38,38,38	0
56	MG	BA	3453	1/1	0.98	0.04	27,27,27,27	0
56	MG	BA	3456	1/1	0.98	0.12	33,33,33,33	0
56	MG	BA	3457	1/1	0.98	0.06	29,29,29,29	0
56	MG	BA	3225	1/1	0.98	0.05	31,31,31,31	0
56	MG	BA	3029	1/1	0.98	0.07	12,12,12,12	0
56	MG	AA	3030	1/1	0.98	0.09	47,47,47,47	0
56	MG	BB	3011	1/1	0.98	0.05	45,45,45,45	0
56	MG	DA	3546	1/1	0.98	0.06	40,40,40,40	0
56	MG	DA	3177	1/1	0.98	0.06	52,52,52,52	0
56	MG	AA	3162	1/1	0.98	0.06	40,40,40,40	0
56	MG	BA	3032	1/1	0.98	0.04	40,40,40,40	0
56	MG	DA	3180	1/1	0.98	0.06	30,30,30,30	0
56	MG	DA	3181	1/1	0.98	0.05	40,40,40,40	0
56	MG	DA	3182	1/1	0.98	0.05	38,38,38,38	0
56	MG	BA	3015	1/1	0.98	0.04	27,27,27,27	0
56	MG	BA	3364	1/1	0.98	0.05	29,29,29,29	0
56	MG	BA	3114	1/1	0.98	0.12	34,34,34,34	0
56	MG	BA	3291	1/1	0.98	0.08	14,14,14,14	0
56	MG	AA	3050	1/1	0.98	0.04	24,24,24,24	0
56	MG	BD	301	1/1	0.98	0.11	30,30,30,30	0
56	MG	BA	3085	1/1	0.98	0.10	27,27,27,27	0
56	MG	DA	3036	1/1	0.98	0.04	38,38,38,38	0
56	MG	CA	3061	1/1	0.98	0.10	45,45,45,45	0
56	MG	DA	3562	1/1	0.98	0.06	42,42,42,42	0
56	MG	BA	3369	1/1	0.98	0.09	33,33,33,33	0
56	MG	BA	3035	1/1	0.98	0.15	21,21,21,21	0
56	MG	BA	3371	1/1	0.98	0.06	25,25,25,25	0
56	MG	BD	306	1/1	0.98	0.10	36,36,36,36	0
56	MG	DA	3196	1/1	0.98	0.06	33,33,33,33	0
56	MG	DA	3042	1/1	0.98	0.04	32,32,32,32	0
56	MG	DA	3372	1/1	0.98	0.06	21,21,21,21	0
56	MG	BA	3372	1/1	0.98	0.07	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	BA	3475	1/1	0.98	0.07	45,45,45,45	0
56	MG	DA	3200	1/1	0.98	0.08	28,28,28,28	0
56	MG	BA	3119	1/1	0.98	0.08	29,29,29,29	0
56	MG	DA	3202	1/1	0.98	0.13	24,24,24,24	0
56	MG	DA	3378	1/1	0.98	0.08	31,31,31,31	0
56	MG	DA	3380	1/1	0.98	0.04	33,33,33,33	0
56	MG	BA	3477	1/1	0.98	0.06	50,50,50,50	0
56	MG	AA	3173	1/1	0.98	0.12	32,32,32,32	0
56	MG	BE	304	1/1	0.98	0.07	13,13,13,13	0
56	MG	DA	3385	1/1	0.98	0.03	45,45,45,45	0
56	MG	BA	3038	1/1	0.98	0.06	30,30,30,30	0
56	MG	BA	3299	1/1	0.98	0.07	36,36,36,36	0
56	MG	DA	3389	1/1	0.98	0.04	42,42,42,42	0
56	MG	DA	3391	1/1	0.98	0.04	42,42,42,42	0
56	MG	BA	3377	1/1	0.98	0.07	31,31,31,31	0
56	MG	BA	3589	1/1	0.98	0.06	27,27,27,27	0
56	MG	BA	3380	1/1	0.98	0.09	17,17,17,17	0
56	MG	BA	3122	1/1	0.98	0.20	39,39,39,39	0
56	MG	BA	3382	1/1	0.98	0.09	27,27,27,27	0
56	MG	AA	3007	1/1	0.98	0.13	30,30,30,30	0
56	MG	BA	3489	1/1	0.98	0.17	41,41,41,41	0
56	MG	BA	3490	1/1	0.98	0.07	38,38,38,38	0
56	MG	DA	3400	1/1	0.98	0.17	38,38,38,38	0
56	MG	DA	3401	1/1	0.98	0.09	55,55,55,55	0
56	MG	DA	3596	1/1	0.98	0.12	54,54,54,54	0
56	MG	BA	3063	1/1	0.98	0.11	47,47,47,47	0
56	MG	DA	3403	1/1	0.98	0.04	39,39,39,39	0
56	MG	BN	3002	1/1	0.98	0.04	27,27,27,27	0
56	MG	BA	3304	1/1	0.98	0.09	43,43,43,43	0
56	MG	BA	3305	1/1	0.98	0.07	28,28,28,28	0
56	MG	BA	3091	1/1	0.98	0.14	19,19,19,19	0
56	MG	BA	3159	1/1	0.98	0.14	27,27,27,27	0
56	MG	BP	204	1/1	0.98	0.08	31,31,31,31	0
56	MG	BA	3196	1/1	0.98	0.10	17,17,17,17	0
56	MG	BQ	202	1/1	0.98	0.04	14,14,14,14	0
56	MG	BA	3160	1/1	0.98	0.09	29,29,29,29	0
56	MG	BR	3001	1/1	0.98	0.04	31,31,31,31	0
56	MG	DA	3229	1/1	0.98	0.16	38,38,38,38	0
56	MG	BR	3002	1/1	0.98	0.04	23,23,23,23	0
56	MG	DA	3231	1/1	0.98	0.05	37,37,37,37	0
56	MG	BA	3198	1/1	0.98	0.07	34,34,34,34	0
56	MG	CA	3095	1/1	0.98	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	BA	3312	1/1	0.98	0.05	18,18,18,18	0
56	MG	DE	3005	1/1	0.98	0.06	20,20,20,20	0
56	MG	BA	3313	1/1	0.98	0.06	17,17,17,17	0
56	MG	DF	302	1/1	0.98	0.05	41,41,41,41	0
56	MG	BU	204	1/1	0.98	0.12	29,29,29,29	0
56	MG	BA	3161	1/1	0.98	0.04	39,39,39,39	0
56	MG	BA	3247	1/1	0.98	0.19	48,48,48,48	0
56	MG	BA	3248	1/1	0.98	0.14	21,21,21,21	0
56	MG	DA	3426	1/1	0.98	0.07	35,35,35,35	0
56	MG	DA	3427	1/1	0.98	0.08	25,25,25,25	0
56	MG	DA	3080	1/1	0.98	0.07	29,29,29,29	0
56	MG	DR	201	1/1	0.98	0.23	36,36,36,36	0
56	MG	DA	3081	1/1	0.98	0.07	44,44,44,44	0
56	MG	BW	3001	1/1	0.98	0.05	25,25,25,25	0
56	MG	BA	3200	1/1	0.98	0.08	25,25,25,25	0
56	MG	BA	3399	1/1	0.98	0.08	42,42,42,42	0
56	MG	DA	3433	1/1	0.98	0.10	33,33,33,33	0
56	MG	DW	3001	1/1	0.98	0.09	38,38,38,38	0
56	MG	DA	3085	1/1	0.98	0.16	40,40,40,40	0
56	MG	DA	3086	1/1	0.98	0.07	41,41,41,41	0
56	MG	BA	3506	1/1	0.98	0.04	39,39,39,39	0
56	MG	CA	3106	1/1	0.98	0.14	40,40,40,40	0
56	MG	BA	3250	1/1	0.98	0.08	33,33,33,33	0
56	MG	DA	3250	1/1	0.98	0.05	37,37,37,37	0
56	MG	BA	3508	1/1	0.98	0.06	25,25,25,25	0
57	SF4	CD	501	8/8	0.98	0.04	58,71,82,82	0
56	MG	AA	3084	1/1	0.98	0.08	43,43,43,43	0
58	ZN	CN	501	1/1	0.98	0.04	82,82,82,82	0
56	MG	BA	3320	1/1	0.98	0.05	44,44,44,44	0
58	ZN	D9	501	1/1	0.98	0.06	54,54,54,54	0
56	MG	CA	3111	1/1	0.98	0.08	43,43,43,43	0
56	MG	BA	3321	1/1	0.98	0.06	53,53,53,53	0
56	MG	AA	3040	1/1	0.99	0.12	27,27,27,27	0
56	MG	AA	3127	1/1	0.99	0.09	68,68,68,68	0
56	MG	BA	3289	1/1	0.99	0.07	28,28,28,28	0
56	MG	BA	3290	1/1	0.99	0.04	36,36,36,36	0
56	MG	BA	3207	1/1	0.99	0.14	36,36,36,36	0
56	MG	BA	3083	1/1	0.99	0.09	34,34,34,34	0
56	MG	BA	3530	1/1	0.99	0.08	36,36,36,36	0
56	MG	BA	3479	1/1	0.99	0.07	45,45,45,45	0
56	MG	AA	3022	1/1	0.99	0.04	39,39,39,39	0
56	MG	BA	3481	1/1	0.99	0.09	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	BA	3534	1/1	0.99	0.09	20,20,20,20	0
56	MG	BA	3482	1/1	0.99	0.03	23,23,23,23	0
56	MG	BA	3294	1/1	0.99	0.04	32,32,32,32	0
56	MG	BF	302	1/1	0.99	0.03	45,45,45,45	0
56	MG	BA	3647	1/1	0.99	0.02	30,30,30,30	0
56	MG	DA	3413	1/1	0.99	0.07	24,24,24,24	0
56	MG	BA	3648	1/1	0.99	0.05	28,28,28,28	0
56	MG	BA	3433	1/1	0.99	0.04	33,33,33,33	0
56	MG	DA	3334	1/1	0.99	0.03	24,24,24,24	0
56	MG	BA	3065	1/1	0.99	0.08	29,29,29,29	0
56	MG	BA	3397	1/1	0.99	0.03	30,30,30,30	0
56	MG	BA	3436	1/1	0.99	0.04	35,35,35,35	0
56	MG	BA	3541	1/1	0.99	0.02	26,26,26,26	0
56	MG	AA	3090	1/1	0.99	0.10	28,28,28,28	0
56	MG	BA	3438	1/1	0.99	0.05	33,33,33,33	0
56	MG	BA	3656	1/1	0.99	0.07	12,12,12,12	0
56	MG	BA	3109	1/1	0.99	0.04	36,36,36,36	0
56	MG	BA	3440	1/1	0.99	0.05	38,38,38,38	0
56	MG	AA	3115	1/1	0.99	0.03	35,35,35,35	0
56	MG	DA	3345	1/1	0.99	0.08	33,33,33,33	0
56	MG	AA	3011	1/1	0.99	0.05	24,24,24,24	0
56	MG	AA	3140	1/1	0.99	0.05	31,31,31,31	0
56	MG	DA	3595	1/1	0.99	0.04	43,43,43,43	0
56	MG	BA	3445	1/1	0.99	0.03	22,22,22,22	0
56	MG	BA	3664	1/1	0.99	0.12	30,30,30,30	0
56	MG	DA	3350	1/1	0.99	0.09	36,36,36,36	0
56	MG	BA	3008	1/1	0.99	0.07	27,27,27,27	0
56	MG	BA	3071	1/1	0.99	0.09	32,32,32,32	0
56	MG	DA	3205	1/1	0.99	0.17	32,32,32,32	0
56	MG	BA	3303	1/1	0.99	0.06	31,31,31,31	0
56	MG	BU	201	1/1	0.99	0.11	32,32,32,32	0
56	MG	BA	3139	1/1	0.99	0.04	31,31,31,31	0
56	MG	BA	3669	1/1	0.99	0.05	29,29,29,29	0
56	MG	BA	3115	1/1	0.99	0.05	34,34,34,34	0
56	MG	DA	3140	1/1	0.99	0.09	37,37,37,37	0
56	MG	BA	3037	1/1	0.99	0.04	24,24,24,24	0
56	MG	BA	3672	1/1	0.99	0.04	46,46,46,46	0
56	MG	BA	3452	1/1	0.99	0.08	38,38,38,38	0
56	MG	BV	203	1/1	0.99	0.03	24,24,24,24	0
56	MG	BA	3275	1/1	0.99	0.05	39,39,39,39	0
56	MG	BA	3454	1/1	0.99	0.08	21,21,21,21	0
56	MG	DA	3289	1/1	0.99	0.09	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DA	3079	1/1	0.99	0.04	54,54,54,54	0
56	MG	BW	3003	1/1	0.99	0.06	27,27,27,27	0
56	MG	BA	3455	1/1	0.99	0.03	21,21,21,21	0
56	MG	DA	3293	1/1	0.99	0.07	34,34,34,34	0
56	MG	AA	3161	1/1	0.99	0.09	66,66,66,66	0
56	MG	BA	3411	1/1	0.99	0.09	25,25,25,25	0
56	MG	BA	3143	1/1	0.99	0.15	36,36,36,36	0
56	MG	DA	3224	1/1	0.99	0.10	22,22,22,22	0
56	MG	BA	3310	1/1	0.99	0.05	35,35,35,35	0
56	MG	BA	3039	1/1	0.99	0.07	31,31,31,31	0
56	MG	BA	3511	1/1	0.99	0.05	38,38,38,38	0
56	MG	DA	3157	1/1	0.99	0.07	40,40,40,40	0
56	MG	DA	3379	1/1	0.99	0.03	26,26,26,26	0
56	MG	AA	3117	1/1	0.99	0.04	47,47,47,47	0
56	MG	BA	3462	1/1	0.99	0.03	44,44,44,44	0
56	MG	AA	3163	1/1	0.99	0.03	49,49,49,49	0
56	MG	DA	3383	1/1	0.99	0.06	47,47,47,47	0
56	MG	BA	3417	1/1	0.99	0.09	24,24,24,24	0
56	MG	BA	3625	1/1	0.99	0.05	25,25,25,25	0
56	MG	BA	3465	1/1	0.99	0.05	37,37,37,37	0
56	MG	BA	3097	1/1	0.99	0.12	53,53,53,53	0
56	MG	D5	502	1/1	0.99	0.20	36,36,36,36	0
56	MG	DA	3388	1/1	0.99	0.03	35,35,35,35	0
56	MG	AA	3118	1/1	0.99	0.11	36,36,36,36	0
56	MG	DA	3390	1/1	0.99	0.04	41,41,41,41	0
57	SF4	AD	501	8/8	0.99	0.04	50,63,78,83	0
56	MG	BA	3059	1/1	0.99	0.04	27,27,27,27	0
58	ZN	AN	501	1/1	0.99	0.04	67,67,67,67	0
58	ZN	BY	501	1/1	0.99	0.02	51,51,51,51	0
56	MG	BA	3100	1/1	0.99	0.06	29,29,29,29	0
56	MG	DA	3312	1/1	0.99	0.03	47,47,47,47	0
58	ZN	DY	501	1/1	0.99	0.04	92,92,92,92	0
56	MG	AA	3143	1/1	0.99	0.05	32,32,32,32	0
58	ZN	D5	501	1/1	0.99	0.04	67,67,67,67	0
58	ZN	D6	501	1/1	0.99	0.06	68,68,68,68	0
56	MG	AX	3008	1/1	0.99	0.08	23,23,23,23	0
56	MG	BA	3424	1/1	0.99	0.06	38,38,38,38	0
56	MG	CA	3128	1/1	0.99	0.03	39,39,39,39	0
58	ZN	B6	501	1/1	1.00	0.01	45,45,45,45	0
58	ZN	B9	501	1/1	1.00	0.03	45,45,45,45	0
56	MG	BA	3663	1/1	1.00	0.01	20,20,20,20	0
56	MG	BA	3378	1/1	1.00	0.06	16,16,16,16	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DA	3542	1/1	1.00	0.03	30,30,30,30	0
56	MG	BA	3552	1/1	1.00	0.03	31,31,31,31	0
56	MG	BA	3379	1/1	1.00	0.05	31,31,31,31	0
56	MG	DA	3154	1/1	1.00	0.07	24,24,24,24	0
56	MG	BA	3442	1/1	1.00	0.05	20,20,20,20	0
58	ZN	B5	501	1/1	1.00	0.02	42,42,42,42	0

6.5 Other polymers (i)

There are no such residues in this entry.