wwPDB X-ray Structure Validation Summary Report (i)

Aug 5, 2026 – 03:58 PM EDT

PDB ID	:	4W2H / pdb_00004w2h
Title	:	Crystal structure of the Thermus thermophilus 70S ribosome in complex with pactamycin (co-crystallized), mRNA and deacylated tRNA in the P site
Authors	:	Polikanov, Y.S.; Osterman, I.A.; Szal, T.; Tashlitsky, V.N.; Serebryakova, M.V.; Kusochek, P.; Bulkley, D.; Malanicheva, I.A.; Efimenko, T.A.; Efremenkova, O.V.; Konevega, A.L.; Shaw, K.J.; Bogdanov, A.A.; Rodnina, M.V.; Dontsova, O.A.; Mankin, A.S.; Steitz, T.A.; Sergiev, P.V.
Deposited on	:	2014-09-12
Resolution	:	2.70 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:

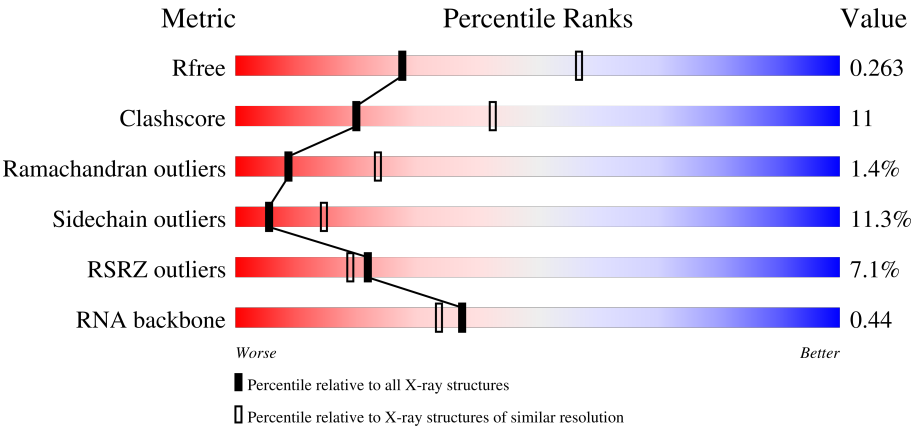
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)

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 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)
RNA backbone	3983	1044 (2.90-2.50)

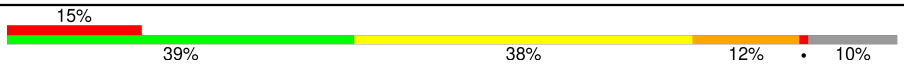
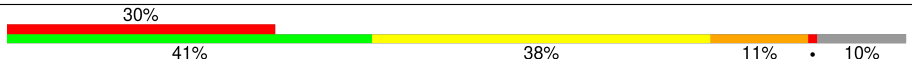
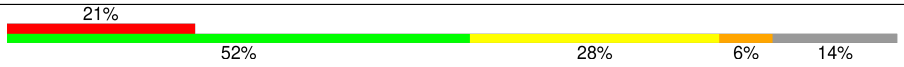
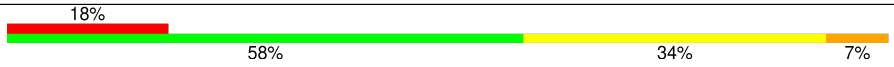
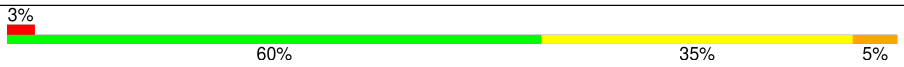
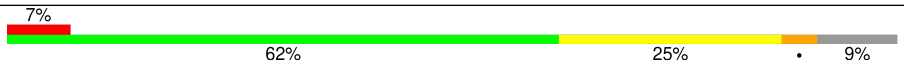
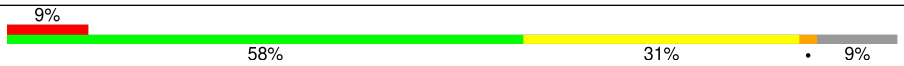
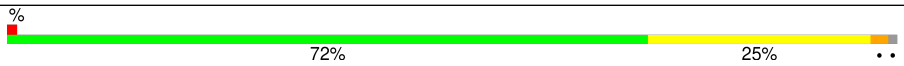
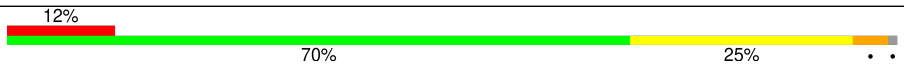
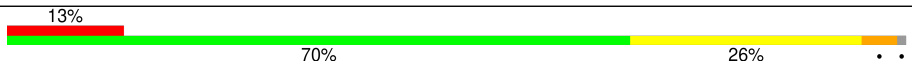
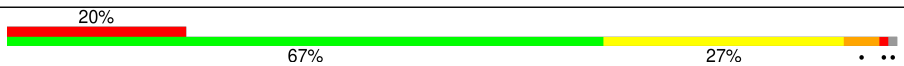
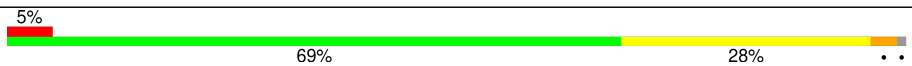
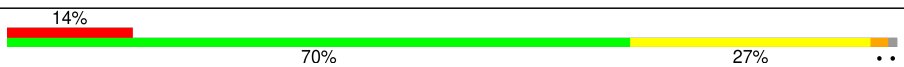
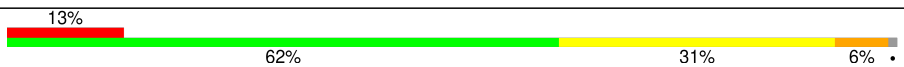
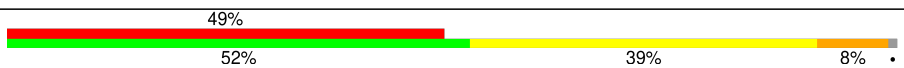
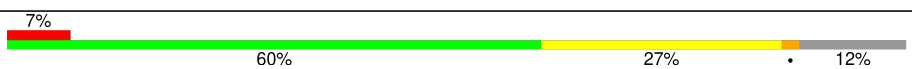
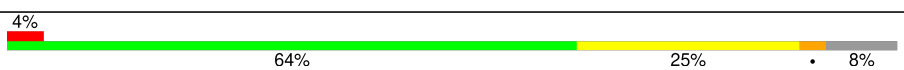
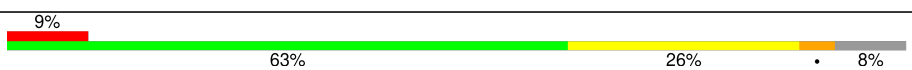
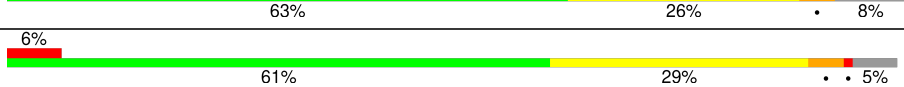
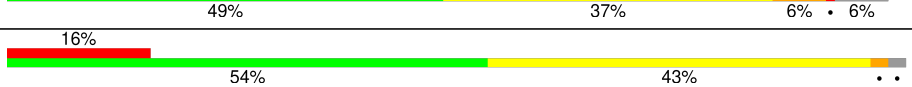
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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% 45% 40% 13%
1	CA	1521	7% 44% 40% 15%

Continued on next page...

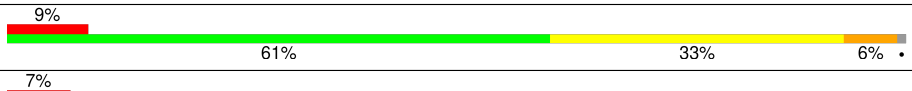
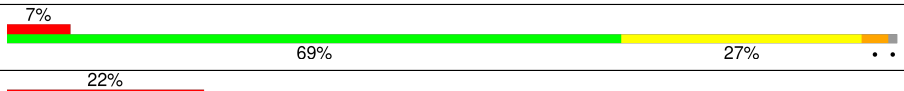
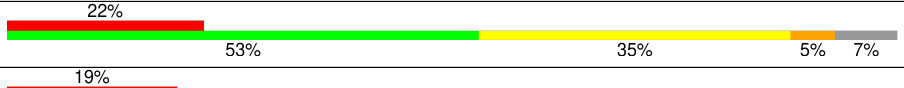
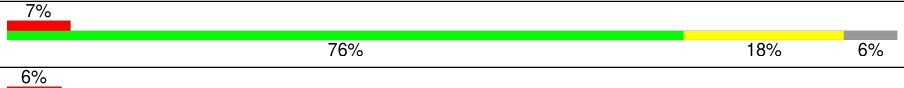
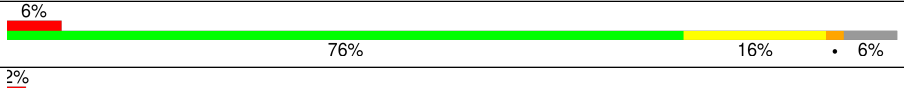
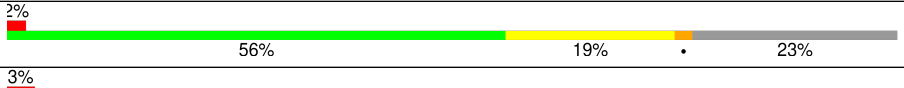
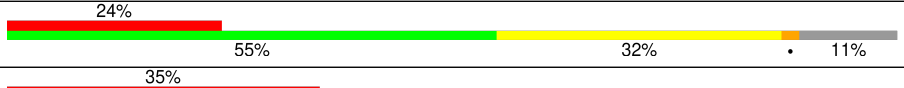
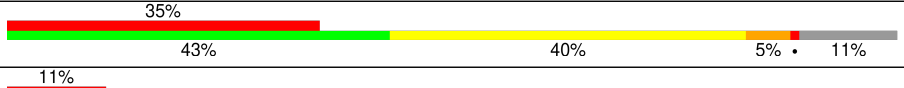
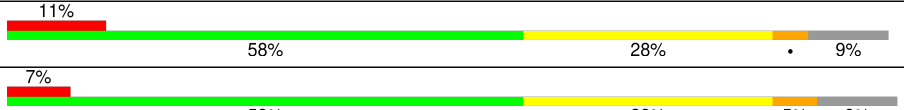
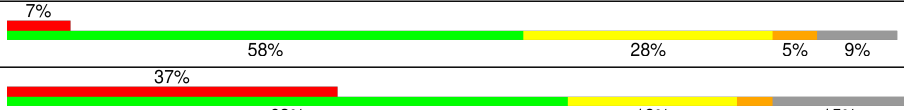
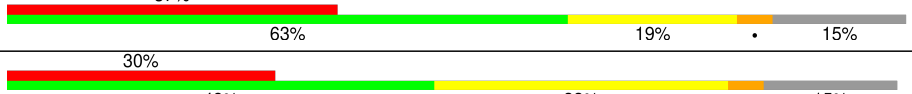
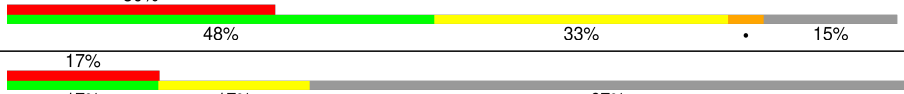
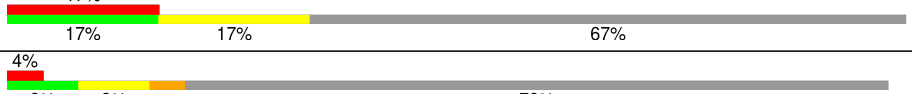
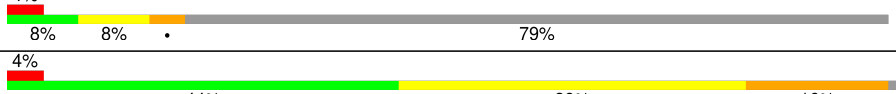
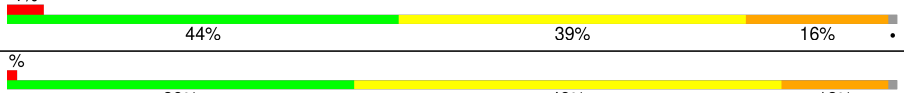
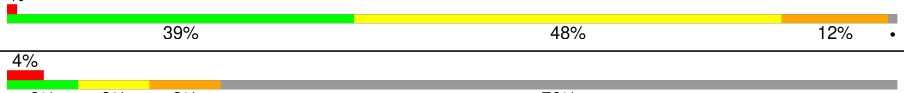
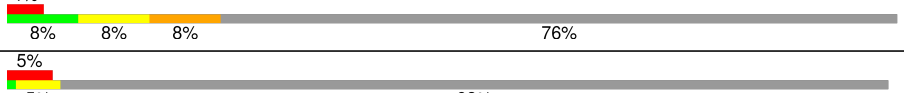
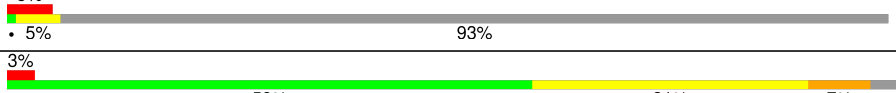
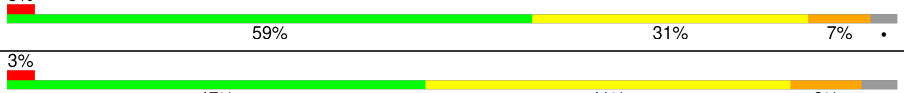
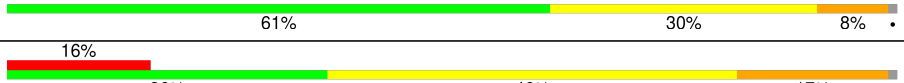
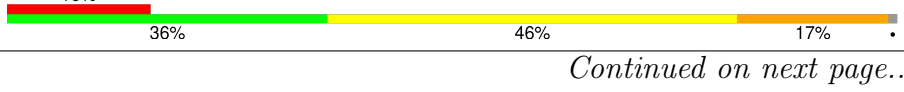
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

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Mol	Chain	Length	Quality of chain
2	AB	256	
2	CB	256	
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	

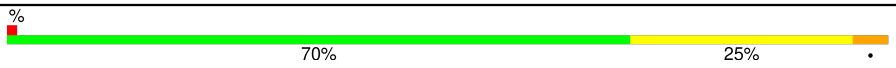
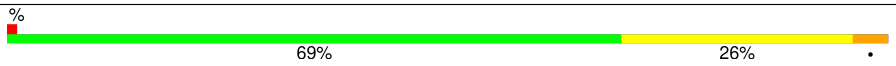
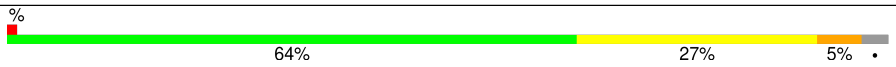
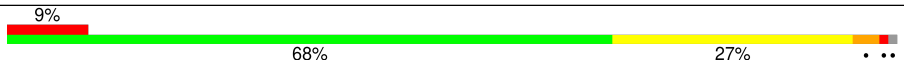
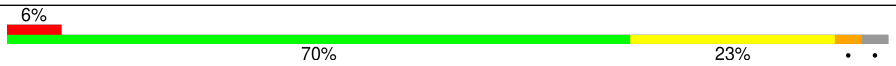
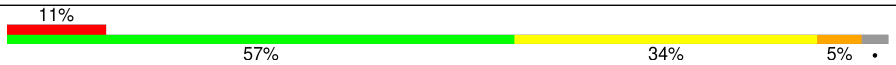
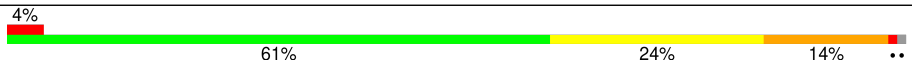
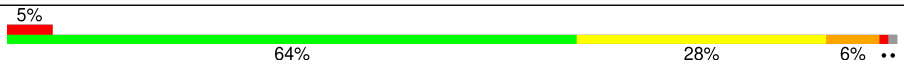
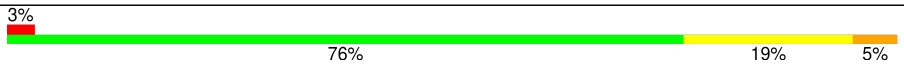
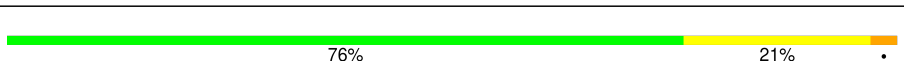
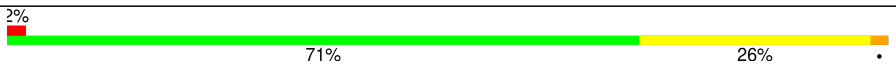
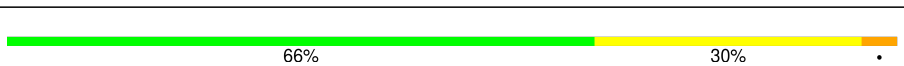
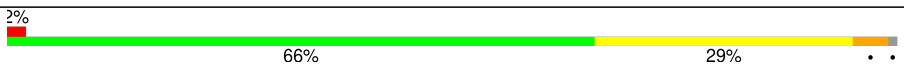
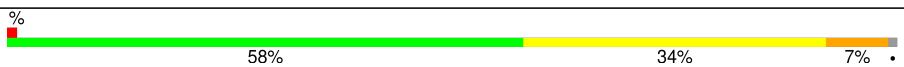
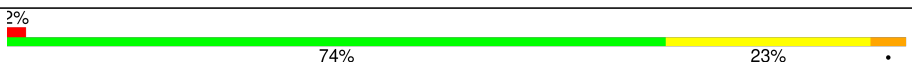
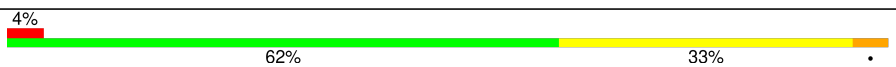
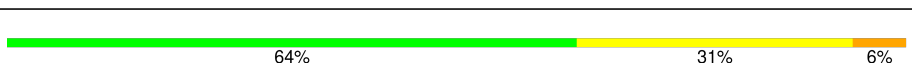
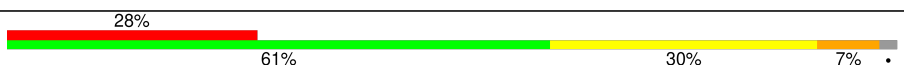
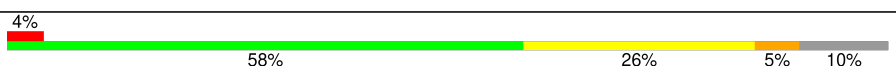
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Mol	Chain	Length	Quality of chain
14	CN	61	
15	AO	89	
15	CO	89	
16	AP	88	
16	CP	88	
17	AQ	105	
17	CQ	105	
18	AR	88	
18	CR	88	
19	AS	93	
19	CS	93	
20	AT	106	
20	CT	106	
21	AU	27	
21	CU	27	
22	AV	24	
22	CV	24	
23	AX	77	
23	CX	77	
24	AY	76	
24	CY	76	
25	BA	2915	
25	DA	2915	
26	BB	121	
26	DB	121	

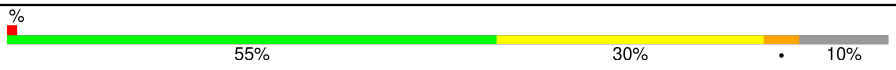
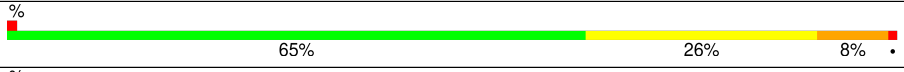
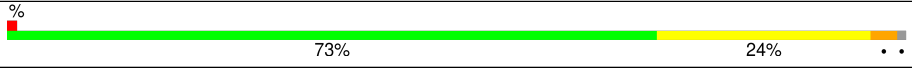
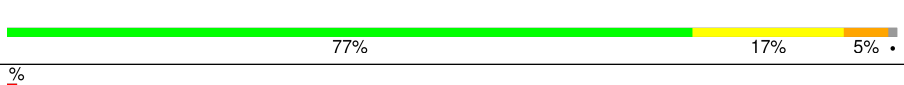
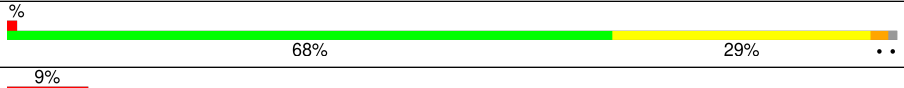
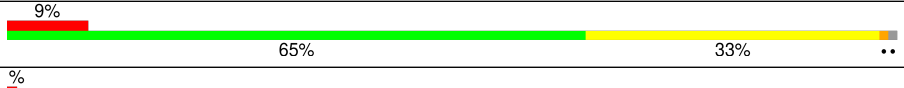
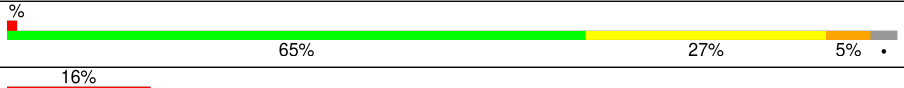
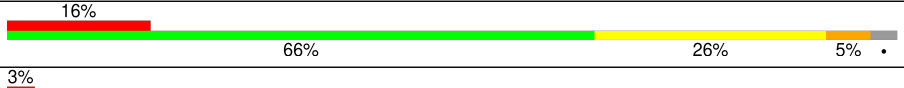
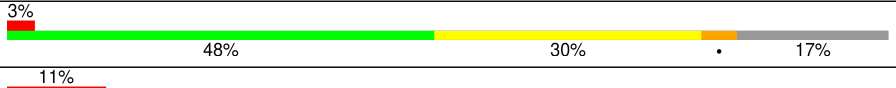
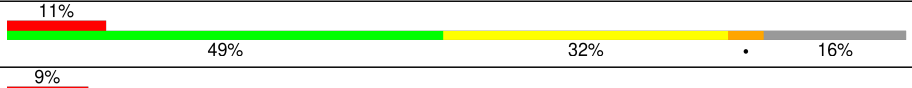
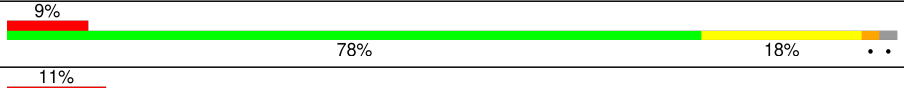
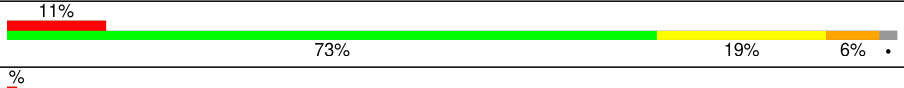
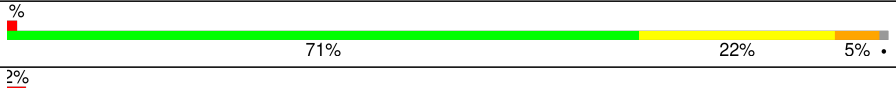
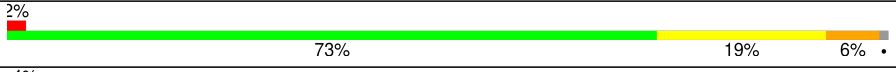
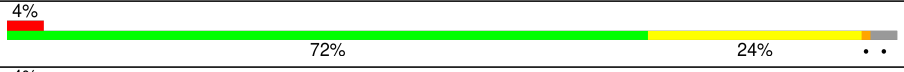
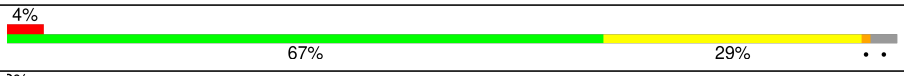
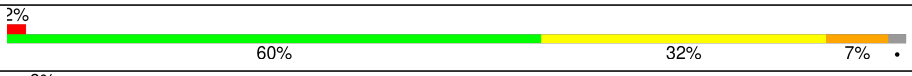
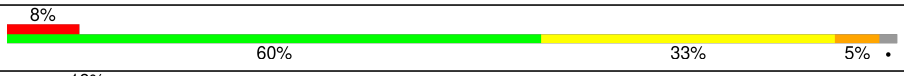
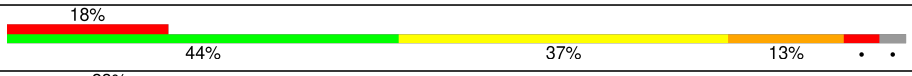
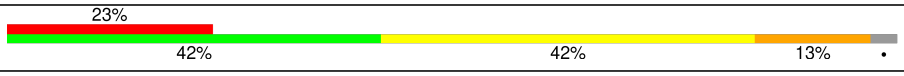
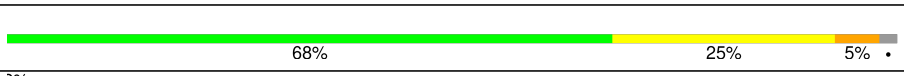
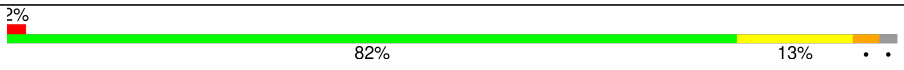
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Mol	Chain	Length	Quality of chain
27	BD	276	
27	DD	276	
28	BE	206	
28	DE	206	
29	BF	210	
29	DF	210	
30	BG	182	
30	DG	182	
31	BH	180	
31	DH	180	
32	BI	148	
32	DI	148	
33	BN	140	
33	DN	140	
34	BO	122	
34	DO	122	
35	BP	150	
35	DP	150	
36	BQ	141	
36	DQ	141	
37	BR	118	
37	DR	118	
38	BS	112	
38	DS	112	
39	BT	146	

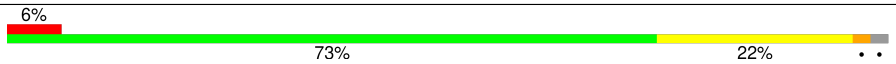
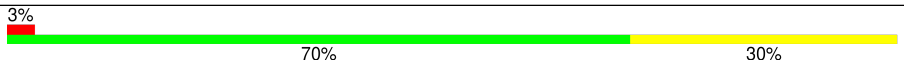
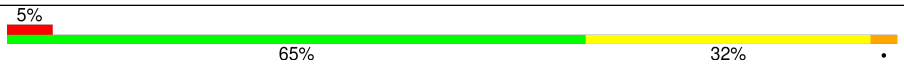
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Mol	Chain	Length	Quality of chain
39	DT	146	
40	BU	118	
40	DU	118	
41	BV	101	
41	DV	101	
42	BW	113	
42	DW	113	
43	BX	96	
43	DX	96	
44	BY	110	
44	DY	110	
45	BZ	206	
45	DZ	206	
46	B0	85	
46	D0	85	
47	B1	98	
47	D1	98	
48	B2	72	
48	D2	72	
49	B3	60	
49	D3	60	
50	B4	71	
50	D4	71	
51	B5	60	
51	D5	60	

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Mol	Chain	Length	Quality of chain
52	B6	54	
52	D6	54	
53	B7	49	
53	D7	49	
54	B8	65	
54	D8	65	
55	B9	37	
55	D9	37	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	CX	3002	-	-	-	X
56	MG	DA	3655	-	-	-	X

2 Entry composition (i)

There are 61 unique types of molecules in this entry. The entry contains 290807 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	1497	Total	C	N	O	P	0	0	0
			32183	14323	5965	10398	1497			
1	CA	1503	Total	C	N	O	P	0	0	0
			32312	14381	5990	10438	1503			

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

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

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

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

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

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

- Molecule 5 is a protein called 30S Ribosomal Protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AE	148	Total	C	N	O	S	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	120	Total 937	C 578	N 194	O 163	S 2	0	0	0
13	CM	118	Total 920	C 566	N 191	O 161	S 2	0	0	0

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

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	8	Total	C	N	O	P	0	0	0
			169	76	29	56	8			
22	CV	5	Total	C	N	O	P	0	0	0
			109	49	22	33	5			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
23	AX	76	Total	C	N	O	P	S	0	0	0
			1625	725	294	529	76	1			
23	CX	76	Total	C	N	O	P	S	0	0	0
			1625	725	294	529	76	1			

- Molecule 24 is a RNA chain called E-site tRNA Acceptor Stem.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	AY	18	Total	C	N	O	P	0	0	0
			385	171	71	125	18			
24	CY	5	Total	C	N	O	P	0	0	0
			104	47	19	33	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	BA	2822	Total	C	N	O	P	0	0	0
			60792	27054	11380	19537	2821			
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
			558	352	102	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	190	Total	Mg	0	0
			190	190		
56	AD	1	Total	Mg	0	0
			1	1		
56	AE	3	Total	Mg	0	0
			3	3		
56	AF	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	AQ	1	Total	Mg	0	0
			1	1		
56	AX	9	Total	Mg	0	0
			9	9		
56	BA	814	Total	Mg	0	0
			814	814		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	BB	22	Total Mg 22 22	0	0
56	BD	9	Total Mg 9 9	0	0
56	BE	7	Total Mg 7 7	0	0
56	BF	9	Total Mg 9 9	0	0
56	BG	2	Total Mg 2 2	0	0
56	BN	7	Total Mg 7 7	0	0
56	BO	1	Total Mg 1 1	0	0
56	BP	4	Total Mg 4 4	0	0
56	BQ	4	Total Mg 4 4	0	0
56	BR	3	Total Mg 3 3	0	0
56	BU	9	Total Mg 9 9	0	0
56	BV	4	Total Mg 4 4	0	0
56	BW	4	Total Mg 4 4	0	0
56	BX	2	Total Mg 2 2	0	0
56	BY	3	Total Mg 3 3	0	0
56	BZ	2	Total Mg 2 2	0	0
56	B0	5	Total Mg 5 5	0	0
56	B2	1	Total Mg 1 1	0	0
56	B3	1	Total Mg 1 1	0	0
56	B4	1	Total Mg 1 1	0	0
56	B5	4	Total Mg 4 4	0	0

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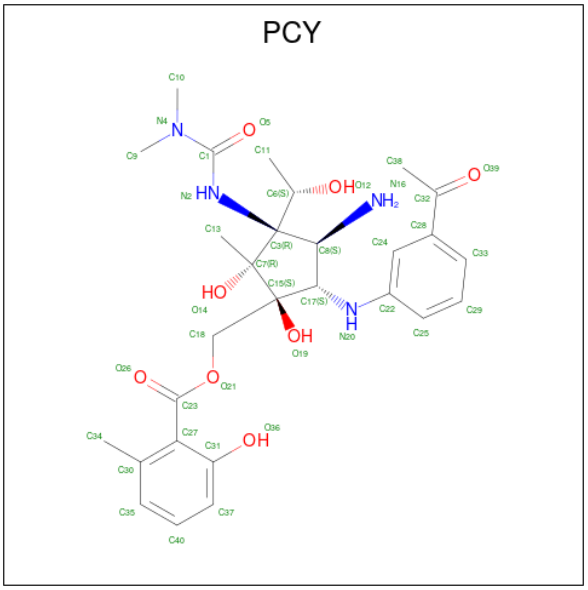
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	B6	2	Total Mg 2 2	0	0
56	B7	5	Total Mg 5 5	0	0
56	B8	2	Total Mg 2 2	0	0
56	B9	1	Total Mg 1 1	0	0
56	CA	175	Total Mg 175 175	0	0
56	CE	2	Total Mg 2 2	0	0
56	CF	1	Total Mg 1 1	0	0
56	CJ	1	Total Mg 1 1	0	0
56	CT	1	Total Mg 1 1	0	0
56	CX	2	Total Mg 2 2	0	0
56	DA	674	Total Mg 674 674	0	0
56	DB	10	Total Mg 10 10	0	0
56	DD	8	Total Mg 8 8	0	0
56	DE	5	Total Mg 5 5	0	0
56	DF	5	Total Mg 5 5	0	0
56	DG	1	Total Mg 1 1	0	0
56	DN	1	Total Mg 1 1	0	0
56	DO	1	Total Mg 1 1	0	0
56	DP	2	Total Mg 2 2	0	0
56	DQ	3	Total Mg 3 3	0	0
56	DR	1	Total Mg 1 1	0	0

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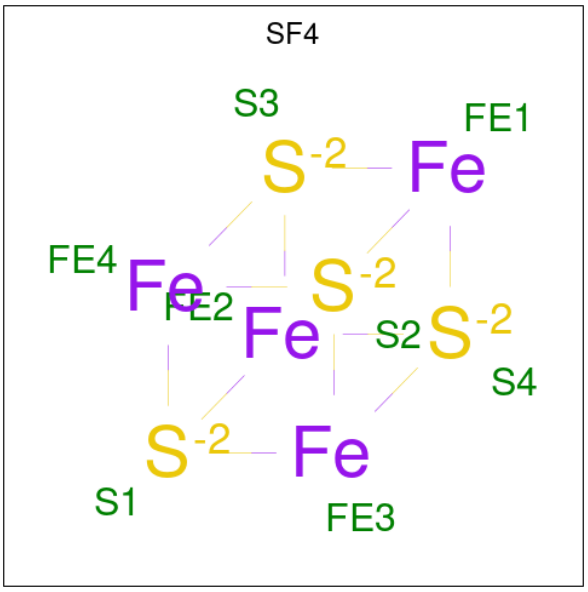
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	DU	4	Total Mg 4 4	0	0
56	DV	3	Total Mg 3 3	0	0
56	DW	2	Total Mg 2 2	0	0
56	DY	1	Total Mg 1 1	0	0
56	D0	2	Total Mg 2 2	0	0
56	D1	1	Total Mg 1 1	0	0
56	D3	1	Total Mg 1 1	0	0
56	D8	1	Total Mg 1 1	0	0

- Molecule 57 is Pactamycin (CCD ID: PCY) (formula: $C_{28}H_{38}N_4O_8$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	AA	1	Total C N O 40 28 4 8	0	0
57	CA	1	Total C N O 40 28 4 8	0	0

- Molecule 58 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



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

- Molecule 59 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	D6	1	Total Zn 1 1	0	0
59	D9	1	Total Zn 1 1	0	0

- Molecule 60 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	AX	1	Total K 1 1	0	0
60	CX	1	Total K 1 1	0	0

- Molecule 61 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	AA	175	Total O 175 175	0	0
61	AJ	2	Total O 2 2	0	0
61	AL	1	Total O 1 1	0	0
61	AM	1	Total O 1 1	0	0
61	AO	1	Total O 1 1	0	0
61	AV	1	Total O 1 1	0	0
61	AX	8	Total O 8 8	0	0
61	BA	1294	Total O 1294 1294	0	0
61	BB	34	Total O 34 34	0	0
61	BD	16	Total O 16 16	0	0
61	BE	12	Total O 12 12	0	0
61	BF	7	Total O 7 7	0	0
61	BG	3	Total O 3 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	BI	1	Total O 1 1	0	0
61	BN	1	Total O 1 1	0	0
61	BO	4	Total O 4 4	0	0
61	BP	15	Total O 15 15	0	0
61	BQ	5	Total O 5 5	0	0
61	BR	1	Total O 1 1	0	0
61	BU	2	Total O 2 2	0	0
61	BV	2	Total O 2 2	0	0
61	BW	3	Total O 3 3	0	0
61	BX	5	Total O 5 5	0	0
61	B0	4	Total O 4 4	0	0
61	B1	1	Total O 1 1	0	0
61	B3	1	Total O 1 1	0	0
61	B5	4	Total O 4 4	0	0
61	B6	1	Total O 1 1	0	0
61	B7	1	Total O 1 1	0	0
61	B8	10	Total O 10 10	0	0
61	CA	137	Total O 137 137	0	0
61	CD	1	Total O 1 1	0	0
61	CJ	2	Total O 2 2	0	0
61	CL	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	CN	1	Total O 1 1	0	0
61	CT	1	Total O 1 1	0	0
61	CX	2	Total O 2 2	0	0
61	DA	924	Total O 924 924	0	0
61	DB	8	Total O 8 8	0	0
61	DD	18	Total O 18 18	0	0
61	DE	9	Total O 9 9	0	0
61	DF	5	Total O 5 5	0	0
61	DN	1	Total O 1 1	0	0
61	DO	1	Total O 1 1	0	0
61	DP	14	Total O 14 14	0	0
61	DR	1	Total O 1 1	0	0
61	DT	1	Total O 1 1	0	0
61	DU	3	Total O 3 3	0	0
61	DV	1	Total O 1 1	0	0
61	DW	1	Total O 1 1	0	0
61	DX	1	Total O 1 1	0	0
61	DY	1	Total O 1 1	0	0
61	D0	7	Total O 7 7	0	0
61	D1	1	Total O 1 1	0	0
61	D3	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	D8	4	Total O 4 4	0	0

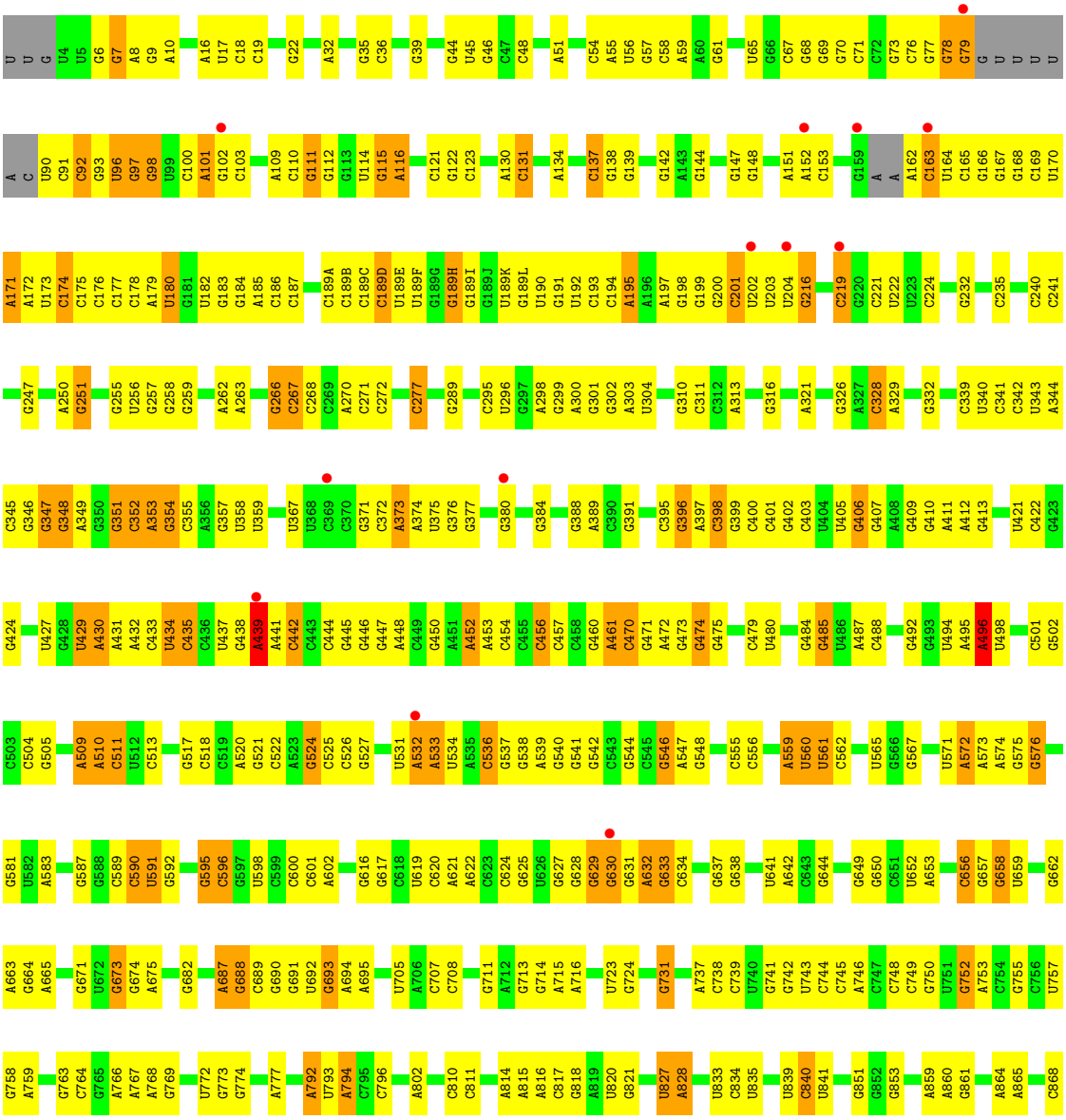
3 Residue-property plots (i)

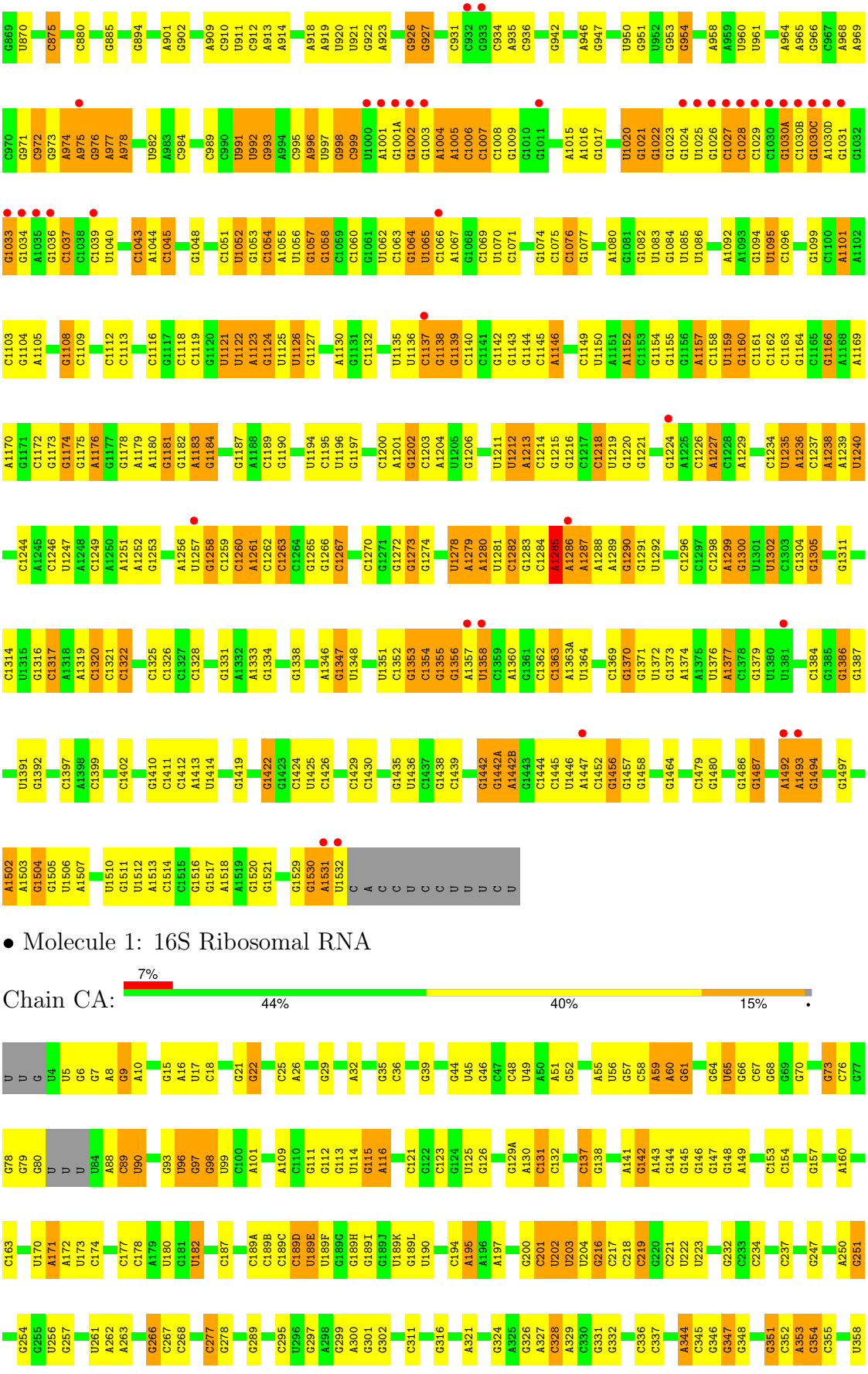
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: 16S Ribosomal RNA

Chain AA:

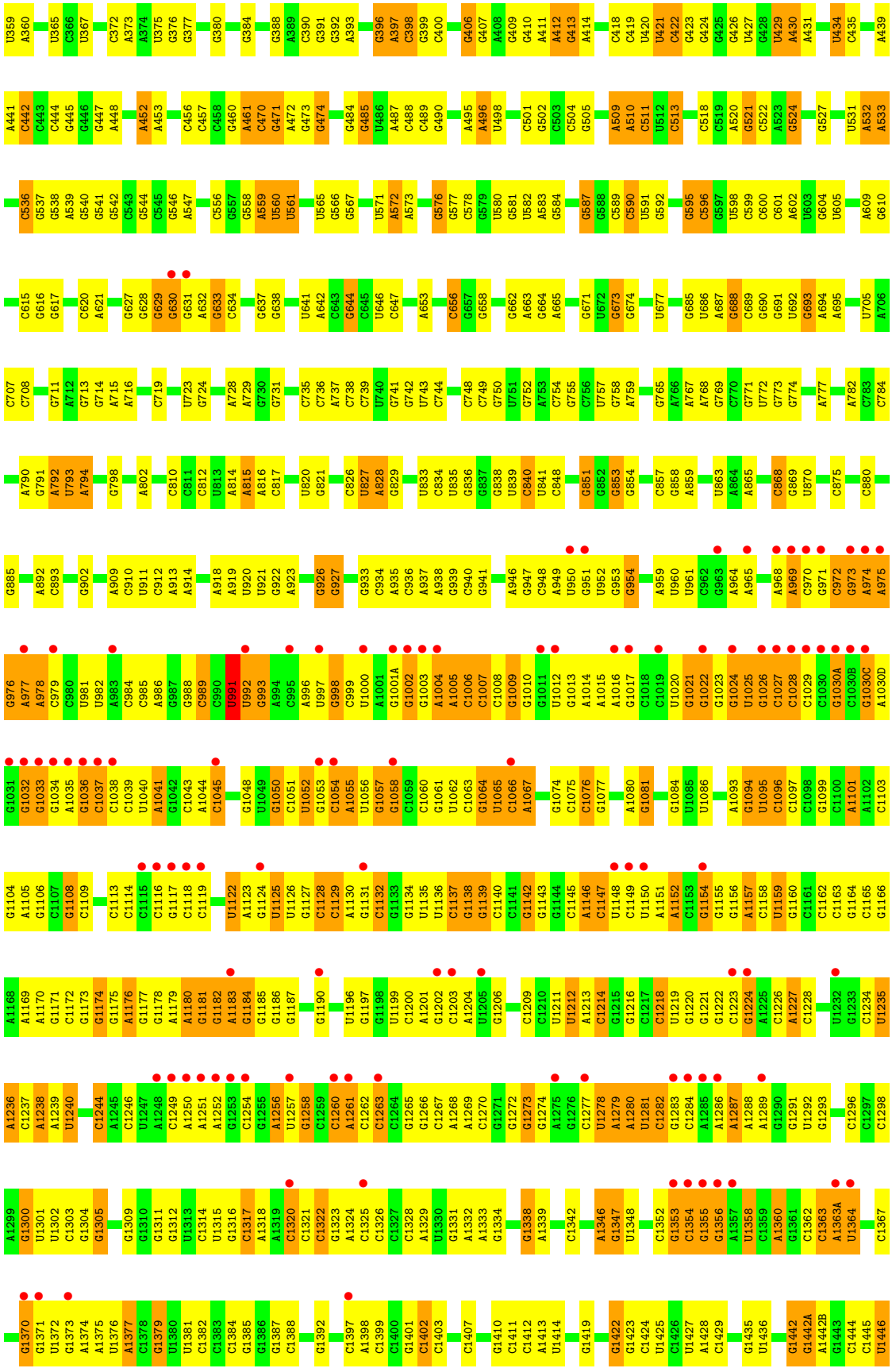


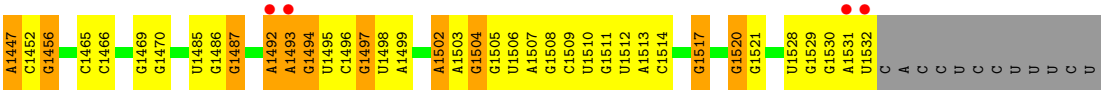




• Molecule 1: 16S Ribosomal RNA

Chain CA:

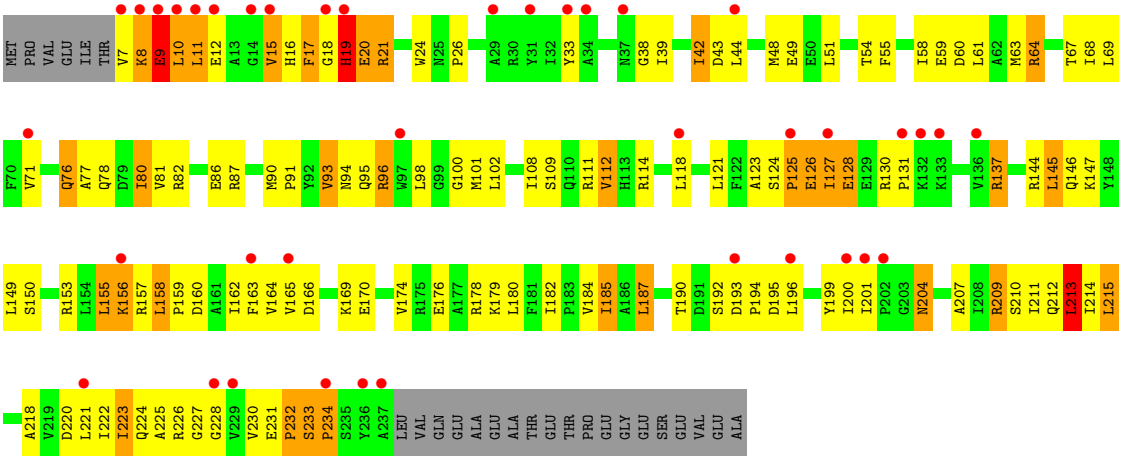




• Molecule 2: 30S Ribosomal Protein S2

Chain AB:

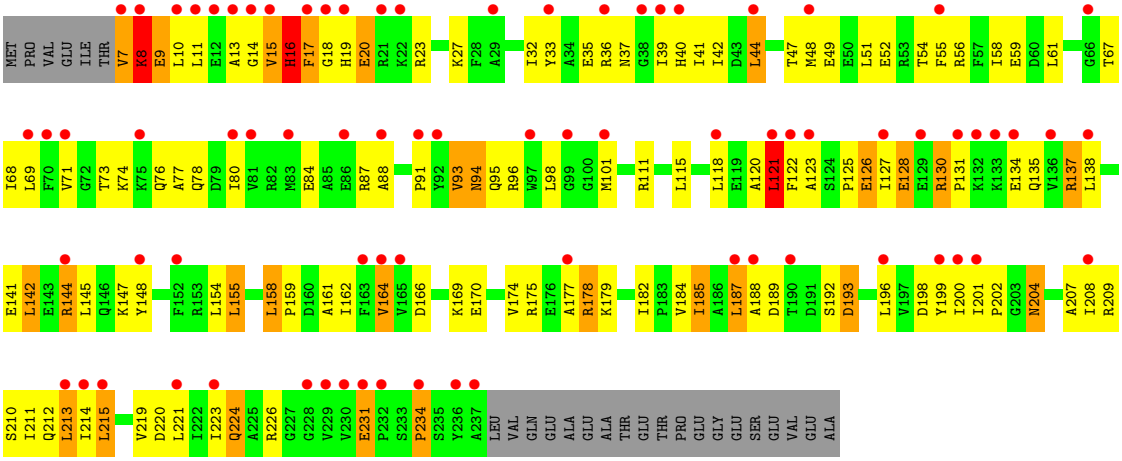




• Molecule 2: 30S Ribosomal Protein S2

Chain CB:

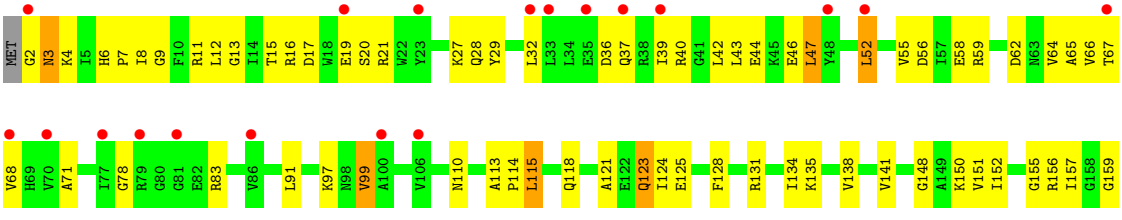


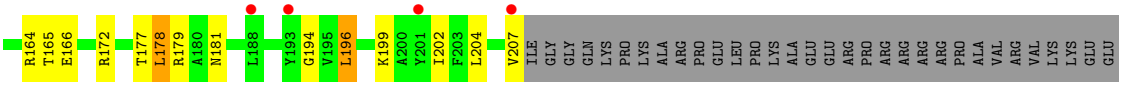


• Molecule 3: 30S Ribosomal Protein S3

Chain AC:



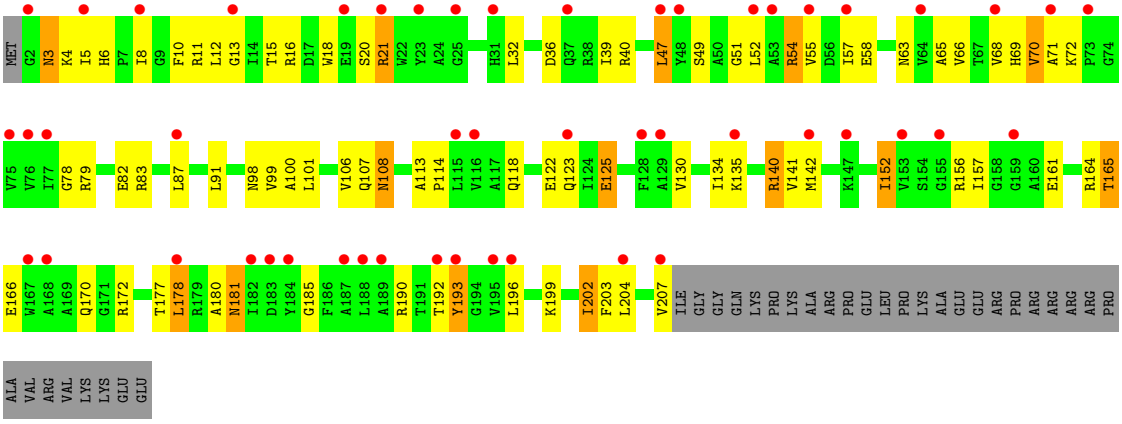




• Molecule 3: 30S Ribosomal Protein S3

Chain CC:

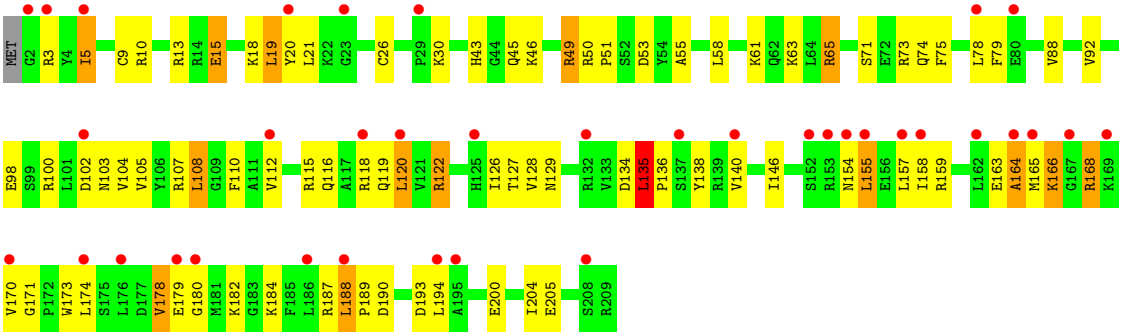




• Molecule 4: 30S Ribosomal Protein S4

Chain AD:

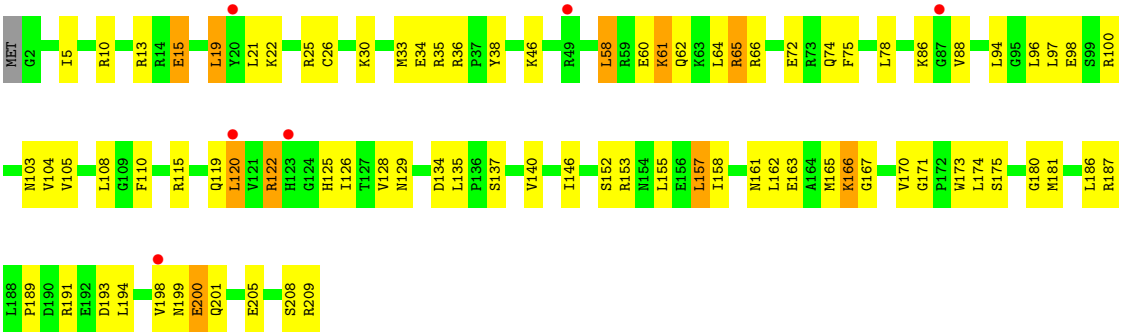




• Molecule 4: 30S Ribosomal Protein S4

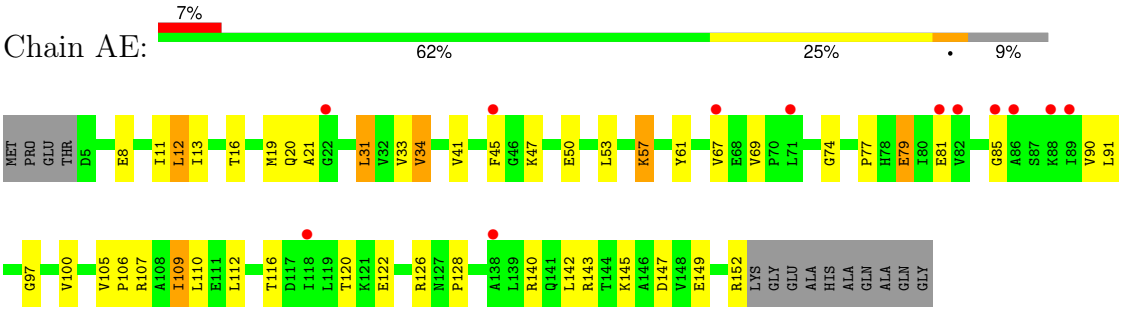
Chain CD:





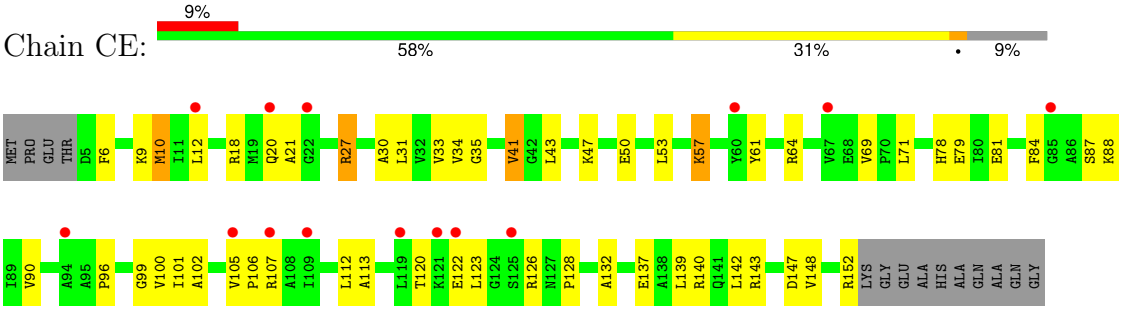
• Molecule 5: 30S Ribosomal Protein S5

Chain AE:



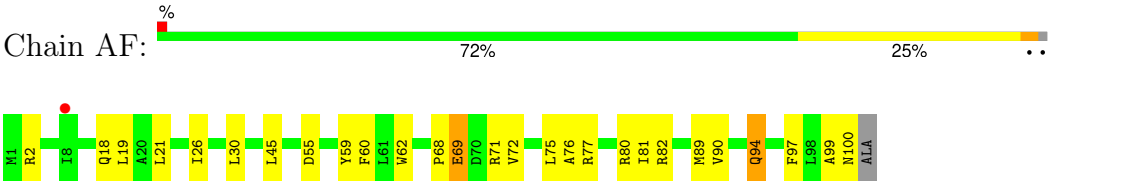
• Molecule 5: 30S Ribosomal Protein S5

Chain CE:



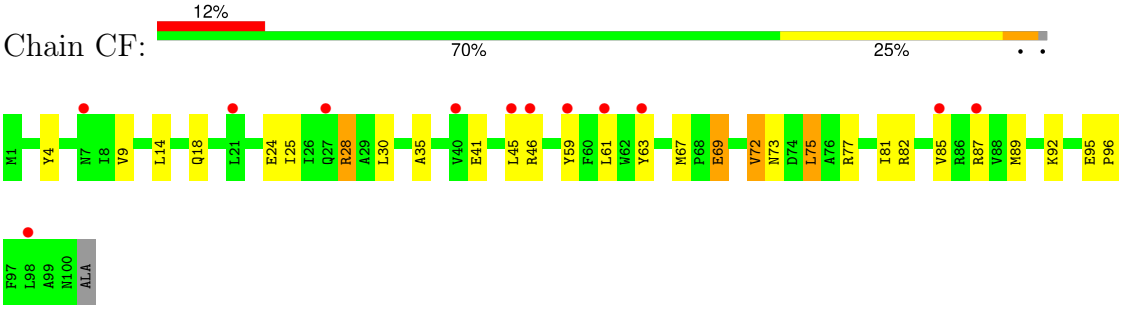
• Molecule 6: 30S Ribosomal Protein S6

Chain AF:



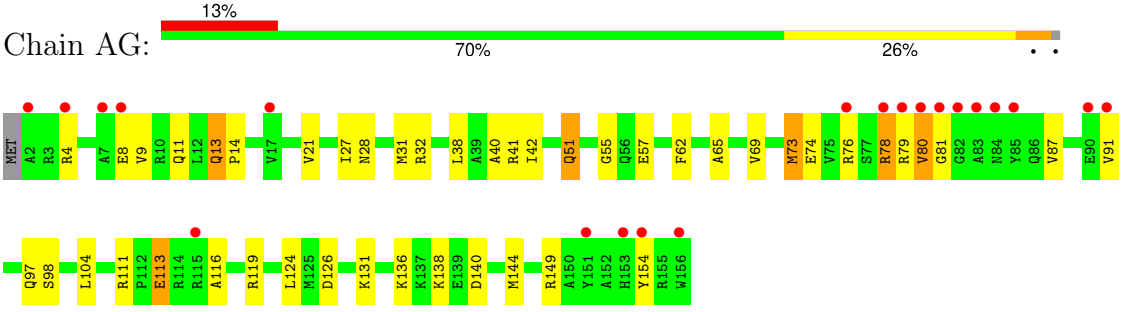
• Molecule 6: 30S Ribosomal Protein S6

Chain CF:



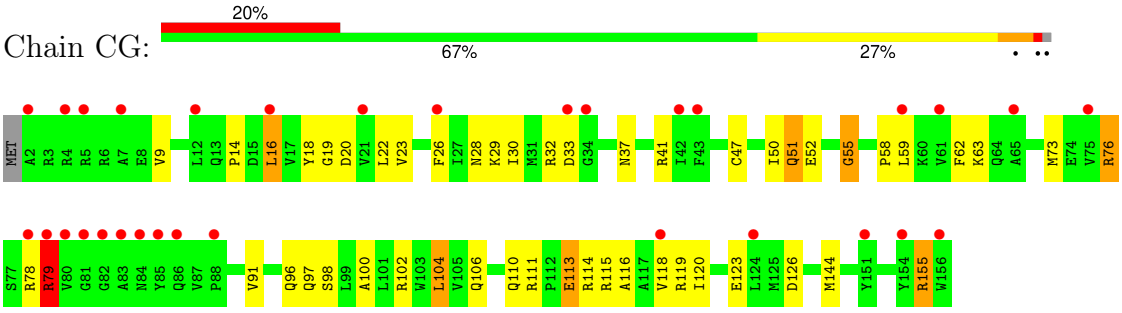
• Molecule 7: 30S Ribosomal Protein S7

Chain AG:



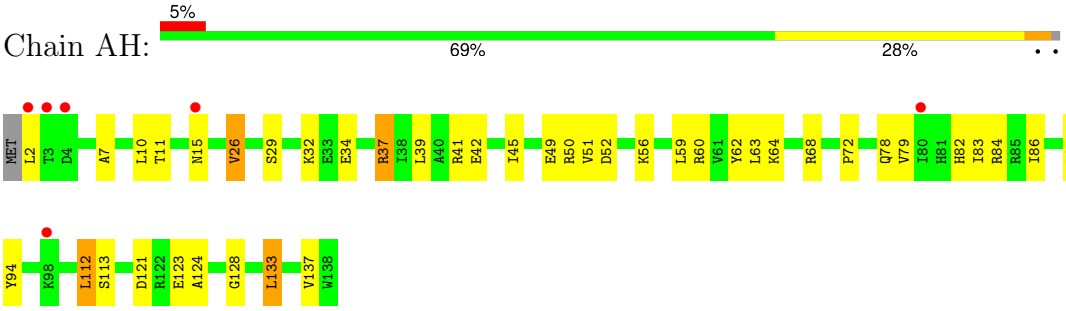
• Molecule 7: 30S Ribosomal Protein S7

Chain CG:



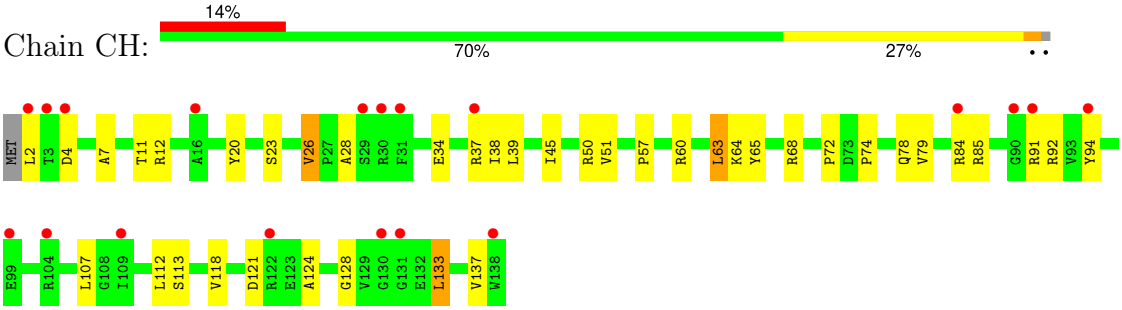
• Molecule 8: 30S Ribosomal Protein S8

Chain AH:



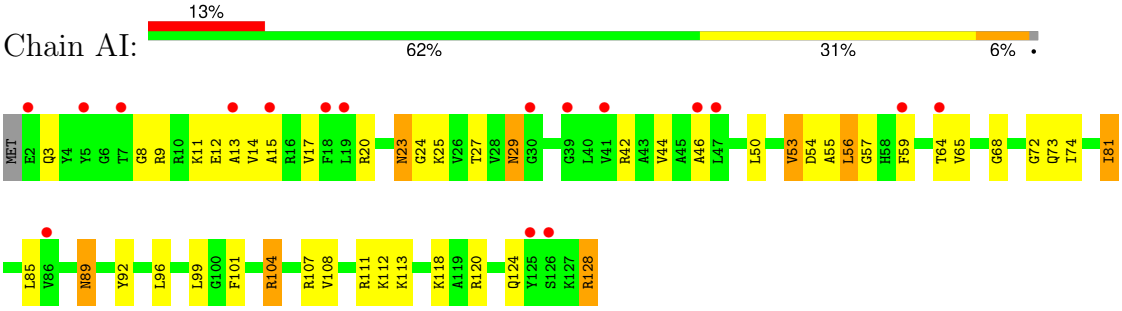
• Molecule 8: 30S Ribosomal Protein S8

Chain CH:



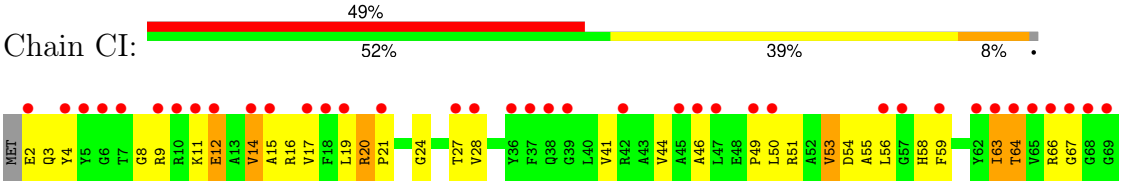
• Molecule 9: 30S Ribosomal Protein S9

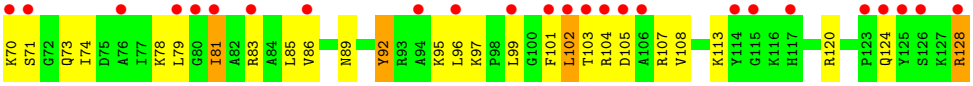
Chain AI:



• Molecule 9: 30S Ribosomal Protein S9

Chain CI:

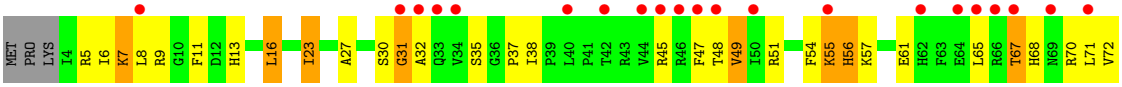


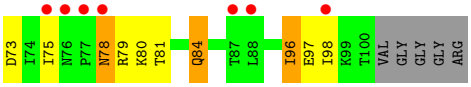


• Molecule 10: 30S Ribosomal Protein S10

Chain AJ:

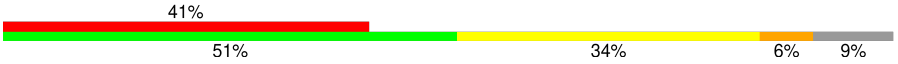


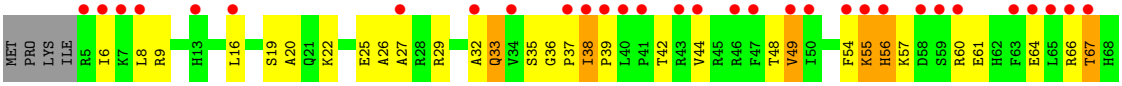


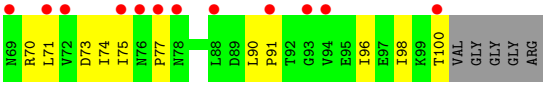


• Molecule 10: 30S Ribosomal Protein S10

Chain CJ:



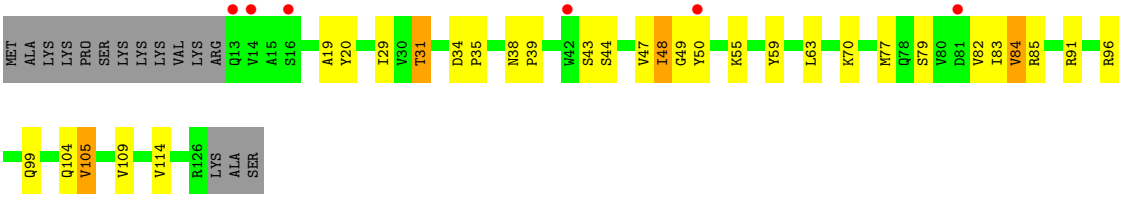




• Molecule 11: 30S Ribosomal Protein S11

Chain AK:

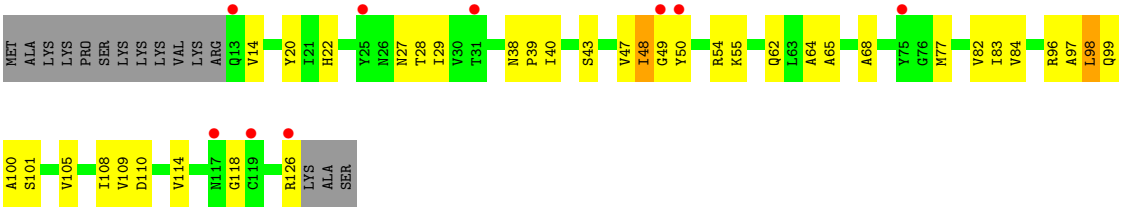




• Molecule 11: 30S Ribosomal Protein S11

Chain CK:





• Molecule 12: 30S Ribosomal Protein S12

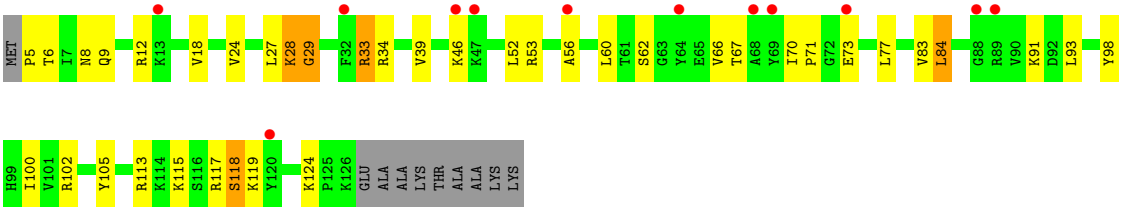
Chain AL:





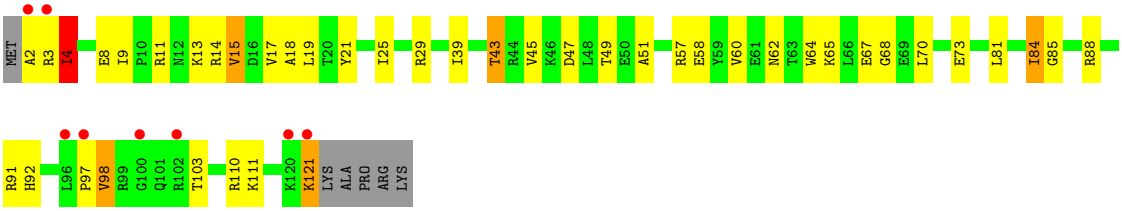
• Molecule 12: 30S Ribosomal Protein S12





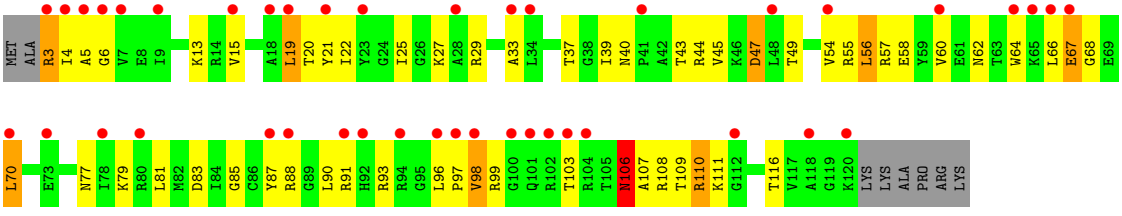
• Molecule 13: 30S Ribosomal Protein S13





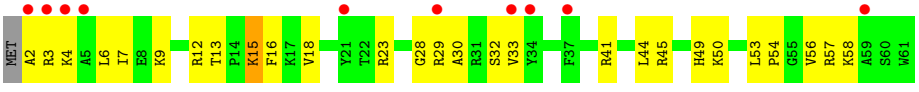
• Molecule 13: 30S Ribosomal Protein S13





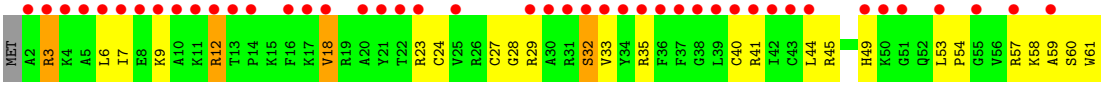
• Molecule 14: 30S Ribosomal Protein S14





• Molecule 14: 30S Ribosomal Protein S14

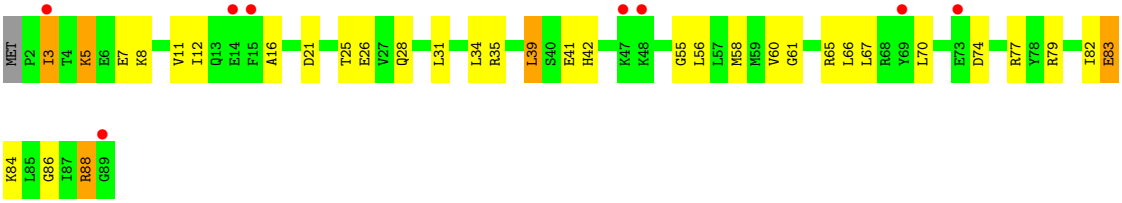




• Molecule 15: 30S Ribosomal Protein S15

Chain AO:

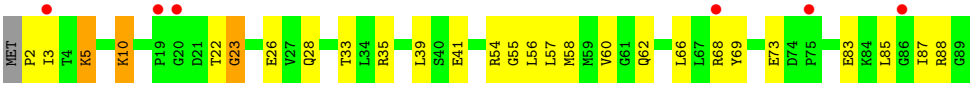




• Molecule 15: 30S Ribosomal Protein S15

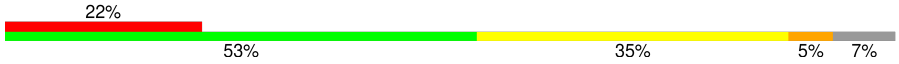
Chain CO:

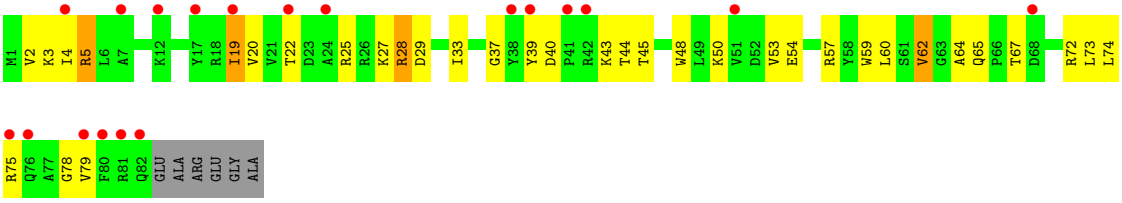




• Molecule 16: 30S Ribosomal Protein S16

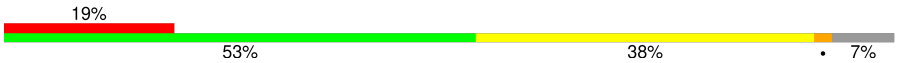
Chain AP:

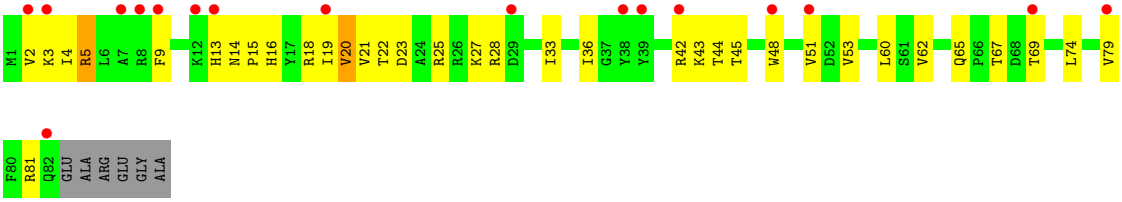




• Molecule 16: 30S Ribosomal Protein S16

Chain CP:

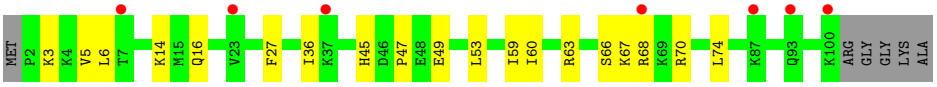




• Molecule 17: 30S Ribosomal Protein S17

Chain AQ:

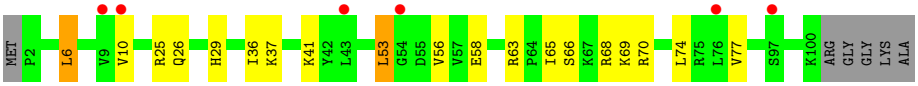




• Molecule 17: 30S Ribosomal Protein S17

Chain CQ:

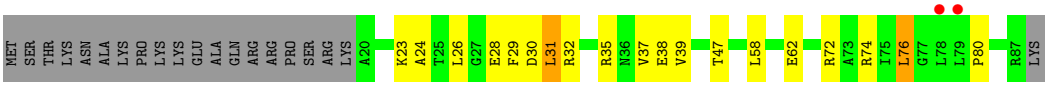




• Molecule 18: 30S Ribosomal Protein S18

Chain AR:

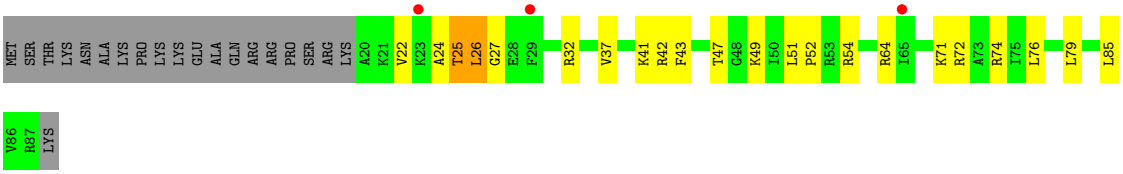




• Molecule 18: 30S Ribosomal Protein S18

Chain CR:

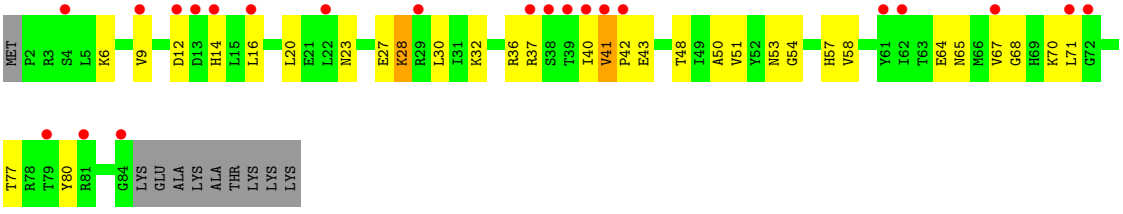




• Molecule 19: 30S Ribosomal Protein S19

Chain AS:

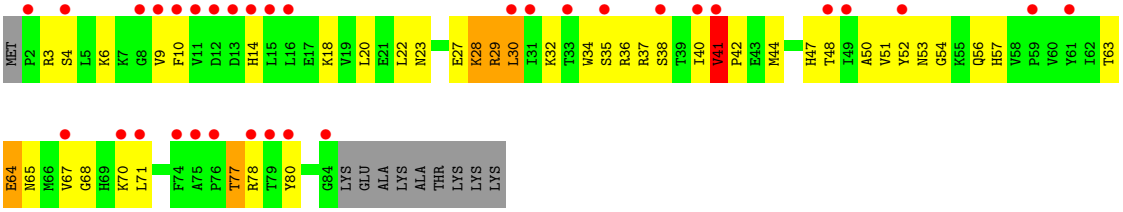




• Molecule 19: 30S Ribosomal Protein S19

Chain CS:

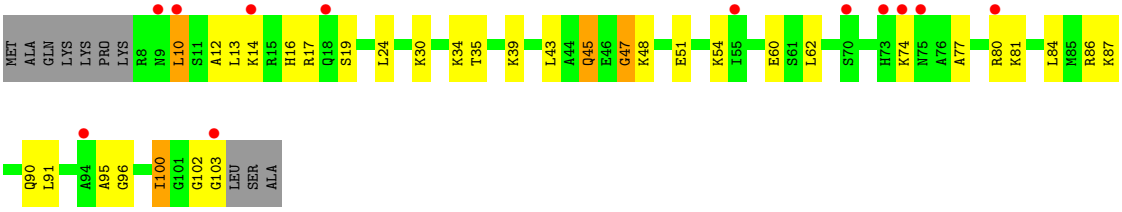




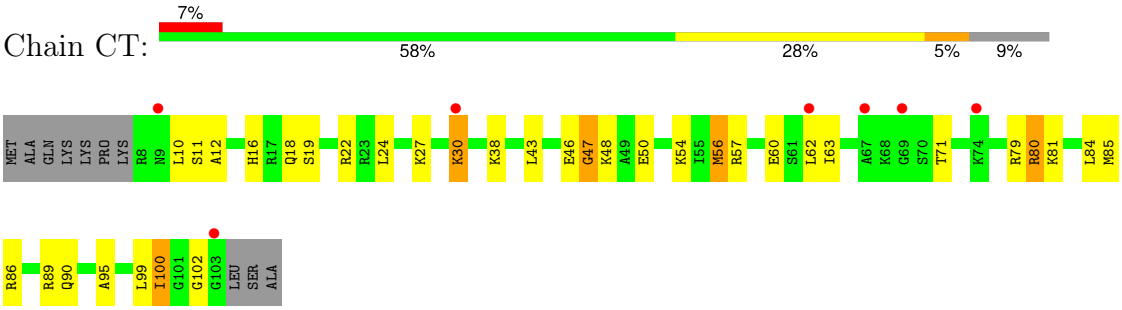
• Molecule 20: 30S Ribosomal Protein S20

Chain AT:

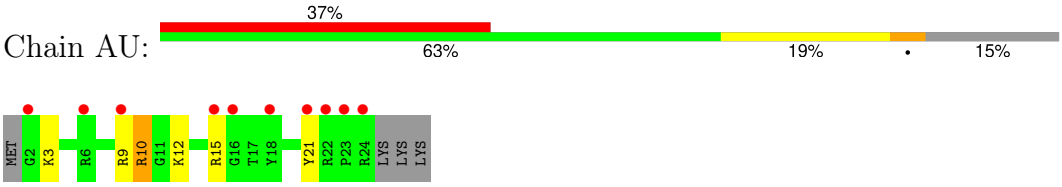




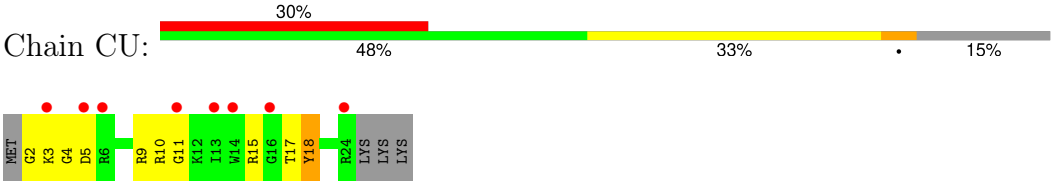
• Molecule 20: 30S Ribosomal Protein S20



• Molecule 21: 30S Ribosomal Protein THX



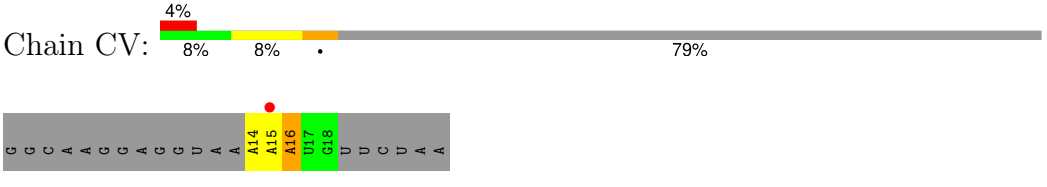
• Molecule 21: 30S Ribosomal Protein THX



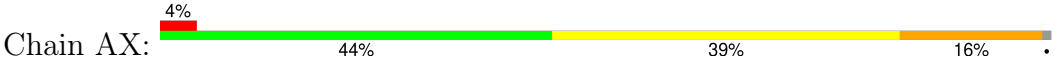
• Molecule 22: mRNA

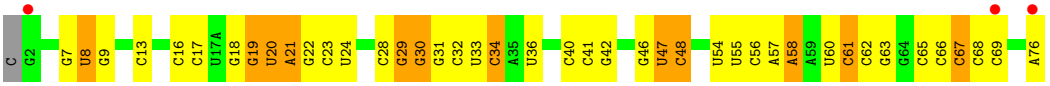


• Molecule 22: mRNA



• Molecule 23: P-site tRNA

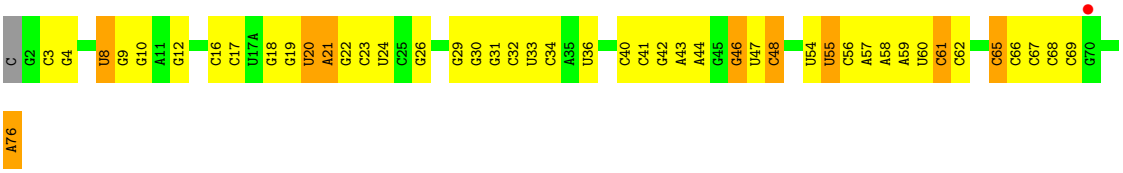




• Molecule 23: P-site tRNA

Chain CX:

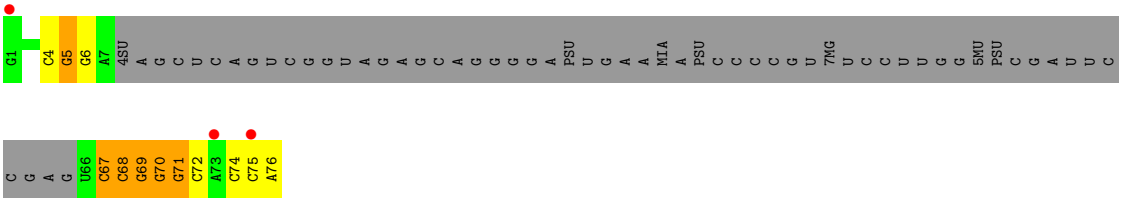




• Molecule 24: E-site tRNA Acceptor Stem

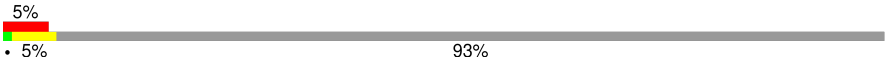
Chain AY:





• Molecule 24: E-site tRNA Acceptor Stem

Chain CY:

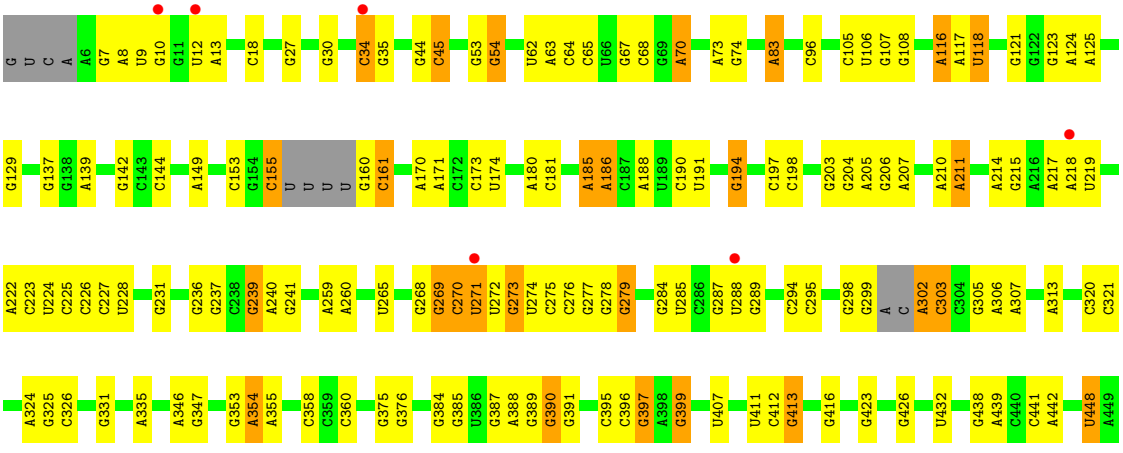


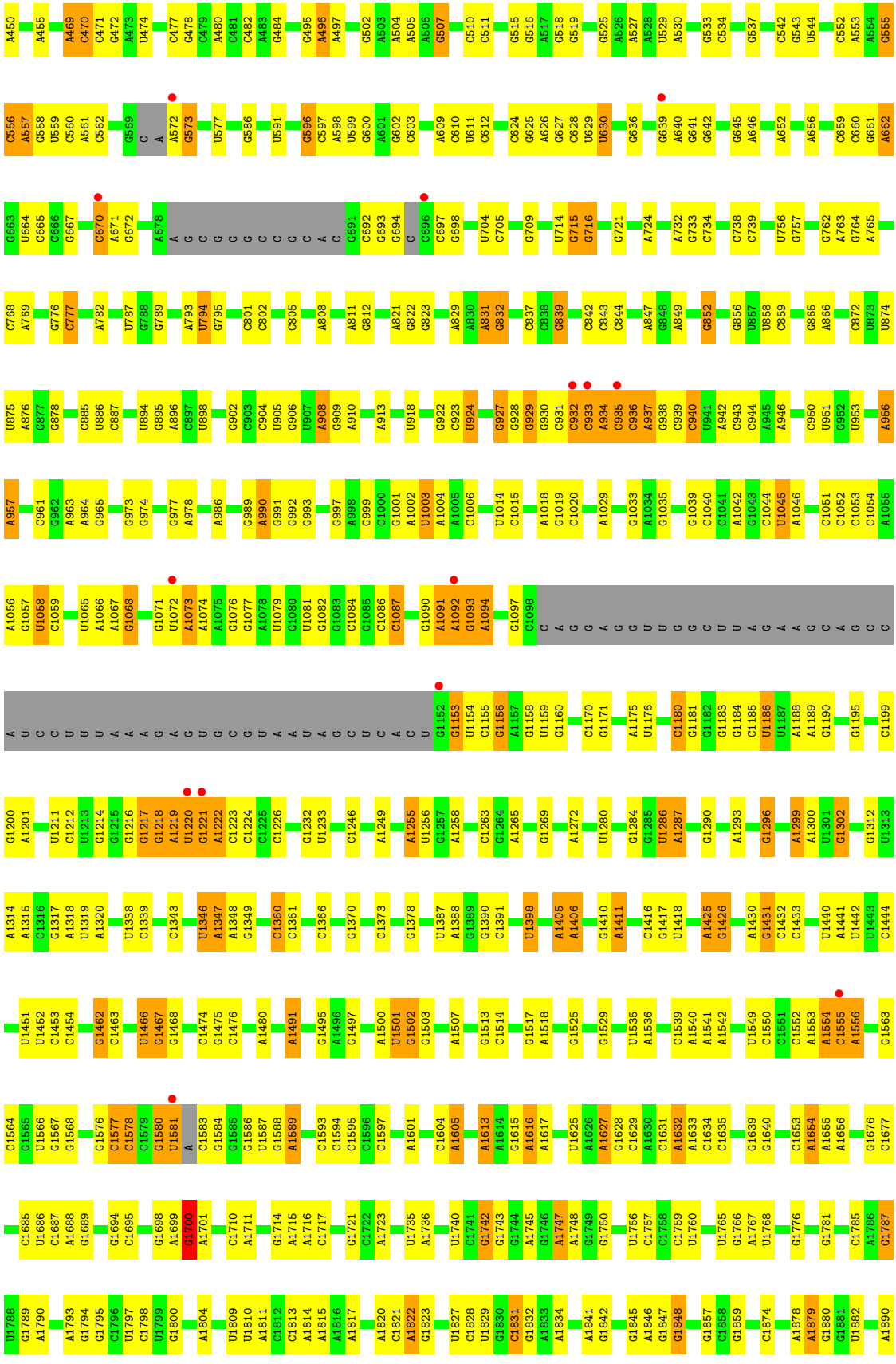


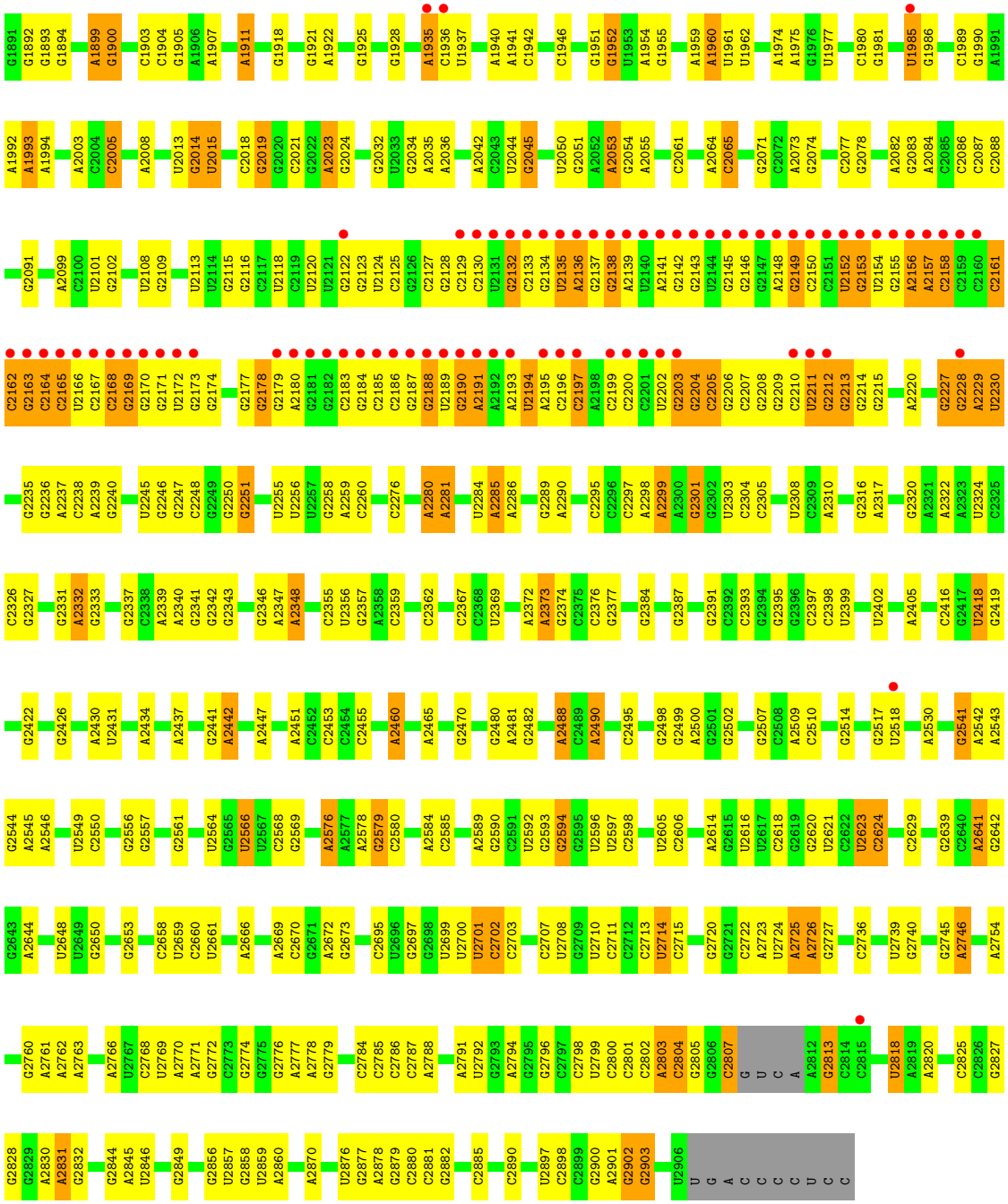
• Molecule 25: 23S Ribosomal RNA

Chain BA:





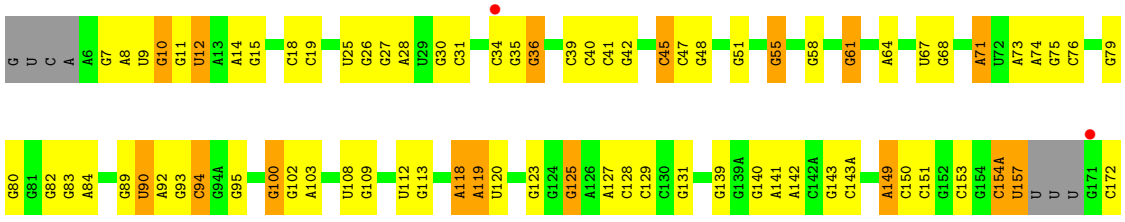


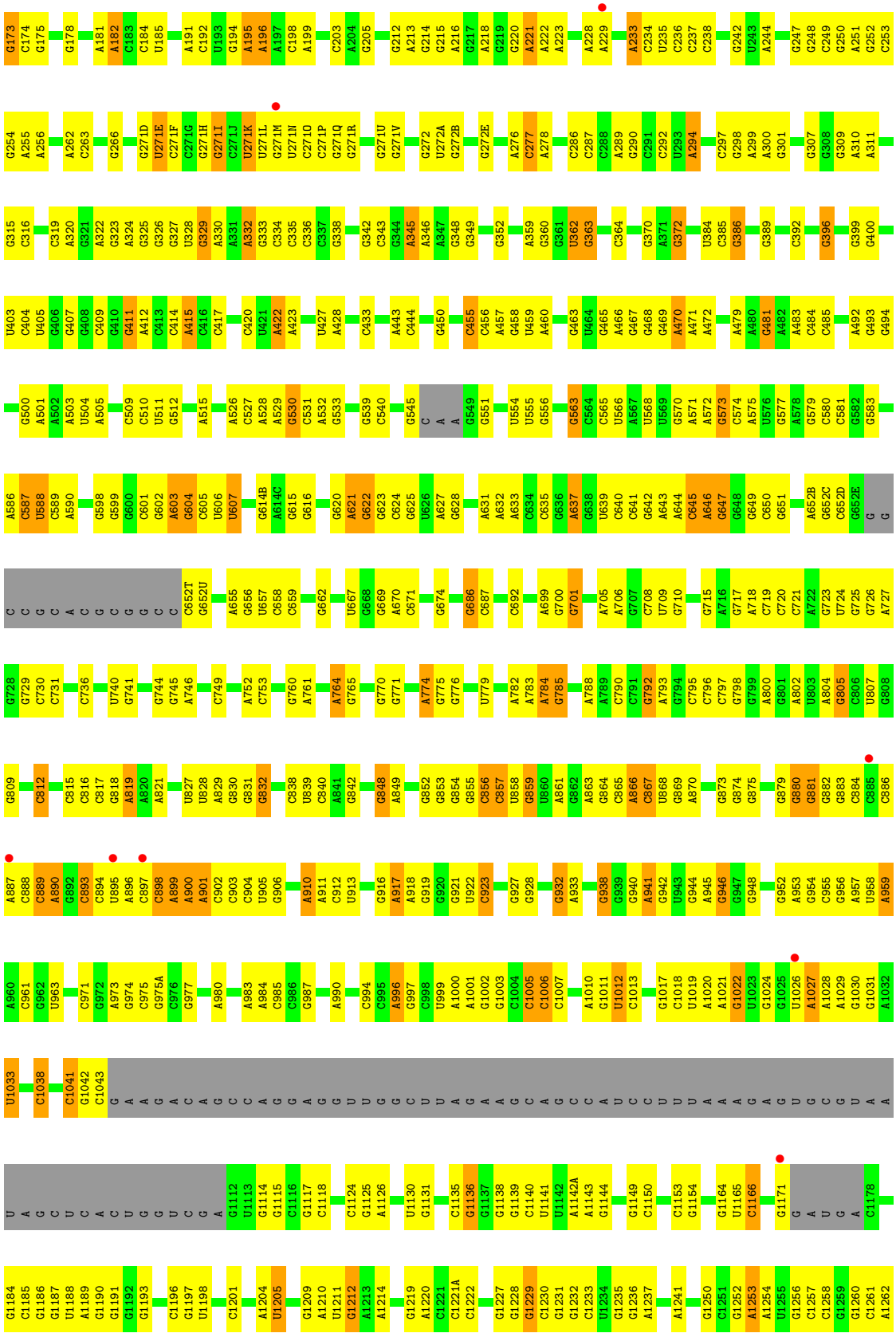


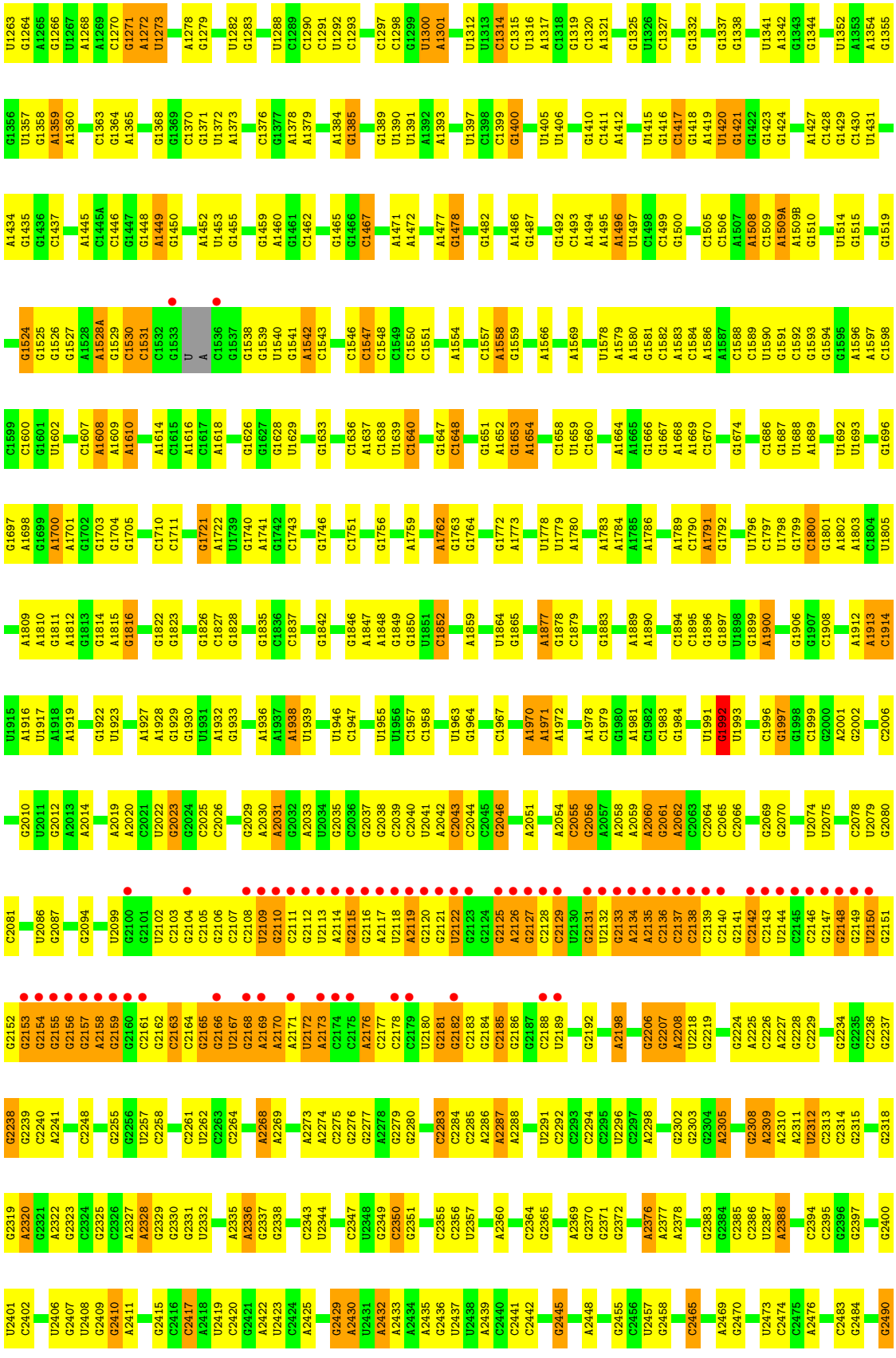
• Molecule 25: 23S Ribosomal RNA

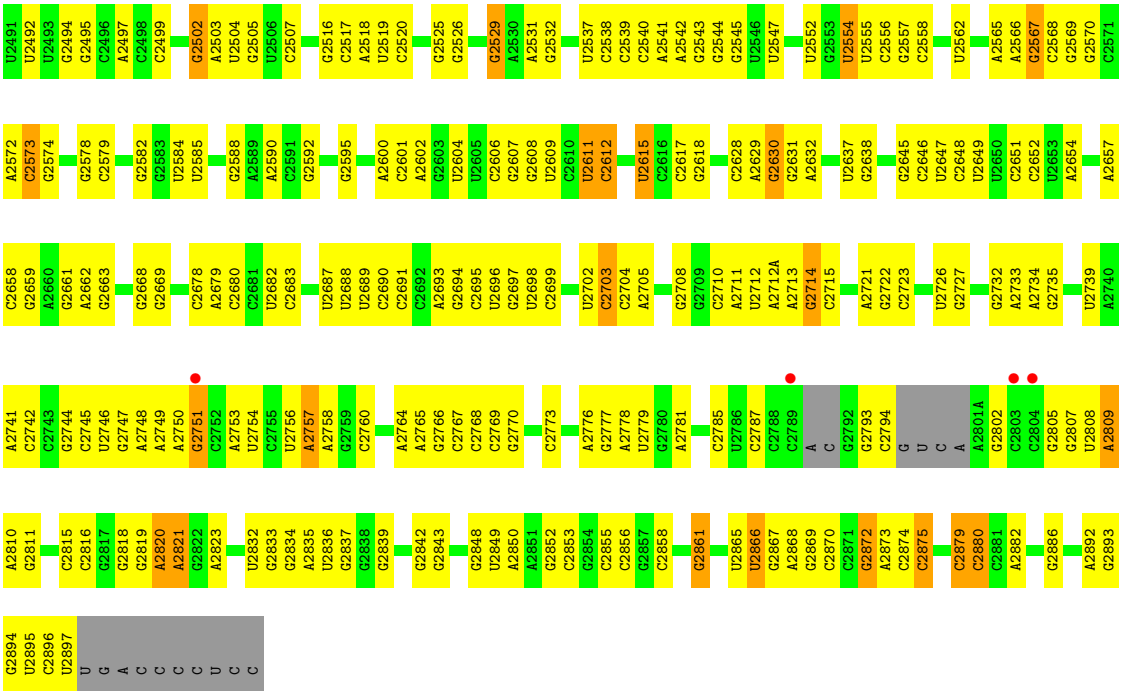
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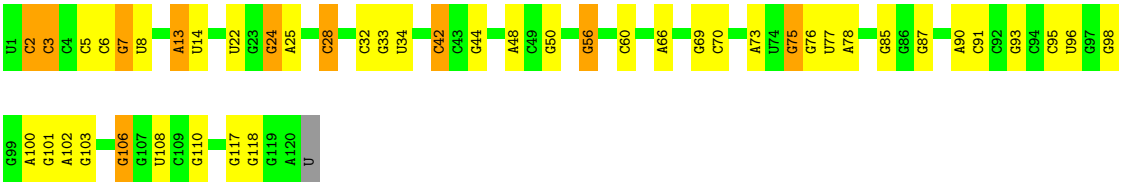




• Molecule 26: 5S Ribosomal RNA

Chain BB:

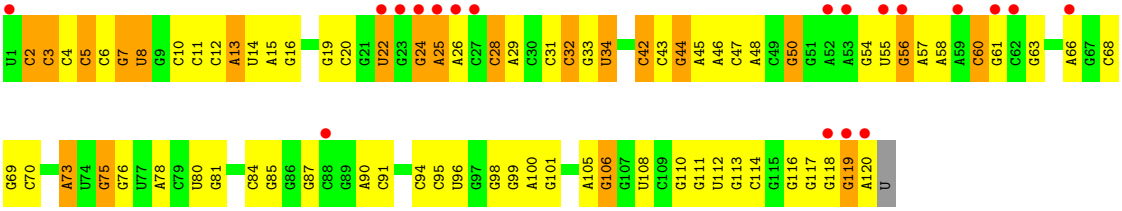




• Molecule 26: 5S Ribosomal RNA

Chain DB:

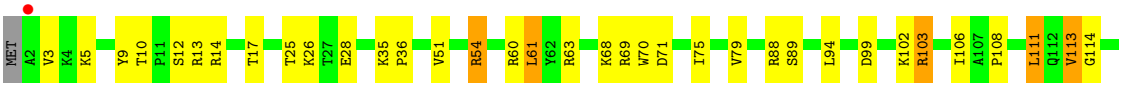


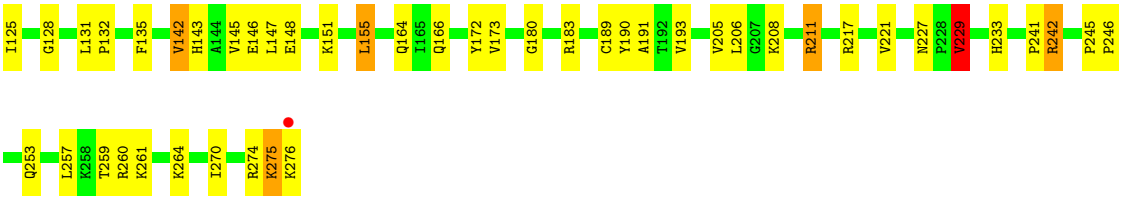


• Molecule 27: 50S Ribosomal Protein L2

Chain BD:



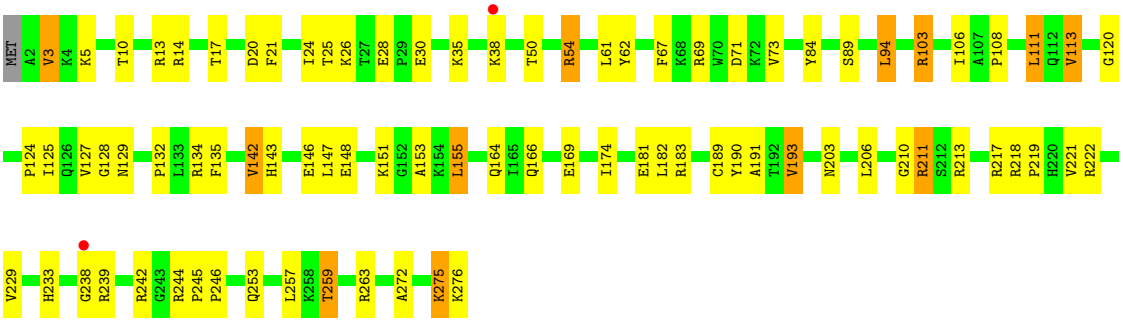




• Molecule 27: 50S Ribosomal Protein L2

Chain DD:

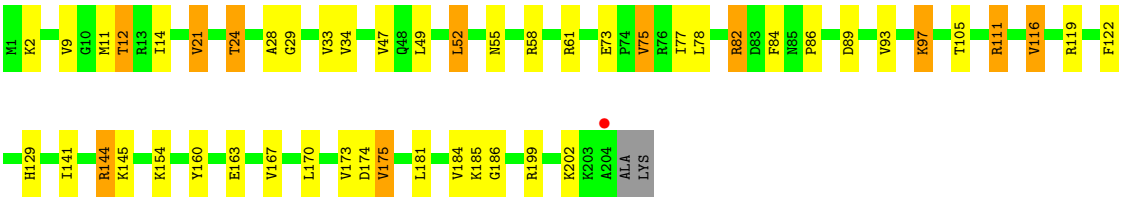




• Molecule 28: 50S Ribosomal Protein L3

Chain BE:

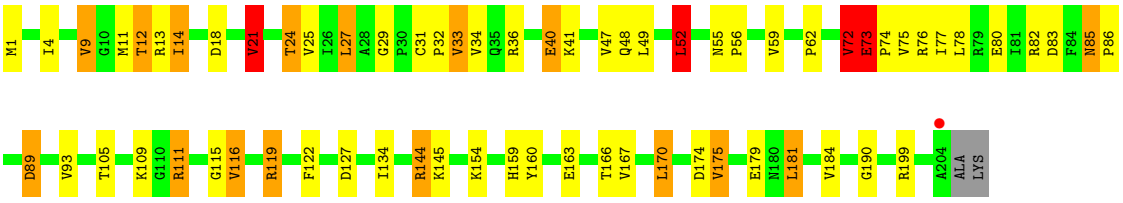




• Molecule 28: 50S Ribosomal Protein L3

Chain DE:



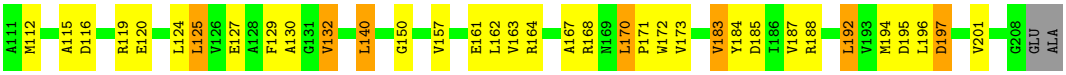


• Molecule 29: 50S Ribosomal Protein L4

Chain BF:



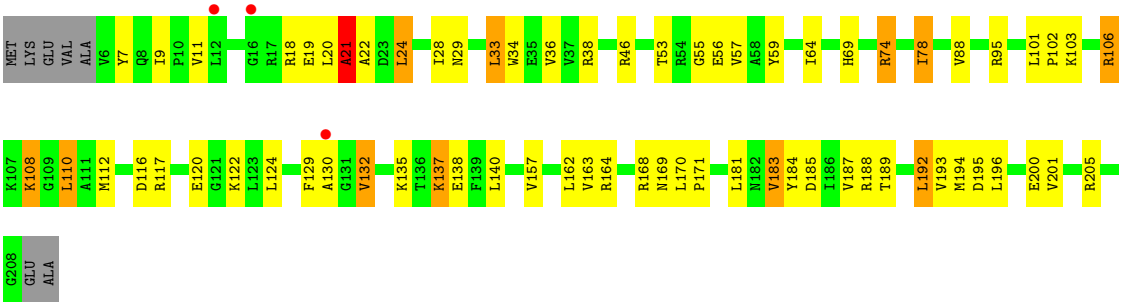




• Molecule 29: 50S Ribosomal Protein L4

Chain DF:

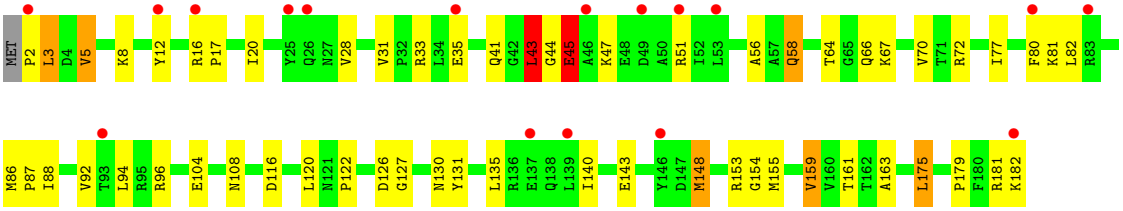




• Molecule 30: 50S Ribosomal Protein L5

Chain BG:

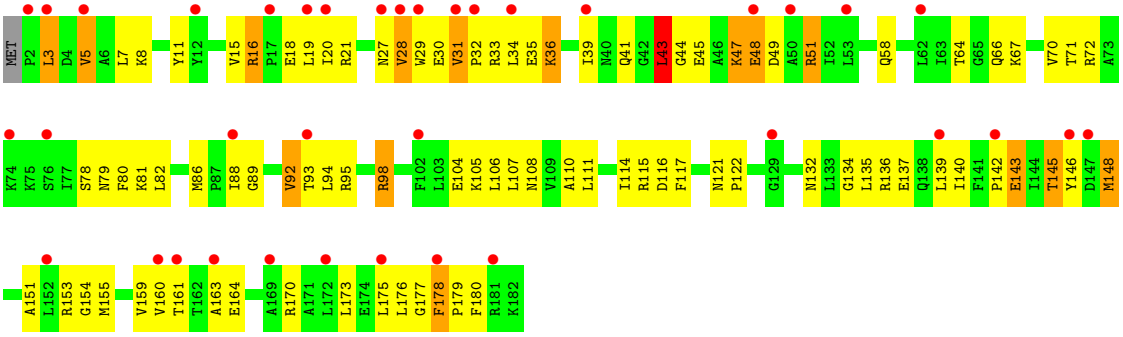




• Molecule 30: 50S Ribosomal Protein L5

Chain DG:

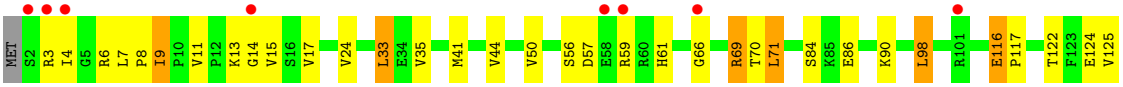




• Molecule 31: 50S Ribosomal Protein L6

Chain BH:





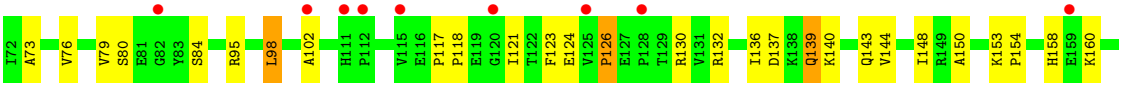


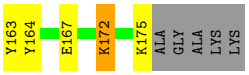
• Molecule 31: 50S Ribosomal Protein L6

Chain DH:





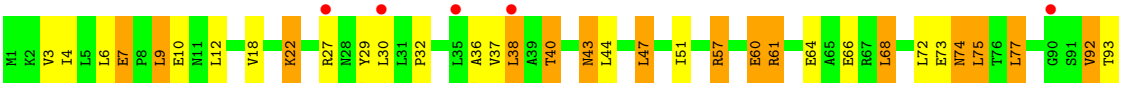


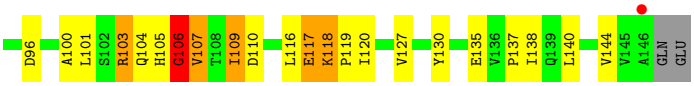


• Molecule 32: 50S Ribosomal Protein L9

Chain BI:



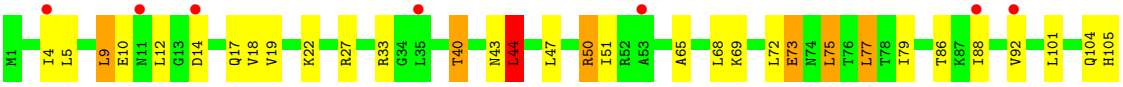


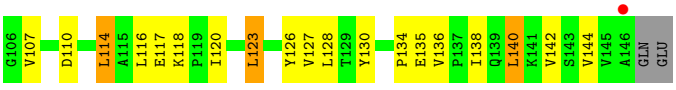


• Molecule 32: 50S Ribosomal Protein L9

Chain DI:



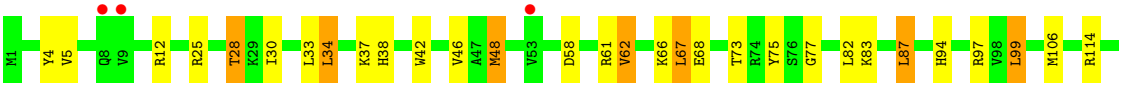


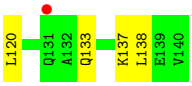


• Molecule 33: 50S Ribosomal Protein L13

Chain BN:

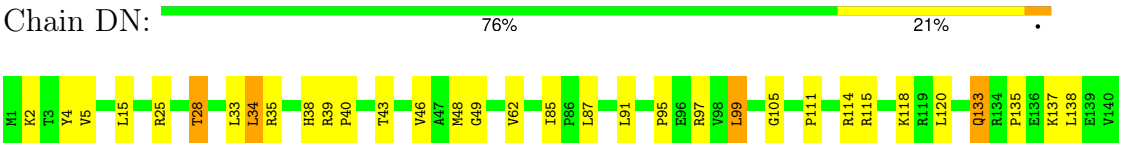






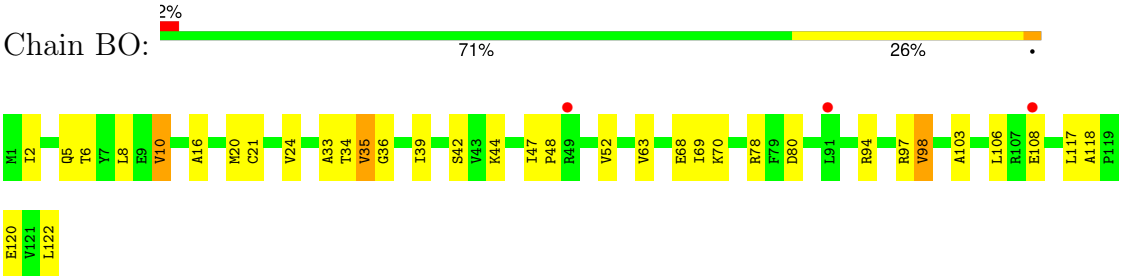
• Molecule 33: 50S Ribosomal Protein L13

Chain DN:



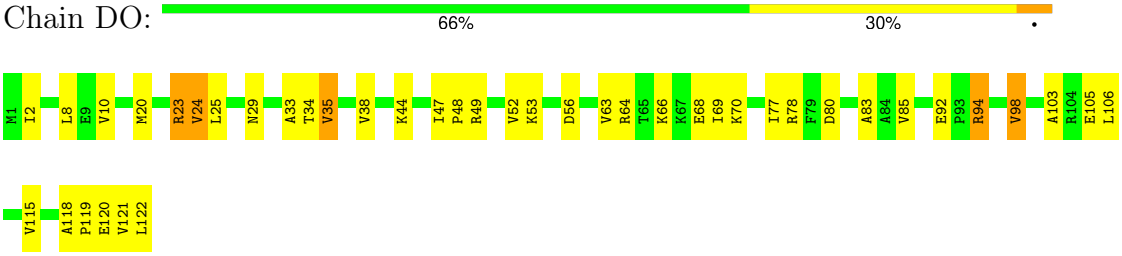
• Molecule 34: 50S Ribosomal Protein L14

Chain BO:



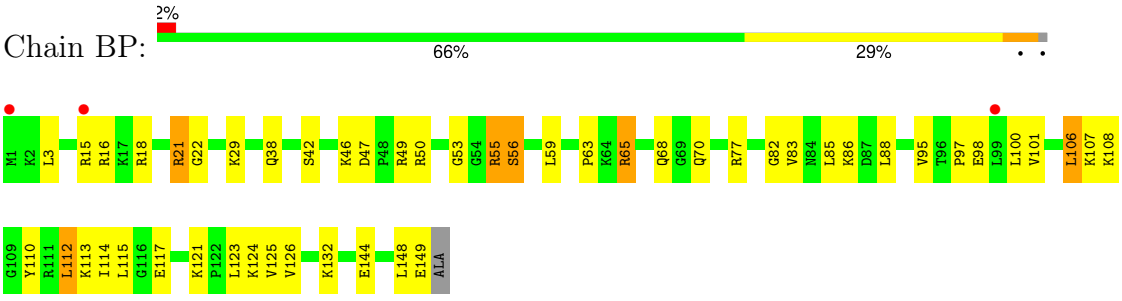
• Molecule 34: 50S Ribosomal Protein L14

Chain DO:



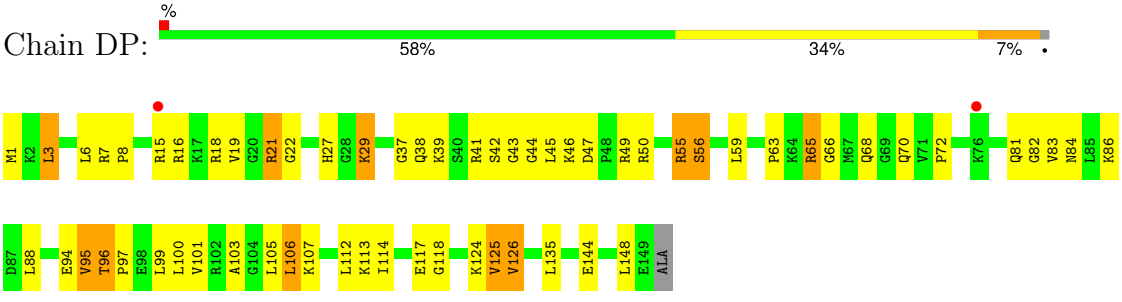
• Molecule 35: 50S Ribosomal Protein L15

Chain BP:



• Molecule 35: 50S Ribosomal Protein L15

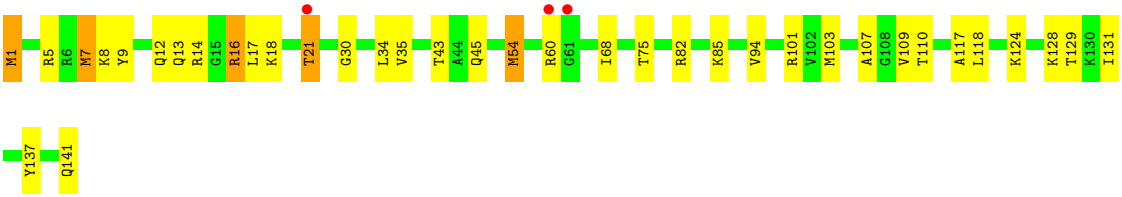
Chain DP:



• Molecule 36: 50S Ribosomal Protein L16

Chain BQ:

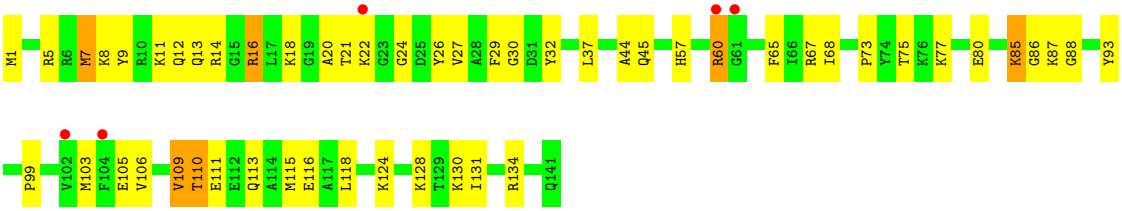




• Molecule 36: 50S Ribosomal Protein L16

Chain DQ:

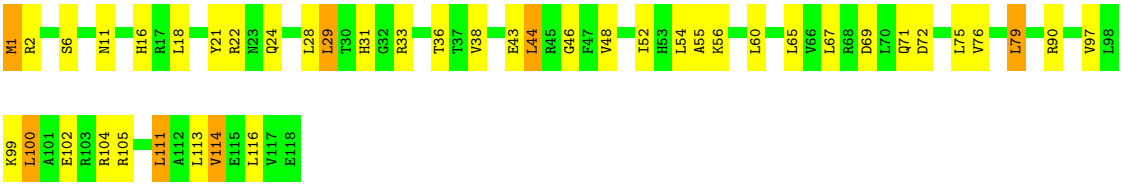




• Molecule 37: 50S Ribosomal Protein L17

Chain BR:

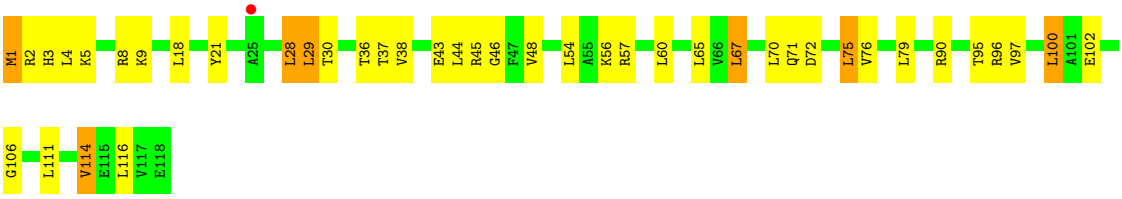




• Molecule 37: 50S Ribosomal Protein L17

Chain DR:

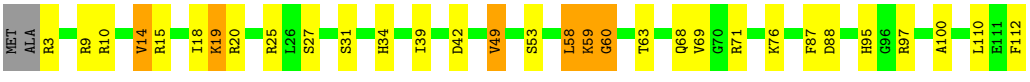




• Molecule 38: 50S Ribosomal Protein L18

Chain BS:

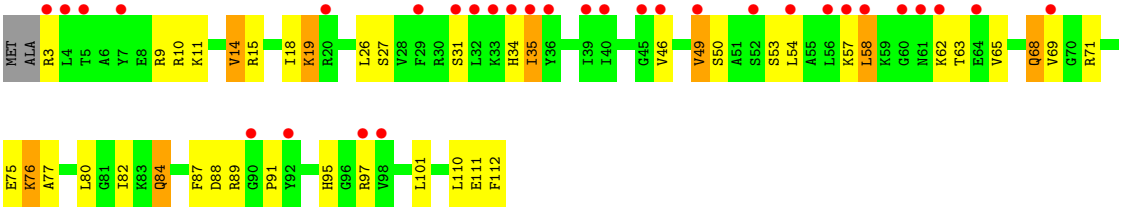




• Molecule 38: 50S Ribosomal Protein L18

Chain DS:

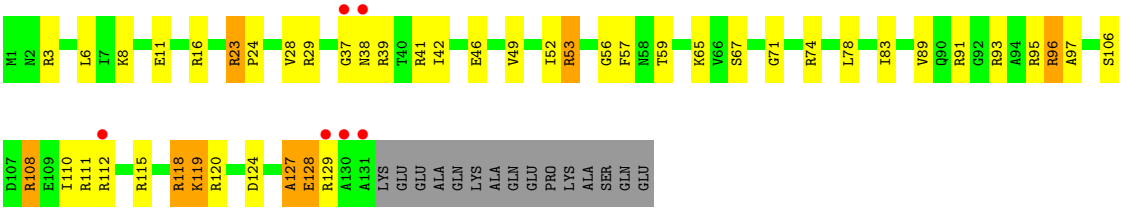




• Molecule 39: 50S Ribosomal Protein L19

Chain BT:

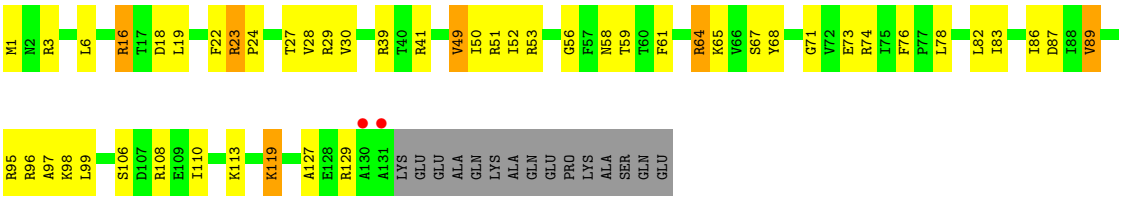




• Molecule 39: 50S Ribosomal Protein L19

Chain DT:

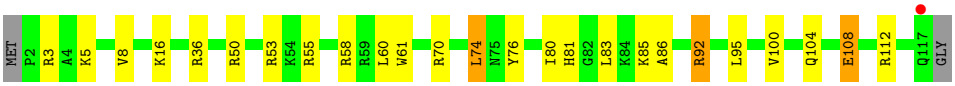




• Molecule 40: 50S Ribosomal Protein L20

Chain BU:

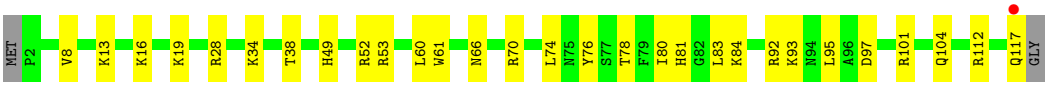




• Molecule 40: 50S Ribosomal Protein L20

Chain DU:

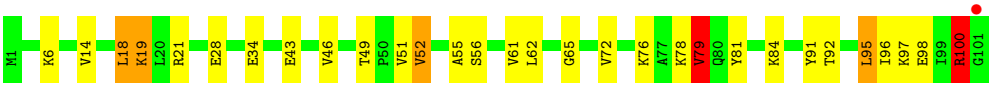




• Molecule 41: 50S Ribosomal Protein L21

Chain BV:

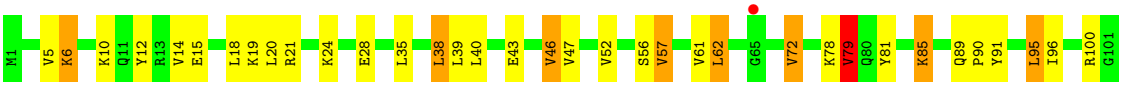




• Molecule 41: 50S Ribosomal Protein L21

Chain DV:

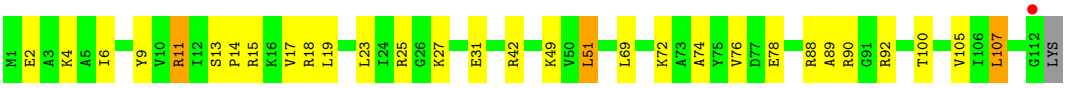




• Molecule 42: 50S Ribosomal Protein L22

Chain BW:

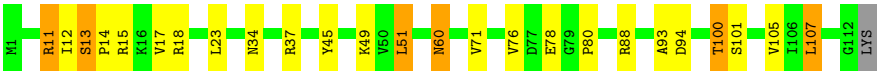




• Molecule 42: 50S Ribosomal Protein L22

Chain DW:

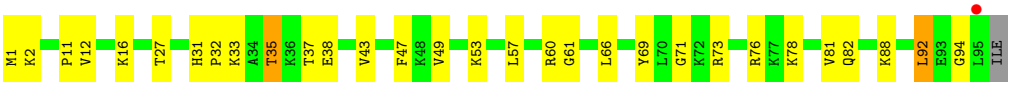




• Molecule 43: 50S Ribosomal Protein L23

Chain BX:

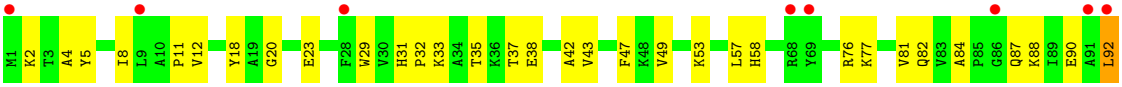




• Molecule 43: 50S Ribosomal Protein L23

Chain DX:



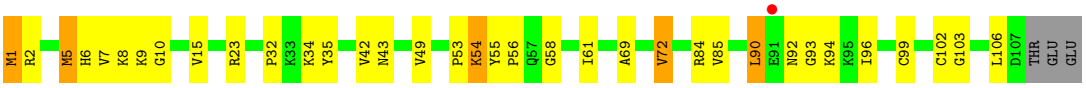




• Molecule 44: 50S Ribosomal Protein L24

Chain BY:

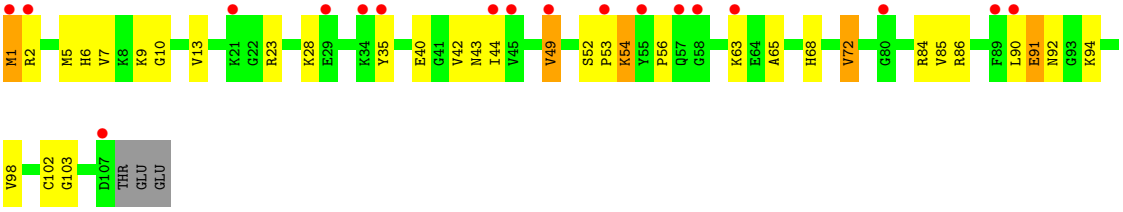




• Molecule 44: 50S Ribosomal Protein L24

Chain DY:

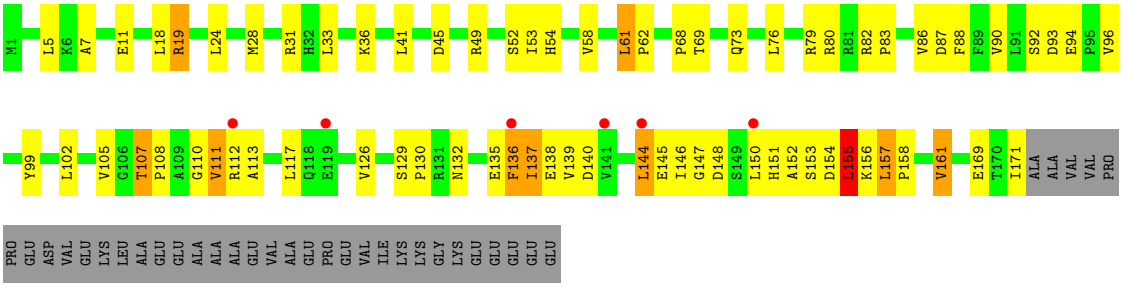




• Molecule 45: 50S Ribosomal Protein L25

Chain BZ:

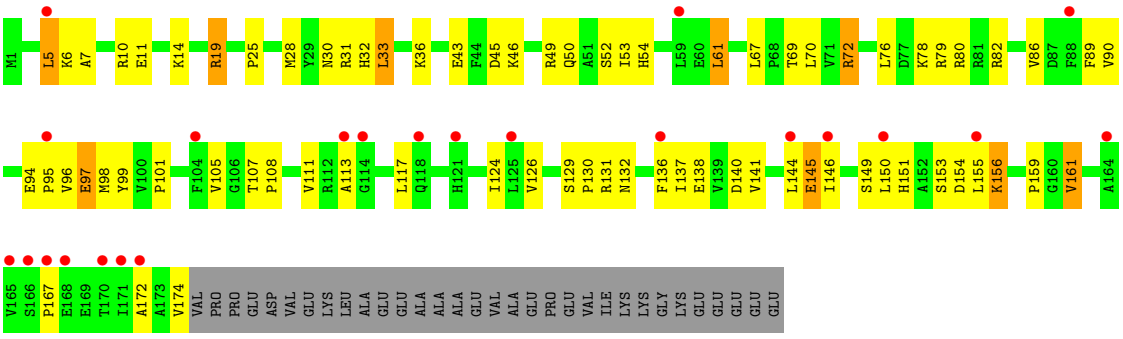




• Molecule 45: 50S Ribosomal Protein L25

Chain DZ:





• Molecule 46: 50S Ribosomal Protein L27

Chain B0:

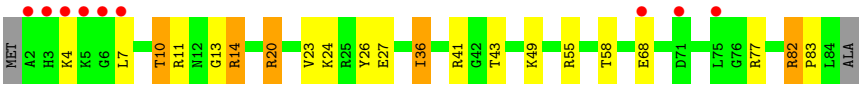




• Molecule 46: 50S Ribosomal Protein L27

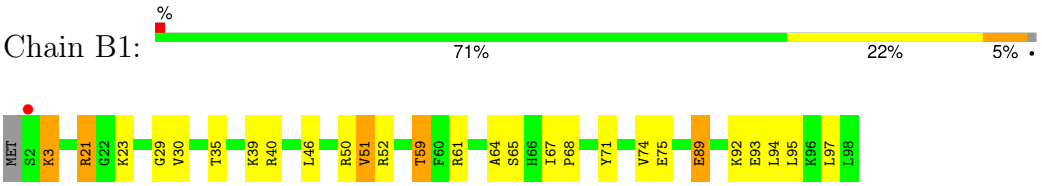
Chain D0:





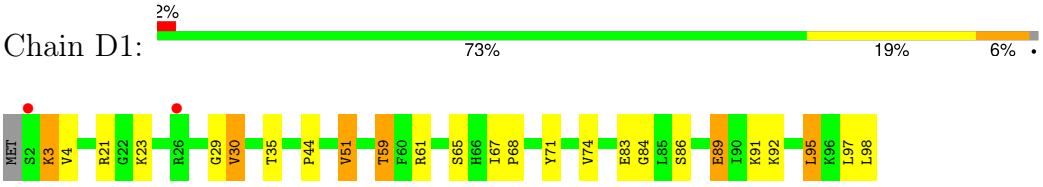
• Molecule 47: 50S Ribosomal Protein L28

Chain B1:



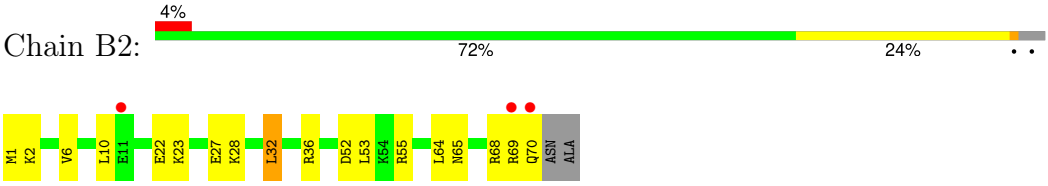
• Molecule 47: 50S Ribosomal Protein L28

Chain D1:



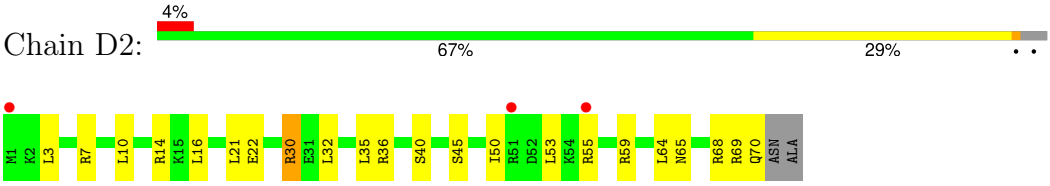
• Molecule 48: 50S Ribosomal Protein L29

Chain B2:



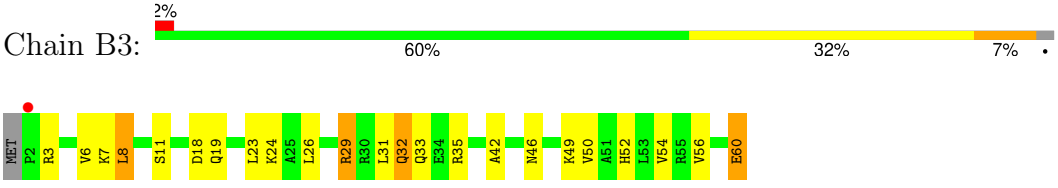
• Molecule 48: 50S Ribosomal Protein L29

Chain D2:



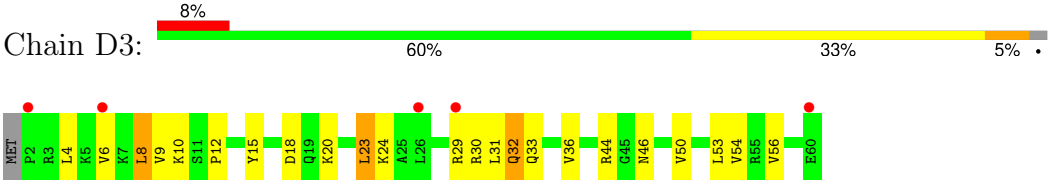
• Molecule 49: 50S Ribosomal Protein L30

Chain B3:



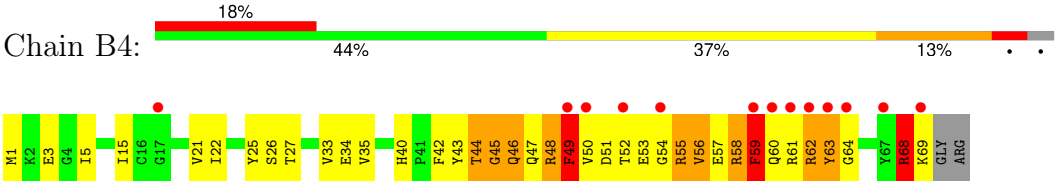
• Molecule 49: 50S Ribosomal Protein L30

Chain D3:



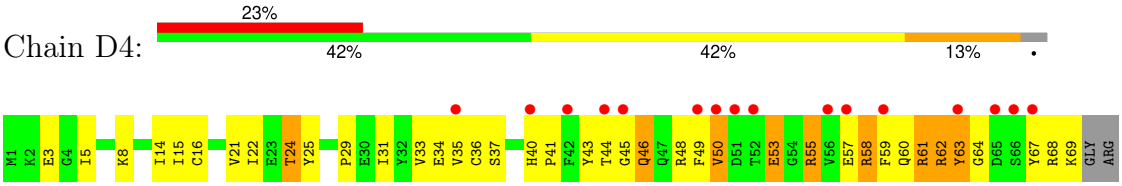
• Molecule 50: 50S Ribosomal Protein L31

Chain B4:



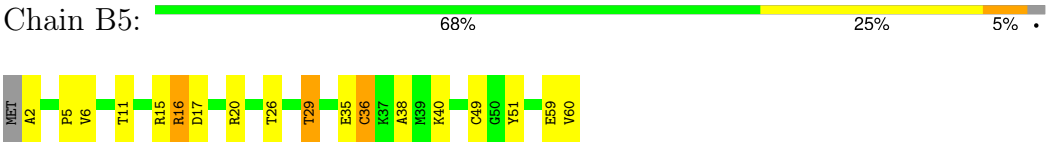
• Molecule 50: 50S Ribosomal Protein L31

Chain D4:



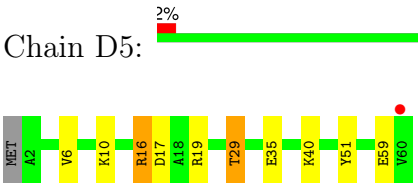
• Molecule 51: 50S Ribosomal Protein L32

Chain B5:



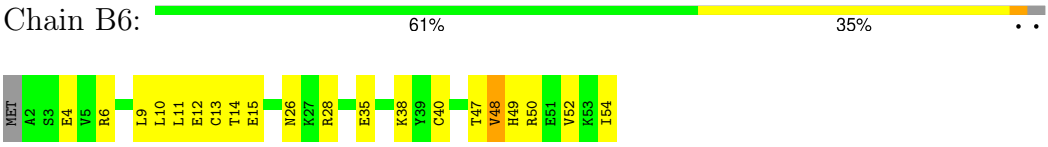
• Molecule 51: 50S Ribosomal Protein L32

Chain D5:



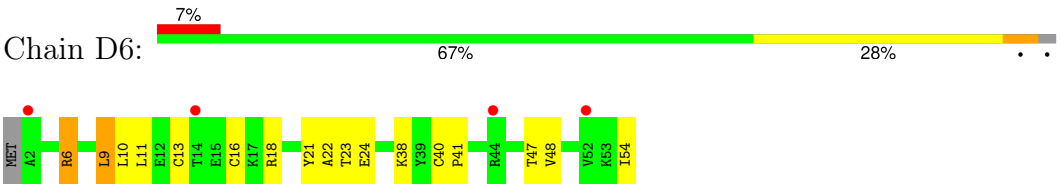
• Molecule 52: 50S Ribosomal Protein L33

Chain B6:



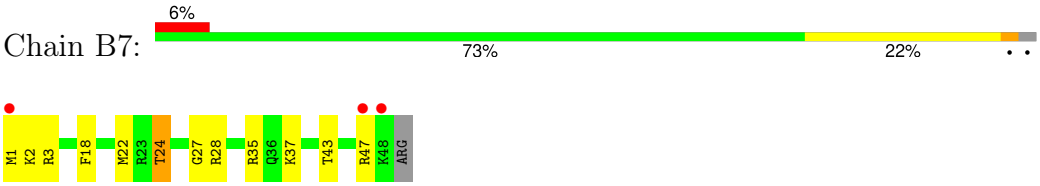
• Molecule 52: 50S Ribosomal Protein L33

Chain D6:



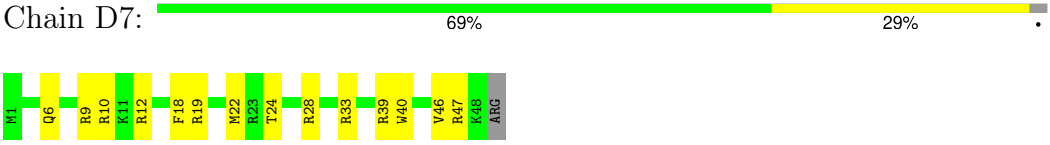
• Molecule 53: 50S Ribosomal Protein L34

Chain B7:



• Molecule 53: 50S Ribosomal Protein L34

Chain D7:



• Molecule 54: 50S Ribosomal Protein L35

Chain B8:

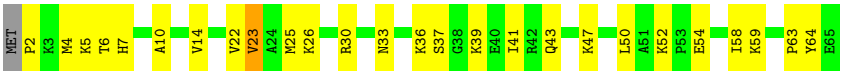




• Molecule 54: 50S Ribosomal Protein L35

Chain D8:

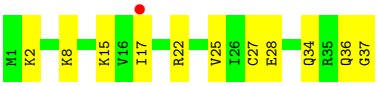




• Molecule 55: 50S Ribosomal Protein L36

Chain B9:

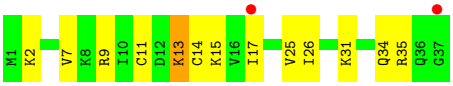




• Molecule 55: 50S Ribosomal Protein L36

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	208.93Å 446.95Å 619.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	144.86 – 2.70 144.86 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.6 (144.86-2.70) 99.6 (144.86-2.70)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.32 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.215 , 0.262 0.216 , 0.263	Depositor DCC
R_{free} test set	78302 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	53.5	Xtriage
Anisotropy	0.258	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 55.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	290807	wwPDB-VP
Average B, all atoms (Å^2)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.51% 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: MG, ZN, 5MC, PSU, PCY, K, 5MU, SF4, 4SU

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	0.51	14/36024 (0.0%)	0.47	7/56222 (0.0%)
1	CA	0.24	0/36170	0.46	1/56452 (0.0%)
2	AB	0.43	0/1881	1.03	10/2542 (0.4%)
2	CB	0.45	0/1860	1.05	8/2518 (0.3%)
3	AC	0.40	0/1576	0.88	2/2130 (0.1%)
3	CC	0.43	0/1566	0.99	4/2119 (0.2%)
4	AD	0.42	0/1689	0.89	2/2267 (0.1%)
4	CD	0.40	0/1704	0.87	2/2284 (0.1%)
5	AE	0.42	0/1145	0.87	0/1543
5	CE	0.42	0/1149	0.97	3/1548 (0.2%)
6	AF	0.39	0/819	0.80	0/1111
6	CF	0.42	0/829	0.84	0/1123
7	AG	0.39	0/1250	0.86	0/1679
7	CG	0.38	0/1254	0.93	2/1683 (0.1%)
8	AH	0.40	0/1108	0.87	0/1494
8	CH	0.38	0/1108	0.87	0/1494
9	AI	0.37	0/1002	0.87	2/1346 (0.1%)
9	CI	0.43	0/997	0.95	5/1343 (0.4%)
10	AJ	0.42	0/722	0.93	0/982
10	CJ	0.48	0/727	1.02	2/988 (0.2%)
11	AK	0.43	0/844	0.88	0/1145
11	CK	0.39	0/848	0.90	1/1149 (0.1%)
12	AL	0.42	0/946	0.82	0/1274
12	CL	0.41	0/946	0.94	4/1274 (0.3%)
13	AM	0.38	0/947	0.92	1/1272 (0.1%)
13	CM	0.41	0/930	0.87	0/1250
14	AN	0.37	0/501	0.93	2/664 (0.3%)
14	CN	0.38	0/501	0.84	0/664
15	AO	0.41	0/739	0.86	0/985
15	CO	0.37	0/739	0.82	0/985
16	AP	0.41	0/697	0.83	0/939
16	CP	0.42	0/693	0.83	0/935

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	AQ	0.39	0/836	0.81	0/1117
17	CQ	0.35	0/836	0.79	2/1117 (0.2%)
18	AR	0.39	0/560	0.83	0/746
18	CR	0.36	0/560	0.78	0/746
19	AS	0.39	0/667	0.86	0/900
19	CS	0.46	0/661	1.03	3/893 (0.3%)
20	AT	0.39	0/730	0.94	0/965
20	CT	0.40	0/729	0.88	1/965 (0.1%)
21	AU	0.36	0/203	0.83	0/266
21	CU	0.42	0/203	0.88	1/266 (0.4%)
22	AV	0.31	0/188	0.52	0/290
22	CV	0.30	0/122	0.48	0/188
23	AX	0.29	0/1725	0.45	0/2689
23	CX	0.29	0/1725	0.47	0/2689
24	AY	0.28	0/428	0.35	0/661
24	CY	0.26	0/115	0.31	0/176
25	BA	0.37	0/68083	0.51	2/106274 (0.0%)
25	DA	0.28	0/67542	0.48	1/105428 (0.0%)
26	BB	0.29	0/2878	0.45	0/4490
26	DB	0.30	0/2878	0.48	0/4490
27	BD	0.57	0/2186	0.92	3/2944 (0.1%)
27	DD	0.49	0/2186	0.92	3/2944 (0.1%)
28	BE	0.60	0/1592	0.93	2/2149 (0.1%)
28	DE	0.49	0/1592	1.02	11/2149 (0.5%)
29	BF	0.55	0/1619	0.88	0/2193
29	DF	0.45	0/1615	0.95	5/2188 (0.2%)
30	BG	0.43	0/1450	0.90	3/1959 (0.2%)
30	DG	0.43	0/1449	0.98	4/1958 (0.2%)
31	BH	0.48	0/1356	0.88	1/1834 (0.1%)
31	DH	0.42	0/1356	0.93	3/1834 (0.2%)
32	BI	0.44	0/1100	0.95	8/1501 (0.5%)
32	DI	0.41	0/1076	0.88	1/1471 (0.1%)
33	BN	0.53	0/1144	0.84	0/1543
33	DN	0.43	0/1144	0.89	0/1543
34	BO	0.59	0/943	0.88	2/1269 (0.2%)
34	DO	0.46	0/943	0.88	2/1269 (0.2%)
35	BP	0.55	0/1152	0.87	2/1533 (0.1%)
35	DP	0.45	0/1152	1.00	8/1533 (0.5%)
36	BQ	0.57	0/1143	0.84	0/1527
36	DQ	0.46	0/1143	0.88	0/1527
37	BR	0.62	1/982 (0.1%)	0.90	0/1312
37	DR	0.46	0/982	0.81	1/1312 (0.1%)
38	BS	0.47	0/887	0.92	0/1180

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
38	DS	0.44	0/880	0.91	0/1172
39	BT	0.49	0/1105	0.87	0/1477
39	DT	0.44	0/1097	0.84	0/1468
40	BU	0.60	0/977	0.86	0/1301
40	DU	0.41	0/977	0.80	0/1301
41	BV	0.55	0/782	0.88	0/1049
41	DV	0.41	0/782	0.84	0/1049
42	BW	0.67	0/897	0.87	0/1205
42	DW	0.47	0/897	0.83	2/1205 (0.2%)
43	BX	0.55	0/764	0.87	1/1025 (0.1%)
43	DX	0.42	0/764	0.82	0/1025
44	BY	0.50	0/819	0.91	0/1095
44	DY	0.39	0/819	0.91	1/1095 (0.1%)
45	BZ	0.49	0/1379	1.01	5/1873 (0.3%)
45	DZ	0.40	0/1390	0.94	4/1890 (0.2%)
46	B0	0.54	0/662	0.91	1/881 (0.1%)
46	D0	0.40	0/662	0.86	3/881 (0.3%)
47	B1	0.50	0/762	0.82	0/1014
47	D1	0.44	0/762	0.86	0/1014
48	B2	0.49	0/590	0.88	0/781
48	D2	0.35	0/590	0.80	0/781
49	B3	0.54	0/474	0.96	2/635 (0.3%)
49	D3	0.40	0/469	0.88	0/630
50	B4	0.46	0/571	1.07	5/768 (0.7%)
50	D4	0.42	0/545	0.99	3/737 (0.4%)
51	B5	0.62	0/469	0.98	0/635
51	D5	0.45	0/469	0.80	0/635
52	B6	0.65	0/460	0.91	0/613
52	D6	0.45	0/456	0.78	0/608
53	B7	0.61	0/426	0.84	0/561
53	D7	0.52	0/426	0.87	2/561 (0.4%)
54	B8	0.59	0/519	0.87	0/684
54	D8	0.47	0/525	0.81	0/691
55	B9	0.58	0/310	0.91	1/407 (0.2%)
55	D9	0.46	0/310	0.90	0/407
All	All	0.39	15/310558 (0.0%)	0.62	157/464586 (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
1	AA	0	1
7	CG	0	2
38	BS	0	1
50	B4	0	1
50	D4	0	1
All	All	0	6

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	439	A	C5-C4	50.86	2.40	1.38
1	AA	496	A	C6-N1	40.12	2.15	1.35
1	AA	496	A	C2-N3	24.68	1.82	1.33
1	AA	439	A	C5-C6	18.99	1.79	1.41
1	AA	439	A	C6-N1	18.63	1.72	1.35

The worst 5 of 157 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	496	A	C2-N3-C4	16.17	159.12	110.60
1	AA	496	A	N1-C2-N3	-15.00	84.31	129.30
2	CB	231	GLU	CA-C-N	-12.93	107.23	120.03
2	CB	231	GLU	C-N-CA	-12.93	107.23	120.03
1	AA	496	A	C5-C6-N6	-9.80	94.30	123.70

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	439	A	Sidechain
50	B4	59	PHE	Peptide
38	BS	58	LEU	Peptide
7	CG	78	ARG	Peptide
7	CG	79	ARG	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	32183	0	16244	644	0
1	CA	32312	0	16308	680	0
2	AB	1846	0	1867	91	0
2	CB	1825	0	1828	92	0
3	AC	1552	0	1546	53	0
3	CC	1542	0	1517	53	0
4	AD	1659	0	1676	75	0
4	CD	1674	0	1714	54	0
5	AE	1129	0	1185	32	0
5	CE	1133	0	1191	37	0
6	AF	806	0	793	19	0
6	CF	816	0	808	17	0
7	AG	1231	0	1238	25	0
7	CG	1235	0	1249	39	0
8	AH	1088	0	1126	28	0
8	CH	1088	0	1126	26	0
9	AI	983	0	986	31	0
9	CI	978	0	966	47	0
10	AJ	709	0	650	35	0
10	CJ	714	0	672	34	0
11	AK	829	0	825	21	0
11	CK	833	0	836	18	0
12	AL	930	0	980	25	0
12	CL	930	0	980	28	0
13	AM	937	0	977	28	0
13	CM	920	0	950	37	0
14	AN	492	0	529	22	0
14	CN	492	0	529	24	0
15	AO	728	0	760	23	0
15	CO	728	0	760	23	0
16	AP	681	0	697	23	0
16	CP	677	0	686	17	0
17	AQ	823	0	891	11	0
17	CQ	823	0	891	11	0
18	AR	555	0	618	13	0
18	CR	555	0	618	14	0
19	AS	652	0	662	25	0
19	CS	646	0	644	41	0
20	AT	728	0	798	21	0
20	CT	727	0	796	17	0
21	AU	199	0	208	5	0
21	CU	199	0	208	9	0
22	AV	169	0	86	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	CV	109	0	55	5	0
23	AX	1625	0	828	20	0
23	CX	1625	0	829	26	0
24	AY	385	0	199	11	0
24	CY	104	0	56	6	0
25	BA	60792	0	30653	707	0
25	DA	60311	0	30414	1002	0
26	BB	2573	0	1306	23	0
26	DB	2573	0	1306	73	0
27	BD	2136	0	2218	61	0
27	DD	2136	0	2218	67	0
28	BE	1559	0	1618	26	0
28	DE	1559	0	1618	46	0
29	BF	1584	0	1625	48	0
29	DF	1580	0	1619	52	0
30	BG	1425	0	1443	45	0
30	DG	1424	0	1434	69	0
31	BH	1330	0	1407	24	0
31	DH	1330	0	1407	50	0
32	BI	1085	0	1114	39	0
32	DI	1061	0	1080	30	0
33	BN	1117	0	1183	20	0
33	DN	1117	0	1184	17	0
34	BO	933	0	996	24	0
34	DO	933	0	996	28	0
35	BP	1135	0	1212	34	0
35	DP	1135	0	1212	54	0
36	BQ	1122	0	1179	27	0
36	DQ	1122	0	1179	39	0
37	BR	968	0	1033	22	0
37	DR	968	0	1033	28	0
38	BS	877	0	938	26	0
38	DS	870	0	923	29	0
39	BT	1091	0	1151	38	0
39	DT	1083	0	1136	38	0
40	BU	959	0	1019	18	0
40	DU	959	0	1019	19	0
41	BV	771	0	830	14	0
41	DV	771	0	830	19	0
42	BW	886	0	940	19	0
42	DW	886	0	940	16	0
43	BX	750	0	814	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	DX	750	0	814	19	0
44	BY	806	0	881	22	0
44	DY	806	0	881	22	0
45	BZ	1349	0	1355	46	0
45	DZ	1360	0	1363	47	0
46	B0	653	0	674	15	0
46	D0	653	0	674	23	0
47	B1	755	0	826	23	0
47	D1	755	0	826	19	0
48	B2	588	0	643	10	0
48	D2	588	0	643	12	0
49	B3	469	0	518	11	0
49	D3	464	0	514	12	0
50	B4	558	0	544	37	0
50	D4	532	0	503	26	0
51	B5	455	0	465	10	0
51	D5	455	0	465	8	0
52	B6	453	0	473	9	0
52	D6	449	0	469	10	0
53	B7	418	0	467	9	0
53	D7	418	0	467	9	0
54	B8	511	0	571	22	0
54	D8	517	0	582	17	0
55	B9	307	0	335	9	0
55	D9	307	0	335	7	0
56	AA	190	0	0	0	0
56	AD	1	0	0	0	0
56	AE	3	0	0	0	0
56	AF	1	0	0	0	0
56	AM	1	0	0	0	0
56	AN	1	0	0	0	0
56	AQ	1	0	0	0	0
56	AX	9	0	0	0	0
56	B0	5	0	0	0	0
56	B2	1	0	0	0	0
56	B3	1	0	0	0	0
56	B4	1	0	0	0	0
56	B5	4	0	0	0	0
56	B6	2	0	0	0	0
56	B7	5	0	0	0	0
56	B8	2	0	0	0	0
56	B9	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	BA	814	0	0	0	0
56	BB	22	0	0	0	0
56	BD	9	0	0	0	0
56	BE	7	0	0	0	0
56	BF	9	0	0	0	0
56	BG	2	0	0	0	0
56	BN	7	0	0	0	0
56	BO	1	0	0	0	0
56	BP	4	0	0	0	0
56	BQ	4	0	0	0	0
56	BR	3	0	0	0	0
56	BU	9	0	0	0	0
56	BV	4	0	0	0	0
56	BW	4	0	0	0	0
56	BX	2	0	0	0	0
56	BY	3	0	0	0	0
56	BZ	2	0	0	0	0
56	CA	175	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	CT	1	0	0	0	0
56	CX	2	0	0	0	0
56	D0	2	0	0	0	0
56	D1	1	0	0	0	0
56	D3	1	0	0	0	0
56	D8	1	0	0	0	0
56	DA	674	0	0	0	0
56	DB	10	0	0	0	0
56	DD	8	0	0	0	0
56	DE	5	0	0	0	0
56	DF	5	0	0	0	0
56	DG	1	0	0	0	0
56	DN	1	0	0	0	0
56	DO	1	0	0	0	0
56	DP	2	0	0	0	0
56	DQ	3	0	0	0	0
56	DR	1	0	0	0	0
56	DU	4	0	0	0	0
56	DV	3	0	0	0	0
56	DW	2	0	0	0	0
56	DY	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	AA	40	0	38	6	0
57	CA	40	0	38	4	0
58	AD	8	0	0	1	0
58	CD	8	0	0	0	0
59	AN	1	0	0	0	0
59	B4	1	0	0	0	0
59	B5	1	0	0	0	0
59	B6	1	0	0	0	0
59	B9	1	0	0	0	0
59	BY	1	0	0	0	0
59	CN	1	0	0	0	0
59	D4	1	0	0	0	0
59	D5	1	0	0	0	0
59	D6	1	0	0	0	0
59	D9	1	0	0	0	0
59	DY	1	0	0	0	0
60	AX	1	0	0	0	0
60	CX	1	0	0	0	0
61	AA	175	0	0	13	0
61	AJ	2	0	0	0	0
61	AL	1	0	0	0	0
61	AM	1	0	0	0	0
61	AO	1	0	0	0	0
61	AV	1	0	0	0	0
61	AX	8	0	0	0	0
61	B0	4	0	0	0	0
61	B1	1	0	0	0	0
61	B3	1	0	0	0	0
61	B5	4	0	0	1	0
61	B6	1	0	0	0	0
61	B7	1	0	0	0	0
61	B8	10	0	0	1	0
61	BA	1294	0	0	49	0
61	BB	34	0	0	1	0
61	BD	16	0	0	1	0
61	BE	12	0	0	1	0
61	BF	7	0	0	1	0
61	BG	3	0	0	0	0
61	BI	1	0	0	0	0
61	BN	1	0	0	0	0
61	BO	4	0	0	0	0
61	BP	15	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	BQ	5	0	0	0	0
61	BR	1	0	0	0	0
61	BU	2	0	0	0	0
61	BV	2	0	0	0	0
61	BW	3	0	0	0	0
61	BX	5	0	0	0	0
61	CA	137	0	0	12	0
61	CD	1	0	0	0	0
61	CJ	2	0	0	0	0
61	CL	1	0	0	1	0
61	CN	1	0	0	0	0
61	CT	1	0	0	0	0
61	CX	2	0	0	0	0
61	D0	7	0	0	0	0
61	D1	1	0	0	0	0
61	D3	1	0	0	0	0
61	D8	4	0	0	0	0
61	DA	924	0	0	75	0
61	DB	8	0	0	0	0
61	DD	18	0	0	3	0
61	DE	9	0	0	1	0
61	DF	5	0	0	0	0
61	DN	1	0	0	0	0
61	DO	1	0	0	0	0
61	DP	14	0	0	1	0
61	DR	1	0	0	0	0
61	DT	1	0	0	0	0
61	DU	3	0	0	0	0
61	DV	1	0	0	0	0
61	DW	1	0	0	0	0
61	DX	1	0	0	0	0
61	DY	1	0	0	0	0
All	All	290807	0	193177	5227	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 11.

The worst 5 of 5227 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:439:A:N3	1:AA:439:A:C2	1.68	1.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:439:A:C5	1:AA:439:A:C6	1.79	1.62
1:AA:439:A:N3	1:AA:439:A:C4	1.70	1.56
1:AA:439:A:C6	1:AA:439:A:N1	1.72	1.55
1:AA:439:A:C2	1:AA:439:A:N1	1.70	1.54

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%)	194 (85%)	24 (10%)	11 (5%)	2 3
2	CB	229/256 (90%)	195 (85%)	24 (10%)	10 (4%)	2 4
3	AC	204/239 (85%)	179 (88%)	23 (11%)	2 (1%)	12 32
3	CC	204/239 (85%)	178 (87%)	23 (11%)	3 (2%)	8 22
4	AD	206/209 (99%)	189 (92%)	15 (7%)	2 (1%)	12 32
4	CD	206/209 (99%)	190 (92%)	14 (7%)	2 (1%)	12 32
5	AE	146/162 (90%)	139 (95%)	5 (3%)	2 (1%)	9 23
5	CE	146/162 (90%)	136 (93%)	8 (6%)	2 (1%)	9 23
6	AF	98/101 (97%)	88 (90%)	10 (10%)	0	100 100
6	CF	98/101 (97%)	91 (93%)	7 (7%)	0	100 100
7	AG	153/156 (98%)	139 (91%)	11 (7%)	3 (2%)	6 16
7	CG	153/156 (98%)	137 (90%)	15 (10%)	1 (1%)	18 41
8	AH	135/138 (98%)	130 (96%)	5 (4%)	0	100 100
8	CH	135/138 (98%)	129 (96%)	5 (4%)	1 (1%)	18 41
9	AI	125/128 (98%)	107 (86%)	14 (11%)	4 (3%)	3 7
9	CI	125/128 (98%)	109 (87%)	12 (10%)	4 (3%)	3 7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
10	AJ	95/105 (90%)	80 (84%)	9 (10%)	6 (6%)	1 2
10	CJ	94/105 (90%)	83 (88%)	6 (6%)	5 (5%)	1 3
11	AK	112/129 (87%)	103 (92%)	7 (6%)	2 (2%)	6 18
11	CK	112/129 (87%)	101 (90%)	8 (7%)	3 (3%)	4 10
12	AL	120/132 (91%)	111 (92%)	9 (8%)	0	100 100
12	CL	120/132 (91%)	113 (94%)	7 (6%)	0	100 100
13	AM	118/126 (94%)	103 (87%)	13 (11%)	2 (2%)	7 19
13	CM	116/126 (92%)	101 (87%)	11 (10%)	4 (3%)	3 7
14	AN	58/61 (95%)	55 (95%)	3 (5%)	0	100 100
14	CN	58/61 (95%)	55 (95%)	3 (5%)	0	100 100
15	AO	86/89 (97%)	80 (93%)	6 (7%)	0	100 100
15	CO	86/89 (97%)	78 (91%)	7 (8%)	1 (1%)	10 27
16	AP	80/88 (91%)	73 (91%)	7 (9%)	0	100 100
16	CP	80/88 (91%)	74 (92%)	5 (6%)	1 (1%)	9 25
17	AQ	97/105 (92%)	92 (95%)	5 (5%)	0	100 100
17	CQ	97/105 (92%)	90 (93%)	7 (7%)	0	100 100
18	AR	66/88 (75%)	63 (96%)	3 (4%)	0	100 100
18	CR	66/88 (75%)	64 (97%)	1 (2%)	1 (2%)	8 22
19	AS	81/93 (87%)	70 (86%)	11 (14%)	0	100 100
19	CS	81/93 (87%)	68 (84%)	11 (14%)	2 (2%)	4 11
20	AT	94/106 (89%)	82 (87%)	6 (6%)	6 (6%)	1 1
20	CT	94/106 (89%)	84 (89%)	5 (5%)	5 (5%)	1 3
21	AU	21/27 (78%)	17 (81%)	4 (19%)	0	100 100
21	CU	21/27 (78%)	16 (76%)	4 (19%)	1 (5%)	2 3
27	BD	273/276 (99%)	258 (94%)	14 (5%)	1 (0%)	30 54
27	DD	273/276 (99%)	257 (94%)	14 (5%)	2 (1%)	18 41
28	BE	202/206 (98%)	194 (96%)	7 (4%)	1 (0%)	24 48
28	DE	202/206 (98%)	193 (96%)	7 (4%)	2 (1%)	12 32
29	BF	201/210 (96%)	196 (98%)	4 (2%)	1 (0%)	24 48
29	DF	201/210 (96%)	195 (97%)	4 (2%)	2 (1%)	12 32
30	BG	179/182 (98%)	165 (92%)	11 (6%)	3 (2%)	7 19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
30	DG	179/182 (98%)	161 (90%)	14 (8%)	4 (2%)	5 14
31	BH	172/180 (96%)	161 (94%)	10 (6%)	1 (1%)	21 44
31	DH	172/180 (96%)	160 (93%)	11 (6%)	1 (1%)	21 44
32	BI	144/148 (97%)	129 (90%)	12 (8%)	3 (2%)	5 15
32	DI	144/148 (97%)	130 (90%)	12 (8%)	2 (1%)	9 23
33	BN	138/140 (99%)	135 (98%)	3 (2%)	0	100 100
33	DN	138/140 (99%)	133 (96%)	4 (3%)	1 (1%)	18 41
34	BO	120/122 (98%)	114 (95%)	5 (4%)	1 (1%)	16 37
34	DO	120/122 (98%)	115 (96%)	5 (4%)	0	100 100
35	BP	147/150 (98%)	140 (95%)	6 (4%)	1 (1%)	18 41
35	DP	147/150 (98%)	137 (93%)	9 (6%)	1 (1%)	18 41
36	BQ	139/141 (99%)	132 (95%)	6 (4%)	1 (1%)	18 41
36	DQ	139/141 (99%)	132 (95%)	5 (4%)	2 (1%)	9 23
37	BR	116/118 (98%)	109 (94%)	7 (6%)	0	100 100
37	DR	116/118 (98%)	110 (95%)	5 (4%)	1 (1%)	14 35
38	BS	108/112 (96%)	98 (91%)	9 (8%)	1 (1%)	14 35
38	DS	108/112 (96%)	98 (91%)	9 (8%)	1 (1%)	14 35
39	BT	129/146 (88%)	122 (95%)	5 (4%)	2 (2%)	7 20
39	DT	129/146 (88%)	125 (97%)	4 (3%)	0	100 100
40	BU	114/118 (97%)	113 (99%)	1 (1%)	0	100 100
40	DU	114/118 (97%)	112 (98%)	2 (2%)	0	100 100
41	BV	99/101 (98%)	92 (93%)	5 (5%)	2 (2%)	6 16
41	DV	99/101 (98%)	94 (95%)	4 (4%)	1 (1%)	12 32
42	BW	110/113 (97%)	109 (99%)	1 (1%)	0	100 100
42	DW	110/113 (97%)	109 (99%)	1 (1%)	0	100 100
43	BX	93/96 (97%)	88 (95%)	4 (4%)	1 (1%)	11 29
43	DX	93/96 (97%)	88 (95%)	3 (3%)	2 (2%)	5 14
44	BY	105/110 (96%)	97 (92%)	6 (6%)	2 (2%)	6 17
44	DY	105/110 (96%)	99 (94%)	5 (5%)	1 (1%)	12 32
45	BZ	169/206 (82%)	147 (87%)	18 (11%)	4 (2%)	4 12
45	DZ	172/206 (84%)	154 (90%)	17 (10%)	1 (1%)	21 44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
46	B0	81/85 (95%)	76 (94%)	4 (5%)	1 (1%)	10 27
46	D0	81/85 (95%)	76 (94%)	5 (6%)	0	100 100
47	B1	95/98 (97%)	92 (97%)	2 (2%)	1 (1%)	11 29
47	D1	95/98 (97%)	92 (97%)	2 (2%)	1 (1%)	11 29
48	B2	68/72 (94%)	68 (100%)	0	0	100 100
48	D2	68/72 (94%)	68 (100%)	0	0	100 100
49	B3	57/60 (95%)	55 (96%)	2 (4%)	0	100 100
49	D3	57/60 (95%)	54 (95%)	3 (5%)	0	100 100
50	B4	67/71 (94%)	50 (75%)	10 (15%)	7 (10%)	0 0
50	D4	67/71 (94%)	53 (79%)	7 (10%)	7 (10%)	0 0
51	B5	57/60 (95%)	56 (98%)	1 (2%)	0	100 100
51	D5	57/60 (95%)	56 (98%)	1 (2%)	0	100 100
52	B6	51/54 (94%)	49 (96%)	1 (2%)	1 (2%)	6 16
52	D6	51/54 (94%)	48 (94%)	3 (6%)	0	100 100
53	B7	46/49 (94%)	45 (98%)	1 (2%)	0	100 100
53	D7	46/49 (94%)	45 (98%)	0	1 (2%)	5 14
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%)	34 (97%)	1 (3%)	0	100 100
55	D9	35/37 (95%)	33 (94%)	2 (6%)	0	100 100
All	All	11402/12128 (94%)	10561 (93%)	687 (6%)	154 (1%)	9 23

5 of 154 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	9	GLU
2	AB	10	LEU
2	AB	125	PRO
4	AD	166	LYS
7	AG	80	VAL

5.3.2 Protein sidechains (i)

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

resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	AB	192/220 (87%)	152 (79%)	40 (21%)	1 3
2	CB	187/220 (85%)	154 (82%)	33 (18%)	2 5
3	AC	143/188 (76%)	128 (90%)	15 (10%)	6 17
3	CC	140/188 (74%)	121 (86%)	19 (14%)	3 9
4	AD	170/181 (94%)	150 (88%)	20 (12%)	5 13
4	CD	173/181 (96%)	156 (90%)	17 (10%)	7 19
5	AE	113/123 (92%)	103 (91%)	10 (9%)	9 23
5	CE	114/123 (93%)	102 (90%)	12 (10%)	6 17
6	AF	83/90 (92%)	78 (94%)	5 (6%)	17 41
6	CF	85/90 (94%)	79 (93%)	6 (7%)	13 33
7	AG	119/127 (94%)	105 (88%)	14 (12%)	5 13
7	CG	120/127 (94%)	108 (90%)	12 (10%)	7 19
8	AH	114/119 (96%)	104 (91%)	10 (9%)	9 23
8	CH	114/119 (96%)	104 (91%)	10 (9%)	9 23
9	AI	90/99 (91%)	78 (87%)	12 (13%)	4 10
9	CI	89/99 (90%)	79 (89%)	10 (11%)	6 15
10	AJ	66/92 (72%)	58 (88%)	8 (12%)	5 12
10	CJ	69/92 (75%)	62 (90%)	7 (10%)	7 18
11	AK	82/99 (83%)	75 (92%)	7 (8%)	10 25
11	CK	83/99 (84%)	74 (89%)	9 (11%)	6 16
12	AL	97/109 (89%)	89 (92%)	8 (8%)	10 27
12	CL	97/109 (89%)	90 (93%)	7 (7%)	13 32
13	AM	91/101 (90%)	78 (86%)	13 (14%)	3 8
13	CM	89/101 (88%)	76 (85%)	13 (15%)	3 8
14	AN	49/50 (98%)	42 (86%)	7 (14%)	3 8
14	CN	49/50 (98%)	41 (84%)	8 (16%)	2 6
15	AO	78/80 (98%)	69 (88%)	9 (12%)	5 14
15	CO	78/80 (98%)	72 (92%)	6 (8%)	12 30
16	AP	69/74 (93%)	58 (84%)	11 (16%)	2 7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
16	CP	68/74 (92%)	58 (85%)	10 (15%)	3 8
17	AQ	94/97 (97%)	88 (94%)	6 (6%)	16 38
17	CQ	94/97 (97%)	89 (95%)	5 (5%)	20 46
18	AR	59/77 (77%)	53 (90%)	6 (10%)	7 18
18	CR	59/77 (77%)	53 (90%)	6 (10%)	7 18
19	AS	69/80 (86%)	64 (93%)	5 (7%)	13 32
19	CS	67/80 (84%)	59 (88%)	8 (12%)	5 13
20	AT	70/82 (85%)	63 (90%)	7 (10%)	7 19
20	CT	70/82 (85%)	61 (87%)	9 (13%)	4 10
21	AU	18/22 (82%)	16 (89%)	2 (11%)	6 15
21	CU	18/22 (82%)	18 (100%)	0	100 100
27	BD	215/218 (99%)	195 (91%)	20 (9%)	8 21
27	DD	215/218 (99%)	197 (92%)	18 (8%)	10 26
28	BE	164/166 (99%)	140 (85%)	24 (15%)	3 8
28	DE	164/166 (99%)	137 (84%)	27 (16%)	2 6
29	BF	160/166 (96%)	139 (87%)	21 (13%)	4 10
29	DF	159/166 (96%)	139 (87%)	20 (13%)	4 11
30	BG	143/156 (92%)	126 (88%)	17 (12%)	5 13
30	DG	142/156 (91%)	124 (87%)	18 (13%)	4 11
31	BH	144/148 (97%)	130 (90%)	14 (10%)	8 20
31	DH	144/148 (97%)	131 (91%)	13 (9%)	9 23
32	BI	110/124 (89%)	86 (78%)	24 (22%)	1 3
32	DI	104/124 (84%)	87 (84%)	17 (16%)	2 6
33	BN	118/119 (99%)	102 (86%)	16 (14%)	3 9
33	DN	118/119 (99%)	105 (89%)	13 (11%)	6 15
34	BO	100/100 (100%)	93 (93%)	7 (7%)	14 34
34	DO	100/100 (100%)	91 (91%)	9 (9%)	9 23
35	BP	115/116 (99%)	101 (88%)	14 (12%)	5 12
35	DP	115/116 (99%)	102 (89%)	13 (11%)	5 14
36	BQ	111/111 (100%)	100 (90%)	11 (10%)	7 19
36	DQ	111/111 (100%)	101 (91%)	10 (9%)	9 23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
37	BR	101/101 (100%)	83 (82%)	18 (18%)	2 5
37	DR	101/101 (100%)	84 (83%)	17 (17%)	2 6
38	BS	87/88 (99%)	79 (91%)	8 (9%)	8 22
38	DS	85/88 (97%)	74 (87%)	11 (13%)	4 10
39	BT	115/127 (91%)	103 (90%)	12 (10%)	7 17
39	DT	113/127 (89%)	102 (90%)	11 (10%)	8 20
40	BU	93/94 (99%)	84 (90%)	9 (10%)	8 20
40	DU	93/94 (99%)	87 (94%)	6 (6%)	15 37
41	BV	80/82 (98%)	65 (81%)	15 (19%)	1 4
41	DV	80/82 (98%)	64 (80%)	16 (20%)	1 4
42	BW	90/92 (98%)	84 (93%)	6 (7%)	15 36
42	DW	90/92 (98%)	83 (92%)	7 (8%)	11 29
43	BX	77/78 (99%)	72 (94%)	5 (6%)	15 37
43	DX	77/78 (99%)	72 (94%)	5 (6%)	15 37
44	BY	85/91 (93%)	77 (91%)	8 (9%)	8 21
44	DY	85/91 (93%)	79 (93%)	6 (7%)	13 33
45	BZ	145/179 (81%)	129 (89%)	16 (11%)	6 15
45	DZ	145/179 (81%)	129 (89%)	16 (11%)	6 15
46	B0	65/67 (97%)	61 (94%)	4 (6%)	16 39
46	D0	65/67 (97%)	60 (92%)	5 (8%)	12 30
47	B1	80/83 (96%)	72 (90%)	8 (10%)	7 19
47	D1	80/83 (96%)	73 (91%)	7 (9%)	9 23
48	B2	65/67 (97%)	60 (92%)	5 (8%)	12 30
48	D2	65/67 (97%)	58 (89%)	7 (11%)	6 16
49	B3	51/52 (98%)	43 (84%)	8 (16%)	2 7
49	D3	50/52 (96%)	43 (86%)	7 (14%)	3 9
50	B4	60/63 (95%)	50 (83%)	10 (17%)	2 6
50	D4	53/63 (84%)	45 (85%)	8 (15%)	3 7
51	B5	50/52 (96%)	41 (82%)	9 (18%)	2 5
51	D5	50/52 (96%)	45 (90%)	5 (10%)	7 19
52	B6	51/52 (98%)	45 (88%)	6 (12%)	5 13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
52	D6	50/52 (96%)	46 (92%)	4 (8%)	11 28
53	B7	41/42 (98%)	39 (95%)	2 (5%)	22 49
53	D7	41/42 (98%)	41 (100%)	0	100 100
54	B8	53/55 (96%)	48 (91%)	5 (9%)	8 21
54	D8	54/55 (98%)	48 (89%)	6 (11%)	6 15
55	B9	34/34 (100%)	33 (97%)	1 (3%)	37 67
55	D9	34/34 (100%)	30 (88%)	4 (12%)	5 13
All	All	9315/10066 (92%)	8264 (89%)	1051 (11%)	5 14

5 of 1051 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
38	DS	69	VAL
41	DV	28	GLU
38	DS	68	GLN
52	D6	48	VAL
37	BR	29	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 184 such sidechains are listed below:

Mol	Chain	Res	Type
6	CF	73	ASN
27	DD	87	ASN
7	CG	64	GLN
12	CL	78	GLN
29	DF	40	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1494/1521 (98%)	367 (24%)	26 (1%)
1	CA	1501/1521 (98%)	374 (24%)	32 (2%)
22	AV	7/24 (29%)	0	0
22	CV	4/24 (16%)	1 (25%)	0
23	AX	75/77 (97%)	25 (33%)	0
23	CX	75/77 (97%)	23 (30%)	0
24	AY	16/76 (21%)	7 (43%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
24	CY	4/76 (5%)	0	0
25	BA	2814/2915 (96%)	477 (16%)	31 (1%)
25	DA	2791/2915 (95%)	524 (18%)	27 (0%)
26	BB	119/121 (98%)	24 (20%)	0
26	DB	119/121 (98%)	25 (21%)	0
All	All	9019/9468 (95%)	1847 (20%)	116 (1%)

5 of 1847 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	6	G
1	AA	7	G
1	AA	9	G
1	AA	22	G
1	AA	32	A

5 of 116 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	CA	60	A
25	DA	2126	A
1	CA	992	U
25	DA	2110	G
25	DA	856	C

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
23	PSU	CX	55	23	18,21,22	1.39	2 (11%)	21,30,33	1.94	5 (23%)
23	PSU	AX	55	23	18,21,22	1.36	2 (11%)	21,30,33	2.05	4 (19%)
23	4SU	AX	8	23	18,21,22	2.29	5 (27%)	25,30,33	1.69	4 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	5MU	AX	54	23	19,22,23	1.51	4 (21%)	27,32,35	1.63	5 (18%)
23	5MU	CX	54	23	19,22,23	1.42	4 (21%)	27,32,35	2.00	6 (22%)
23	5MC	CX	32	23	19,22,23	1.54	3 (15%)	26,32,35	1.22	4 (15%)
23	5MC	AX	32	23	19,22,23	1.79	3 (15%)	26,32,35	1.38	4 (15%)
23	4SU	CX	8	23	18,21,22	1.99	5 (27%)	25,30,33	1.36	4 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	PSU	CX	55	23	-	0/7/25/26	0/2/2/2
23	PSU	AX	55	23	-	0/7/25/26	0/2/2/2
23	4SU	AX	8	23	-	0/7/25/26	0/2/2/2
23	5MU	AX	54	23	-	0/7/25/26	0/2/2/2
23	5MU	CX	54	23	-	0/7/25/26	0/2/2/2
23	5MC	CX	32	23	-	0/7/25/26	0/2/2/2
23	5MC	AX	32	23	-	0/7/25/26	0/2/2/2
23	4SU	CX	8	23	-	0/7/25/26	0/2/2/2

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	AX	32	5MC	C5-C4	6.40	1.49	1.44
23	AX	8	4SU	C4-N3	-5.59	1.31	1.37
23	CX	32	5MC	C5-C4	5.41	1.48	1.44
23	AX	8	4SU	C4-S4	-4.96	1.59	1.68
23	CX	8	4SU	C4-N3	-4.63	1.32	1.37

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	AX	55	PSU	N1-C2-N3	6.18	121.68	115.17
23	CX	55	PSU	N1-C2-N3	6.13	121.63	115.17
23	CX	54	5MU	N3-C2-N1	5.12	121.56	114.89
23	AX	8	4SU	C6-C5-C4	-5.10	115.54	119.95
23	CX	54	5MU	C4-N3-C2	-4.63	121.27	127.34

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	CX	55	PSU	1	0
23	AX	8	4SU	1	0
23	CX	8	4SU	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2061 ligands modelled in this entry, 2057 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
57	PCY	CA	3176	-	34,42,42	1.77	5 (14%)	41,65,65	0.95	3 (7%)
58	SF4	AD	501	4	0,12,12	-	-	-		
57	PCY	AA	3191	-	34,42,42	1.94	5 (14%)	41,65,65	1.51	8 (19%)
58	SF4	CD	501	4	0,12,12	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	PCY	CA	3176	-	-	6/33/67/67	0/3/3/3
58	SF4	AD	501	4	-	-	0/6/5/5
57	PCY	AA	3191	-	-	18/33/67/67	0/3/3/3
58	SF4	CD	501	4	-	-	0/6/5/5

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	AA	3191	PCY	C34-C30	-6.06	1.39	1.51
57	CA	3176	PCY	C34-C30	-5.75	1.40	1.51
57	AA	3191	PCY	C28-C32	-5.38	1.39	1.49
57	AA	3191	PCY	C17-N20	4.78	1.51	1.45
57	CA	3176	PCY	C28-C32	-4.73	1.40	1.49

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
57	AA	3191	PCY	O21-C18-C15	4.06	115.29	107.79
57	AA	3191	PCY	O21-C23-C27	4.04	121.35	112.35
57	AA	3191	PCY	C18-O21-C23	-2.84	110.93	116.55
57	AA	3191	PCY	C30-C27-C23	2.45	127.43	120.47
57	CA	3176	PCY	C18-O21-C23	-2.35	111.90	116.55

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
57	AA	3191	PCY	N2-C3-C6-C11
57	AA	3191	PCY	N2-C3-C6-O12
57	AA	3191	PCY	C7-C3-C6-C11
57	AA	3191	PCY	C7-C3-C6-O12
57	AA	3191	PCY	C8-C3-C6-C11

There are no ring outliers.

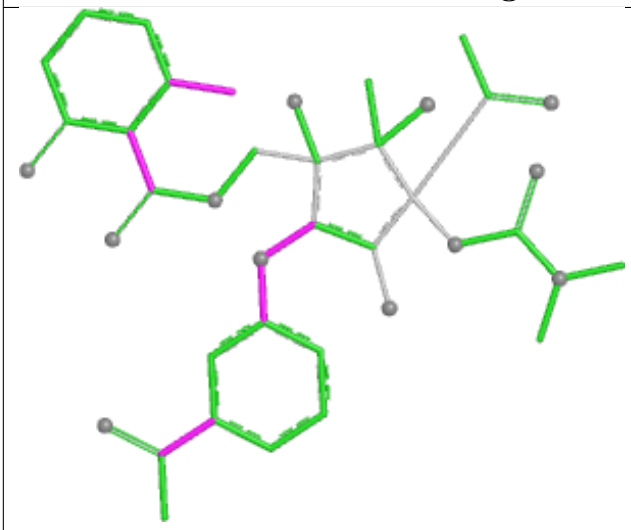
3 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	CA	3176	PCY	4	0
58	AD	501	SF4	1	0
57	AA	3191	PCY	6	0

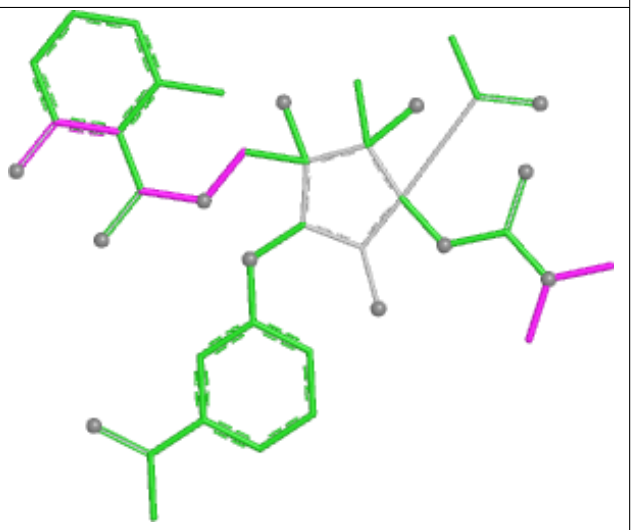
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

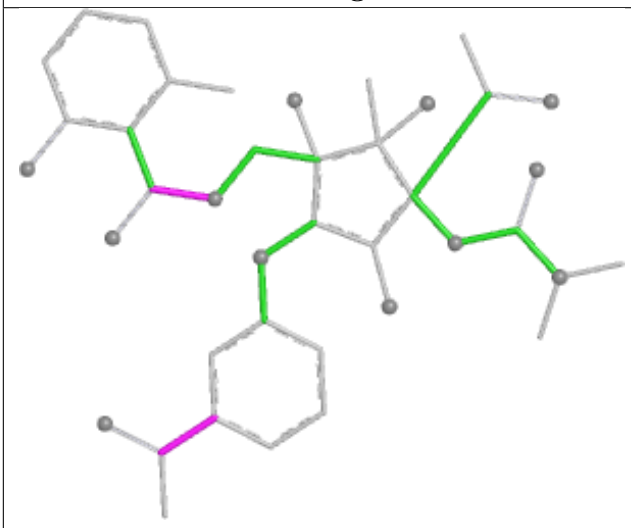
Ligand PCY CA 3176



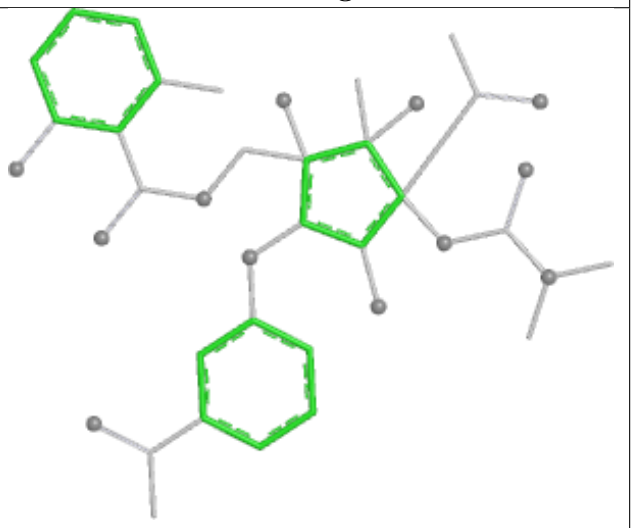
Bond lengths



Bond angles

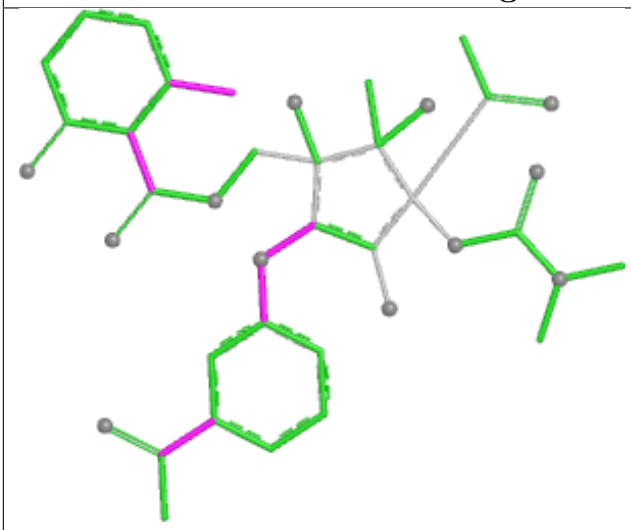


Torsions

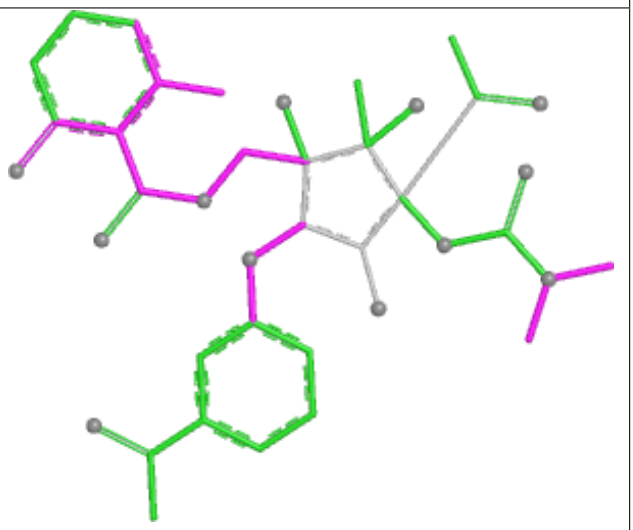


Rings

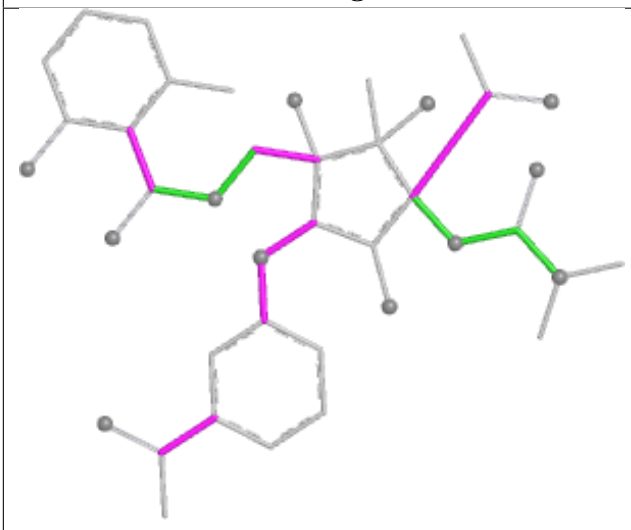
Ligand PCY AA 3191



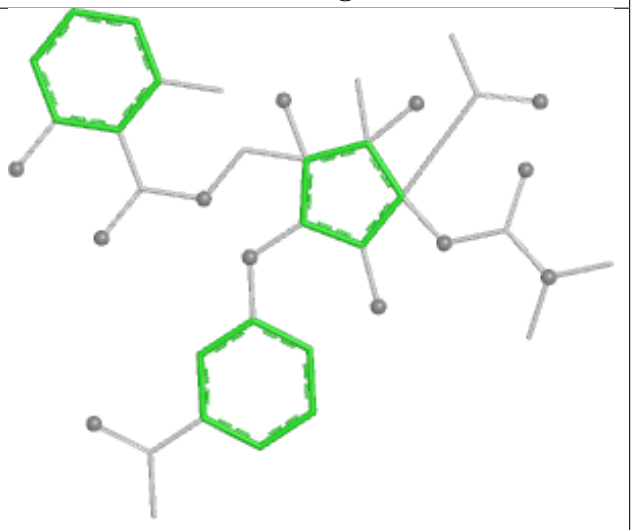
Bond lengths



Bond angles



Torsions



Rings

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	1497/1521 (98%)	0.50	52 (3%) 47 43	40, 76, 97, 113	0
1	CA	1503/1521 (98%)	0.57	106 (7%) 22 19	42, 77, 97, 113	0
2	AB	231/256 (90%)	1.24	39 (16%) 4 3	71, 85, 93, 98	0
2	CB	231/256 (90%)	1.71	77 (33%) 1 1	71, 86, 94, 98	0
3	AC	206/239 (86%)	1.06	23 (11%) 10 8	69, 83, 91, 95	0
3	CC	206/239 (86%)	1.55	50 (24%) 2 1	69, 84, 92, 96	0
4	AD	208/209 (99%)	1.30	37 (17%) 4 3	60, 76, 86, 91	0
4	CD	208/209 (99%)	0.77	6 (2%) 53 50	60, 76, 84, 89	0
5	AE	148/162 (91%)	0.86	12 (8%) 18 15	56, 72, 81, 88	0
5	CE	148/162 (91%)	1.04	14 (9%) 14 11	58, 74, 83, 89	0
6	AF	100/101 (99%)	0.71	1 (1%) 79 78	61, 74, 82, 85	0
6	CF	100/101 (99%)	1.05	12 (12%) 9 7	62, 75, 83, 86	0
7	AG	155/156 (99%)	1.00	21 (13%) 7 6	69, 79, 89, 98	0
7	CG	155/156 (99%)	1.42	31 (20%) 3 2	70, 80, 90, 99	0
8	AH	137/138 (99%)	0.81	7 (5%) 33 29	61, 74, 81, 85	0
8	CH	137/138 (99%)	1.19	19 (13%) 6 5	63, 75, 83, 88	0
9	AI	127/128 (99%)	1.21	17 (13%) 7 6	63, 85, 91, 94	0
9	CI	127/128 (99%)	2.05	63 (49%) 0 0	70, 86, 92, 96	0
10	AJ	97/105 (92%)	1.57	28 (28%) 1 1	73, 87, 94, 97	0
10	CJ	96/105 (91%)	2.02	43 (44%) 0 0	76, 89, 95, 96	0
11	AK	114/129 (88%)	0.79	6 (5%) 32 28	52, 72, 84, 87	0
11	CK	114/129 (88%)	0.85	9 (7%) 18 16	54, 74, 84, 87	0
12	AL	122/132 (92%)	0.78	5 (4%) 41 37	52, 67, 77, 81	0
12	CL	122/132 (92%)	0.92	12 (9%) 13 11	53, 67, 76, 81	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	AM	120/126 (95%)	1.03	8 (6%) 24 21	53, 75, 85, 93	0
13	CM	118/126 (93%)	1.74	42 (35%) 1 1	71, 88, 94, 98	0
14	AN	60/61 (98%)	1.26	10 (16%) 4 3	74, 80, 88, 90	0
14	CN	60/61 (98%)	2.63	44 (73%) 0 0	75, 83, 88, 92	0
15	AO	88/89 (98%)	0.99	8 (9%) 15 12	55, 69, 81, 85	0
15	CO	88/89 (98%)	0.82	6 (6%) 23 20	58, 71, 82, 86	0
16	AP	82/88 (93%)	1.54	19 (23%) 2 2	64, 75, 84, 91	0
16	CP	82/88 (93%)	1.39	17 (20%) 2 2	63, 73, 83, 89	0
17	AQ	99/105 (94%)	0.86	7 (7%) 22 19	55, 70, 79, 81	0
17	CQ	99/105 (94%)	1.07	6 (6%) 27 24	58, 71, 80, 84	0
18	AR	68/88 (77%)	0.74	2 (2%) 53 50	62, 74, 84, 89	0
18	CR	68/88 (77%)	0.83	3 (4%) 39 35	64, 74, 84, 91	0
19	AS	83/93 (89%)	1.65	22 (26%) 1 1	75, 85, 93, 94	0
19	CS	83/93 (89%)	1.95	33 (39%) 1 0	78, 87, 93, 96	0
20	AT	96/106 (90%)	1.01	12 (12%) 8 7	63, 72, 82, 87	0
20	CT	96/106 (90%)	1.06	7 (7%) 21 18	61, 73, 82, 87	0
21	AU	23/27 (85%)	1.79	10 (43%) 0 0	71, 77, 79, 81	0
21	CU	23/27 (85%)	1.88	8 (34%) 1 1	72, 79, 81, 83	0
22	AV	8/24 (33%)	1.70	4 (50%) 0 0	62, 89, 94, 97	0
22	CV	5/24 (20%)	1.40	1 (20%) 3 2	65, 73, 91, 96	0
23	AX	72/77 (93%)	0.54	3 (4%) 40 37	40, 71, 88, 98	0
23	CX	72/77 (93%)	0.39	1 (1%) 73 72	43, 74, 90, 97	0
24	AY	18/76 (23%)	1.35	3 (16%) 4 3	62, 104, 109, 109	0
24	CY	5/76 (6%)	2.61	4 (80%) 0 0	74, 101, 102, 106	0
25	BA	2822/2915 (96%)	-0.29	97 (3%) 48 44	18, 41, 91, 109	0
25	DA	2800/2915 (96%)	-0.29	79 (2%) 55 51	22, 45, 91, 112	0
26	BB	120/121 (99%)	0.17	0 100 100	31, 63, 75, 88	0
26	DB	120/121 (99%)	1.07	19 (15%) 5 4	38, 69, 81, 91	0
27	BD	275/276 (99%)	0.02	2 (0%) 84 83	20, 39, 58, 77	0
27	DD	275/276 (99%)	-0.07	2 (0%) 84 83	22, 42, 60, 78	0
28	BE	204/206 (99%)	0.11	1 (0%) 87 86	19, 44, 64, 86	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
28	DE	204/206 (99%)	0.13	1 (0%) 87 86	22, 48, 66, 86	0
29	BF	203/210 (96%)	0.19	1 (0%) 87 86	21, 50, 74, 91	0
29	DF	203/210 (96%)	0.16	3 (1%) 72 70	24, 55, 77, 90	0
30	BG	181/182 (99%)	0.94	17 (9%) 14 12	55, 71, 83, 96	0
30	DG	181/182 (99%)	1.32	37 (20%) 3 2	60, 75, 84, 95	0
31	BH	174/180 (96%)	0.82	10 (5%) 29 26	45, 64, 75, 84	0
31	DH	174/180 (96%)	1.14	20 (11%) 9 8	53, 68, 79, 86	0
32	BI	146/148 (98%)	0.65	6 (4%) 41 37	48, 75, 84, 88	0
32	DI	146/148 (98%)	0.87	8 (5%) 30 27	51, 75, 84, 88	0
33	BN	140/140 (100%)	0.44	4 (2%) 53 50	28, 45, 69, 79	0
33	DN	140/140 (100%)	0.37	0 100 100	33, 49, 71, 81	0
34	BO	122/122 (100%)	0.06	3 (2%) 58 55	31, 45, 63, 70	0
34	DO	122/122 (100%)	0.00	0 100 100	34, 48, 64, 70	0
35	BP	149/150 (99%)	0.36	3 (2%) 65 62	18, 53, 74, 82	0
35	DP	149/150 (99%)	0.32	2 (1%) 75 73	20, 56, 76, 84	0
36	BQ	141/141 (100%)	0.26	3 (2%) 63 61	29, 48, 65, 77	0
36	DQ	141/141 (100%)	0.41	5 (3%) 47 43	32, 52, 69, 78	0
37	BR	118/118 (100%)	-0.34	0 100 100	19, 32, 49, 62	0
37	DR	118/118 (100%)	0.20	1 (0%) 82 81	35, 53, 66, 78	0
38	BS	110/112 (98%)	0.01	0 100 100	30, 47, 65, 70	0
38	DS	110/112 (98%)	1.50	31 (28%) 1 1	63, 77, 88, 93	0
39	BT	131/146 (89%)	0.03	6 (4%) 37 34	30, 43, 71, 85	0
39	DT	131/146 (89%)	0.44	2 (1%) 72 70	43, 59, 78, 88	0
40	BU	116/118 (98%)	-0.45	1 (0%) 81 80	15, 27, 48, 62	0
40	DU	116/118 (98%)	0.38	1 (0%) 81 80	38, 59, 76, 87	0
41	BV	101/101 (100%)	-0.46	1 (0%) 79 78	14, 35, 57, 76	0
41	DV	101/101 (100%)	0.48	1 (0%) 79 78	43, 71, 84, 90	0
42	BW	112/113 (99%)	-0.49	1 (0%) 81 80	17, 28, 50, 75	0
42	DW	112/113 (99%)	0.04	0 100 100	34, 50, 68, 92	0
43	BX	95/96 (98%)	-0.20	1 (1%) 78 76	17, 35, 65, 78	0
43	DX	95/96 (98%)	0.88	9 (9%) 14 11	44, 62, 77, 90	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
44	BY	107/110 (97%)	0.18	1 (0%) 81 80	28, 47, 67, 85	0
44	DY	107/110 (97%)	1.16	18 (16%) 4 3	51, 72, 83, 88	0
45	BZ	171/206 (83%)	0.50	6 (3%) 47 43	36, 62, 81, 90	0
45	DZ	174/206 (84%)	1.28	23 (13%) 7 6	66, 83, 93, 96	0
46	B0	83/85 (97%)	0.02	8 (9%) 13 11	12, 33, 66, 84	0
46	D0	83/85 (97%)	0.87	9 (10%) 11 9	34, 64, 78, 91	0
47	B1	97/98 (98%)	0.01	1 (1%) 79 78	19, 43, 69, 72	0
47	D1	97/98 (98%)	0.45	2 (2%) 63 61	37, 57, 78, 82	0
48	B2	70/72 (97%)	0.08	3 (4%) 40 36	30, 46, 63, 77	0
48	D2	70/72 (97%)	0.83	3 (4%) 40 36	56, 71, 80, 85	0
49	B3	59/60 (98%)	-0.31	1 (1%) 69 67	20, 31, 56, 83	0
49	D3	59/60 (98%)	0.58	5 (8%) 16 14	47, 62, 77, 91	0
50	B4	69/71 (97%)	1.02	13 (18%) 3 3	55, 77, 92, 99	0
50	D4	69/71 (97%)	1.41	16 (23%) 2 2	77, 91, 99, 105	0
51	B5	59/60 (98%)	-0.47	0 100 100	11, 28, 53, 67	0
51	D5	59/60 (98%)	-0.02	1 (1%) 69 67	27, 52, 68, 81	0
52	B6	53/54 (98%)	-0.17	0 100 100	27, 39, 56, 66	0
52	D6	53/54 (98%)	0.66	4 (7%) 20 17	45, 62, 73, 79	0
53	B7	48/49 (97%)	-0.09	3 (6%) 26 23	16, 23, 52, 68	0
53	D7	48/49 (97%)	-0.13	0 100 100	29, 40, 64, 77	0
54	B8	64/65 (98%)	-0.27	0 100 100	24, 31, 43, 61	0
54	D8	64/65 (98%)	0.41	0 100 100	44, 53, 63, 72	0
55	B9	37/37 (100%)	0.27	1 (2%) 56 53	28, 45, 67, 72	0
55	D9	37/37 (100%)	0.72	2 (5%) 31 27	44, 55, 68, 75	0
All	All	20640/21596 (95%)	0.41	1468 (7%) 22 19	11, 64, 91, 113	0

The worst 5 of 1468 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
20	CT	9	ASN	7.6
25	BA	2143	G	7.5
14	CN	2	ALA	6.6
2	CB	165	VAL	6.3
25	BA	2135	U	6.1

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
23	4SU	CX	8	20/21	0.81	0.11	73,81,98,100	0
23	PSU	CX	55	20/21	0.82	0.13	56,73,80,86	0
23	5MU	CX	54	21/22	0.84	0.13	69,80,93,106	0
23	PSU	AX	55	20/21	0.91	0.11	56,70,78,80	0
23	5MC	CX	32	21/22	0.91	0.12	66,75,83,86	0
23	5MU	AX	54	21/22	0.92	0.11	60,72,80,91	0
23	4SU	AX	8	20/21	0.94	0.10	47,67,77,84	0
23	5MC	AX	32	21/22	0.95	0.13	38,59,69,83	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	AA	3147	1/1	0.56	0.18	72,72,72,72	0
56	MG	CJ	5001	1/1	0.58	0.14	94,94,94,94	0
56	MG	DB	3001	1/1	0.58	0.13	77,77,77,77	0
56	MG	AA	3177	1/1	0.62	0.23	80,80,80,80	0
56	MG	DA	3640	1/1	0.64	0.19	64,64,64,64	0
56	MG	DA	3533	1/1	0.64	0.14	52,52,52,52	0
56	MG	DA	3655	1/1	0.67	0.54	74,74,74,74	0
56	MG	DA	3612	1/1	0.67	0.21	58,58,58,58	0
56	MG	BA	3447	1/1	0.68	0.21	59,59,59,59	0
56	MG	CA	3124	1/1	0.68	0.20	75,75,75,75	0
56	MG	DA	3607	1/1	0.69	0.22	63,63,63,63	0
56	MG	BE	306	1/1	0.69	0.28	93,93,93,93	0
56	MG	DA	3634	1/1	0.69	0.19	61,61,61,61	0
56	MG	DA	3657	1/1	0.70	0.20	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	CA	3174	1/1	0.70	0.15	80,80,80,80	0
56	MG	CA	3054	1/1	0.72	0.39	70,70,70,70	0
56	MG	BA	3657	1/1	0.72	0.27	52,52,52,52	0
56	MG	AA	3171	1/1	0.72	0.18	67,67,67,67	0
56	MG	CA	3131	1/1	0.73	0.35	81,81,81,81	0
56	MG	CX	3002	1/1	0.73	0.43	81,81,81,81	0
56	MG	CA	3084	1/1	0.74	0.28	71,71,71,71	0
56	MG	AA	3067	1/1	0.74	0.40	72,72,72,72	0
57	PCY	CA	3176	40/40	0.74	0.22	72,89,98,102	0
56	MG	BA	3703	1/1	0.75	0.14	57,57,57,57	0
56	MG	DA	3562	1/1	0.75	0.19	72,72,72,72	0
56	MG	BA	3598	1/1	0.75	0.24	53,53,53,53	0
56	MG	AA	3059	1/1	0.75	0.27	64,64,64,64	0
56	MG	DA	3466	1/1	0.75	0.24	66,66,66,66	0
56	MG	AA	3040	1/1	0.76	0.16	72,72,72,72	0
56	MG	BA	3659	1/1	0.76	0.32	67,67,67,67	0
56	MG	BA	3671	1/1	0.76	0.23	59,59,59,59	0
56	MG	AA	3163	1/1	0.76	0.24	58,58,58,58	0
56	MG	CE	201	1/1	0.76	0.30	73,73,73,73	0
56	MG	BA	3555	1/1	0.76	0.11	61,61,61,61	0
56	MG	AA	3043	1/1	0.76	0.32	76,76,76,76	0
56	MG	DA	3211	1/1	0.76	0.15	53,53,53,53	0
56	MG	CA	3082	1/1	0.76	0.32	73,73,73,73	0
56	MG	DA	3484	1/1	0.76	0.16	32,32,32,32	0
56	MG	AA	3153	1/1	0.77	0.19	81,81,81,81	0
56	MG	BA	3692	1/1	0.77	0.15	51,51,51,51	0
56	MG	BA	3521	1/1	0.77	0.19	29,29,29,29	0
56	MG	BA	3768	1/1	0.77	0.12	61,61,61,61	0
56	MG	AA	3179	1/1	0.77	0.26	61,61,61,61	0
57	PCY	AA	3191	40/40	0.77	0.21	59,86,97,99	0
56	MG	DA	3319	1/1	0.77	0.15	52,52,52,52	0
56	MG	BA	3737	1/1	0.78	0.16	70,70,70,70	0
56	MG	BA	3498	1/1	0.78	0.21	43,43,43,43	0
56	MG	BA	3505	1/1	0.78	0.18	33,33,33,33	0
56	MG	AA	3125	1/1	0.78	0.14	72,72,72,72	0
56	MG	CA	3063	1/1	0.78	0.32	70,70,70,70	0
56	MG	BA	3384	1/1	0.78	0.22	63,63,63,63	0
56	MG	AA	3100	1/1	0.78	0.26	66,66,66,66	0
56	MG	DA	3110	1/1	0.79	0.33	64,64,64,64	0
56	MG	CA	3144	1/1	0.79	0.26	68,68,68,68	0
56	MG	CA	3171	1/1	0.79	0.24	65,65,65,65	0
56	MG	CA	3100	1/1	0.79	0.17	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	AA	3184	1/1	0.79	0.13	66,66,66,66	0
56	MG	DA	3527	1/1	0.79	0.15	61,61,61,61	0
56	MG	AA	3034	1/1	0.79	0.21	70,70,70,70	0
56	MG	DA	3537	1/1	0.79	0.25	58,58,58,58	0
56	MG	CA	3142	1/1	0.79	0.17	81,81,81,81	0
56	MG	DA	3567	1/1	0.80	0.19	57,57,57,57	0
56	MG	BA	3514	1/1	0.80	0.11	45,45,45,45	0
56	MG	DA	3341	1/1	0.80	0.20	67,67,67,67	0
56	MG	DA	3435	1/1	0.80	0.30	55,55,55,55	0
56	MG	BA	3512	1/1	0.80	0.23	47,47,47,47	0
56	MG	BA	3626	1/1	0.80	0.17	43,43,43,43	0
56	MG	BA	3650	1/1	0.80	0.21	48,48,48,48	0
56	MG	DA	3103	1/1	0.80	0.15	71,71,71,71	0
56	MG	CA	3149	1/1	0.80	0.31	74,74,74,74	0
56	MG	B4	502	1/1	0.80	0.21	77,77,77,77	0
56	MG	BA	3592	1/1	0.81	0.22	64,64,64,64	0
56	MG	AA	3169	1/1	0.81	0.18	73,73,73,73	0
56	MG	AA	3170	1/1	0.81	0.25	73,73,73,73	0
56	MG	DA	3559	1/1	0.81	0.21	61,61,61,61	0
56	MG	CA	3091	1/1	0.81	0.24	70,70,70,70	0
56	MG	BA	3760	1/1	0.81	0.14	43,43,43,43	0
56	MG	CA	3107	1/1	0.81	0.12	77,77,77,77	0
56	MG	DA	3175	1/1	0.81	0.18	51,51,51,51	0
56	MG	AX	3002	1/1	0.81	0.18	69,69,69,69	0
56	MG	BB	205	1/1	0.81	0.29	76,76,76,76	0
56	MG	AA	3127	1/1	0.81	0.17	79,79,79,79	0
56	MG	BA	3437	1/1	0.81	0.20	61,61,61,61	0
56	MG	DA	3438	1/1	0.81	0.15	55,55,55,55	0
56	MG	CA	3043	1/1	0.81	0.31	67,67,67,67	0
56	MG	AA	3094	1/1	0.81	0.29	66,66,66,66	0
56	MG	CA	3019	1/1	0.82	0.29	62,62,62,62	0
56	MG	CT	3001	1/1	0.82	0.31	59,59,59,59	0
56	MG	BA	3725	1/1	0.82	0.17	44,44,44,44	0
56	MG	AA	3049	1/1	0.82	0.15	64,64,64,64	0
56	MG	DA	3109	1/1	0.82	0.30	68,68,68,68	0
56	MG	AA	3105	1/1	0.82	0.23	71,71,71,71	0
56	MG	BA	3663	1/1	0.82	0.26	65,65,65,65	0
56	MG	DA	3202	1/1	0.82	0.19	52,52,52,52	0
56	MG	BA	3108	1/1	0.82	0.27	64,64,64,64	0
56	MG	DA	3222	1/1	0.82	0.12	46,46,46,46	0
56	MG	CA	3159	1/1	0.82	0.25	71,71,71,71	0
56	MG	DA	3324	1/1	0.82	0.15	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	BA	3288	1/1	0.82	0.14	44,44,44,44	0
56	MG	DA	3402	1/1	0.82	0.14	56,56,56,56	0
56	MG	DA	3426	1/1	0.82	0.12	39,39,39,39	0
56	MG	DB	3008	1/1	0.82	0.17	64,64,64,64	0
56	MG	DD	308	1/1	0.82	0.33	72,72,72,72	0
56	MG	DV	3003	1/1	0.82	0.09	55,55,55,55	0
56	MG	CA	3096	1/1	0.82	0.17	65,65,65,65	0
56	MG	BA	3525	1/1	0.82	0.13	23,23,23,23	0
56	MG	BA	3579	1/1	0.83	0.17	43,43,43,43	0
56	MG	DA	3469	1/1	0.83	0.11	53,53,53,53	0
56	MG	CA	3083	1/1	0.83	0.29	72,72,72,72	0
56	MG	DA	3488	1/1	0.83	0.16	51,51,51,51	0
56	MG	DA	3499	1/1	0.83	0.23	61,61,61,61	0
56	MG	BA	3583	1/1	0.83	0.14	56,56,56,56	0
56	MG	BA	3518	1/1	0.83	0.17	65,65,65,65	0
56	MG	AA	3185	1/1	0.83	0.15	61,61,61,61	0
56	MG	BP	203	1/1	0.83	0.16	49,49,49,49	0
56	MG	DA	3150	1/1	0.83	0.22	52,52,52,52	0
56	MG	B0	101	1/1	0.83	0.15	55,55,55,55	0
56	MG	DA	3606	1/1	0.83	0.12	48,48,48,48	0
56	MG	DA	3185	1/1	0.83	0.16	55,55,55,55	0
56	MG	CA	3122	1/1	0.83	0.26	65,65,65,65	0
56	MG	DA	3626	1/1	0.83	0.18	56,56,56,56	0
56	MG	BA	3607	1/1	0.83	0.22	51,51,51,51	0
56	MG	BA	3693	1/1	0.83	0.16	74,74,74,74	0
56	MG	CA	3025	1/1	0.83	0.31	61,61,61,61	0
56	MG	BA	3617	1/1	0.83	0.17	44,44,44,44	0
56	MG	CA	3053	1/1	0.83	0.27	55,55,55,55	0
56	MG	DA	3400	1/1	0.83	0.18	56,56,56,56	0
56	MG	BA	3265	1/1	0.83	0.15	49,49,49,49	0
56	MG	BA	3389	1/1	0.83	0.16	56,56,56,56	0
56	MG	CA	3067	1/1	0.83	0.24	72,72,72,72	0
56	MG	CA	3078	1/1	0.83	0.28	64,64,64,64	0
56	MG	AX	3007	1/1	0.84	0.20	69,69,69,69	0
56	MG	DA	3221	1/1	0.84	0.17	52,52,52,52	0
56	MG	BA	3677	1/1	0.84	0.18	56,56,56,56	0
56	MG	DA	3257	1/1	0.84	0.37	57,57,57,57	0
56	MG	BA	3296	1/1	0.84	0.17	47,47,47,47	0
56	MG	DA	3599	1/1	0.84	0.15	47,47,47,47	0
56	MG	BA	3066	1/1	0.84	0.23	52,52,52,52	0
56	MG	CA	3090	1/1	0.84	0.27	67,67,67,67	0
56	MG	CA	3011	1/1	0.84	0.27	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	BA	3097	1/1	0.84	0.26	52,52,52,52	0
56	MG	AA	3157	1/1	0.84	0.19	84,84,84,84	0
56	MG	BA	3112	1/1	0.84	0.11	42,42,42,42	0
56	MG	DA	3437	1/1	0.84	0.12	36,36,36,36	0
56	MG	BA	3558	1/1	0.84	0.28	57,57,57,57	0
56	MG	BA	3221	1/1	0.84	0.10	39,39,39,39	0
56	MG	AA	3020	1/1	0.84	0.44	71,71,71,71	0
56	MG	CA	3134	1/1	0.84	0.18	65,65,65,65	0
56	MG	CA	3138	1/1	0.84	0.24	65,65,65,65	0
56	MG	CA	3139	1/1	0.84	0.28	69,69,69,69	0
56	MG	BB	211	1/1	0.84	0.13	81,81,81,81	0
56	MG	DA	3229	1/1	0.85	0.28	64,64,64,64	0
56	MG	DA	3249	1/1	0.85	0.29	65,65,65,65	0
56	MG	CA	3030	1/1	0.85	0.11	56,56,56,56	0
56	MG	DA	3268	1/1	0.85	0.20	56,56,56,56	0
56	MG	BA	3420	1/1	0.85	0.22	46,46,46,46	0
56	MG	BA	3605	1/1	0.85	0.14	44,44,44,44	0
56	MG	DA	3059	1/1	0.85	0.09	40,40,40,40	0
56	MG	DA	3583	1/1	0.85	0.09	56,56,56,56	0
56	MG	DA	3364	1/1	0.85	0.16	57,57,57,57	0
56	MG	DA	3389	1/1	0.85	0.12	50,50,50,50	0
56	MG	BA	3506	1/1	0.85	0.10	31,31,31,31	0
56	MG	B5	105	1/1	0.85	0.14	66,66,66,66	0
56	MG	DA	3412	1/1	0.85	0.14	56,56,56,56	0
56	MG	DA	3629	1/1	0.85	0.13	61,61,61,61	0
56	MG	DA	3631	1/1	0.85	0.20	57,57,57,57	0
56	MG	DA	3417	1/1	0.85	0.19	62,62,62,62	0
56	MG	DA	3418	1/1	0.85	0.12	44,44,44,44	0
56	MG	CA	3007	1/1	0.85	0.21	42,42,42,42	0
56	MG	CA	3158	1/1	0.85	0.15	75,75,75,75	0
56	MG	CA	3116	1/1	0.85	0.13	54,54,54,54	0
56	MG	CA	3164	1/1	0.85	0.19	73,73,73,73	0
56	MG	CA	3169	1/1	0.85	0.15	52,52,52,52	0
56	MG	BA	3392	1/1	0.85	0.15	41,41,41,41	0
56	MG	BA	3721	1/1	0.85	0.08	9,9,9,9	0
56	MG	BA	3503	1/1	0.85	0.22	64,64,64,64	0
56	MG	AA	3141	1/1	0.86	0.20	50,50,50,50	0
56	MG	AA	3080	1/1	0.86	0.42	71,71,71,71	0
56	MG	BA	3455	1/1	0.86	0.10	32,32,32,32	0
56	MG	B7	104	1/1	0.86	0.19	64,64,64,64	0
56	MG	CA	3151	1/1	0.86	0.20	60,60,60,60	0
56	MG	DA	3423	1/1	0.86	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	CA	3152	1/1	0.86	0.12	54,54,54,54	0
56	MG	DA	3433	1/1	0.86	0.13	34,34,34,34	0
56	MG	CA	3155	1/1	0.86	0.22	76,76,76,76	0
56	MG	BA	3458	1/1	0.86	0.38	66,66,66,66	0
56	MG	BA	3109	1/1	0.86	0.35	56,56,56,56	0
56	MG	AA	3150	1/1	0.86	0.18	66,66,66,66	0
56	MG	BA	3165	1/1	0.86	0.24	50,50,50,50	0
56	MG	DA	3479	1/1	0.86	0.18	35,35,35,35	0
56	MG	BA	3175	1/1	0.86	0.20	57,57,57,57	0
56	MG	BA	3199	1/1	0.86	0.18	51,51,51,51	0
56	MG	CA	3052	1/1	0.86	0.16	69,69,69,69	0
56	MG	DA	3502	1/1	0.86	0.08	48,48,48,48	0
56	MG	BA	3216	1/1	0.86	0.13	62,62,62,62	0
56	MG	AA	3122	1/1	0.86	0.14	80,80,80,80	0
56	MG	CA	3061	1/1	0.86	0.16	64,64,64,64	0
56	MG	BA	3698	1/1	0.86	0.16	50,50,50,50	0
56	MG	BA	3699	1/1	0.86	0.14	48,48,48,48	0
56	MG	AA	3183	1/1	0.86	0.22	73,73,73,73	0
56	MG	DA	3569	1/1	0.86	0.13	59,59,59,59	0
56	MG	BA	3274	1/1	0.86	0.18	51,51,51,51	0
56	MG	AA	3138	1/1	0.86	0.10	73,73,73,73	0
56	MG	DA	3603	1/1	0.86	0.23	55,55,55,55	0
56	MG	AA	3139	1/1	0.86	0.13	72,72,72,72	0
56	MG	BA	3744	1/1	0.86	0.14	61,61,61,61	0
56	MG	BA	3381	1/1	0.86	0.12	45,45,45,45	0
56	MG	DA	3621	1/1	0.86	0.33	50,50,50,50	0
56	MG	BA	3767	1/1	0.86	0.20	57,57,57,57	0
56	MG	CA	3099	1/1	0.86	0.14	58,58,58,58	0
56	MG	AA	3166	1/1	0.86	0.16	74,74,74,74	0
56	MG	CA	3103	1/1	0.86	0.11	79,79,79,79	0
56	MG	BA	3770	1/1	0.86	0.20	47,47,47,47	0
56	MG	DA	3648	1/1	0.86	0.09	31,31,31,31	0
56	MG	DA	3650	1/1	0.86	0.14	46,46,46,46	0
56	MG	BA	3813	1/1	0.86	0.13	58,58,58,58	0
56	MG	AA	3167	1/1	0.86	0.19	61,61,61,61	0
56	MG	DA	3670	1/1	0.86	0.13	49,49,49,49	0
56	MG	BB	209	1/1	0.86	0.29	69,69,69,69	0
56	MG	CA	3129	1/1	0.86	0.19	69,69,69,69	0
56	MG	DD	302	1/1	0.86	0.17	73,73,73,73	0
56	MG	BA	3595	1/1	0.86	0.46	43,43,43,43	0
56	MG	AA	3140	1/1	0.86	0.22	36,36,36,36	0
56	MG	DY	502	1/1	0.86	0.16	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DA	3377	1/1	0.86	0.19	62,62,62,62	0
56	MG	BA	3083	1/1	0.86	0.12	51,51,51,51	0
56	MG	BA	3711	1/1	0.87	0.22	51,51,51,51	0
56	MG	BA	3044	1/1	0.87	0.14	61,61,61,61	0
56	MG	AA	3173	1/1	0.87	0.25	60,60,60,60	0
56	MG	BA	3728	1/1	0.87	0.12	60,60,60,60	0
56	MG	BA	3082	1/1	0.87	0.30	55,55,55,55	0
56	MG	DA	3455	1/1	0.87	0.23	46,46,46,46	0
56	MG	DA	3458	1/1	0.87	0.12	57,57,57,57	0
56	MG	AA	3098	1/1	0.87	0.24	71,71,71,71	0
56	MG	BA	3745	1/1	0.87	0.17	58,58,58,58	0
56	MG	BA	3755	1/1	0.87	0.14	52,52,52,52	0
56	MG	BA	3759	1/1	0.87	0.10	36,36,36,36	0
56	MG	DA	3044	1/1	0.87	0.13	49,49,49,49	0
56	MG	AA	3016	1/1	0.87	0.30	55,55,55,55	0
56	MG	BA	3294	1/1	0.87	0.24	67,67,67,67	0
56	MG	DA	3525	1/1	0.87	0.17	44,44,44,44	0
56	MG	BA	3612	1/1	0.87	0.19	58,58,58,58	0
56	MG	AA	3102	1/1	0.87	0.17	64,64,64,64	0
56	MG	CA	3093	1/1	0.87	0.28	65,65,65,65	0
56	MG	DA	3547	1/1	0.87	0.12	45,45,45,45	0
56	MG	BA	3793	1/1	0.87	0.19	52,52,52,52	0
56	MG	BA	3359	1/1	0.87	0.21	40,40,40,40	0
56	MG	BA	3648	1/1	0.87	0.18	65,65,65,65	0
56	MG	BA	3371	1/1	0.87	0.14	40,40,40,40	0
56	MG	DA	3575	1/1	0.87	0.16	51,51,51,51	0
56	MG	AA	3073	1/1	0.87	0.20	71,71,71,71	0
56	MG	BB	220	1/1	0.87	0.09	51,51,51,51	0
56	MG	CA	3117	1/1	0.87	0.20	58,58,58,58	0
56	MG	BB	221	1/1	0.87	0.12	43,43,43,43	0
56	MG	AA	3038	1/1	0.87	0.20	61,61,61,61	0
56	MG	DA	3266	1/1	0.87	0.31	56,56,56,56	0
56	MG	AA	3084	1/1	0.87	0.31	62,62,62,62	0
56	MG	DA	3276	1/1	0.87	0.14	54,54,54,54	0
56	MG	DA	3290	1/1	0.87	0.12	46,46,46,46	0
56	MG	AA	3012	1/1	0.87	0.11	50,50,50,50	0
56	MG	DA	3632	1/1	0.87	0.12	50,50,50,50	0
56	MG	BA	3673	1/1	0.87	0.11	28,28,28,28	0
56	MG	DA	3330	1/1	0.87	0.20	54,54,54,54	0
56	MG	DA	3339	1/1	0.87	0.16	60,60,60,60	0
56	MG	BA	3027	1/1	0.87	0.09	45,45,45,45	0
56	MG	DA	3347	1/1	0.87	0.09	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	BA	3690	1/1	0.87	0.11	52,52,52,52	0
56	MG	BA	3427	1/1	0.87	0.14	52,52,52,52	0
56	MG	CA	3009	1/1	0.87	0.31	66,66,66,66	0
56	MG	CA	3148	1/1	0.87	0.12	88,88,88,88	0
56	MG	BA	3561	1/1	0.87	0.18	55,55,55,55	0
56	MG	CA	3013	1/1	0.87	0.16	54,54,54,54	0
56	MG	BA	3571	1/1	0.87	0.12	46,46,46,46	0
56	MG	BA	3575	1/1	0.87	0.13	27,27,27,27	0
56	MG	DA	3419	1/1	0.87	0.15	45,45,45,45	0
56	MG	BA	3434	1/1	0.87	0.16	40,40,40,40	0
56	MG	BA	3624	1/1	0.88	0.14	37,37,37,37	0
56	MG	DA	3420	1/1	0.88	0.14	40,40,40,40	0
56	MG	AA	3078	1/1	0.88	0.13	72,72,72,72	0
56	MG	BA	3644	1/1	0.88	0.15	50,50,50,50	0
56	MG	DA	3431	1/1	0.88	0.12	64,64,64,64	0
56	MG	CA	3062	1/1	0.88	0.26	67,67,67,67	0
56	MG	BA	3766	1/1	0.88	0.13	59,59,59,59	0
56	MG	BA	3378	1/1	0.88	0.11	47,47,47,47	0
56	MG	CA	3075	1/1	0.88	0.29	67,67,67,67	0
56	MG	DA	3446	1/1	0.88	0.15	44,44,44,44	0
56	MG	AA	3180	1/1	0.88	0.14	49,49,49,49	0
56	MG	CA	3081	1/1	0.88	0.25	58,58,58,58	0
56	MG	DA	3465	1/1	0.88	0.21	49,49,49,49	0
56	MG	DA	3034	1/1	0.88	0.12	45,45,45,45	0
56	MG	BA	3185	1/1	0.88	0.13	52,52,52,52	0
56	MG	DA	3478	1/1	0.88	0.20	67,67,67,67	0
56	MG	BA	3772	1/1	0.88	0.17	56,56,56,56	0
56	MG	DA	3062	1/1	0.88	0.25	51,51,51,51	0
56	MG	DA	3083	1/1	0.88	0.23	63,63,63,63	0
56	MG	DA	3098	1/1	0.88	0.11	57,57,57,57	0
56	MG	BA	3194	1/1	0.88	0.22	62,62,62,62	0
56	MG	DA	3524	1/1	0.88	0.22	59,59,59,59	0
56	MG	CA	3086	1/1	0.88	0.33	76,76,76,76	0
56	MG	CA	3087	1/1	0.88	0.14	62,62,62,62	0
56	MG	DA	3124	1/1	0.88	0.16	50,50,50,50	0
56	MG	DA	3534	1/1	0.88	0.11	67,67,67,67	0
56	MG	DA	3131	1/1	0.88	0.18	52,52,52,52	0
56	MG	DA	3541	1/1	0.88	0.14	40,40,40,40	0
56	MG	CA	3088	1/1	0.88	0.23	66,66,66,66	0
56	MG	AA	3124	1/1	0.88	0.21	71,71,71,71	0
56	MG	BB	201	1/1	0.88	0.21	65,65,65,65	0
56	MG	DA	3563	1/1	0.88	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	CA	3092	1/1	0.88	0.30	61,61,61,61	0
56	MG	AA	3047	1/1	0.88	0.24	63,63,63,63	0
56	MG	BA	3096	1/1	0.88	0.25	61,61,61,61	0
56	MG	DA	3582	1/1	0.88	0.13	64,64,64,64	0
56	MG	BA	3566	1/1	0.88	0.17	50,50,50,50	0
56	MG	DA	3589	1/1	0.88	0.12	53,53,53,53	0
56	MG	DA	3590	1/1	0.88	0.14	66,66,66,66	0
56	MG	BA	3241	1/1	0.88	0.09	45,45,45,45	0
56	MG	BA	3259	1/1	0.88	0.19	59,59,59,59	0
56	MG	DA	3255	1/1	0.88	0.26	62,62,62,62	0
56	MG	BA	3440	1/1	0.88	0.12	29,29,29,29	0
56	MG	DA	3609	1/1	0.88	0.24	61,61,61,61	0
56	MG	BO	5001	1/1	0.88	0.12	55,55,55,55	0
56	MG	BA	3580	1/1	0.88	0.15	48,48,48,48	0
56	MG	DA	3623	1/1	0.88	0.22	66,66,66,66	0
56	MG	BA	3262	1/1	0.88	0.34	54,54,54,54	0
56	MG	DA	3286	1/1	0.88	0.15	54,54,54,54	0
56	MG	AA	3048	1/1	0.88	0.27	59,59,59,59	0
56	MG	CA	3128	1/1	0.88	0.24	68,68,68,68	0
56	MG	DA	3321	1/1	0.88	0.06	30,30,30,30	0
56	MG	AA	3136	1/1	0.88	0.18	62,62,62,62	0
56	MG	BA	3716	1/1	0.88	0.20	39,39,39,39	0
56	MG	DA	3649	1/1	0.88	0.17	53,53,53,53	0
56	MG	CA	3005	1/1	0.88	0.36	73,73,73,73	0
56	MG	BA	3477	1/1	0.88	0.17	59,59,59,59	0
56	MG	DA	3656	1/1	0.88	0.09	57,57,57,57	0
56	MG	BA	3604	1/1	0.88	0.16	46,46,46,46	0
56	MG	DA	3666	1/1	0.88	0.20	47,47,47,47	0
56	MG	AA	3074	1/1	0.88	0.25	51,51,51,51	0
56	MG	BA	3111	1/1	0.88	0.17	57,57,57,57	0
56	MG	BA	3738	1/1	0.88	0.16	60,60,60,60	0
56	MG	DA	3392	1/1	0.88	0.09	50,50,50,50	0
56	MG	AA	3109	1/1	0.88	0.21	67,67,67,67	0
56	MG	BA	3135	1/1	0.88	0.08	61,61,61,61	0
56	MG	CA	3042	1/1	0.88	0.30	70,70,70,70	0
56	MG	BA	3747	1/1	0.88	0.14	33,33,33,33	0
56	MG	BA	3748	1/1	0.88	0.15	69,69,69,69	0
56	MG	BA	3028	1/1	0.89	0.26	52,52,52,52	0
56	MG	CA	3006	1/1	0.89	0.11	59,59,59,59	0
56	MG	BA	3697	1/1	0.89	0.10	46,46,46,46	0
56	MG	BA	3161	1/1	0.89	0.21	46,46,46,46	0
56	MG	BA	3029	1/1	0.89	0.13	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	BA	3040	1/1	0.89	0.15	52,52,52,52	0
56	MG	CA	3014	1/1	0.89	0.14	57,57,57,57	0
56	MG	BA	3704	1/1	0.89	0.24	36,36,36,36	0
56	MG	CA	3021	1/1	0.89	0.24	65,65,65,65	0
56	MG	BA	3567	1/1	0.89	0.11	45,45,45,45	0
56	MG	CA	3168	1/1	0.89	0.27	60,60,60,60	0
56	MG	BA	3387	1/1	0.89	0.12	45,45,45,45	0
56	MG	CA	3036	1/1	0.89	0.34	72,72,72,72	0
56	MG	DA	3445	1/1	0.89	0.15	50,50,50,50	0
56	MG	BA	3717	1/1	0.89	0.17	54,54,54,54	0
56	MG	DA	3454	1/1	0.89	0.13	56,56,56,56	0
56	MG	AA	3004	1/1	0.89	0.14	66,66,66,66	0
56	MG	CA	3045	1/1	0.89	0.31	68,68,68,68	0
56	MG	DA	3459	1/1	0.89	0.12	44,44,44,44	0
56	MG	CA	3047	1/1	0.89	0.13	59,59,59,59	0
56	MG	CA	3049	1/1	0.89	0.12	71,71,71,71	0
56	MG	DA	3017	1/1	0.89	0.15	56,56,56,56	0
56	MG	DA	3472	1/1	0.89	0.20	60,60,60,60	0
56	MG	BA	3576	1/1	0.89	0.13	36,36,36,36	0
56	MG	BA	3055	1/1	0.89	0.31	55,55,55,55	0
56	MG	DA	3057	1/1	0.89	0.09	55,55,55,55	0
56	MG	BA	3396	1/1	0.89	0.09	41,41,41,41	0
56	MG	DA	3494	1/1	0.89	0.20	57,57,57,57	0
56	MG	CA	3058	1/1	0.89	0.19	59,59,59,59	0
56	MG	BA	3059	1/1	0.89	0.15	49,49,49,49	0
56	MG	DA	3510	1/1	0.89	0.09	55,55,55,55	0
56	MG	DA	3512	1/1	0.89	0.10	48,48,48,48	0
56	MG	BA	3740	1/1	0.89	0.10	35,35,35,35	0
56	MG	BA	3741	1/1	0.89	0.12	50,50,50,50	0
56	MG	BA	3584	1/1	0.89	0.14	34,34,34,34	0
56	MG	AA	3162	1/1	0.89	0.14	59,59,59,59	0
56	MG	DA	3115	1/1	0.89	0.17	46,46,46,46	0
56	MG	DA	3118	1/1	0.89	0.20	43,43,43,43	0
56	MG	AA	3104	1/1	0.89	0.33	70,70,70,70	0
56	MG	DA	3542	1/1	0.89	0.23	58,58,58,58	0
56	MG	BA	3225	1/1	0.89	0.13	31,31,31,31	0
56	MG	DA	3132	1/1	0.89	0.12	54,54,54,54	0
56	MG	DA	3146	1/1	0.89	0.18	49,49,49,49	0
56	MG	AA	3097	1/1	0.89	0.41	71,71,71,71	0
56	MG	BA	3242	1/1	0.89	0.09	47,47,47,47	0
56	MG	BA	3606	1/1	0.89	0.19	67,67,67,67	0
56	MG	BA	3452	1/1	0.89	0.18	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	BA	3255	1/1	0.89	0.14	41,41,41,41	0
56	MG	DA	3218	1/1	0.89	0.14	30,30,30,30	0
56	MG	BA	3457	1/1	0.89	0.17	47,47,47,47	0
56	MG	BA	3092	1/1	0.89	0.13	53,53,53,53	0
56	MG	DA	3225	1/1	0.89	0.12	49,49,49,49	0
56	MG	BA	3464	1/1	0.89	0.10	46,46,46,46	0
56	MG	DA	3240	1/1	0.89	0.09	42,42,42,42	0
56	MG	BA	3634	1/1	0.89	0.21	47,47,47,47	0
56	MG	BA	3639	1/1	0.89	0.11	54,54,54,54	0
56	MG	AA	3142	1/1	0.89	0.14	46,46,46,46	0
56	MG	DA	3264	1/1	0.89	0.24	50,50,50,50	0
56	MG	AA	3130	1/1	0.89	0.15	56,56,56,56	0
56	MG	AA	3055	1/1	0.89	0.40	69,69,69,69	0
56	MG	AX	3003	1/1	0.89	0.29	66,66,66,66	0
56	MG	DA	3630	1/1	0.89	0.16	51,51,51,51	0
56	MG	BA	3292	1/1	0.89	0.17	40,40,40,40	0
56	MG	AA	3001	1/1	0.89	0.16	77,77,77,77	0
56	MG	DA	3309	1/1	0.89	0.13	46,46,46,46	0
56	MG	DA	3637	1/1	0.89	0.06	70,70,70,70	0
56	MG	BA	3666	1/1	0.89	0.09	47,47,47,47	0
56	MG	CA	3118	1/1	0.89	0.19	60,60,60,60	0
56	MG	DA	3322	1/1	0.89	0.17	53,53,53,53	0
56	MG	BF	304	1/1	0.89	0.12	35,35,35,35	0
56	MG	DA	3654	1/1	0.89	0.14	50,50,50,50	0
56	MG	BA	3295	1/1	0.89	0.18	49,49,49,49	0
56	MG	CA	3127	1/1	0.89	0.32	65,65,65,65	0
56	MG	AA	3156	1/1	0.89	0.13	67,67,67,67	0
56	MG	DA	3665	1/1	0.89	0.14	48,48,48,48	0
56	MG	BA	3315	1/1	0.89	0.21	59,59,59,59	0
56	MG	B0	105	1/1	0.89	0.13	64,64,64,64	0
56	MG	DA	3673	1/1	0.89	0.18	68,68,68,68	0
56	MG	DA	3365	1/1	0.89	0.11	56,56,56,56	0
56	MG	DA	3376	1/1	0.89	0.15	51,51,51,51	0
56	MG	CA	3132	1/1	0.89	0.24	55,55,55,55	0
56	MG	DA	3388	1/1	0.89	0.10	52,52,52,52	0
56	MG	DG	3001	1/1	0.89	0.15	57,57,57,57	0
56	MG	DP	202	1/1	0.89	0.23	55,55,55,55	0
56	MG	DV	3002	1/1	0.89	0.20	48,48,48,48	0
56	MG	BA	3682	1/1	0.89	0.19	39,39,39,39	0
56	MG	DW	201	1/1	0.89	0.12	67,67,67,67	0
56	MG	BA	3125	1/1	0.89	0.15	49,49,49,49	0
56	MG	DA	3399	1/1	0.89	0.12	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	BA	3547	1/1	0.89	0.09	64,64,64,64	0
60	K	CX	3001	1/1	0.89	0.14	77,77,77,77	0
56	MG	BA	3290	1/1	0.90	0.23	50,50,50,50	0
56	MG	AA	3025	1/1	0.90	0.30	69,69,69,69	0
56	MG	CA	3163	1/1	0.90	0.10	78,78,78,78	0
56	MG	BA	3121	1/1	0.90	0.14	45,45,45,45	0
56	MG	AA	3026	1/1	0.90	0.18	71,71,71,71	0
56	MG	AA	3008	1/1	0.90	0.07	56,56,56,56	0
56	MG	BA	3529	1/1	0.90	0.15	25,25,25,25	0
56	MG	BA	3310	1/1	0.90	0.10	42,42,42,42	0
56	MG	CA	3032	1/1	0.90	0.11	57,57,57,57	0
56	MG	BA	3312	1/1	0.90	0.12	35,35,35,35	0
56	MG	BA	3706	1/1	0.90	0.08	63,63,63,63	0
56	MG	BA	3039	1/1	0.90	0.22	58,58,58,58	0
56	MG	BA	3319	1/1	0.90	0.12	39,39,39,39	0
56	MG	DA	3442	1/1	0.90	0.10	37,37,37,37	0
56	MG	DA	3443	1/1	0.90	0.17	38,38,38,38	0
56	MG	DA	3032	1/1	0.90	0.08	47,47,47,47	0
56	MG	DA	3033	1/1	0.90	0.11	54,54,54,54	0
56	MG	DA	3453	1/1	0.90	0.18	56,56,56,56	0
56	MG	BA	3356	1/1	0.90	0.19	52,52,52,52	0
56	MG	BA	3162	1/1	0.90	0.15	53,53,53,53	0
56	MG	BA	3363	1/1	0.90	0.10	66,66,66,66	0
56	MG	AA	3149	1/1	0.90	0.12	68,68,68,68	0
56	MG	BA	3733	1/1	0.90	0.08	46,46,46,46	0
56	MG	DA	3076	1/1	0.90	0.11	39,39,39,39	0
56	MG	BA	3377	1/1	0.90	0.17	48,48,48,48	0
56	MG	DA	3089	1/1	0.90	0.14	47,47,47,47	0
56	MG	CA	3059	1/1	0.90	0.15	75,75,75,75	0
56	MG	DA	3100	1/1	0.90	0.29	66,66,66,66	0
56	MG	BA	3578	1/1	0.90	0.13	20,20,20,20	0
56	MG	AA	3174	1/1	0.90	0.11	54,54,54,54	0
56	MG	DA	3489	1/1	0.90	0.12	45,45,45,45	0
56	MG	DA	3493	1/1	0.90	0.25	63,63,63,63	0
56	MG	BA	3048	1/1	0.90	0.21	47,47,47,47	0
56	MG	BA	3193	1/1	0.90	0.27	62,62,62,62	0
56	MG	CA	3072	1/1	0.90	0.34	62,62,62,62	0
56	MG	AA	3091	1/1	0.90	0.13	40,40,40,40	0
56	MG	BA	3587	1/1	0.90	0.09	54,54,54,54	0
56	MG	BA	3590	1/1	0.90	0.20	60,60,60,60	0
56	MG	DA	3135	1/1	0.90	0.24	46,46,46,46	0
56	MG	BA	3195	1/1	0.90	0.26	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	DA	3531	1/1	0.90	0.14	62,62,62,62	0
56	MG	BA	3056	1/1	0.90	0.08	50,50,50,50	0
56	MG	BA	3204	1/1	0.90	0.13	55,55,55,55	0
56	MG	DA	3184	1/1	0.90	0.15	49,49,49,49	0
56	MG	CA	3085	1/1	0.90	0.23	73,73,73,73	0
56	MG	DA	3194	1/1	0.90	0.18	54,54,54,54	0
56	MG	DA	3201	1/1	0.90	0.31	64,64,64,64	0
56	MG	DA	3548	1/1	0.90	0.12	55,55,55,55	0
56	MG	DA	3549	1/1	0.90	0.12	32,32,32,32	0
56	MG	BA	3399	1/1	0.90	0.15	61,61,61,61	0
56	MG	BA	3211	1/1	0.90	0.18	41,41,41,41	0
56	MG	DA	3212	1/1	0.90	0.17	54,54,54,54	0
56	MG	DA	3214	1/1	0.90	0.27	51,51,51,51	0
56	MG	BA	3422	1/1	0.90	0.15	53,53,53,53	0
56	MG	DA	3570	1/1	0.90	0.11	59,59,59,59	0
56	MG	AA	3057	1/1	0.90	0.43	66,66,66,66	0
56	MG	BA	3219	1/1	0.90	0.12	62,62,62,62	0
56	MG	BA	3789	1/1	0.90	0.16	37,37,37,37	0
56	MG	DA	3226	1/1	0.90	0.17	57,57,57,57	0
56	MG	AA	3096	1/1	0.90	0.39	60,60,60,60	0
56	MG	DA	3233	1/1	0.90	0.14	40,40,40,40	0
56	MG	DA	3234	1/1	0.90	0.22	56,56,56,56	0
56	MG	DA	3239	1/1	0.90	0.20	51,51,51,51	0
56	MG	BA	3806	1/1	0.90	0.32	33,33,33,33	0
56	MG	BA	3618	1/1	0.90	0.11	56,56,56,56	0
56	MG	AA	3010	1/1	0.90	0.13	63,63,63,63	0
56	MG	DA	3616	1/1	0.90	0.10	43,43,43,43	0
56	MG	BA	3237	1/1	0.90	0.37	63,63,63,63	0
56	MG	DA	3260	1/1	0.90	0.30	55,55,55,55	0
56	MG	DA	3624	1/1	0.90	0.23	46,46,46,46	0
56	MG	BA	3631	1/1	0.90	0.21	49,49,49,49	0
56	MG	AA	3158	1/1	0.90	0.12	71,71,71,71	0
56	MG	BA	3636	1/1	0.90	0.14	52,52,52,52	0
56	MG	BA	3453	1/1	0.90	0.21	52,52,52,52	0
56	MG	DA	3278	1/1	0.90	0.12	37,37,37,37	0
56	MG	DA	3282	1/1	0.90	0.19	42,42,42,42	0
56	MG	AA	3066	1/1	0.90	0.23	58,58,58,58	0
56	MG	DA	3639	1/1	0.90	0.15	52,52,52,52	0
56	MG	CA	3123	1/1	0.90	0.16	67,67,67,67	0
56	MG	DA	3643	1/1	0.90	0.18	49,49,49,49	0
56	MG	DA	3305	1/1	0.90	0.13	45,45,45,45	0
56	MG	BA	3250	1/1	0.90	0.22	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	CA	3125	1/1	0.90	0.08	63,63,63,63	0
56	MG	DA	3652	1/1	0.90	0.18	53,53,53,53	0
56	MG	DA	3320	1/1	0.90	0.12	34,34,34,34	0
56	MG	AD	502	1/1	0.90	0.28	56,56,56,56	0
56	MG	BA	3654	1/1	0.90	0.13	49,49,49,49	0
56	MG	BU	201	1/1	0.90	0.12	36,36,36,36	0
56	MG	BU	206	1/1	0.90	0.42	61,61,61,61	0
56	MG	BZ	301	1/1	0.90	0.13	58,58,58,58	0
56	MG	AA	3017	1/1	0.90	0.34	69,69,69,69	0
56	MG	DA	3343	1/1	0.90	0.14	42,42,42,42	0
56	MG	DA	3344	1/1	0.90	0.13	46,46,46,46	0
56	MG	DB	3002	1/1	0.90	0.20	58,58,58,58	0
56	MG	DA	3345	1/1	0.90	0.13	38,38,38,38	0
56	MG	BA	3103	1/1	0.90	0.11	44,44,44,44	0
56	MG	BA	3479	1/1	0.90	0.11	53,53,53,53	0
56	MG	DE	302	1/1	0.90	0.10	33,33,33,33	0
56	MG	BA	3495	1/1	0.90	0.11	58,58,58,58	0
56	MG	DP	201	1/1	0.90	0.24	58,58,58,58	0
56	MG	CA	3143	1/1	0.90	0.24	77,77,77,77	0
56	MG	AA	3019	1/1	0.90	0.14	66,66,66,66	0
56	MG	AX	3006	1/1	0.90	0.17	71,71,71,71	0
56	MG	BA	3277	1/1	0.90	0.20	54,54,54,54	0
56	MG	BA	3678	1/1	0.90	0.28	35,35,35,35	0
56	MG	DA	3398	1/1	0.90	0.29	52,52,52,52	0
56	MG	AA	3011	1/1	0.90	0.20	56,56,56,56	0
56	MG	CA	3010	1/1	0.90	0.24	57,57,57,57	0
56	MG	BA	3019	1/1	0.91	0.11	39,39,39,39	0
56	MG	CA	3160	1/1	0.91	0.20	61,61,61,61	0
56	MG	CA	3162	1/1	0.91	0.08	42,42,42,42	0
56	MG	BA	3318	1/1	0.91	0.08	25,25,25,25	0
56	MG	DA	3391	1/1	0.91	0.07	44,44,44,44	0
56	MG	BA	3020	1/1	0.91	0.13	36,36,36,36	0
56	MG	BA	3685	1/1	0.91	0.14	51,51,51,51	0
56	MG	BA	3687	1/1	0.91	0.18	53,53,53,53	0
56	MG	BA	3321	1/1	0.91	0.11	21,21,21,21	0
56	MG	BA	3534	1/1	0.91	0.12	44,44,44,44	0
56	MG	DA	3405	1/1	0.91	0.10	41,41,41,41	0
56	MG	BA	3355	1/1	0.91	0.14	28,28,28,28	0
56	MG	AA	3095	1/1	0.91	0.17	50,50,50,50	0
56	MG	BA	3180	1/1	0.91	0.24	46,46,46,46	0
56	MG	AA	3168	1/1	0.91	0.10	57,57,57,57	0
56	MG	CX	3003	1/1	0.91	0.14	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DA	3014	1/1	0.91	0.07	43,43,43,43	0
56	MG	DA	3424	1/1	0.91	0.12	41,41,41,41	0
56	MG	DA	3015	1/1	0.91	0.21	48,48,48,48	0
56	MG	BA	3700	1/1	0.91	0.11	53,53,53,53	0
56	MG	DA	3019	1/1	0.91	0.11	48,48,48,48	0
56	MG	BA	3368	1/1	0.91	0.12	35,35,35,35	0
56	MG	BA	3186	1/1	0.91	0.13	47,47,47,47	0
56	MG	AA	3033	1/1	0.91	0.30	58,58,58,58	0
56	MG	DA	3037	1/1	0.91	0.09	34,34,34,34	0
56	MG	AA	3021	1/1	0.91	0.19	62,62,62,62	0
56	MG	DA	3046	1/1	0.91	0.21	56,56,56,56	0
56	MG	CA	3041	1/1	0.91	0.34	62,62,62,62	0
56	MG	BA	3715	1/1	0.91	0.13	51,51,51,51	0
56	MG	AA	3070	1/1	0.91	0.18	65,65,65,65	0
56	MG	DA	3066	1/1	0.91	0.21	47,47,47,47	0
56	MG	DA	3068	1/1	0.91	0.14	47,47,47,47	0
56	MG	AA	3022	1/1	0.91	0.07	54,54,54,54	0
56	MG	BA	3719	1/1	0.91	0.11	36,36,36,36	0
56	MG	DA	3087	1/1	0.91	0.10	50,50,50,50	0
56	MG	BA	3720	1/1	0.91	0.12	45,45,45,45	0
56	MG	DA	3091	1/1	0.91	0.15	46,46,46,46	0
56	MG	AA	3054	1/1	0.91	0.15	62,62,62,62	0
56	MG	BA	3724	1/1	0.91	0.09	25,25,25,25	0
56	MG	DA	3482	1/1	0.91	0.12	42,42,42,42	0
56	MG	BA	3050	1/1	0.91	0.15	46,46,46,46	0
56	MG	CA	3057	1/1	0.91	0.16	52,52,52,52	0
56	MG	AA	3076	1/1	0.91	0.08	56,56,56,56	0
56	MG	BA	3731	1/1	0.91	0.07	26,26,26,26	0
56	MG	DA	3116	1/1	0.91	0.13	48,48,48,48	0
56	MG	BA	3395	1/1	0.91	0.14	36,36,36,36	0
56	MG	BA	3735	1/1	0.91	0.08	20,20,20,20	0
56	MG	DA	3128	1/1	0.91	0.23	57,57,57,57	0
56	MG	DA	3511	1/1	0.91	0.15	54,54,54,54	0
56	MG	DA	3129	1/1	0.91	0.14	42,42,42,42	0
56	MG	DA	3517	1/1	0.91	0.09	57,57,57,57	0
56	MG	BA	3736	1/1	0.91	0.10	42,42,42,42	0
56	MG	BA	3585	1/1	0.91	0.08	58,58,58,58	0
56	MG	CA	3068	1/1	0.91	0.30	64,64,64,64	0
56	MG	AA	3077	1/1	0.91	0.25	54,54,54,54	0
56	MG	CA	3073	1/1	0.91	0.16	55,55,55,55	0
56	MG	DA	3168	1/1	0.91	0.07	47,47,47,47	0
56	MG	DA	3536	1/1	0.91	0.08	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	AA	3039	1/1	0.91	0.09	46,46,46,46	0
56	MG	DA	3181	1/1	0.91	0.27	54,54,54,54	0
56	MG	DA	3182	1/1	0.91	0.07	43,43,43,43	0
56	MG	CA	3077	1/1	0.91	0.31	61,61,61,61	0
56	MG	BA	3411	1/1	0.91	0.17	30,30,30,30	0
56	MG	DA	3186	1/1	0.91	0.27	54,54,54,54	0
56	MG	DA	3556	1/1	0.91	0.14	55,55,55,55	0
56	MG	DA	3187	1/1	0.91	0.27	51,51,51,51	0
56	MG	AA	3181	1/1	0.91	0.19	63,63,63,63	0
56	MG	DA	3200	1/1	0.91	0.21	57,57,57,57	0
56	MG	DA	3565	1/1	0.91	0.18	45,45,45,45	0
56	MG	BA	3596	1/1	0.91	0.20	68,68,68,68	0
56	MG	BA	3597	1/1	0.91	0.13	40,40,40,40	0
56	MG	DA	3210	1/1	0.91	0.14	53,53,53,53	0
56	MG	DA	3574	1/1	0.91	0.12	55,55,55,55	0
56	MG	BA	3229	1/1	0.91	0.13	44,44,44,44	0
56	MG	BA	3754	1/1	0.91	0.17	60,60,60,60	0
56	MG	AA	3182	1/1	0.91	0.25	64,64,64,64	0
56	MG	BA	3431	1/1	0.91	0.10	63,63,63,63	0
56	MG	AA	3155	1/1	0.91	0.15	49,49,49,49	0
56	MG	AA	3056	1/1	0.91	0.29	54,54,54,54	0
56	MG	AA	3002	1/1	0.91	0.15	63,63,63,63	0
56	MG	BA	3615	1/1	0.91	0.13	60,60,60,60	0
56	MG	BA	3254	1/1	0.91	0.22	55,55,55,55	0
56	MG	DA	3608	1/1	0.91	0.07	47,47,47,47	0
56	MG	CA	3094	1/1	0.91	0.40	68,68,68,68	0
56	MG	BA	3771	1/1	0.91	0.19	52,52,52,52	0
56	MG	AA	3187	1/1	0.91	0.14	54,54,54,54	0
56	MG	BA	3778	1/1	0.91	0.14	41,41,41,41	0
56	MG	DA	3242	1/1	0.91	0.28	68,68,68,68	0
56	MG	BA	3781	1/1	0.91	0.14	47,47,47,47	0
56	MG	BA	3622	1/1	0.91	0.10	29,29,29,29	0
56	MG	DA	3627	1/1	0.91	0.11	64,64,64,64	0
56	MG	DA	3256	1/1	0.91	0.13	46,46,46,46	0
56	MG	CA	3112	1/1	0.91	0.16	56,56,56,56	0
56	MG	AA	3085	1/1	0.91	0.26	66,66,66,66	0
56	MG	BA	3800	1/1	0.91	0.09	41,41,41,41	0
56	MG	AE	202	1/1	0.91	0.09	74,74,74,74	0
56	MG	DA	3635	1/1	0.91	0.19	47,47,47,47	0
56	MG	AF	3001	1/1	0.91	0.16	56,56,56,56	0
56	MG	AA	3087	1/1	0.91	0.34	53,53,53,53	0
56	MG	BA	3461	1/1	0.91	0.08	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DA	3279	1/1	0.91	0.27	54,54,54,54	0
56	MG	DA	3646	1/1	0.91	0.15	54,54,54,54	0
56	MG	DA	3280	1/1	0.91	0.28	62,62,62,62	0
56	MG	BB	206	1/1	0.91	0.18	58,58,58,58	0
56	MG	AA	3018	1/1	0.91	0.17	50,50,50,50	0
56	MG	BA	3280	1/1	0.91	0.08	32,32,32,32	0
56	MG	DA	3293	1/1	0.91	0.20	57,57,57,57	0
56	MG	DA	3294	1/1	0.91	0.08	36,36,36,36	0
56	MG	BB	216	1/1	0.91	0.21	63,63,63,63	0
56	MG	BB	219	1/1	0.91	0.11	74,74,74,74	0
56	MG	DA	3664	1/1	0.91	0.25	50,50,50,50	0
56	MG	DA	3310	1/1	0.91	0.10	49,49,49,49	0
56	MG	DA	3316	1/1	0.91	0.08	34,34,34,34	0
56	MG	BA	3646	1/1	0.91	0.12	57,57,57,57	0
56	MG	BA	3120	1/1	0.91	0.09	50,50,50,50	0
56	MG	BA	3649	1/1	0.91	0.09	44,44,44,44	0
56	MG	BE	307	1/1	0.91	0.08	31,31,31,31	0
56	MG	BA	3492	1/1	0.91	0.09	47,47,47,47	0
56	MG	DB	3009	1/1	0.91	0.21	58,58,58,58	0
56	MG	DB	3010	1/1	0.91	0.23	53,53,53,53	0
56	MG	DA	3326	1/1	0.91	0.15	47,47,47,47	0
56	MG	AA	3165	1/1	0.91	0.16	49,49,49,49	0
56	MG	DA	3338	1/1	0.91	0.13	43,43,43,43	0
56	MG	AA	3061	1/1	0.91	0.19	54,54,54,54	0
56	MG	CA	3147	1/1	0.91	0.24	70,70,70,70	0
56	MG	BA	3133	1/1	0.91	0.12	48,48,48,48	0
56	MG	AX	3009	1/1	0.91	0.18	74,74,74,74	0
56	MG	BA	3137	1/1	0.91	0.21	40,40,40,40	0
56	MG	BA	3147	1/1	0.91	0.09	41,41,41,41	0
56	MG	AX	3010	1/1	0.91	0.11	59,59,59,59	0
56	MG	BA	3674	1/1	0.91	0.14	55,55,55,55	0
56	MG	DA	3369	1/1	0.91	0.09	37,37,37,37	0
56	MG	DA	3370	1/1	0.91	0.08	50,50,50,50	0
56	MG	DA	3415	1/1	0.92	0.13	59,59,59,59	0
56	MG	BA	3632	1/1	0.92	0.21	43,43,43,43	0
56	MG	DA	3079	1/1	0.92	0.08	32,32,32,32	0
56	MG	BA	3633	1/1	0.92	0.14	59,59,59,59	0
56	MG	AA	3029	1/1	0.92	0.17	43,43,43,43	0
56	MG	AA	3144	1/1	0.92	0.19	59,59,59,59	0
56	MG	AA	3189	1/1	0.92	0.32	62,62,62,62	0
56	MG	BA	3643	1/1	0.92	0.13	58,58,58,58	0
56	MG	DA	3430	1/1	0.92	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	3360	1/1	0.92	0.09	21,21,21,21	0
56	MG	BA	3645	1/1	0.92	0.09	50,50,50,50	0
56	MG	DA	3106	1/1	0.92	0.07	52,52,52,52	0
56	MG	DA	3107	1/1	0.92	0.12	43,43,43,43	0
56	MG	BA	3222	1/1	0.92	0.08	48,48,48,48	0
56	MG	BA	3779	1/1	0.92	0.09	45,45,45,45	0
56	MG	CA	3079	1/1	0.92	0.48	67,67,67,67	0
56	MG	BA	3122	1/1	0.92	0.23	46,46,46,46	0
56	MG	AA	3146	1/1	0.92	0.23	53,53,53,53	0
56	MG	DA	3450	1/1	0.92	0.12	41,41,41,41	0
56	MG	BA	3792	1/1	0.92	0.11	52,52,52,52	0
56	MG	BA	3231	1/1	0.92	0.12	51,51,51,51	0
56	MG	BA	3795	1/1	0.92	0.18	43,43,43,43	0
56	MG	BA	3796	1/1	0.92	0.15	47,47,47,47	0
56	MG	AA	3041	1/1	0.92	0.14	64,64,64,64	0
56	MG	BA	3656	1/1	0.92	0.14	64,64,64,64	0
56	MG	CA	3089	1/1	0.92	0.28	67,67,67,67	0
56	MG	DA	3147	1/1	0.92	0.17	53,53,53,53	0
56	MG	BA	3807	1/1	0.92	0.18	66,66,66,66	0
56	MG	DA	3152	1/1	0.92	0.10	62,62,62,62	0
56	MG	BA	3054	1/1	0.92	0.18	43,43,43,43	0
56	MG	DA	3170	1/1	0.92	0.20	46,46,46,46	0
56	MG	BA	3537	1/1	0.92	0.12	21,21,21,21	0
56	MG	BA	3538	1/1	0.92	0.10	26,26,26,26	0
56	MG	BA	3545	1/1	0.92	0.07	36,36,36,36	0
56	MG	AA	3030	1/1	0.92	0.12	63,63,63,63	0
56	MG	BA	3551	1/1	0.92	0.16	49,49,49,49	0
56	MG	BA	3246	1/1	0.92	0.09	47,47,47,47	0
56	MG	DA	3501	1/1	0.92	0.08	46,46,46,46	0
56	MG	BA	3247	1/1	0.92	0.18	50,50,50,50	0
56	MG	DA	3504	1/1	0.92	0.12	41,41,41,41	0
56	MG	DA	3192	1/1	0.92	0.08	57,57,57,57	0
56	MG	BA	3559	1/1	0.92	0.08	59,59,59,59	0
56	MG	BA	3144	1/1	0.92	0.12	43,43,43,43	0
56	MG	DA	3513	1/1	0.92	0.08	30,30,30,30	0
56	MG	BA	3251	1/1	0.92	0.32	52,52,52,52	0
56	MG	BA	3252	1/1	0.92	0.17	44,44,44,44	0
56	MG	AA	3064	1/1	0.92	0.07	54,54,54,54	0
56	MG	CA	3120	1/1	0.92	0.18	65,65,65,65	0
56	MG	BF	306	1/1	0.92	0.20	30,30,30,30	0
56	MG	DA	3213	1/1	0.92	0.09	46,46,46,46	0
56	MG	BG	3002	1/1	0.92	0.08	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DA	3215	1/1	0.92	0.31	49,49,49,49	0
56	MG	BN	3002	1/1	0.92	0.12	57,57,57,57	0
56	MG	BA	3572	1/1	0.92	0.10	52,52,52,52	0
56	MG	BA	3401	1/1	0.92	0.15	34,34,34,34	0
56	MG	DA	3545	1/1	0.92	0.11	51,51,51,51	0
56	MG	BA	3151	1/1	0.92	0.08	37,37,37,37	0
56	MG	BA	3417	1/1	0.92	0.13	32,32,32,32	0
56	MG	BA	3419	1/1	0.92	0.09	25,25,25,25	0
56	MG	DA	3554	1/1	0.92	0.13	47,47,47,47	0
56	MG	DA	3230	1/1	0.92	0.21	52,52,52,52	0
56	MG	BZ	302	1/1	0.92	0.23	56,56,56,56	0
56	MG	BA	3256	1/1	0.92	0.13	54,54,54,54	0
56	MG	DA	3236	1/1	0.92	0.10	42,42,42,42	0
56	MG	DA	3564	1/1	0.92	0.08	50,50,50,50	0
56	MG	BA	3157	1/1	0.92	0.39	36,36,36,36	0
56	MG	DA	3566	1/1	0.92	0.11	62,62,62,62	0
56	MG	AA	3129	1/1	0.92	0.14	70,70,70,70	0
56	MG	DA	3568	1/1	0.92	0.08	66,66,66,66	0
56	MG	B5	101	1/1	0.92	0.25	39,39,39,39	0
56	MG	DA	3243	1/1	0.92	0.10	47,47,47,47	0
56	MG	DA	3244	1/1	0.92	0.30	59,59,59,59	0
56	MG	BA	3062	1/1	0.92	0.09	48,48,48,48	0
56	MG	DA	3577	1/1	0.92	0.11	49,49,49,49	0
56	MG	AA	3154	1/1	0.92	0.18	50,50,50,50	0
56	MG	CA	3002	1/1	0.92	0.14	62,62,62,62	0
56	MG	DA	3584	1/1	0.92	0.12	31,31,31,31	0
56	MG	BA	3168	1/1	0.92	0.10	39,39,39,39	0
56	MG	DA	3258	1/1	0.92	0.32	51,51,51,51	0
56	MG	DA	3594	1/1	0.92	0.11	54,54,54,54	0
56	MG	DA	3597	1/1	0.92	0.07	49,49,49,49	0
56	MG	DA	3259	1/1	0.92	0.30	53,53,53,53	0
56	MG	BA	3439	1/1	0.92	0.10	71,71,71,71	0
56	MG	DA	3605	1/1	0.92	0.10	54,54,54,54	0
56	MG	BA	3172	1/1	0.92	0.12	52,52,52,52	0
56	MG	CA	3008	1/1	0.92	0.40	60,60,60,60	0
56	MG	CA	3153	1/1	0.92	0.13	52,52,52,52	0
56	MG	AA	3176	1/1	0.92	0.14	57,57,57,57	0
56	MG	CA	3157	1/1	0.92	0.19	61,61,61,61	0
56	MG	AA	3046	1/1	0.92	0.27	56,56,56,56	0
56	MG	AA	3134	1/1	0.92	0.10	65,65,65,65	0
56	MG	AA	3103	1/1	0.92	0.20	48,48,48,48	0
56	MG	BA	3192	1/1	0.92	0.10	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	3625	1/1	0.92	0.15	56,56,56,56	0
56	MG	CA	3016	1/1	0.92	0.21	53,53,53,53	0
56	MG	DA	3291	1/1	0.92	0.11	41,41,41,41	0
56	MG	BA	3726	1/1	0.92	0.17	65,65,65,65	0
56	MG	AA	3092	1/1	0.92	0.36	54,54,54,54	0
56	MG	CA	3024	1/1	0.92	0.23	58,58,58,58	0
56	MG	BA	3100	1/1	0.92	0.27	53,53,53,53	0
56	MG	CA	3026	1/1	0.92	0.18	55,55,55,55	0
56	MG	CA	3029	1/1	0.92	0.15	58,58,58,58	0
56	MG	BA	3611	1/1	0.92	0.09	45,45,45,45	0
56	MG	DA	3638	1/1	0.92	0.10	42,42,42,42	0
56	MG	BA	3026	1/1	0.92	0.17	49,49,49,49	0
56	MG	BA	3613	1/1	0.92	0.19	55,55,55,55	0
56	MG	CA	3039	1/1	0.92	0.20	55,55,55,55	0
56	MG	DA	3645	1/1	0.92	0.08	38,38,38,38	0
56	MG	DA	3002	1/1	0.92	0.19	55,55,55,55	0
56	MG	DA	3325	1/1	0.92	0.08	37,37,37,37	0
56	MG	DA	3006	1/1	0.92	0.40	58,58,58,58	0
56	MG	CA	3040	1/1	0.92	0.15	45,45,45,45	0
56	MG	BA	3614	1/1	0.92	0.30	59,59,59,59	0
56	MG	BA	3197	1/1	0.92	0.25	51,51,51,51	0
56	MG	BA	3739	1/1	0.92	0.12	46,46,46,46	0
56	MG	DA	3026	1/1	0.92	0.11	52,52,52,52	0
56	MG	BA	3616	1/1	0.92	0.13	51,51,51,51	0
56	MG	BA	3478	1/1	0.92	0.13	59,59,59,59	0
56	MG	AA	3015	1/1	0.92	0.07	65,65,65,65	0
56	MG	DA	3360	1/1	0.92	0.14	37,37,37,37	0
56	MG	DA	3036	1/1	0.92	0.14	46,46,46,46	0
56	MG	CA	3051	1/1	0.92	0.32	55,55,55,55	0
56	MG	DA	3367	1/1	0.92	0.14	55,55,55,55	0
56	MG	DA	3043	1/1	0.92	0.12	52,52,52,52	0
56	MG	DB	3003	1/1	0.92	0.10	56,56,56,56	0
56	MG	DB	3004	1/1	0.92	0.20	53,53,53,53	0
56	MG	DB	3006	1/1	0.92	0.26	60,60,60,60	0
56	MG	AA	3106	1/1	0.92	0.09	61,61,61,61	0
56	MG	DA	3372	1/1	0.92	0.09	24,24,24,24	0
56	MG	AA	3079	1/1	0.92	0.33	55,55,55,55	0
56	MG	DA	3052	1/1	0.92	0.05	26,26,26,26	0
56	MG	DD	306	1/1	0.92	0.46	48,48,48,48	0
56	MG	DA	3385	1/1	0.92	0.06	32,32,32,32	0
56	MG	DA	3054	1/1	0.92	0.08	39,39,39,39	0
56	MG	BA	3496	1/1	0.92	0.14	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DO	5001	1/1	0.92	0.18	55,55,55,55	0
56	MG	CA	3055	1/1	0.92	0.23	55,55,55,55	0
56	MG	DA	3061	1/1	0.92	0.06	41,41,41,41	0
56	MG	DR	5001	1/1	0.92	0.12	51,51,51,51	0
56	MG	DU	3001	1/1	0.92	0.21	55,55,55,55	0
56	MG	DU	3004	1/1	0.92	0.18	59,59,59,59	0
56	MG	DA	3393	1/1	0.92	0.07	48,48,48,48	0
56	MG	BA	3750	1/1	0.92	0.16	42,42,42,42	0
56	MG	BA	3629	1/1	0.92	0.20	57,57,57,57	0
56	MG	DW	202	1/1	0.92	0.15	46,46,46,46	0
56	MG	BA	3344	1/1	0.92	0.23	55,55,55,55	0
56	MG	D1	101	1/1	0.92	0.13	50,50,50,50	0
56	MG	D8	5001	1/1	0.92	0.18	52,52,52,52	0
56	MG	DA	3070	1/1	0.92	0.14	51,51,51,51	0
56	MG	DA	3073	1/1	0.92	0.25	55,55,55,55	0
56	MG	DA	3074	1/1	0.92	0.14	56,56,56,56	0
56	MG	BA	3485	1/1	0.93	0.09	55,55,55,55	0
56	MG	DA	3148	1/1	0.93	0.17	43,43,43,43	0
56	MG	DA	3444	1/1	0.93	0.09	46,46,46,46	0
56	MG	CA	3121	1/1	0.93	0.09	81,81,81,81	0
56	MG	BA	3366	1/1	0.93	0.09	42,42,42,42	0
56	MG	DA	3163	1/1	0.93	0.21	54,54,54,54	0
56	MG	DA	3166	1/1	0.93	0.17	35,35,35,35	0
56	MG	BA	3190	1/1	0.93	0.19	50,50,50,50	0
56	MG	BA	3191	1/1	0.93	0.18	43,43,43,43	0
56	MG	DA	3457	1/1	0.93	0.11	43,43,43,43	0
56	MG	DA	3172	1/1	0.93	0.11	31,31,31,31	0
56	MG	CA	3001	1/1	0.93	0.08	59,59,59,59	0
56	MG	DA	3180	1/1	0.93	0.12	58,58,58,58	0
56	MG	BA	3375	1/1	0.93	0.12	38,38,38,38	0
56	MG	DA	3467	1/1	0.93	0.25	48,48,48,48	0
56	MG	AA	3006	1/1	0.93	0.10	71,71,71,71	0
56	MG	DA	3470	1/1	0.93	0.15	31,31,31,31	0
56	MG	BA	3257	1/1	0.93	0.24	54,54,54,54	0
56	MG	BA	3002	1/1	0.93	0.14	57,57,57,57	0
56	MG	BA	3018	1/1	0.93	0.19	63,63,63,63	0
56	MG	AA	3101	1/1	0.93	0.18	49,49,49,49	0
56	MG	DA	3191	1/1	0.93	0.18	46,46,46,46	0
56	MG	DA	3485	1/1	0.93	0.11	43,43,43,43	0
56	MG	DA	3486	1/1	0.93	0.11	50,50,50,50	0
56	MG	CA	3135	1/1	0.93	0.16	63,63,63,63	0
56	MG	DA	3193	1/1	0.93	0.20	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DA	3491	1/1	0.93	0.07	42,42,42,42	0
56	MG	CA	3136	1/1	0.93	0.09	55,55,55,55	0
56	MG	DA	3195	1/1	0.93	0.14	58,58,58,58	0
56	MG	DA	3497	1/1	0.93	0.12	36,36,36,36	0
56	MG	DA	3198	1/1	0.93	0.10	49,49,49,49	0
56	MG	BA	3065	1/1	0.93	0.19	41,41,41,41	0
56	MG	BA	3519	1/1	0.93	0.20	53,53,53,53	0
56	MG	BA	3276	1/1	0.93	0.07	42,42,42,42	0
56	MG	DA	3508	1/1	0.93	0.12	41,41,41,41	0
56	MG	DA	3509	1/1	0.93	0.14	55,55,55,55	0
56	MG	DA	3203	1/1	0.93	0.11	50,50,50,50	0
56	MG	BA	3523	1/1	0.93	0.17	47,47,47,47	0
56	MG	AA	3014	1/1	0.93	0.25	62,62,62,62	0
56	MG	CA	3146	1/1	0.93	0.18	65,65,65,65	0
56	MG	BA	3025	1/1	0.93	0.19	48,48,48,48	0
56	MG	DA	3518	1/1	0.93	0.15	58,58,58,58	0
56	MG	BA	3398	1/1	0.93	0.11	51,51,51,51	0
56	MG	CA	3022	1/1	0.93	0.30	60,60,60,60	0
56	MG	CA	3023	1/1	0.93	0.05	39,39,39,39	0
56	MG	DA	3220	1/1	0.93	0.09	50,50,50,50	0
56	MG	BA	3536	1/1	0.93	0.11	36,36,36,36	0
56	MG	BA	3637	1/1	0.93	0.14	54,54,54,54	0
56	MG	CA	3154	1/1	0.93	0.17	54,54,54,54	0
56	MG	BA	3638	1/1	0.93	0.18	56,56,56,56	0
56	MG	CA	3028	1/1	0.93	0.27	55,55,55,55	0
56	MG	AA	3044	1/1	0.93	0.34	55,55,55,55	0
56	MG	DA	3544	1/1	0.93	0.09	39,39,39,39	0
56	MG	DA	3231	1/1	0.93	0.17	38,38,38,38	0
56	MG	BA	3640	1/1	0.93	0.11	42,42,42,42	0
56	MG	CA	3031	1/1	0.93	0.14	59,59,59,59	0
56	MG	BA	3150	1/1	0.93	0.13	56,56,56,56	0
56	MG	CA	3034	1/1	0.93	0.18	51,51,51,51	0
56	MG	BA	3539	1/1	0.93	0.12	29,29,29,29	0
56	MG	DA	3241	1/1	0.93	0.10	48,48,48,48	0
56	MG	DA	3561	1/1	0.93	0.11	58,58,58,58	0
56	MG	CA	3165	1/1	0.93	0.10	60,60,60,60	0
56	MG	CA	3038	1/1	0.93	0.12	63,63,63,63	0
56	MG	BA	3764	1/1	0.93	0.13	44,44,44,44	0
56	MG	DA	3248	1/1	0.93	0.16	49,49,49,49	0
56	MG	BA	3541	1/1	0.93	0.15	55,55,55,55	0
56	MG	DA	3250	1/1	0.93	0.21	40,40,40,40	0
56	MG	BA	3544	1/1	0.93	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	CA	3175	1/1	0.93	0.20	46,46,46,46	0
56	MG	BA	3410	1/1	0.93	0.16	31,31,31,31	0
56	MG	AA	3081	1/1	0.93	0.22	51,51,51,51	0
56	MG	AE	203	1/1	0.93	0.24	73,73,73,73	0
56	MG	DA	3576	1/1	0.93	0.17	50,50,50,50	0
56	MG	BA	3651	1/1	0.93	0.07	52,52,52,52	0
56	MG	DA	3580	1/1	0.93	0.09	46,46,46,46	0
56	MG	DA	3262	1/1	0.93	0.14	46,46,46,46	0
56	MG	CA	3048	1/1	0.93	0.13	77,77,77,77	0
56	MG	AA	3062	1/1	0.93	0.21	67,67,67,67	0
56	MG	DA	3586	1/1	0.93	0.09	39,39,39,39	0
56	MG	CA	3050	1/1	0.93	0.19	52,52,52,52	0
56	MG	DA	3011	1/1	0.93	0.12	51,51,51,51	0
56	MG	DA	3593	1/1	0.93	0.07	50,50,50,50	0
56	MG	AQ	3001	1/1	0.93	0.20	52,52,52,52	0
56	MG	BA	3780	1/1	0.93	0.12	54,54,54,54	0
56	MG	BA	3297	1/1	0.93	0.22	46,46,46,46	0
56	MG	BA	3786	1/1	0.93	0.14	58,58,58,58	0
56	MG	DA	3285	1/1	0.93	0.25	52,52,52,52	0
56	MG	DA	3024	1/1	0.93	0.37	37,37,37,37	0
56	MG	BA	3787	1/1	0.93	0.20	57,57,57,57	0
56	MG	BA	3307	1/1	0.93	0.20	50,50,50,50	0
56	MG	DA	3292	1/1	0.93	0.12	40,40,40,40	0
56	MG	BA	3660	1/1	0.93	0.18	51,51,51,51	0
56	MG	DA	3615	1/1	0.93	0.09	50,50,50,50	0
56	MG	BA	3662	1/1	0.93	0.10	52,52,52,52	0
56	MG	BA	3430	1/1	0.93	0.11	31,31,31,31	0
56	MG	AA	3032	1/1	0.93	0.26	59,59,59,59	0
56	MG	DA	3039	1/1	0.93	0.11	44,44,44,44	0
56	MG	BA	3668	1/1	0.93	0.21	48,48,48,48	0
56	MG	DA	3318	1/1	0.93	0.10	33,33,33,33	0
56	MG	BA	3166	1/1	0.93	0.16	46,46,46,46	0
56	MG	BA	3233	1/1	0.93	0.16	61,61,61,61	0
56	MG	AA	3135	1/1	0.93	0.10	60,60,60,60	0
56	MG	DA	3053	1/1	0.93	0.19	37,37,37,37	0
56	MG	BA	3238	1/1	0.93	0.14	41,41,41,41	0
56	MG	DA	3056	1/1	0.93	0.21	60,60,60,60	0
56	MG	BA	3445	1/1	0.93	0.13	48,48,48,48	0
56	MG	BA	3446	1/1	0.93	0.10	31,31,31,31	0
56	MG	DA	3060	1/1	0.93	0.10	48,48,48,48	0
56	MG	BA	3169	1/1	0.93	0.14	50,50,50,50	0
56	MG	BA	3340	1/1	0.93	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	BA	3342	1/1	0.93	0.06	33,33,33,33	0
56	MG	DA	3644	1/1	0.93	0.10	40,40,40,40	0
56	MG	DA	3067	1/1	0.93	0.14	45,45,45,45	0
56	MG	BA	3046	1/1	0.93	0.15	34,34,34,34	0
56	MG	DA	3069	1/1	0.93	0.16	55,55,55,55	0
56	MG	BA	3586	1/1	0.93	0.11	60,60,60,60	0
56	MG	DA	3362	1/1	0.93	0.20	59,59,59,59	0
56	MG	DA	3071	1/1	0.93	0.09	48,48,48,48	0
56	MG	DA	3653	1/1	0.93	0.18	32,32,32,32	0
56	MG	BA	3696	1/1	0.93	0.08	45,45,45,45	0
56	MG	BA	3351	1/1	0.93	0.12	59,59,59,59	0
56	MG	BA	3588	1/1	0.93	0.06	29,29,29,29	0
56	MG	DA	3077	1/1	0.93	0.08	47,47,47,47	0
56	MG	DA	3659	1/1	0.93	0.18	39,39,39,39	0
56	MG	DA	3662	1/1	0.93	0.11	38,38,38,38	0
56	MG	BF	302	1/1	0.93	0.27	56,56,56,56	0
56	MG	BF	303	1/1	0.93	0.17	43,43,43,43	0
56	MG	BA	3353	1/1	0.93	0.12	49,49,49,49	0
56	MG	DA	3379	1/1	0.93	0.10	50,50,50,50	0
56	MG	DA	3672	1/1	0.93	0.12	59,59,59,59	0
56	MG	BA	3459	1/1	0.93	0.08	47,47,47,47	0
56	MG	DA	3387	1/1	0.93	0.13	39,39,39,39	0
56	MG	BF	309	1/1	0.93	0.07	45,45,45,45	0
56	MG	DA	3094	1/1	0.93	0.22	52,52,52,52	0
56	MG	DA	3097	1/1	0.93	0.14	57,57,57,57	0
56	MG	DB	3005	1/1	0.93	0.22	48,48,48,48	0
56	MG	BA	3460	1/1	0.93	0.14	58,58,58,58	0
56	MG	AA	3107	1/1	0.93	0.19	63,63,63,63	0
56	MG	DA	3102	1/1	0.93	0.12	49,49,49,49	0
56	MG	BN	3007	1/1	0.93	0.18	50,50,50,50	0
56	MG	BA	3178	1/1	0.93	0.33	42,42,42,42	0
56	MG	CA	3097	1/1	0.93	0.12	64,64,64,64	0
56	MG	BA	3473	1/1	0.93	0.17	52,52,52,52	0
56	MG	DA	3411	1/1	0.93	0.13	46,46,46,46	0
56	MG	BR	201	1/1	0.93	0.16	40,40,40,40	0
56	MG	DA	3113	1/1	0.93	0.20	50,50,50,50	0
56	MG	BA	3712	1/1	0.93	0.21	29,29,29,29	0
56	MG	CA	3104	1/1	0.93	0.08	60,60,60,60	0
56	MG	CA	3105	1/1	0.93	0.13	51,51,51,51	0
56	MG	DA	3122	1/1	0.93	0.22	53,53,53,53	0
56	MG	DU	3003	1/1	0.93	0.15	53,53,53,53	0
56	MG	BA	3714	1/1	0.93	0.12	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	DA	3126	1/1	0.93	0.09	46,46,46,46	0
56	MG	BA	3603	1/1	0.93	0.19	42,42,42,42	0
56	MG	CA	3113	1/1	0.93	0.16	49,49,49,49	0
56	MG	CA	3115	1/1	0.93	0.15	60,60,60,60	0
56	MG	AA	3027	1/1	0.93	0.16	46,46,46,46	0
56	MG	BA	3119	1/1	0.93	0.13	29,29,29,29	0
56	MG	DA	3436	1/1	0.93	0.10	70,70,70,70	0
56	MG	DA	3142	1/1	0.93	0.14	50,50,50,50	0
56	MG	AA	3113	1/1	0.93	0.18	67,67,67,67	0
59	ZN	B5	104	1/1	0.93	0.10	82,82,82,82	0
56	MG	DA	3440	1/1	0.93	0.12	51,51,51,51	0
56	MG	DA	3023	1/1	0.94	0.07	44,44,44,44	0
56	MG	CA	3069	1/1	0.94	0.17	59,59,59,59	0
56	MG	DA	3025	1/1	0.94	0.26	52,52,52,52	0
56	MG	CA	3071	1/1	0.94	0.15	57,57,57,57	0
56	MG	AA	3005	1/1	0.94	0.37	77,77,77,77	0
56	MG	AN	502	1/1	0.94	0.08	56,56,56,56	0
56	MG	CA	3074	1/1	0.94	0.22	57,57,57,57	0
56	MG	DA	3035	1/1	0.94	0.06	40,40,40,40	0
56	MG	BA	3308	1/1	0.94	0.15	49,49,49,49	0
56	MG	BA	3099	1/1	0.94	0.21	67,67,67,67	0
56	MG	BA	3412	1/1	0.94	0.18	19,19,19,19	0
56	MG	DA	3041	1/1	0.94	0.21	56,56,56,56	0
56	MG	BF	305	1/1	0.94	0.06	45,45,45,45	0
56	MG	DA	3506	1/1	0.94	0.06	40,40,40,40	0
56	MG	BA	3620	1/1	0.94	0.17	62,62,62,62	0
56	MG	BA	3621	1/1	0.94	0.10	39,39,39,39	0
56	MG	DA	3252	1/1	0.94	0.08	38,38,38,38	0
56	MG	DA	3051	1/1	0.94	0.07	45,45,45,45	0
56	MG	BA	3034	1/1	0.94	0.09	34,34,34,34	0
56	MG	BA	3101	1/1	0.94	0.09	39,39,39,39	0
56	MG	DA	3514	1/1	0.94	0.07	45,45,45,45	0
56	MG	AA	3178	1/1	0.94	0.12	59,59,59,59	0
56	MG	DA	3055	1/1	0.94	0.09	54,54,54,54	0
56	MG	BA	3106	1/1	0.94	0.11	44,44,44,44	0
56	MG	BA	3630	1/1	0.94	0.15	43,43,43,43	0
56	MG	DA	3263	1/1	0.94	0.17	44,44,44,44	0
56	MG	AA	3112	1/1	0.94	0.13	60,60,60,60	0
56	MG	BA	3327	1/1	0.94	0.11	37,37,37,37	0
56	MG	BU	204	1/1	0.94	0.09	43,43,43,43	0
56	MG	DA	3269	1/1	0.94	0.21	54,54,54,54	0
56	MG	DA	3271	1/1	0.94	0.21	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DA	3540	1/1	0.94	0.08	56,56,56,56	0
56	MG	DA	3274	1/1	0.94	0.11	54,54,54,54	0
56	MG	BA	3331	1/1	0.94	0.14	38,38,38,38	0
56	MG	BV	204	1/1	0.94	0.18	47,47,47,47	0
56	MG	BW	201	1/1	0.94	0.19	45,45,45,45	0
56	MG	BA	3336	1/1	0.94	0.17	50,50,50,50	0
56	MG	DA	3281	1/1	0.94	0.11	49,49,49,49	0
56	MG	AA	3133	1/1	0.94	0.08	66,66,66,66	0
56	MG	BA	3548	1/1	0.94	0.10	40,40,40,40	0
56	MG	B0	103	1/1	0.94	0.11	38,38,38,38	0
56	MG	DA	3557	1/1	0.94	0.10	44,44,44,44	0
56	MG	DA	3558	1/1	0.94	0.08	43,43,43,43	0
56	MG	DA	3072	1/1	0.94	0.23	52,52,52,52	0
56	MG	DA	3560	1/1	0.94	0.07	47,47,47,47	0
56	MG	AA	3068	1/1	0.94	0.34	62,62,62,62	0
56	MG	B2	3001	1/1	0.94	0.08	49,49,49,49	0
56	MG	BA	3047	1/1	0.94	0.11	43,43,43,43	0
56	MG	BA	3187	1/1	0.94	0.21	48,48,48,48	0
56	MG	DA	3296	1/1	0.94	0.07	35,35,35,35	0
56	MG	DA	3300	1/1	0.94	0.11	41,41,41,41	0
56	MG	BA	3642	1/1	0.94	0.08	36,36,36,36	0
56	MG	DA	3308	1/1	0.94	0.12	49,49,49,49	0
56	MG	DA	3080	1/1	0.94	0.09	49,49,49,49	0
56	MG	CA	3108	1/1	0.94	0.13	52,52,52,52	0
56	MG	BA	3113	1/1	0.94	0.14	39,39,39,39	0
56	MG	B8	101	1/1	0.94	0.12	36,36,36,36	0
56	MG	DA	3090	1/1	0.94	0.20	48,48,48,48	0
56	MG	AA	3115	1/1	0.94	0.22	45,45,45,45	0
56	MG	DA	3578	1/1	0.94	0.08	40,40,40,40	0
56	MG	BA	3562	1/1	0.94	0.11	44,44,44,44	0
56	MG	AA	3119	1/1	0.94	0.06	65,65,65,65	0
56	MG	BA	3647	1/1	0.94	0.12	49,49,49,49	0
56	MG	CA	3119	1/1	0.94	0.14	51,51,51,51	0
56	MG	DA	3585	1/1	0.94	0.16	43,43,43,43	0
56	MG	BA	3751	1/1	0.94	0.08	55,55,55,55	0
56	MG	BA	3358	1/1	0.94	0.09	40,40,40,40	0
56	MG	DA	3333	1/1	0.94	0.09	51,51,51,51	0
56	MG	DA	3337	1/1	0.94	0.07	44,44,44,44	0
56	MG	DA	3104	1/1	0.94	0.09	39,39,39,39	0
56	MG	BA	3454	1/1	0.94	0.07	29,29,29,29	0
56	MG	DA	3340	1/1	0.94	0.07	30,30,30,30	0
56	MG	AA	3009	1/1	0.94	0.08	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	BA	3258	1/1	0.94	0.28	61,61,61,61	0
56	MG	BA	3761	1/1	0.94	0.21	53,53,53,53	0
56	MG	DA	3111	1/1	0.94	0.07	53,53,53,53	0
56	MG	CA	3126	1/1	0.94	0.08	57,57,57,57	0
56	MG	DA	3357	1/1	0.94	0.06	38,38,38,38	0
56	MG	DA	3610	1/1	0.94	0.09	49,49,49,49	0
56	MG	DA	3611	1/1	0.94	0.13	45,45,45,45	0
56	MG	DA	3358	1/1	0.94	0.08	28,28,28,28	0
56	MG	BA	3763	1/1	0.94	0.10	39,39,39,39	0
56	MG	CA	3015	1/1	0.94	0.17	58,58,58,58	0
56	MG	DA	3617	1/1	0.94	0.07	45,45,45,45	0
56	MG	DA	3619	1/1	0.94	0.12	54,54,54,54	0
56	MG	BA	3361	1/1	0.94	0.11	61,61,61,61	0
56	MG	DA	3622	1/1	0.94	0.10	35,35,35,35	0
56	MG	CA	3017	1/1	0.94	0.12	76,76,76,76	0
56	MG	BA	3765	1/1	0.94	0.11	53,53,53,53	0
56	MG	CA	3133	1/1	0.94	0.08	45,45,45,45	0
56	MG	BA	3577	1/1	0.94	0.17	18,18,18,18	0
56	MG	AA	3082	1/1	0.94	0.33	51,51,51,51	0
56	MG	DA	3628	1/1	0.94	0.07	47,47,47,47	0
56	MG	BA	3006	1/1	0.94	0.10	52,52,52,52	0
56	MG	BA	3264	1/1	0.94	0.22	45,45,45,45	0
56	MG	BA	3582	1/1	0.94	0.12	19,19,19,19	0
56	MG	DA	3381	1/1	0.94	0.07	34,34,34,34	0
56	MG	DA	3141	1/1	0.94	0.17	46,46,46,46	0
56	MG	BA	3016	1/1	0.94	0.07	37,37,37,37	0
56	MG	BA	3372	1/1	0.94	0.08	56,56,56,56	0
56	MG	BA	3476	1/1	0.94	0.12	48,48,48,48	0
56	MG	BA	3373	1/1	0.94	0.07	42,42,42,42	0
56	MG	AA	3093	1/1	0.94	0.23	51,51,51,51	0
56	MG	BA	3785	1/1	0.94	0.13	81,81,81,81	0
56	MG	DA	3156	1/1	0.94	0.25	50,50,50,50	0
56	MG	DA	3158	1/1	0.94	0.16	30,30,30,30	0
56	MG	CA	3033	1/1	0.94	0.16	60,60,60,60	0
56	MG	DA	3647	1/1	0.94	0.09	53,53,53,53	0
56	MG	DA	3164	1/1	0.94	0.24	47,47,47,47	0
56	MG	BA	3376	1/1	0.94	0.11	43,43,43,43	0
56	MG	DA	3408	1/1	0.94	0.10	51,51,51,51	0
56	MG	DA	3651	1/1	0.94	0.09	40,40,40,40	0
56	MG	DA	3409	1/1	0.94	0.20	55,55,55,55	0
56	MG	BA	3480	1/1	0.94	0.07	50,50,50,50	0
56	MG	CA	3037	1/1	0.94	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	AA	3172	1/1	0.94	0.09	55,55,55,55	0
56	MG	DA	3173	1/1	0.94	0.12	51,51,51,51	0
56	MG	BA	3593	1/1	0.94	0.12	47,47,47,47	0
56	MG	DA	3177	1/1	0.94	0.12	46,46,46,46	0
56	MG	DA	3179	1/1	0.94	0.10	57,57,57,57	0
56	MG	CA	3156	1/1	0.94	0.13	41,41,41,41	0
56	MG	BA	3683	1/1	0.94	0.09	43,43,43,43	0
56	MG	DA	3425	1/1	0.94	0.19	52,52,52,52	0
56	MG	DA	3668	1/1	0.94	0.55	51,51,51,51	0
56	MG	BA	3489	1/1	0.94	0.25	44,44,44,44	0
56	MG	DA	3183	1/1	0.94	0.07	40,40,40,40	0
56	MG	BA	3206	1/1	0.94	0.10	37,37,37,37	0
56	MG	DA	3674	1/1	0.94	0.23	43,43,43,43	0
56	MG	BA	3798	1/1	0.94	0.07	51,51,51,51	0
56	MG	BA	3799	1/1	0.94	0.27	50,50,50,50	0
56	MG	AA	3050	1/1	0.94	0.09	77,77,77,77	0
56	MG	DA	3189	1/1	0.94	0.12	41,41,41,41	0
56	MG	BA	3801	1/1	0.94	0.15	39,39,39,39	0
56	MG	DA	3439	1/1	0.94	0.15	46,46,46,46	0
56	MG	BA	3382	1/1	0.94	0.10	41,41,41,41	0
56	MG	BA	3599	1/1	0.94	0.12	45,45,45,45	0
56	MG	BA	3281	1/1	0.94	0.12	56,56,56,56	0
56	MG	BA	3071	1/1	0.94	0.10	40,40,40,40	0
56	MG	DA	3197	1/1	0.94	0.20	55,55,55,55	0
56	MG	DD	307	1/1	0.94	0.10	50,50,50,50	0
56	MG	BA	3217	1/1	0.94	0.13	47,47,47,47	0
56	MG	BA	3080	1/1	0.94	0.26	51,51,51,51	0
56	MG	DE	304	1/1	0.94	0.16	40,40,40,40	0
56	MG	BA	3509	1/1	0.94	0.07	39,39,39,39	0
56	MG	CE	202	1/1	0.94	0.08	74,74,74,74	0
56	MG	CA	3056	1/1	0.94	0.15	60,60,60,60	0
56	MG	BB	210	1/1	0.94	0.23	55,55,55,55	0
56	MG	DQ	3003	1/1	0.94	0.09	52,52,52,52	0
56	MG	BA	3702	1/1	0.94	0.15	53,53,53,53	0
56	MG	AE	201	1/1	0.94	0.34	64,64,64,64	0
56	MG	DA	3461	1/1	0.94	0.16	57,57,57,57	0
56	MG	DA	3463	1/1	0.94	0.06	32,32,32,32	0
56	MG	BB	217	1/1	0.94	0.10	41,41,41,41	0
56	MG	DA	3003	1/1	0.94	0.18	48,48,48,48	0
56	MG	AA	3128	1/1	0.94	0.10	67,67,67,67	0
56	MG	DA	3468	1/1	0.94	0.12	37,37,37,37	0
56	MG	AA	3160	1/1	0.94	0.18	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	CA	3064	1/1	0.94	0.18	59,59,59,59	0
56	MG	CA	3066	1/1	0.94	0.15	47,47,47,47	0
56	MG	BA	3707	1/1	0.94	0.09	43,43,43,43	0
56	MG	DA	3018	1/1	0.94	0.13	51,51,51,51	0
56	MG	DA	3481	1/1	0.94	0.07	24,24,24,24	0
59	ZN	D4	501	1/1	0.94	0.07	151,151,151,151	0
56	MG	BD	3306	1/1	0.94	0.19	38,38,38,38	0
56	MG	BA	3367	1/1	0.95	0.09	34,34,34,34	0
56	MG	BB	218	1/1	0.95	0.07	31,31,31,31	0
56	MG	DA	3434	1/1	0.95	0.07	27,27,27,27	0
56	MG	DA	3143	1/1	0.95	0.27	36,36,36,36	0
56	MG	BA	3077	1/1	0.95	0.21	29,29,29,29	0
56	MG	BA	3369	1/1	0.95	0.11	40,40,40,40	0
56	MG	CA	3106	1/1	0.95	0.07	58,58,58,58	0
56	MG	BA	3526	1/1	0.95	0.11	35,35,35,35	0
56	MG	DA	3151	1/1	0.95	0.09	33,33,33,33	0
56	MG	DA	3441	1/1	0.95	0.06	30,30,30,30	0
56	MG	BD	3304	1/1	0.95	0.07	25,25,25,25	0
56	MG	DA	3153	1/1	0.95	0.12	38,38,38,38	0
56	MG	DA	3154	1/1	0.95	0.20	52,52,52,52	0
56	MG	BA	3153	1/1	0.95	0.07	50,50,50,50	0
56	MG	DA	3157	1/1	0.95	0.13	42,42,42,42	0
56	MG	DA	3447	1/1	0.95	0.11	41,41,41,41	0
56	MG	BD	3307	1/1	0.95	0.27	56,56,56,56	0
56	MG	DA	3160	1/1	0.95	0.20	38,38,38,38	0
56	MG	BA	3530	1/1	0.95	0.12	25,25,25,25	0
56	MG	BA	3532	1/1	0.95	0.16	30,30,30,30	0
56	MG	DA	3165	1/1	0.95	0.17	42,42,42,42	0
56	MG	BF	301	1/1	0.95	0.18	32,32,32,32	0
56	MG	BA	3533	1/1	0.95	0.09	38,38,38,38	0
56	MG	DA	3169	1/1	0.95	0.21	44,44,44,44	0
56	MG	BA	3670	1/1	0.95	0.12	47,47,47,47	0
56	MG	AA	3110	1/1	0.95	0.17	46,46,46,46	0
56	MG	BA	3024	1/1	0.95	0.17	45,45,45,45	0
56	MG	AA	3190	1/1	0.95	0.11	48,48,48,48	0
56	MG	DA	3176	1/1	0.95	0.12	44,44,44,44	0
56	MG	BF	308	1/1	0.95	0.14	45,45,45,45	0
56	MG	DA	3178	1/1	0.95	0.07	53,53,53,53	0
56	MG	DA	3471	1/1	0.95	0.18	54,54,54,54	0
56	MG	BA	3675	1/1	0.95	0.15	29,29,29,29	0
56	MG	DA	3474	1/1	0.95	0.07	30,30,30,30	0
56	MG	DA	3477	1/1	0.95	0.06	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	BG	3001	1/1	0.95	0.21	51,51,51,51	0
56	MG	BA	3676	1/1	0.95	0.12	37,37,37,37	0
56	MG	BA	3088	1/1	0.95	0.14	49,49,49,49	0
56	MG	BN	3004	1/1	0.95	0.20	61,61,61,61	0
56	MG	BN	3006	1/1	0.95	0.17	47,47,47,47	0
56	MG	AA	3148	1/1	0.95	0.12	58,58,58,58	0
56	MG	BA	3679	1/1	0.95	0.29	56,56,56,56	0
56	MG	BA	3093	1/1	0.95	0.17	48,48,48,48	0
56	MG	DA	3188	1/1	0.95	0.07	26,26,26,26	0
56	MG	BP	204	1/1	0.95	0.09	54,54,54,54	0
56	MG	BA	3380	1/1	0.95	0.05	36,36,36,36	0
56	MG	BA	3094	1/1	0.95	0.17	44,44,44,44	0
56	MG	BU	202	1/1	0.95	0.06	29,29,29,29	0
56	MG	BA	3171	1/1	0.95	0.17	54,54,54,54	0
56	MG	BU	205	1/1	0.95	0.11	43,43,43,43	0
56	MG	AA	3088	1/1	0.95	0.18	42,42,42,42	0
56	MG	BV	203	1/1	0.95	0.20	31,31,31,31	0
56	MG	CA	3145	1/1	0.95	0.10	68,68,68,68	0
56	MG	DA	3507	1/1	0.95	0.09	57,57,57,57	0
56	MG	BA	3549	1/1	0.95	0.10	36,36,36,36	0
56	MG	BA	3385	1/1	0.95	0.20	41,41,41,41	0
56	MG	BY	202	1/1	0.95	0.17	48,48,48,48	0
56	MG	DA	3209	1/1	0.95	0.12	46,46,46,46	0
56	MG	BY	204	1/1	0.95	0.26	52,52,52,52	0
56	MG	BA	3695	1/1	0.95	0.11	37,37,37,37	0
56	MG	BA	3554	1/1	0.95	0.09	24,24,24,24	0
56	MG	DA	3516	1/1	0.95	0.07	52,52,52,52	0
56	MG	BA	3386	1/1	0.95	0.16	47,47,47,47	0
56	MG	B0	102	1/1	0.95	0.15	50,50,50,50	0
56	MG	DA	3519	1/1	0.95	0.10	32,32,32,32	0
56	MG	DA	3520	1/1	0.95	0.05	44,44,44,44	0
56	MG	DA	3521	1/1	0.95	0.14	55,55,55,55	0
56	MG	BA	3557	1/1	0.95	0.14	37,37,37,37	0
56	MG	BA	3260	1/1	0.95	0.07	42,42,42,42	0
56	MG	DA	3219	1/1	0.95	0.10	36,36,36,36	0
56	MG	DA	3530	1/1	0.95	0.12	47,47,47,47	0
56	MG	AA	3089	1/1	0.95	0.28	57,57,57,57	0
56	MG	BA	3176	1/1	0.95	0.07	44,44,44,44	0
56	MG	BA	3394	1/1	0.95	0.05	20,20,20,20	0
56	MG	DA	3535	1/1	0.95	0.09	59,59,59,59	0
56	MG	DA	3224	1/1	0.95	0.10	47,47,47,47	0
56	MG	B5	102	1/1	0.95	0.15	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	B5	103	1/1	0.95	0.06	41,41,41,41	0
56	MG	BA	3563	1/1	0.95	0.07	44,44,44,44	0
56	MG	BA	3098	1/1	0.95	0.15	38,38,38,38	0
56	MG	BA	3269	1/1	0.95	0.22	42,42,42,42	0
56	MG	CA	3166	1/1	0.95	0.09	52,52,52,52	0
56	MG	DA	3546	1/1	0.95	0.07	47,47,47,47	0
56	MG	CA	3167	1/1	0.95	0.06	47,47,47,47	0
56	MG	BA	3709	1/1	0.95	0.20	28,28,28,28	0
56	MG	DA	3237	1/1	0.95	0.05	43,43,43,43	0
56	MG	BA	3569	1/1	0.95	0.20	56,56,56,56	0
56	MG	AA	3152	1/1	0.95	0.07	48,48,48,48	0
56	MG	BA	3032	1/1	0.95	0.17	42,42,42,42	0
56	MG	BA	3573	1/1	0.95	0.08	24,24,24,24	0
56	MG	AA	3090	1/1	0.95	0.19	41,41,41,41	0
56	MG	AA	3065	1/1	0.95	0.09	55,55,55,55	0
56	MG	DA	3245	1/1	0.95	0.10	47,47,47,47	0
56	MG	BA	3105	1/1	0.95	0.10	39,39,39,39	0
56	MG	BA	3282	1/1	0.95	0.23	41,41,41,41	0
56	MG	CA	3012	1/1	0.95	0.17	51,51,51,51	0
56	MG	BA	3283	1/1	0.95	0.07	30,30,30,30	0
56	MG	DA	3254	1/1	0.95	0.18	35,35,35,35	0
56	MG	DA	3001	1/1	0.95	0.07	40,40,40,40	0
56	MG	BA	3722	1/1	0.95	0.07	17,17,17,17	0
56	MG	BA	3286	1/1	0.95	0.26	41,41,41,41	0
56	MG	AA	3013	1/1	0.95	0.12	57,57,57,57	0
56	MG	BA	3041	1/1	0.95	0.12	35,35,35,35	0
56	MG	BA	3424	1/1	0.95	0.11	55,55,55,55	0
56	MG	CA	3020	1/1	0.95	0.18	46,46,46,46	0
56	MG	DA	3016	1/1	0.95	0.10	42,42,42,42	0
56	MG	AA	3123	1/1	0.95	0.12	51,51,51,51	0
56	MG	AA	3003	1/1	0.95	0.12	63,63,63,63	0
56	MG	DA	3267	1/1	0.95	0.14	41,41,41,41	0
56	MG	AX	3005	1/1	0.95	0.24	64,64,64,64	0
56	MG	AA	3023	1/1	0.95	0.27	48,48,48,48	0
56	MG	DA	3270	1/1	0.95	0.39	56,56,56,56	0
56	MG	BA	3114	1/1	0.95	0.13	34,34,34,34	0
56	MG	DA	3273	1/1	0.95	0.12	39,39,39,39	0
56	MG	BA	3300	1/1	0.95	0.20	28,28,28,28	0
56	MG	DA	3592	1/1	0.95	0.10	40,40,40,40	0
56	MG	BA	3200	1/1	0.95	0.14	41,41,41,41	0
56	MG	DA	3277	1/1	0.95	0.25	54,54,54,54	0
56	MG	DA	3030	1/1	0.95	0.07	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DA	3031	1/1	0.95	0.24	44,44,44,44	0
56	MG	DA	3600	1/1	0.95	0.09	43,43,43,43	0
56	MG	DA	3602	1/1	0.95	0.08	51,51,51,51	0
56	MG	BA	3117	1/1	0.95	0.22	35,35,35,35	0
56	MG	AA	3159	1/1	0.95	0.10	59,59,59,59	0
56	MG	BA	3742	1/1	0.95	0.15	21,21,21,21	0
56	MG	DA	3283	1/1	0.95	0.11	43,43,43,43	0
56	MG	BA	3207	1/1	0.95	0.07	44,44,44,44	0
56	MG	BA	3449	1/1	0.95	0.11	32,32,32,32	0
56	MG	DA	3287	1/1	0.95	0.06	39,39,39,39	0
56	MG	AA	3028	1/1	0.95	0.20	49,49,49,49	0
56	MG	BA	3214	1/1	0.95	0.14	44,44,44,44	0
56	MG	DA	3614	1/1	0.95	0.16	61,61,61,61	0
56	MG	AA	3161	1/1	0.95	0.19	59,59,59,59	0
56	MG	AA	3143	1/1	0.95	0.09	57,57,57,57	0
56	MG	BA	3323	1/1	0.95	0.09	43,43,43,43	0
56	MG	DA	3618	1/1	0.95	0.06	64,64,64,64	0
56	MG	BA	3324	1/1	0.95	0.15	42,42,42,42	0
56	MG	DA	3620	1/1	0.95	0.15	59,59,59,59	0
56	MG	DA	3297	1/1	0.95	0.11	24,24,24,24	0
56	MG	DA	3047	1/1	0.95	0.05	39,39,39,39	0
56	MG	DA	3304	1/1	0.95	0.07	40,40,40,40	0
56	MG	DA	3048	1/1	0.95	0.21	51,51,51,51	0
56	MG	DA	3049	1/1	0.95	0.17	53,53,53,53	0
56	MG	BA	3756	1/1	0.95	0.11	56,56,56,56	0
56	MG	BA	3758	1/1	0.95	0.11	44,44,44,44	0
56	MG	DA	3313	1/1	0.95	0.06	46,46,46,46	0
56	MG	BA	3610	1/1	0.95	0.08	39,39,39,39	0
56	MG	AA	3086	1/1	0.95	0.19	48,48,48,48	0
56	MG	BA	3330	1/1	0.95	0.10	52,52,52,52	0
56	MG	BA	3127	1/1	0.95	0.07	36,36,36,36	0
56	MG	DA	3633	1/1	0.95	0.07	56,56,56,56	0
56	MG	BA	3128	1/1	0.95	0.07	44,44,44,44	0
56	MG	BA	3467	1/1	0.95	0.09	49,49,49,49	0
56	MG	DA	3636	1/1	0.95	0.19	52,52,52,52	0
56	MG	BA	3472	1/1	0.95	0.13	38,38,38,38	0
56	MG	BA	3337	1/1	0.95	0.10	46,46,46,46	0
56	MG	BA	3338	1/1	0.95	0.21	43,43,43,43	0
56	MG	DA	3327	1/1	0.95	0.09	47,47,47,47	0
56	MG	DA	3642	1/1	0.95	0.06	48,48,48,48	0
56	MG	DA	3328	1/1	0.95	0.10	41,41,41,41	0
56	MG	BA	3769	1/1	0.95	0.07	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DA	3332	1/1	0.95	0.11	50,50,50,50	0
56	MG	BA	3224	1/1	0.95	0.22	50,50,50,50	0
56	MG	BA	3130	1/1	0.95	0.22	41,41,41,41	0
56	MG	BA	3227	1/1	0.95	0.08	34,34,34,34	0
56	MG	BA	3777	1/1	0.95	0.17	44,44,44,44	0
56	MG	BA	3346	1/1	0.95	0.08	29,29,29,29	0
56	MG	BA	3483	1/1	0.95	0.14	41,41,41,41	0
56	MG	BA	3348	1/1	0.95	0.07	24,24,24,24	0
56	MG	BA	3014	1/1	0.95	0.07	38,38,38,38	0
56	MG	BA	3783	1/1	0.95	0.06	43,43,43,43	0
56	MG	CA	3065	1/1	0.95	0.21	64,64,64,64	0
56	MG	DA	3353	1/1	0.95	0.12	42,42,42,42	0
56	MG	DA	3355	1/1	0.95	0.12	35,35,35,35	0
56	MG	DA	3078	1/1	0.95	0.09	35,35,35,35	0
56	MG	BA	3490	1/1	0.95	0.10	60,60,60,60	0
56	MG	BA	3491	1/1	0.95	0.12	45,45,45,45	0
56	MG	DA	3081	1/1	0.95	0.10	48,48,48,48	0
56	MG	BA	3352	1/1	0.95	0.10	45,45,45,45	0
56	MG	BA	3494	1/1	0.95	0.05	47,47,47,47	0
56	MG	CA	3070	1/1	0.95	0.13	49,49,49,49	0
56	MG	DA	3671	1/1	0.95	0.08	37,37,37,37	0
56	MG	BA	3790	1/1	0.95	0.17	29,29,29,29	0
56	MG	BA	3635	1/1	0.95	0.10	51,51,51,51	0
56	MG	BA	3134	1/1	0.95	0.16	36,36,36,36	0
56	MG	DA	3096	1/1	0.95	0.17	48,48,48,48	0
56	MG	AA	3164	1/1	0.95	0.10	51,51,51,51	0
56	MG	BA	3234	1/1	0.95	0.19	32,32,32,32	0
56	MG	BA	3499	1/1	0.95	0.10	19,19,19,19	0
56	MG	DA	3382	1/1	0.95	0.06	31,31,31,31	0
56	MG	BA	3501	1/1	0.95	0.07	43,43,43,43	0
56	MG	BA	3502	1/1	0.95	0.05	20,20,20,20	0
56	MG	BA	3357	1/1	0.95	0.09	46,46,46,46	0
56	MG	DA	3105	1/1	0.95	0.06	41,41,41,41	0
56	MG	AA	3145	1/1	0.95	0.12	65,65,65,65	0
56	MG	DD	303	1/1	0.95	0.17	51,51,51,51	0
56	MG	AA	3072	1/1	0.95	0.21	45,45,45,45	0
56	MG	BA	3808	1/1	0.95	0.08	40,40,40,40	0
56	MG	BA	3507	1/1	0.95	0.18	35,35,35,35	0
56	MG	BA	3814	1/1	0.95	0.16	42,42,42,42	0
56	MG	DE	303	1/1	0.95	0.13	62,62,62,62	0
56	MG	BA	3240	1/1	0.95	0.06	30,30,30,30	0
56	MG	DE	305	1/1	0.95	0.14	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DF	301	1/1	0.95	0.26	47,47,47,47	0
56	MG	DF	303	1/1	0.95	0.05	52,52,52,52	0
56	MG	DF	305	1/1	0.95	0.17	44,44,44,44	0
56	MG	DA	3114	1/1	0.95	0.12	55,55,55,55	0
56	MG	DN	5001	1/1	0.95	0.06	54,54,54,54	0
56	MG	DA	3403	1/1	0.95	0.08	56,56,56,56	0
56	MG	DA	3404	1/1	0.95	0.08	40,40,40,40	0
56	MG	BB	202	1/1	0.95	0.14	45,45,45,45	0
56	MG	BB	203	1/1	0.95	0.16	44,44,44,44	0
56	MG	BA	3072	1/1	0.95	0.08	58,58,58,58	0
56	MG	DA	3410	1/1	0.95	0.06	46,46,46,46	0
56	MG	BA	3362	1/1	0.95	0.10	40,40,40,40	0
56	MG	BB	207	1/1	0.95	0.17	39,39,39,39	0
56	MG	DV	3001	1/1	0.95	0.10	61,61,61,61	0
56	MG	BA	3073	1/1	0.95	0.23	45,45,45,45	0
56	MG	DA	3416	1/1	0.95	0.06	22,22,22,22	0
56	MG	BA	3245	1/1	0.95	0.14	61,61,61,61	0
56	MG	CA	3095	1/1	0.95	0.11	56,56,56,56	0
56	MG	DA	3130	1/1	0.95	0.21	54,54,54,54	0
56	MG	BA	3520	1/1	0.95	0.09	50,50,50,50	0
56	MG	D3	3001	1/1	0.95	0.13	60,60,60,60	0
56	MG	BB	212	1/1	0.95	0.09	42,42,42,42	0
56	MG	DA	3133	1/1	0.95	0.14	52,52,52,52	0
56	MG	DA	3134	1/1	0.95	0.08	48,48,48,48	0
56	MG	BA	3655	1/1	0.95	0.12	54,54,54,54	0
59	ZN	B6	103	1/1	0.95	0.06	62,62,62,62	0
59	ZN	CN	501	1/1	0.95	0.07	103,103,103,103	0
56	MG	DA	3429	1/1	0.95	0.07	45,45,45,45	0
56	MG	DA	3140	1/1	0.95	0.13	44,44,44,44	0
56	MG	BQ	201	1/1	0.96	0.15	35,35,35,35	0
56	MG	CA	3141	1/1	0.96	0.14	53,53,53,53	0
56	MG	BQ	203	1/1	0.96	0.11	36,36,36,36	0
56	MG	BQ	204	1/1	0.96	0.15	43,43,43,43	0
56	MG	AA	3058	1/1	0.96	0.12	61,61,61,61	0
56	MG	DA	3451	1/1	0.96	0.10	20,20,20,20	0
56	MG	BA	3035	1/1	0.96	0.11	42,42,42,42	0
56	MG	BA	3390	1/1	0.96	0.08	25,25,25,25	0
56	MG	BA	3701	1/1	0.96	0.10	20,20,20,20	0
56	MG	DA	3456	1/1	0.96	0.15	54,54,54,54	0
56	MG	BA	3391	1/1	0.96	0.06	26,26,26,26	0
56	MG	BA	3267	1/1	0.96	0.14	45,45,45,45	0
56	MG	CA	3150	1/1	0.96	0.12	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	BU	208	1/1	0.96	0.15	28,28,28,28	0
56	MG	BA	3268	1/1	0.96	0.29	57,57,57,57	0
56	MG	BA	3705	1/1	0.96	0.18	28,28,28,28	0
56	MG	BA	3170	1/1	0.96	0.35	52,52,52,52	0
56	MG	BW	202	1/1	0.96	0.13	41,41,41,41	0
56	MG	BY	201	1/1	0.96	0.07	52,52,52,52	0
56	MG	BA	3271	1/1	0.96	0.17	38,38,38,38	0
56	MG	DA	3196	1/1	0.96	0.20	45,45,45,45	0
56	MG	BA	3565	1/1	0.96	0.04	43,43,43,43	0
56	MG	BA	3038	1/1	0.96	0.14	40,40,40,40	0
56	MG	DA	3199	1/1	0.96	0.21	55,55,55,55	0
56	MG	AA	3069	1/1	0.96	0.06	52,52,52,52	0
56	MG	BA	3713	1/1	0.96	0.13	26,26,26,26	0
56	MG	BA	3568	1/1	0.96	0.12	26,26,26,26	0
56	MG	DA	3480	1/1	0.96	0.05	38,38,38,38	0
56	MG	BA	3174	1/1	0.96	0.08	50,50,50,50	0
56	MG	DA	3204	1/1	0.96	0.10	50,50,50,50	0
56	MG	DA	3483	1/1	0.96	0.11	32,32,32,32	0
56	MG	DA	3205	1/1	0.96	0.18	34,34,34,34	0
56	MG	DA	3207	1/1	0.96	0.23	36,36,36,36	0
56	MG	DA	3208	1/1	0.96	0.12	44,44,44,44	0
56	MG	BA	3403	1/1	0.96	0.04	22,22,22,22	0
56	MG	AX	3008	1/1	0.96	0.10	37,37,37,37	0
56	MG	AA	3045	1/1	0.96	0.31	54,54,54,54	0
56	MG	AA	3083	1/1	0.96	0.19	53,53,53,53	0
56	MG	BA	3416	1/1	0.96	0.12	36,36,36,36	0
56	MG	DA	3496	1/1	0.96	0.15	35,35,35,35	0
56	MG	BA	3179	1/1	0.96	0.08	41,41,41,41	0
56	MG	CA	3173	1/1	0.96	0.12	58,58,58,58	0
56	MG	DA	3500	1/1	0.96	0.16	51,51,51,51	0
56	MG	DA	3217	1/1	0.96	0.09	34,34,34,34	0
56	MG	BA	3418	1/1	0.96	0.09	34,34,34,34	0
56	MG	DA	3503	1/1	0.96	0.09	31,31,31,31	0
56	MG	B6	102	1/1	0.96	0.20	51,51,51,51	0
56	MG	BA	3284	1/1	0.96	0.20	33,33,33,33	0
56	MG	BA	3285	1/1	0.96	0.20	54,54,54,54	0
56	MG	CF	3001	1/1	0.96	0.12	55,55,55,55	0
56	MG	DA	3223	1/1	0.96	0.20	41,41,41,41	0
56	MG	B9	502	1/1	0.96	0.10	47,47,47,47	0
56	MG	BA	3102	1/1	0.96	0.30	61,61,61,61	0
56	MG	BA	3045	1/1	0.96	0.10	38,38,38,38	0
56	MG	DA	3227	1/1	0.96	0.07	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	3001	1/1	0.96	0.11	31,31,31,31	0
56	MG	DA	3515	1/1	0.96	0.06	39,39,39,39	0
56	MG	BA	3291	1/1	0.96	0.10	50,50,50,50	0
56	MG	AA	3071	1/1	0.96	0.13	51,51,51,51	0
56	MG	DA	3232	1/1	0.96	0.14	45,45,45,45	0
56	MG	BA	3004	1/1	0.96	0.09	26,26,26,26	0
56	MG	BA	3435	1/1	0.96	0.09	26,26,26,26	0
56	MG	DA	3235	1/1	0.96	0.15	35,35,35,35	0
56	MG	DA	3522	1/1	0.96	0.12	53,53,53,53	0
56	MG	DA	3007	1/1	0.96	0.11	43,43,43,43	0
56	MG	DA	3010	1/1	0.96	0.10	45,45,45,45	0
56	MG	BA	3049	1/1	0.96	0.15	34,34,34,34	0
56	MG	BA	3438	1/1	0.96	0.06	21,21,21,21	0
56	MG	AA	3060	1/1	0.96	0.11	52,52,52,52	0
56	MG	BA	3051	1/1	0.96	0.14	18,18,18,18	0
56	MG	BA	3443	1/1	0.96	0.10	27,27,27,27	0
56	MG	BA	3444	1/1	0.96	0.17	43,43,43,43	0
56	MG	BA	3746	1/1	0.96	0.09	55,55,55,55	0
56	MG	DA	3247	1/1	0.96	0.07	34,34,34,34	0
56	MG	BA	3010	1/1	0.96	0.12	41,41,41,41	0
56	MG	BA	3305	1/1	0.96	0.07	46,46,46,46	0
56	MG	BA	3749	1/1	0.96	0.07	29,29,29,29	0
56	MG	DA	3543	1/1	0.96	0.15	52,52,52,52	0
56	MG	BA	3600	1/1	0.96	0.11	50,50,50,50	0
56	MG	DA	3253	1/1	0.96	0.14	47,47,47,47	0
56	MG	BA	3602	1/1	0.96	0.12	32,32,32,32	0
56	MG	BA	3753	1/1	0.96	0.08	27,27,27,27	0
56	MG	AA	3117	1/1	0.96	0.16	34,34,34,34	0
56	MG	AA	3118	1/1	0.96	0.10	39,39,39,39	0
56	MG	BA	3450	1/1	0.96	0.07	10,10,10,10	0
56	MG	CA	3027	1/1	0.96	0.29	61,61,61,61	0
56	MG	BA	3757	1/1	0.96	0.06	45,45,45,45	0
56	MG	BA	3198	1/1	0.96	0.13	28,28,28,28	0
56	MG	DA	3038	1/1	0.96	0.12	28,28,28,28	0
56	MG	BA	3057	1/1	0.96	0.06	53,53,53,53	0
56	MG	DA	3040	1/1	0.96	0.14	58,58,58,58	0
56	MG	BA	3314	1/1	0.96	0.14	44,44,44,44	0
56	MG	DA	3042	1/1	0.96	0.21	46,46,46,46	0
56	MG	BA	3017	1/1	0.96	0.14	52,52,52,52	0
56	MG	BA	3762	1/1	0.96	0.15	53,53,53,53	0
56	MG	BA	3317	1/1	0.96	0.08	41,41,41,41	0
56	MG	DA	3272	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	3201	1/1	0.96	0.18	41,41,41,41	0
56	MG	BA	3202	1/1	0.96	0.06	38,38,38,38	0
56	MG	DA	3275	1/1	0.96	0.22	58,58,58,58	0
56	MG	DA	3571	1/1	0.96	0.10	51,51,51,51	0
56	MG	DA	3573	1/1	0.96	0.10	27,27,27,27	0
56	MG	BA	3320	1/1	0.96	0.07	55,55,55,55	0
56	MG	BA	3203	1/1	0.96	0.18	38,38,38,38	0
56	MG	BA	3322	1/1	0.96	0.21	48,48,48,48	0
56	MG	BA	3061	1/1	0.96	0.24	49,49,49,49	0
56	MG	BA	3468	1/1	0.96	0.08	45,45,45,45	0
56	MG	AA	3051	1/1	0.96	0.18	60,60,60,60	0
56	MG	BA	3325	1/1	0.96	0.13	51,51,51,51	0
56	MG	CA	3046	1/1	0.96	0.17	50,50,50,50	0
56	MG	DA	3284	1/1	0.96	0.19	37,37,37,37	0
56	MG	BA	3774	1/1	0.96	0.07	37,37,37,37	0
56	MG	BA	3776	1/1	0.96	0.09	48,48,48,48	0
56	MG	BA	3623	1/1	0.96	0.04	33,33,33,33	0
56	MG	DA	3289	1/1	0.96	0.06	39,39,39,39	0
56	MG	BA	3475	1/1	0.96	0.10	45,45,45,45	0
56	MG	DA	3063	1/1	0.96	0.21	54,54,54,54	0
56	MG	DA	3064	1/1	0.96	0.14	56,56,56,56	0
56	MG	DA	3065	1/1	0.96	0.10	41,41,41,41	0
56	MG	BA	3326	1/1	0.96	0.07	22,22,22,22	0
56	MG	BA	3627	1/1	0.96	0.19	57,57,57,57	0
56	MG	BA	3628	1/1	0.96	0.06	34,34,34,34	0
56	MG	DA	3299	1/1	0.96	0.10	40,40,40,40	0
56	MG	DA	3604	1/1	0.96	0.08	47,47,47,47	0
56	MG	BA	3124	1/1	0.96	0.09	35,35,35,35	0
56	MG	DA	3303	1/1	0.96	0.08	55,55,55,55	0
56	MG	BA	3328	1/1	0.96	0.09	11,11,11,11	0
56	MG	BA	3064	1/1	0.96	0.10	33,33,33,33	0
56	MG	BA	3213	1/1	0.96	0.07	35,35,35,35	0
56	MG	BA	3335	1/1	0.96	0.14	42,42,42,42	0
56	MG	BA	3126	1/1	0.96	0.12	47,47,47,47	0
56	MG	DA	3312	1/1	0.96	0.06	41,41,41,41	0
56	MG	DA	3075	1/1	0.96	0.07	43,43,43,43	0
56	MG	DA	3314	1/1	0.96	0.07	45,45,45,45	0
56	MG	DA	3315	1/1	0.96	0.06	44,44,44,44	0
56	MG	AA	3121	1/1	0.96	0.08	33,33,33,33	0
56	MG	DA	3317	1/1	0.96	0.06	38,38,38,38	0
56	MG	AA	3175	1/1	0.96	0.09	66,66,66,66	0
56	MG	BA	3067	1/1	0.96	0.16	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	3131	1/1	0.96	0.17	39,39,39,39	0
56	MG	BA	3797	1/1	0.96	0.09	19,19,19,19	0
56	MG	BA	3132	1/1	0.96	0.16	49,49,49,49	0
56	MG	DA	3082	1/1	0.96	0.06	40,40,40,40	0
56	MG	BA	3223	1/1	0.96	0.06	39,39,39,39	0
56	MG	BA	3641	1/1	0.96	0.06	54,54,54,54	0
56	MG	BA	3347	1/1	0.96	0.09	37,37,37,37	0
56	MG	BA	3804	1/1	0.96	0.06	35,35,35,35	0
56	MG	BA	3805	1/1	0.96	0.16	30,30,30,30	0
56	MG	DA	3331	1/1	0.96	0.09	49,49,49,49	0
56	MG	DA	3093	1/1	0.96	0.14	54,54,54,54	0
56	MG	BA	3068	1/1	0.96	0.25	46,46,46,46	0
56	MG	DA	3335	1/1	0.96	0.07	43,43,43,43	0
56	MG	DA	3095	1/1	0.96	0.07	43,43,43,43	0
56	MG	BA	3349	1/1	0.96	0.16	49,49,49,49	0
56	MG	BA	3350	1/1	0.96	0.10	28,28,28,28	0
56	MG	BA	3810	1/1	0.96	0.08	43,43,43,43	0
56	MG	DA	3099	1/1	0.96	0.13	45,45,45,45	0
56	MG	DA	3342	1/1	0.96	0.06	46,46,46,46	0
56	MG	BA	3811	1/1	0.96	0.24	41,41,41,41	0
56	MG	DA	3641	1/1	0.96	0.08	49,49,49,49	0
56	MG	DA	3101	1/1	0.96	0.13	55,55,55,55	0
56	MG	AA	3052	1/1	0.96	0.17	49,49,49,49	0
56	MG	AM	201	1/1	0.96	0.04	59,59,59,59	0
56	MG	DA	3349	1/1	0.96	0.09	31,31,31,31	0
56	MG	DA	3350	1/1	0.96	0.06	53,53,53,53	0
56	MG	CA	3080	1/1	0.96	0.13	56,56,56,56	0
56	MG	DA	3354	1/1	0.96	0.07	48,48,48,48	0
56	MG	AA	3075	1/1	0.96	0.32	49,49,49,49	0
56	MG	BA	3139	1/1	0.96	0.08	53,53,53,53	0
56	MG	BA	3232	1/1	0.96	0.10	51,51,51,51	0
56	MG	DA	3359	1/1	0.96	0.11	39,39,39,39	0
56	MG	BB	204	1/1	0.96	0.07	42,42,42,42	0
56	MG	BA	3508	1/1	0.96	0.05	34,34,34,34	0
56	MG	DA	3363	1/1	0.96	0.13	49,49,49,49	0
56	MG	BA	3652	1/1	0.96	0.09	61,61,61,61	0
56	MG	DA	3112	1/1	0.96	0.18	37,37,37,37	0
56	MG	DA	3658	1/1	0.96	0.08	55,55,55,55	0
56	MG	DA	3366	1/1	0.96	0.05	38,38,38,38	0
56	MG	DA	3661	1/1	0.96	0.09	54,54,54,54	0
56	MG	BA	3653	1/1	0.96	0.09	39,39,39,39	0
56	MG	BA	3140	1/1	0.96	0.16	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	BA	3141	1/1	0.96	0.16	42,42,42,42	0
56	MG	BA	3236	1/1	0.96	0.11	34,34,34,34	0
56	MG	DA	3117	1/1	0.96	0.10	42,42,42,42	0
56	MG	BA	3142	1/1	0.96	0.15	29,29,29,29	0
56	MG	DA	3121	1/1	0.96	0.10	40,40,40,40	0
56	MG	BB	214	1/1	0.96	0.17	53,53,53,53	0
56	MG	AA	3024	1/1	0.96	0.26	55,55,55,55	0
56	MG	DA	3383	1/1	0.96	0.08	31,31,31,31	0
56	MG	DA	3125	1/1	0.96	0.08	40,40,40,40	0
56	MG	DA	3386	1/1	0.96	0.06	23,23,23,23	0
56	MG	BA	3239	1/1	0.96	0.16	40,40,40,40	0
56	MG	BA	3079	1/1	0.96	0.25	49,49,49,49	0
56	MG	BA	3522	1/1	0.96	0.10	16,16,16,16	0
56	MG	DA	3390	1/1	0.96	0.06	19,19,19,19	0
56	MG	BA	3365	1/1	0.96	0.13	37,37,37,37	0
56	MG	AA	3042	1/1	0.96	0.20	55,55,55,55	0
56	MG	BA	3669	1/1	0.96	0.09	36,36,36,36	0
56	MG	DA	3396	1/1	0.96	0.07	47,47,47,47	0
56	MG	BD	3305	1/1	0.96	0.09	31,31,31,31	0
56	MG	DD	305	1/1	0.96	0.36	39,39,39,39	0
56	MG	AA	3007	1/1	0.96	0.13	54,54,54,54	0
56	MG	BA	3527	1/1	0.96	0.06	27,27,27,27	0
56	MG	DA	3138	1/1	0.96	0.07	63,63,63,63	0
56	MG	BD	3308	1/1	0.96	0.20	60,60,60,60	0
56	MG	BD	3309	1/1	0.96	0.09	40,40,40,40	0
56	MG	BE	301	1/1	0.96	0.10	27,27,27,27	0
56	MG	BE	302	1/1	0.96	0.20	40,40,40,40	0
56	MG	BE	303	1/1	0.96	0.33	32,32,32,32	0
56	MG	DF	302	1/1	0.96	0.09	44,44,44,44	0
56	MG	BE	304	1/1	0.96	0.12	43,43,43,43	0
56	MG	DF	304	1/1	0.96	0.16	40,40,40,40	0
56	MG	BA	3672	1/1	0.96	0.07	62,62,62,62	0
56	MG	DA	3149	1/1	0.96	0.26	37,37,37,37	0
56	MG	BA	3152	1/1	0.96	0.16	42,42,42,42	0
56	MG	BA	3030	1/1	0.96	0.09	40,40,40,40	0
56	MG	BA	3531	1/1	0.96	0.09	43,43,43,43	0
56	MG	BA	3154	1/1	0.96	0.17	37,37,37,37	0
56	MG	DQ	3001	1/1	0.96	0.07	45,45,45,45	0
56	MG	BA	3248	1/1	0.96	0.30	52,52,52,52	0
56	MG	BA	3155	1/1	0.96	0.26	30,30,30,30	0
56	MG	DA	3422	1/1	0.96	0.07	51,51,51,51	0
56	MG	BA	3087	1/1	0.96	0.32	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	BF	307	1/1	0.96	0.18	40,40,40,40	0
56	MG	DA	3159	1/1	0.96	0.06	42,42,42,42	0
56	MG	BA	3158	1/1	0.96	0.10	40,40,40,40	0
56	MG	DA	3161	1/1	0.96	0.13	37,37,37,37	0
56	MG	DA	3162	1/1	0.96	0.06	37,37,37,37	0
56	MG	BA	3159	1/1	0.96	0.11	40,40,40,40	0
56	MG	BA	3160	1/1	0.96	0.17	40,40,40,40	0
56	MG	D0	102	1/1	0.96	0.13	51,51,51,51	0
56	MG	BA	3379	1/1	0.96	0.11	39,39,39,39	0
56	MG	BN	3001	1/1	0.96	0.34	52,52,52,52	0
56	MG	BA	3688	1/1	0.96	0.06	16,16,16,16	0
56	MG	BA	3031	1/1	0.96	0.13	28,28,28,28	0
56	MG	BA	3090	1/1	0.96	0.07	27,27,27,27	0
56	MG	DA	3171	1/1	0.96	0.13	53,53,53,53	0
56	MG	BA	3163	1/1	0.96	0.11	34,34,34,34	0
56	MG	BA	3164	1/1	0.96	0.25	35,35,35,35	0
56	MG	AA	3036	1/1	0.96	0.40	69,69,69,69	0
60	K	AX	3001	1/1	0.96	0.12	65,65,65,65	0
56	MG	BA	3033	1/1	0.96	0.28	42,42,42,42	0
56	MG	AA	3099	1/1	0.97	0.25	47,47,47,47	0
56	MG	CA	3140	1/1	0.97	0.11	75,75,75,75	0
56	MG	DA	3295	1/1	0.97	0.06	30,30,30,30	0
56	MG	DA	3123	1/1	0.97	0.13	52,52,52,52	0
56	MG	B7	105	1/1	0.97	0.12	46,46,46,46	0
56	MG	BA	3095	1/1	0.97	0.11	30,30,30,30	0
56	MG	BA	3661	1/1	0.97	0.09	48,48,48,48	0
56	MG	DA	3301	1/1	0.97	0.09	51,51,51,51	0
56	MG	BA	3279	1/1	0.97	0.27	45,45,45,45	0
56	MG	BA	3167	1/1	0.97	0.14	43,43,43,43	0
56	MG	CA	3004	1/1	0.97	0.05	67,67,67,67	0
56	MG	DA	3307	1/1	0.97	0.06	27,27,27,27	0
56	MG	BA	3782	1/1	0.97	0.29	30,30,30,30	0
56	MG	BA	3015	1/1	0.97	0.19	50,50,50,50	0
56	MG	DA	3523	1/1	0.97	0.06	52,52,52,52	0
56	MG	BA	3784	1/1	0.97	0.08	23,23,23,23	0
56	MG	BA	3667	1/1	0.97	0.13	39,39,39,39	0
56	MG	BA	3129	1/1	0.97	0.30	38,38,38,38	0
56	MG	DA	3136	1/1	0.97	0.26	43,43,43,43	0
56	MG	BA	3564	1/1	0.97	0.13	50,50,50,50	0
56	MG	DA	3532	1/1	0.97	0.08	61,61,61,61	0
56	MG	DA	3139	1/1	0.97	0.06	41,41,41,41	0
56	MG	BA	3456	1/1	0.97	0.05	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	AA	3114	1/1	0.97	0.09	45,45,45,45	0
56	MG	AA	3053	1/1	0.97	0.13	46,46,46,46	0
56	MG	BA	3070	1/1	0.97	0.16	39,39,39,39	0
56	MG	DA	3538	1/1	0.97	0.06	44,44,44,44	0
56	MG	DA	3144	1/1	0.97	0.06	39,39,39,39	0
56	MG	DA	3145	1/1	0.97	0.13	38,38,38,38	0
56	MG	DA	3323	1/1	0.97	0.09	29,29,29,29	0
56	MG	BA	3173	1/1	0.97	0.25	41,41,41,41	0
56	MG	BA	3570	1/1	0.97	0.11	35,35,35,35	0
56	MG	BA	3287	1/1	0.97	0.16	28,28,28,28	0
56	MG	BA	3462	1/1	0.97	0.10	49,49,49,49	0
56	MG	BA	3226	1/1	0.97	0.16	25,25,25,25	0
56	MG	DA	3329	1/1	0.97	0.13	47,47,47,47	0
56	MG	BA	3466	1/1	0.97	0.10	44,44,44,44	0
56	MG	DA	3552	1/1	0.97	0.07	36,36,36,36	0
56	MG	BA	3681	1/1	0.97	0.12	50,50,50,50	0
56	MG	DA	3555	1/1	0.97	0.05	56,56,56,56	0
56	MG	BA	3803	1/1	0.97	0.13	33,33,33,33	0
56	MG	AA	3116	1/1	0.97	0.06	32,32,32,32	0
56	MG	BA	3228	1/1	0.97	0.30	56,56,56,56	0
56	MG	DA	3336	1/1	0.97	0.05	39,39,39,39	0
56	MG	BA	3684	1/1	0.97	0.13	51,51,51,51	0
56	MG	BA	3469	1/1	0.97	0.10	41,41,41,41	0
56	MG	BA	3686	1/1	0.97	0.07	41,41,41,41	0
56	MG	BA	3809	1/1	0.97	0.06	41,41,41,41	0
56	MG	BA	3471	1/1	0.97	0.07	27,27,27,27	0
56	MG	AA	3037	1/1	0.97	0.20	46,46,46,46	0
56	MG	BA	3812	1/1	0.97	0.09	31,31,31,31	0
56	MG	BA	3689	1/1	0.97	0.09	53,53,53,53	0
56	MG	BA	3581	1/1	0.97	0.05	37,37,37,37	0
56	MG	DA	3346	1/1	0.97	0.10	48,48,48,48	0
56	MG	CA	3035	1/1	0.97	0.13	52,52,52,52	0
56	MG	DA	3167	1/1	0.97	0.14	38,38,38,38	0
56	MG	DA	3572	1/1	0.97	0.06	68,68,68,68	0
56	MG	BA	3691	1/1	0.97	0.08	68,68,68,68	0
56	MG	DA	3352	1/1	0.97	0.06	27,27,27,27	0
56	MG	BA	3293	1/1	0.97	0.09	40,40,40,40	0
56	MG	BA	3053	1/1	0.97	0.09	23,23,23,23	0
56	MG	BA	3694	1/1	0.97	0.15	54,54,54,54	0
56	MG	DA	3356	1/1	0.97	0.14	37,37,37,37	0
56	MG	DA	3579	1/1	0.97	0.06	52,52,52,52	0
56	MG	BA	3075	1/1	0.97	0.10	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	BA	3104	1/1	0.97	0.13	23,23,23,23	0
56	MG	DA	3005	1/1	0.97	0.12	26,26,26,26	0
56	MG	BA	3076	1/1	0.97	0.12	34,34,34,34	0
56	MG	DA	3361	1/1	0.97	0.05	25,25,25,25	0
56	MG	BA	3298	1/1	0.97	0.24	49,49,49,49	0
56	MG	DA	3588	1/1	0.97	0.05	65,65,65,65	0
56	MG	DA	3008	1/1	0.97	0.09	40,40,40,40	0
56	MG	CA	3044	1/1	0.97	0.10	44,44,44,44	0
56	MG	DA	3591	1/1	0.97	0.05	59,59,59,59	0
56	MG	BA	3299	1/1	0.97	0.05	44,44,44,44	0
56	MG	DA	3012	1/1	0.97	0.04	39,39,39,39	0
56	MG	BA	3481	1/1	0.97	0.13	44,44,44,44	0
56	MG	DA	3595	1/1	0.97	0.08	39,39,39,39	0
56	MG	BA	3181	1/1	0.97	0.11	26,26,26,26	0
56	MG	DA	3598	1/1	0.97	0.08	30,30,30,30	0
56	MG	BB	213	1/1	0.97	0.09	30,30,30,30	0
56	MG	DA	3371	1/1	0.97	0.07	22,22,22,22	0
56	MG	BA	3484	1/1	0.97	0.10	51,51,51,51	0
56	MG	DA	3374	1/1	0.97	0.05	31,31,31,31	0
56	MG	DA	3375	1/1	0.97	0.06	37,37,37,37	0
56	MG	BA	3301	1/1	0.97	0.06	48,48,48,48	0
56	MG	BA	3302	1/1	0.97	0.12	24,24,24,24	0
56	MG	DA	3020	1/1	0.97	0.05	32,32,32,32	0
56	MG	DA	3021	1/1	0.97	0.18	40,40,40,40	0
56	MG	DA	3190	1/1	0.97	0.10	41,41,41,41	0
56	MG	BA	3304	1/1	0.97	0.05	37,37,37,37	0
56	MG	BA	3182	1/1	0.97	0.07	21,21,21,21	0
56	MG	AA	3186	1/1	0.97	0.11	42,42,42,42	0
56	MG	DA	3613	1/1	0.97	0.04	55,55,55,55	0
56	MG	BA	3708	1/1	0.97	0.20	36,36,36,36	0
56	MG	DA	3028	1/1	0.97	0.14	45,45,45,45	0
56	MG	BB	222	1/1	0.97	0.14	50,50,50,50	0
56	MG	BD	3301	1/1	0.97	0.11	37,37,37,37	0
56	MG	BD	3302	1/1	0.97	0.05	46,46,46,46	0
56	MG	BA	3021	1/1	0.97	0.07	22,22,22,22	0
56	MG	CA	3060	1/1	0.97	0.08	47,47,47,47	0
56	MG	AA	3126	1/1	0.97	0.14	57,57,57,57	0
56	MG	BA	3388	1/1	0.97	0.05	27,27,27,27	0
56	MG	BA	3311	1/1	0.97	0.08	23,23,23,23	0
56	MG	BA	3188	1/1	0.97	0.15	46,46,46,46	0
56	MG	DA	3401	1/1	0.97	0.04	43,43,43,43	0
56	MG	BA	3189	1/1	0.97	0.17	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DA	3206	1/1	0.97	0.16	46,46,46,46	0
56	MG	BA	3243	1/1	0.97	0.12	56,56,56,56	0
56	MG	BA	3609	1/1	0.97	0.07	54,54,54,54	0
56	MG	BA	3718	1/1	0.97	0.13	53,53,53,53	0
56	MG	BA	3244	1/1	0.97	0.25	39,39,39,39	0
56	MG	BA	3146	1/1	0.97	0.06	19,19,19,19	0
56	MG	DA	3045	1/1	0.97	0.32	60,60,60,60	0
56	MG	BA	3110	1/1	0.97	0.06	46,46,46,46	0
56	MG	DA	3413	1/1	0.97	0.04	34,34,34,34	0
56	MG	DA	3414	1/1	0.97	0.06	38,38,38,38	0
56	MG	BA	3148	1/1	0.97	0.06	49,49,49,49	0
56	MG	BA	3081	1/1	0.97	0.09	33,33,33,33	0
56	MG	BA	3249	1/1	0.97	0.09	40,40,40,40	0
56	MG	DA	3050	1/1	0.97	0.08	37,37,37,37	0
56	MG	BA	3510	1/1	0.97	0.07	42,42,42,42	0
56	MG	CA	3076	1/1	0.97	0.17	35,35,35,35	0
56	MG	BA	3511	1/1	0.97	0.16	43,43,43,43	0
56	MG	BA	3729	1/1	0.97	0.04	27,27,27,27	0
56	MG	BA	3402	1/1	0.97	0.06	25,25,25,25	0
56	MG	BA	3732	1/1	0.97	0.06	41,41,41,41	0
56	MG	BA	3619	1/1	0.97	0.07	33,33,33,33	0
56	MG	DA	3427	1/1	0.97	0.04	45,45,45,45	0
56	MG	DA	3428	1/1	0.97	0.05	26,26,26,26	0
56	MG	DA	3058	1/1	0.97	0.07	50,50,50,50	0
56	MG	AA	3188	1/1	0.97	0.19	49,49,49,49	0
56	MG	DA	3228	1/1	0.97	0.14	46,46,46,46	0
56	MG	BA	3517	1/1	0.97	0.08	49,49,49,49	0
56	MG	BA	3406	1/1	0.97	0.06	32,32,32,32	0
56	MG	BA	3408	1/1	0.97	0.05	21,21,21,21	0
56	MG	BA	3058	1/1	0.97	0.09	27,27,27,27	0
56	MG	BA	3196	1/1	0.97	0.07	40,40,40,40	0
56	MG	BA	3086	1/1	0.97	0.17	49,49,49,49	0
56	MG	BA	3115	1/1	0.97	0.07	33,33,33,33	0
56	MG	DA	3660	1/1	0.97	0.04	28,28,28,28	0
56	MG	BA	3116	1/1	0.97	0.05	35,35,35,35	0
56	MG	BA	3156	1/1	0.97	0.08	32,32,32,32	0
56	MG	AA	3111	1/1	0.97	0.15	61,61,61,61	0
56	MG	BQ	202	1/1	0.97	0.14	37,37,37,37	0
56	MG	BA	3528	1/1	0.97	0.10	46,46,46,46	0
56	MG	DA	3667	1/1	0.97	0.10	66,66,66,66	0
56	MG	BA	3332	1/1	0.97	0.12	36,36,36,36	0
56	MG	DA	3669	1/1	0.97	0.12	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	3421	1/1	0.97	0.14	48,48,48,48	0
56	MG	BR	202	1/1	0.97	0.15	42,42,42,42	0
56	MG	DA	3449	1/1	0.97	0.05	33,33,33,33	0
56	MG	CA	3098	1/1	0.97	0.10	44,44,44,44	0
56	MG	BR	203	1/1	0.97	0.16	34,34,34,34	0
56	MG	DA	3452	1/1	0.97	0.05	37,37,37,37	0
56	MG	BA	3060	1/1	0.97	0.18	26,26,26,26	0
56	MG	CA	3102	1/1	0.97	0.12	49,49,49,49	0
56	MG	BA	3089	1/1	0.97	0.14	42,42,42,42	0
56	MG	BA	3752	1/1	0.97	0.07	32,32,32,32	0
56	MG	BA	3042	1/1	0.97	0.09	41,41,41,41	0
56	MG	DB	3007	1/1	0.97	0.10	42,42,42,42	0
56	MG	BA	3263	1/1	0.97	0.28	56,56,56,56	0
56	MG	BA	3205	1/1	0.97	0.14	40,40,40,40	0
56	MG	DA	3460	1/1	0.97	0.07	42,42,42,42	0
56	MG	DA	3084	1/1	0.97	0.07	47,47,47,47	0
56	MG	DA	3462	1/1	0.97	0.05	31,31,31,31	0
56	MG	DD	304	1/1	0.97	0.10	33,33,33,33	0
56	MG	DA	3086	1/1	0.97	0.17	36,36,36,36	0
56	MG	DA	3464	1/1	0.97	0.04	24,24,24,24	0
56	MG	BA	3091	1/1	0.97	0.22	40,40,40,40	0
56	MG	DA	3088	1/1	0.97	0.11	30,30,30,30	0
56	MG	CA	3109	1/1	0.97	0.17	41,41,41,41	0
56	MG	DA	3261	1/1	0.97	0.14	36,36,36,36	0
56	MG	CA	3110	1/1	0.97	0.21	48,48,48,48	0
56	MG	BA	3343	1/1	0.97	0.06	30,30,30,30	0
56	MG	DA	3092	1/1	0.97	0.11	48,48,48,48	0
56	MG	DA	3265	1/1	0.97	0.13	37,37,37,37	0
56	MG	DA	3473	1/1	0.97	0.07	30,30,30,30	0
56	MG	BA	3266	1/1	0.97	0.12	27,27,27,27	0
56	MG	DA	3475	1/1	0.97	0.08	38,38,38,38	0
56	MG	DA	3476	1/1	0.97	0.11	53,53,53,53	0
56	MG	CA	3114	1/1	0.97	0.09	52,52,52,52	0
56	MG	BA	3540	1/1	0.97	0.07	57,57,57,57	0
56	MG	BX	101	1/1	0.97	0.07	36,36,36,36	0
56	MG	BA	3345	1/1	0.97	0.05	28,28,28,28	0
56	MG	BA	3542	1/1	0.97	0.09	20,20,20,20	0
56	MG	BA	3543	1/1	0.97	0.15	23,23,23,23	0
56	MG	BA	3123	1/1	0.97	0.14	28,28,28,28	0
56	MG	BA	3210	1/1	0.97	0.06	43,43,43,43	0
56	MG	DU	3002	1/1	0.97	0.28	52,52,52,52	0
56	MG	BA	3442	1/1	0.97	0.06	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	AA	3031	1/1	0.97	0.21	54,54,54,54	0
56	MG	DA	3487	1/1	0.97	0.09	37,37,37,37	0
56	MG	BA	3270	1/1	0.97	0.24	40,40,40,40	0
56	MG	B0	104	1/1	0.97	0.10	41,41,41,41	0
56	MG	DA	3490	1/1	0.97	0.07	43,43,43,43	0
56	MG	BA	3550	1/1	0.97	0.06	25,25,25,25	0
56	MG	BA	3212	1/1	0.97	0.10	26,26,26,26	0
56	MG	D0	101	1/1	0.97	0.07	50,50,50,50	0
56	MG	DA	3108	1/1	0.97	0.07	46,46,46,46	0
56	MG	B3	3001	1/1	0.97	0.09	38,38,38,38	0
56	MG	BA	3552	1/1	0.97	0.06	46,46,46,46	0
56	MG	CA	3130	1/1	0.97	0.15	51,51,51,51	0
56	MG	BA	3553	1/1	0.97	0.09	53,53,53,53	0
56	MG	BA	3273	1/1	0.97	0.24	41,41,41,41	0
59	ZN	B4	501	1/1	0.97	0.04	99,99,99,99	0
56	MG	AX	3004	1/1	0.97	0.12	53,53,53,53	0
56	MG	DA	3288	1/1	0.97	0.08	48,48,48,48	0
59	ZN	B9	501	1/1	0.97	0.04	49,49,49,49	0
56	MG	BA	3775	1/1	0.97	0.05	34,34,34,34	0
56	MG	B6	101	1/1	0.97	0.08	47,47,47,47	0
56	MG	BA	3658	1/1	0.97	0.08	51,51,51,51	0
56	MG	B7	103	1/1	0.97	0.07	35,35,35,35	0
56	MG	DA	3119	1/1	0.98	0.12	40,40,40,40	0
56	MG	BA	3215	1/1	0.98	0.09	47,47,47,47	0
56	MG	BA	3601	1/1	0.98	0.09	49,49,49,49	0
56	MG	BA	3451	1/1	0.98	0.09	31,31,31,31	0
56	MG	BA	3383	1/1	0.98	0.08	20,20,20,20	0
56	MG	CA	3101	1/1	0.98	0.14	54,54,54,54	0
56	MG	DA	3022	1/1	0.98	0.04	29,29,29,29	0
56	MG	DA	3127	1/1	0.98	0.13	36,36,36,36	0
56	MG	BD	3303	1/1	0.98	0.04	33,33,33,33	0
56	MG	DA	3348	1/1	0.98	0.04	32,32,32,32	0
56	MG	BA	3333	1/1	0.98	0.04	23,23,23,23	0
56	MG	BA	3334	1/1	0.98	0.07	26,26,26,26	0
56	MG	DA	3351	1/1	0.98	0.11	32,32,32,32	0
56	MG	AA	3137	1/1	0.98	0.06	42,42,42,42	0
56	MG	DA	3238	1/1	0.98	0.09	54,54,54,54	0
56	MG	AA	3035	1/1	0.98	0.09	26,26,26,26	0
56	MG	DA	3029	1/1	0.98	0.06	36,36,36,36	0
56	MG	BA	3608	1/1	0.98	0.11	34,34,34,34	0
56	MG	BA	3218	1/1	0.98	0.10	34,34,34,34	0
56	MG	BA	3253	1/1	0.98	0.21	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	3137	1/1	0.98	0.22	43,43,43,43	0
56	MG	BA	3535	1/1	0.98	0.15	31,31,31,31	0
56	MG	DA	3246	1/1	0.98	0.08	31,31,31,31	0
56	MG	CA	3111	1/1	0.98	0.10	56,56,56,56	0
56	MG	BA	3074	1/1	0.98	0.09	31,31,31,31	0
56	MG	CA	3018	1/1	0.98	0.06	52,52,52,52	0
56	MG	DA	3492	1/1	0.98	0.05	44,44,44,44	0
56	MG	BA	3220	1/1	0.98	0.15	40,40,40,40	0
56	MG	DA	3251	1/1	0.98	0.11	46,46,46,46	0
56	MG	BE	305	1/1	0.98	0.07	19,19,19,19	0
56	MG	AA	3120	1/1	0.98	0.07	49,49,49,49	0
56	MG	DA	3498	1/1	0.98	0.05	44,44,44,44	0
56	MG	BA	3136	1/1	0.98	0.07	42,42,42,42	0
56	MG	BA	3043	1/1	0.98	0.05	35,35,35,35	0
56	MG	BA	3465	1/1	0.98	0.06	47,47,47,47	0
56	MG	BA	3138	1/1	0.98	0.20	40,40,40,40	0
56	MG	BA	3397	1/1	0.98	0.06	25,25,25,25	0
56	MG	AA	3063	1/1	0.98	0.09	42,42,42,42	0
56	MG	DA	3505	1/1	0.98	0.07	45,45,45,45	0
56	MG	BA	3261	1/1	0.98	0.04	46,46,46,46	0
56	MG	DA	3378	1/1	0.98	0.05	34,34,34,34	0
56	MG	BA	3470	1/1	0.98	0.11	37,37,37,37	0
56	MG	DA	3380	1/1	0.98	0.05	35,35,35,35	0
56	MG	BA	3400	1/1	0.98	0.05	34,34,34,34	0
56	MG	BA	3118	1/1	0.98	0.27	37,37,37,37	0
56	MG	DA	3155	1/1	0.98	0.25	38,38,38,38	0
56	MG	DA	3384	1/1	0.98	0.09	39,39,39,39	0
56	MG	BA	3625	1/1	0.98	0.04	31,31,31,31	0
56	MG	BA	3078	1/1	0.98	0.06	15,15,15,15	0
56	MG	BA	3474	1/1	0.98	0.04	20,20,20,20	0
56	MG	BA	3303	1/1	0.98	0.17	37,37,37,37	0
56	MG	BN	3003	1/1	0.98	0.09	44,44,44,44	0
56	MG	BA	3404	1/1	0.98	0.10	23,23,23,23	0
56	MG	BN	3005	1/1	0.98	0.10	35,35,35,35	0
56	MG	BA	3005	1/1	0.98	0.06	33,33,33,33	0
56	MG	BA	3143	1/1	0.98	0.05	39,39,39,39	0
56	MG	DA	3395	1/1	0.98	0.04	33,33,33,33	0
56	MG	BA	3354	1/1	0.98	0.04	20,20,20,20	0
56	MG	DA	3397	1/1	0.98	0.03	30,30,30,30	0
56	MG	BP	202	1/1	0.98	0.06	27,27,27,27	0
56	MG	DA	3528	1/1	0.98	0.04	39,39,39,39	0
56	MG	DA	3663	1/1	0.98	0.05	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	3529	1/1	0.98	0.06	57,57,57,57	0
56	MG	BA	3230	1/1	0.98	0.21	36,36,36,36	0
56	MG	BA	3788	1/1	0.98	0.07	10,10,10,10	0
56	MG	AA	3151	1/1	0.98	0.05	56,56,56,56	0
56	MG	BA	3414	1/1	0.98	0.11	33,33,33,33	0
56	MG	BA	3791	1/1	0.98	0.05	18,18,18,18	0
56	MG	BA	3710	1/1	0.98	0.16	28,28,28,28	0
56	MG	BA	3415	1/1	0.98	0.09	34,34,34,34	0
56	MG	DA	3174	1/1	0.98	0.23	50,50,50,50	0
56	MG	BA	3309	1/1	0.98	0.05	50,50,50,50	0
56	MG	DA	3539	1/1	0.98	0.08	38,38,38,38	0
56	MG	BA	3145	1/1	0.98	0.08	41,41,41,41	0
56	MG	BA	3008	1/1	0.98	0.08	26,26,26,26	0
56	MG	BA	3063	1/1	0.98	0.32	54,54,54,54	0
56	MG	BA	3313	1/1	0.98	0.08	34,34,34,34	0
56	MG	AA	3132	1/1	0.98	0.10	36,36,36,36	0
56	MG	BA	3272	1/1	0.98	0.09	22,22,22,22	0
56	MG	BA	3802	1/1	0.98	0.19	23,23,23,23	0
56	MG	BU	209	1/1	0.98	0.21	27,27,27,27	0
56	MG	BV	202	1/1	0.98	0.20	33,33,33,33	0
56	MG	BA	3423	1/1	0.98	0.06	31,31,31,31	0
56	MG	DD	301	1/1	0.98	0.06	43,43,43,43	0
56	MG	DA	3550	1/1	0.98	0.09	22,22,22,22	0
56	MG	DA	3551	1/1	0.98	0.04	47,47,47,47	0
56	MG	BA	3497	1/1	0.98	0.03	44,44,44,44	0
56	MG	DA	3553	1/1	0.98	0.04	46,46,46,46	0
56	MG	BA	3364	1/1	0.98	0.15	29,29,29,29	0
56	MG	BA	3425	1/1	0.98	0.08	48,48,48,48	0
56	MG	BW	204	1/1	0.98	0.19	31,31,31,31	0
56	MG	DE	301	1/1	0.98	0.07	35,35,35,35	0
56	MG	CA	3161	1/1	0.98	0.10	51,51,51,51	0
56	MG	BA	3316	1/1	0.98	0.11	25,25,25,25	0
56	MG	DA	3302	1/1	0.98	0.07	32,32,32,32	0
56	MG	BX	102	1/1	0.98	0.08	36,36,36,36	0
56	MG	BA	3149	1/1	0.98	0.21	36,36,36,36	0
56	MG	BA	3085	1/1	0.98	0.12	23,23,23,23	0
56	MG	DA	3306	1/1	0.98	0.19	35,35,35,35	0
56	MG	DA	3432	1/1	0.98	0.05	37,37,37,37	0
56	MG	BA	3504	1/1	0.98	0.05	40,40,40,40	0
56	MG	BA	3432	1/1	0.98	0.07	35,35,35,35	0
56	MG	BA	3433	1/1	0.98	0.08	31,31,31,31	0
56	MG	BA	3275	1/1	0.98	0.17	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DA	3311	1/1	0.98	0.06	19,19,19,19	0
56	MG	CA	3170	1/1	0.98	0.11	53,53,53,53	0
56	MG	BA	3022	1/1	0.98	0.03	25,25,25,25	0
56	MG	DQ	3002	1/1	0.98	0.10	41,41,41,41	0
56	MG	CA	3172	1/1	0.98	0.08	50,50,50,50	0
56	MG	BA	3436	1/1	0.98	0.09	17,17,17,17	0
56	MG	BA	3177	1/1	0.98	0.06	44,44,44,44	0
56	MG	BA	3278	1/1	0.98	0.21	30,30,30,30	0
56	MG	BA	3023	1/1	0.98	0.09	35,35,35,35	0
56	MG	BA	3374	1/1	0.98	0.04	21,21,21,21	0
56	MG	BA	3036	1/1	0.98	0.12	19,19,19,19	0
56	MG	BA	3589	1/1	0.98	0.07	42,42,42,42	0
56	MG	DA	3448	1/1	0.98	0.06	45,45,45,45	0
56	MG	BB	208	1/1	0.98	0.08	36,36,36,36	0
56	MG	BA	3208	1/1	0.98	0.13	19,19,19,19	0
56	MG	BA	3743	1/1	0.98	0.07	43,43,43,43	0
56	MG	BA	3664	1/1	0.98	0.10	17,17,17,17	0
56	MG	BA	3665	1/1	0.98	0.06	40,40,40,40	0
56	MG	DA	3587	1/1	0.98	0.12	52,52,52,52	0
56	MG	B7	101	1/1	0.98	0.06	47,47,47,47	0
56	MG	B7	102	1/1	0.98	0.10	28,28,28,28	0
56	MG	BA	3052	1/1	0.98	0.12	23,23,23,23	0
56	MG	BA	3011	1/1	0.98	0.04	33,33,33,33	0
58	SF4	AD	501	8/8	0.98	0.05	62,74,91,95	0
58	SF4	CD	501	8/8	0.98	0.04	64,77,89,111	0
59	ZN	AN	501	1/1	0.98	0.05	86,86,86,86	0
56	MG	BA	3012	1/1	0.98	0.18	33,33,33,33	0
56	MG	BA	3183	1/1	0.98	0.08	35,35,35,35	0
56	MG	B8	102	1/1	0.98	0.07	41,41,41,41	0
56	MG	DA	3334	1/1	0.98	0.05	45,45,45,45	0
56	MG	BA	3448	1/1	0.98	0.08	23,23,23,23	0
56	MG	BA	3524	1/1	0.98	0.10	53,53,53,53	0
56	MG	BA	3184	1/1	0.98	0.17	37,37,37,37	0
56	MG	CA	3003	1/1	0.98	0.09	51,51,51,51	0
56	MG	DA	3407	1/1	0.99	0.02	28,28,28,28	0
56	MG	BA	3429	1/1	0.99	0.03	23,23,23,23	0
56	MG	DA	3009	1/1	0.99	0.07	29,29,29,29	0
56	MG	BA	3546	1/1	0.99	0.05	38,38,38,38	0
56	MG	DA	3120	1/1	0.99	0.07	34,34,34,34	0
56	MG	BP	201	1/1	0.99	0.24	28,28,28,28	0
56	MG	BA	3513	1/1	0.99	0.03	43,43,43,43	0
56	MG	DA	3013	1/1	0.99	0.04	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	BB	215	1/1	0.99	0.04	35,35,35,35	0
56	MG	BA	3341	1/1	0.99	0.03	43,43,43,43	0
56	MG	BA	3515	1/1	0.99	0.06	35,35,35,35	0
56	MG	BA	3482	1/1	0.99	0.08	42,42,42,42	0
56	MG	DA	3298	1/1	0.99	0.04	55,55,55,55	0
56	MG	BA	3407	1/1	0.99	0.09	40,40,40,40	0
56	MG	DA	3421	1/1	0.99	0.02	31,31,31,31	0
56	MG	BA	3007	1/1	0.99	0.06	35,35,35,35	0
56	MG	BA	3409	1/1	0.99	0.07	21,21,21,21	0
56	MG	BA	3486	1/1	0.99	0.05	22,22,22,22	0
56	MG	BA	3591	1/1	0.99	0.08	48,48,48,48	0
56	MG	BA	3289	1/1	0.99	0.30	35,35,35,35	0
56	MG	BA	3556	1/1	0.99	0.06	48,48,48,48	0
56	MG	BU	203	1/1	0.99	0.13	27,27,27,27	0
56	MG	BA	3594	1/1	0.99	0.11	33,33,33,33	0
56	MG	DA	3027	1/1	0.99	0.15	42,42,42,42	0
56	MG	DA	3495	1/1	0.99	0.12	39,39,39,39	0
56	MG	BA	3037	1/1	0.99	0.31	29,29,29,29	0
56	MG	DA	3368	1/1	0.99	0.06	24,24,24,24	0
56	MG	BA	3235	1/1	0.99	0.12	26,26,26,26	0
56	MG	BU	207	1/1	0.99	0.24	29,29,29,29	0
56	MG	DA	3085	1/1	0.99	0.12	38,38,38,38	0
56	MG	BA	3413	1/1	0.99	0.08	27,27,27,27	0
56	MG	DA	3373	1/1	0.99	0.06	39,39,39,39	0
56	MG	BA	3560	1/1	0.99	0.10	38,38,38,38	0
56	MG	BV	201	1/1	0.99	0.19	27,27,27,27	0
56	MG	BA	3493	1/1	0.99	0.06	49,49,49,49	0
56	MG	BA	3463	1/1	0.99	0.03	10,10,10,10	0
56	MG	BA	3393	1/1	0.99	0.05	22,22,22,22	0
56	MG	BA	3003	1/1	0.99	0.05	30,30,30,30	0
56	MG	BA	3107	1/1	0.99	0.18	50,50,50,50	0
56	MG	BW	203	1/1	0.99	0.10	37,37,37,37	0
56	MG	BA	3680	1/1	0.99	0.05	53,53,53,53	0
56	MG	BA	3441	1/1	0.99	0.08	32,32,32,32	0
56	MG	BA	3306	1/1	0.99	0.14	18,18,18,18	0
56	MG	BA	3500	1/1	0.99	0.08	32,32,32,32	0
56	MG	BA	3723	1/1	0.99	0.04	25,25,25,25	0
56	MG	BA	3069	1/1	0.99	0.14	39,39,39,39	0
56	MG	BA	3084	1/1	0.99	0.11	33,33,33,33	0
56	MG	BA	3209	1/1	0.99	0.07	35,35,35,35	0
56	MG	BA	3013	1/1	0.99	0.10	26,26,26,26	0
56	MG	DA	3216	1/1	0.99	0.13	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	3009	1/1	0.99	0.04	25,25,25,25	0
56	MG	BA	3730	1/1	0.99	0.08	13,13,13,13	0
56	MG	DA	3394	1/1	0.99	0.04	40,40,40,40	0
56	MG	BA	3773	1/1	0.99	0.04	38,38,38,38	0
56	MG	BA	3574	1/1	0.99	0.04	28,28,28,28	0
56	MG	DA	3526	1/1	0.99	0.17	28,28,28,28	0
56	MG	BA	3339	1/1	0.99	0.07	23,23,23,23	0
56	MG	BA	3370	1/1	0.99	0.04	27,27,27,27	0
56	MG	DA	3596	1/1	0.99	0.03	65,65,65,65	0
59	ZN	BY	203	1/1	0.99	0.02	54,54,54,54	0
56	MG	BA	3734	1/1	0.99	0.07	18,18,18,18	0
56	MG	AA	3108	1/1	0.99	0.08	58,58,58,58	0
56	MG	BA	3426	1/1	0.99	0.10	20,20,20,20	0
56	MG	DA	3004	1/1	0.99	0.12	25,25,25,25	0
56	MG	BA	3405	1/1	0.99	0.09	22,22,22,22	0
59	ZN	DY	501	1/1	0.99	0.05	97,97,97,97	0
56	MG	CA	3137	1/1	0.99	0.09	50,50,50,50	0
59	ZN	D6	501	1/1	0.99	0.05	66,66,66,66	0
59	ZN	D9	501	1/1	0.99	0.03	65,65,65,65	0
56	MG	BA	3428	1/1	0.99	0.12	36,36,36,36	0
56	MG	DA	3406	1/1	0.99	0.04	33,33,33,33	0
56	MG	AA	3131	1/1	1.00	0.07	29,29,29,29	0
56	MG	DA	3601	1/1	1.00	0.02	26,26,26,26	0
56	MG	BA	3487	1/1	1.00	0.07	23,23,23,23	0
56	MG	BA	3516	1/1	1.00	0.09	28,28,28,28	0
56	MG	BA	3727	1/1	1.00	0.02	34,34,34,34	0
59	ZN	D5	501	1/1	1.00	0.03	52,52,52,52	0
56	MG	BA	3794	1/1	1.00	0.07	29,29,29,29	0
56	MG	DA	3581	1/1	1.00	0.03	35,35,35,35	0
56	MG	BA	3488	1/1	1.00	0.06	16,16,16,16	0
56	MG	BA	3329	1/1	1.00	0.06	24,24,24,24	0

6.5 Other polymers (i)

There are no such residues in this entry.