wwPDB X-ray Structure Validation Summary Report (i)

Aug 6, 2026 – 10:26 AM EDT

PDB ID	:	7JQL / pdb_00007jql
Title	:	Crystal structure of the Thermus thermophilus 70S ribosome in complex with Bac7-001, mRNA, and deacylated P-site tRNA at 3.00A resolution
Authors	:	Mardirossian, M.; Sola, R.; Beckert, B.; Valencic, E.; Collis, D.W.P.; Borisek, J.; Armas, F.; Di Stasi, A.; Buchmann, J.; Syroegin, E.A.; Polikanov, Y.S.; Magistrato, A.; Hilpert, K.; Wilson, D.N.; Scocchi, M.
Deposited on	:	2020-08-11
Resolution	:	3.00 Å(reported)

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

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

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

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

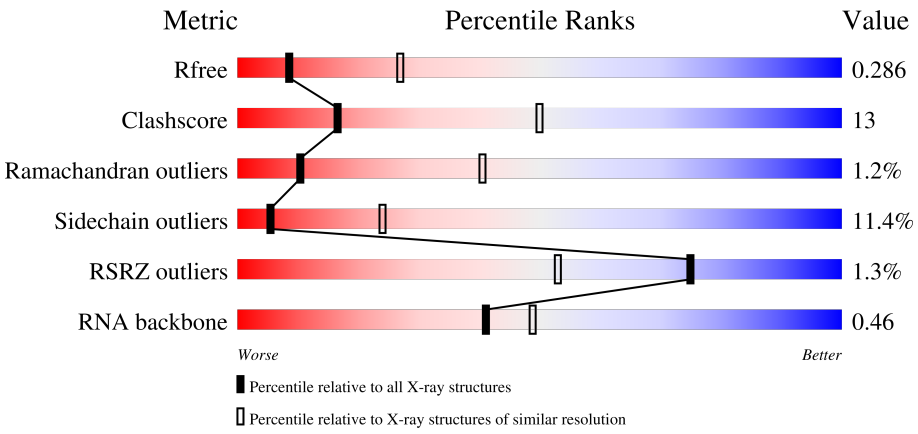
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)
RNA backbone	3983	1109 (3.20-2.80)

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	1A	2915	2% 51% 39% 9% •
1	2A	2915	% 45% 41% 10% •
2	1B	121	60% 33% 7% •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	2B	121	%, 31%, 51%, 17%
3	1D	276	%, 67%, 29%
3	2D	276	%, 63%, 29%, 7%
4	1E	206	67%, 28%, 5%
4	2E	206	54%, 38%, 6%
5	1F	210	60%, 30%, 7%
5	2F	210	%, 53%, 40%
6	1G	182	%, 59%, 36%
6	2G	182	3%, 48%, 42%, 9%
7	1H	180	60%, 32%
7	2H	180	%, 57%, 36%
8	1I	148	%, 64%, 28%, 7%
8	2I	148	57%, 35%, 6%
9	1N	140	74%, 25%
9	2N	140	63%, 33%
10	1O	122	69%, 26%, 5%
10	2O	122	%, 57%, 38%
11	1P	150	58%, 35%, 6%
11	2P	150	2%, 63%, 30%, 7%
12	1Q	141	%, 72%, 26%
12	2Q	141	2%, 57%, 38%, 6%
13	1R	118	%, 69%, 22%, 8%
13	2R	118	%, 59%, 35%, 6%
14	1S	112	70%, 23%, 5%
14	2S	112	52%, 41%, 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
15	1T	146	%, 53%, 32%, 5%, 10%
15	2T	146	2%, 53%, 34%, •, 10%
16	1U	118	61%, 34%, • •
16	2U	118	70%, 27%, • •
17	1V	101	72%, 22%, 6%
17	2V	101	78%, 20%, • •
18	1W	113	%, 61%, 35%, • •
18	2W	113	61%, 34%, • •
19	1X	96	61%, 35%, • •
19	2X	96	2%, 68%, 31%, •
20	1Y	110	%, 59%, 32%, 6%, •
20	2Y	110	3%, 59%, 34%, 5%, •
21	1Z	206	41%, 30%, •, 25%
21	2Z	206	38%, 32%, 7%, 22%
22	10	85	%, 67%, 21%, •, 11%
22	20	85	2%, 62%, 25%, •, 11%
23	11	98	2%, 65%, 34%, •
23	21	98	%, 61%, 34%, • •
24	12	72	62%, 31%, • •
24	22	72	%, 58%, 38%, • •
25	13	60	45%, 47%, 7%, •
25	23	60	65%, 28%, 5%, •
26	14	71	%, 52%, 35%, 8%, • •
26	24	71	6%, 54%, 37%, 7%, •
27	15	60	60%, 37%, • •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
27	25	60	70% 27%
28	16	54	70% 20% 7%
28	26	54	54% 31% 13%
29	17	49	6% 73% 24%
29	27	49	6% 61% 33%
30	18	65	58% 35% 5%
30	28	65	55% 38% 5%
31	19	37	3% 73% 24%
31	29	37	5% 59% 32% 8%
32	1a	1521	% 43% 45% 10%
32	2a	1521	% 43% 47% 9%
33	1b	256	% 48% 36% 6% 10%
33	2b	256	3% 40% 41% 9% 10%
34	1c	239	% 54% 29% 14%
34	2c	239	3% 45% 35% 6% 14%
35	1d	209	% 56% 38% 5%
35	2d	209	57% 40%
36	1e	162	% 53% 35% 9%
36	2e	162	% 55% 34% 9%
37	1f	101	62% 33%
37	2f	101	57% 40%
38	1g	156	% 72% 26%
38	2g	156	% 63% 32%
39	1h	138	% 54% 41%
39	2h	138	% 64% 33%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
40	1i	128	5% 55% 36% 8%
40	2i	128	5% 51% 41% 8%
41	1j	105	2% 52% 35% 8%
41	2j	105	9% 53% 33% 5% 9%
42	1k	129	64% 21% 12%
42	2k	129	50% 35% 12%
43	1l	132	63% 27% 8%
43	2l	132	% 59% 28% 5% 8%
44	1m	126	3% 59% 32% 7%
44	2m	126	3% 44% 44% 8%
45	1n	61	2% 51% 44%
45	2n	61	11% 56% 39%
46	1o	89	% 57% 39%
46	2o	89	61% 31% 7%
47	1p	88	2% 52% 38% 7%
47	2p	88	58% 32% 7%
48	1q	105	% 49% 42% 6%
48	2q	105	3% 50% 44% 6%
49	1r	88	51% 23% 23%
49	2r	88	40% 34% 23%
50	1s	93	55% 33% 11%
50	2s	93	6% 35% 49% 11%
51	1t	106	% 59% 25% 6% 9%
51	2t	106	5% 51% 32% 8% 9%
52	1u	27	48% 33% 15%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
52	2u	27	22% 41% 37% 7% 15%
53	1v	24	8% 17% 29% 8% 46%
53	2v	24	25% 21% 25% 8% 46%
54	1x	77	58% 34% 5%
54	2x	77	49% 36% 13%
55	1z	16	12% 81% 19%
55	2z	16	6% 62% 19% 19%

2 Entry composition (i)

There are 60 unique types of molecules in this entry. The entry contains 293228 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 23S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	1A	2871	61852	27531	11572	19878	2871	0	0	0
1	2A	2800	60322	26848	11284	19390	2800	0	0	0

- Molecule 2 is a RNA chain called 5S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	1B	120	2577	1146	476	835	120	0	0	0
2	2B	120	2575	1146	476	833	120	0	0	0

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	1D	275	2136	1349	423	361	3	0	0	0
3	2D	275	2136	1349	423	361	3	0	0	0

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	1E	204	1559	985	298	270	6	0	0	0
4	2E	204	1559	985	298	270	6	0	0	0

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	1F	203	1584	1009	298	275	2	0	0	1
5	2F	203	1580	1007	297	274	2	0	0	1

- Molecule 6 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	1G	181	1423	913	253	253	4	0	0	0
6	2G	181	1428	913	258	253	4	0	0	0

- Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	1H	174	1330	845	248	236	1	0	0	0
7	2H	174	1330	845	248	236	1	0	0	0

- Molecule 8 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	1I	146	1097	701	191	204	1	0	0	0
8	2I	146	1064	681	186	196	1	0	0	0

- Molecule 9 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
9	1N	140	1117	719	207	187	4	0	0	0
9	2N	140	1117	719	207	187	4	0	0	0

- Molecule 10 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	1O	122	933	588	171	170	4	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	2O	122	933	588	171	170	4	0	0	0

- Molecule 11 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	1P	149	1135	706	230	196	3	0	0	0
			Total	C	N	O	S			
11	2P	149	1135	706	230	196	3	0	0	0

- Molecule 12 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	1Q	141	1122	715	212	188	7	0	0	0
			Total	C	N	O	S			
12	2Q	141	1122	715	212	188	7	0	0	0

- Molecule 13 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
13	1R	118	968	604	203	160	1	0	0	0
			Total	C	N	O	S			
13	2R	118	968	604	203	160	1	0	0	0

- Molecule 14 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
14	1S	110	873	550	174	149	0	0	0
			Total	C	N	O			
14	2S	110	870	549	173	148	0	0	0

- Molecule 15 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
15	1T	131	1091	680	225	185	1	0	0	0
			Total	C	N	O	S			
15	2T	131	1083	675	224	183	1	0	0	0

- Molecule 16 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
16	1U	116	959	608	201	149	1	0	0	0
16	2U	116	959	608	201	149	1	0	0	0

- Molecule 17 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
17	1V	101	771	495	140	135	1	0	0	0
17	2V	101	771	495	140	135	1	0	0	0

- Molecule 18 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
18	1W	112	886	557	174	153	2	0	0	0
18	2W	112	886	557	174	153	2	0	0	0

- Molecule 19 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
19	1X	95	750	488	135	126	1	0	0	0
19	2X	95	750	488	135	126	1	0	0	0

- Molecule 20 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
20	1Y	107	806	517	152	131	6	0	0	0
20	2Y	107	806	517	152	131	6	0	0	0

- Molecule 21 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
21	1Z	154	1240	795	222	220	3	0	0	0
21	2Z	160	1271	814	228	227	2	0	0	0

- Molecule 22 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
22	10	76	604	373	128	102	1	0	0	0
22	20	76	604	373	128	102	1	0	0	0

- Molecule 23 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
23	11	97	755	475	148	131	1	0	0	0
23	21	97	755	475	148	131	1	0	0	0

- Molecule 24 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
24	12	70	588	365	118	103	2	0	0	0
24	22	70	588	365	118	103	2	0	0	0

- Molecule 25 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
25	13	59	469	298	90	81	0	0	0
25	23	59	464	296	90	78	0	0	0

- Molecule 26 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
26	14	69	552	349	99	99	5	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
26	24	69	532	339	97	91	5	0	0	0

- Molecule 27 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
27	15	59	455	285	89	76	5	0	0	0
			Total	C	N	O	S			
27	25	59	455	285	89	76	5	0	0	0

- Molecule 28 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
28	16	53	453	281	91	77	4	0	0	0
			Total	C	N	O	S			
28	26	53	449	279	91	75	4	0	0	0

- Molecule 29 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
29	17	48	418	257	104	55	2	0	0	0
			Total	C	N	O	S			
29	27	48	418	257	104	55	2	0	0	0

- Molecule 30 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
30	18	64	517	331	102	82	2	0	0	0
			Total	C	N	O	S			
30	28	64	517	331	102	82	2	0	0	0

- Molecule 31 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
31	19	37	307	188	68	47	4	0	0	0
			Total	C	N	O	S			
31	29	37	307	188	68	47	4	0	0	0

- Molecule 32 is a RNA chain called 16S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
32	1a	1500	32246	14358	5975	10413	1500	0	0	0
32	2a	1503	32327	14396	5990	10438	1503	0	0	0

- Molecule 33 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
33	1b	231	1846	1179	331	331	5	0	0	0
33	2b	231	1825	1167	326	327	5	0	0	0

- Molecule 34 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
34	1c	206	1548	973	301	273	1	0	0	0
34	2c	206	1542	968	300	273	1	0	0	0

- Molecule 35 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
35	1d	208	1655	1038	326	284	7	0	0	0
35	2d	208	1674	1050	333	284	7	0	0	0

- Molecule 36 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
36	1e	148	1129	714	213	198	4	0	0	0
36	2e	148	1133	716	214	199	4	0	0	0

- Molecule 37 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
37	1f	100	810	514	144	149	3	0	0	0
37	2f	100	816	516	146	151	3	0	0	0

- Molecule 38 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
38	1g	155	1231	766	243	216	6	0	0	0
38	2g	155	1235	769	244	216	6	0	0	0

- Molecule 39 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
39	1h	137	1088	689	206	191	2	0	0	0
39	2h	137	1088	689	206	191	2	0	0	0

- Molecule 40 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
40	1i	127	983	623	193	167	0	0	0
40	2i	127	978	619	190	169	0	0	0

- Molecule 41 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
41	1j	97	709	440	138	131	0	0	0
41	2j	96	714	445	138	131	0	0	0

- Molecule 42 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
42	1k	114	829	516	155	155	3	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
42	2k	114	833	519	156	155	3	0	0	0

- Molecule 43 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
43	1l	122	932	586	185	159	2	0	0	0
43	2l	122	932	586	185	159	2	0	0	0

- Molecule 44 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
44	1m	123	958	592	198	166	2	0	0	0
44	2m	122	950	586	197	165	2	0	0	0

- Molecule 45 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
45	1n	60	492	312	104	72	4	0	0	0
45	2n	60	492	312	104	72	4	0	0	0

- Molecule 46 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
46	1o	88	728	456	144	126	2	0	0	0
46	2o	88	728	456	144	126	2	0	0	0

- Molecule 47 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
47	1p	82	681	433	134	113	1	0	0	0
47	2p	82	677	430	133	113	1	0	0	0

- Molecule 48 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
48	1q	99	823	528	151	142	2	0	0	0
48	2q	99	823	528	151	142	2	0	0	0

- Molecule 49 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
49	1r	68	555	355	108	92	0	0	0
49	2r	68	555	355	108	92	0	0	0

- Molecule 50 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
50	1s	83	652	417	120	113	2	0	0	0
50	2s	83	646	412	119	113	2	0	0	0

- Molecule 51 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
51	1t	96	728	446	156	124	2	0	0	0
51	2t	96	727	446	155	124	2	0	0	0

- Molecule 52 is a protein called 30S ribosomal protein Thx.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
52	1u	23	199	122	48	29	0	0	0
52	2u	23	199	122	48	29	0	0	0

- Molecule 53 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
53	1v	13	277	125	51	88	13	0	0	0
53	2v	13	277	125	51	88	13	0	0	0

- Molecule 54 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
54	1x	76	1625	725	294	529	76	1	0	0	0
54	2x	76	1625	725	294	529	76	1	0	0	0

- Molecule 55 is a protein called Bac7-001.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
55	1z	16	143	92	35	16	0	0	0
55	2z	16	143	92	35	16	0	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
56	1A	1041	1041	1041	0	0
56	1B	31	31	31	0	0
56	1D	10	10	10	0	0
56	1E	9	9	9	0	0
56	1F	9	9	9	0	0
56	1G	4	4	4	0	0
56	1N	2	2	2	0	0
56	1O	2	2	2	0	0
56	1P	4	4	4	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
56	1Q	5	5	5	0	0
56	1R	3	3	3	0	0
56	1S	2	2	2	0	0
56	1T	5	5	5	0	0
56	1U	10	10	10	0	0
56	1V	6	6	6	0	0
56	1W	5	5	5	0	0
56	1X	5	5	5	0	0
56	1Y	1	1	1	0	0
56	1Z	2	2	2	0	0
56	10	8	8	8	0	0
56	11	1	1	1	0	0
56	13	4	4	4	0	0
56	15	7	7	7	0	0
56	16	2	2	2	0	0
56	17	7	7	7	0	0
56	18	3	3	3	0	0
56	19	2	2	2	0	0
56	1a	221	221	221	0	0
56	1b	1	1	1	0	0
56	1e	1	1	1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
56	1f	2	2	2	0	0
56	1h	1	1	1	0	0
56	1l	3	3	3	0	0
56	1m	1	1	1	0	0
56	1n	2	2	2	0	0
56	1s	1	1	1	0	0
56	1t	1	1	1	0	0
56	1v	1	1	1	0	0
56	1x	15	15	15	0	0
56	2A	810	810	810	0	0
56	2B	15	15	15	0	0
56	2D	4	4	4	0	0
56	2E	9	9	9	0	0
56	2F	2	2	2	0	0
56	2G	1	1	1	0	0
56	2O	2	2	2	0	0
56	2P	2	2	2	0	0
56	2Q	2	2	2	0	0
56	2R	4	4	4	0	0
56	2T	4	4	4	0	0
56	2U	2	2	2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
56	2V	2	2	2	0	0
56	2W	2	2	2	0	0
56	2X	2	2	2	0	0
56	2Y	1	1	1	0	0
56	20	3	3	3	0	0
56	23	1	1	1	0	0
56	25	4	4	4	0	0
56	26	1	1	1	0	0
56	27	1	1	1	0	0
56	28	1	1	1	0	0
56	2a	217	217	217	0	0
56	2d	1	1	1	0	0
56	2e	1	1	1	0	0
56	2f	1	1	1	0	0
56	2i	1	1	1	0	0
56	2k	1	1	1	0	0
56	2l	1	1	1	0	0
56	2n	1	1	1	0	0
56	2q	1	1	1	0	0
56	2r	1	1	1	0	0
56	2t	1	1	1	0	0

Continued on next page...

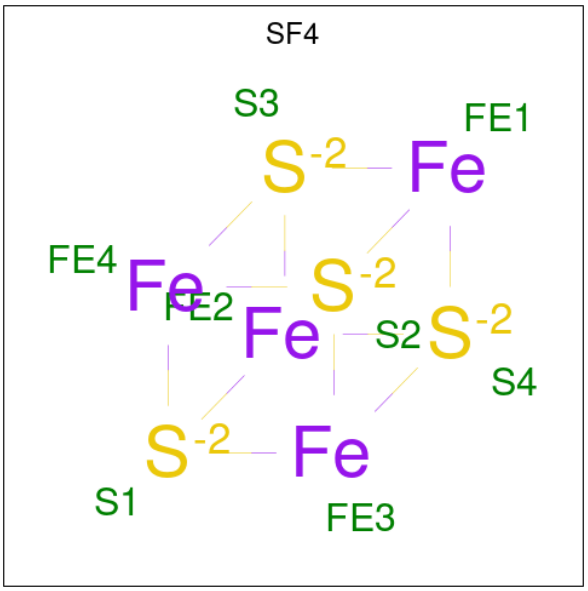
Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	2v	1	Total Mg 1 1	0	0
56	2x	5	Total Mg 5 5	0	0

- Molecule 57 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	1Y	1	Total Zn 1 1	0	0
57	14	1	Total Zn 1 1	0	0
57	15	1	Total Zn 1 1	0	0
57	16	1	Total Zn 1 1	0	0
57	19	1	Total Zn 1 1	0	0
57	1n	1	Total Zn 1 1	0	0
57	2Y	1	Total Zn 1 1	0	0
57	24	1	Total Zn 1 1	0	0
57	25	1	Total Zn 1 1	0	0
57	26	1	Total Zn 1 1	0	0
57	29	1	Total Zn 1 1	0	0
57	2n	1	Total Zn 1 1	0	0

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	1d	1	Total Fe S 8 4 4	0	0
58	2d	1	Total Fe S 8 4 4	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	2A	1	Total K 1 1	0	0

- Molecule 60 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	1A	1949	Total O 1949 1949	0	0
60	1B	50	Total O 50 50	0	0
60	1D	21	Total O 21 21	0	0
60	1E	14	Total O 14 14	0	0
60	1F	9	Total O 9 9	0	0
60	1G	1	Total O 1 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	1N	3	Total O 3 3	0	0
60	1O	4	Total O 4 4	0	0
60	1P	17	Total O 17 17	0	0
60	1Q	3	Total O 3 3	0	0
60	1R	8	Total O 8 8	0	0
60	1S	1	Total O 1 1	0	0
60	1T	3	Total O 3 3	0	0
60	1U	5	Total O 5 5	0	0
60	1V	2	Total O 2 2	0	0
60	1W	5	Total O 5 5	0	0
60	1X	3	Total O 3 3	0	0
60	1Y	1	Total O 1 1	0	0
60	10	5	Total O 5 5	0	0
60	11	6	Total O 6 6	0	0
60	13	5	Total O 5 5	0	0
60	14	1	Total O 1 1	0	0
60	15	5	Total O 5 5	0	0
60	16	1	Total O 1 1	0	0
60	17	7	Total O 7 7	0	0
60	18	12	Total O 12 12	0	0
60	19	1	Total O 1 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	1a	301	Total O 301 301	0	0
60	1b	1	Total O 1 1	0	0
60	1e	1	Total O 1 1	0	0
60	1i	1	Total O 1 1	0	0
60	1l	4	Total O 4 4	0	0
60	1o	1	Total O 1 1	0	0
60	1q	3	Total O 3 3	0	0
60	1v	5	Total O 5 5	0	0
60	1x	16	Total O 16 16	0	0
60	1z	3	Total O 3 3	0	0
60	2A	917	Total O 917 917	0	0
60	2B	4	Total O 4 4	0	0
60	2D	14	Total O 14 14	0	0
60	2E	10	Total O 10 10	0	0
60	2F	12	Total O 12 12	0	0
60	2N	1	Total O 1 1	0	0
60	2O	2	Total O 2 2	0	0
60	2P	8	Total O 8 8	0	0
60	2Q	1	Total O 1 1	0	0
60	2R	2	Total O 2 2	0	0
60	2T	2	Total O 2 2	0	0

Continued on next page...

Continued from previous page...

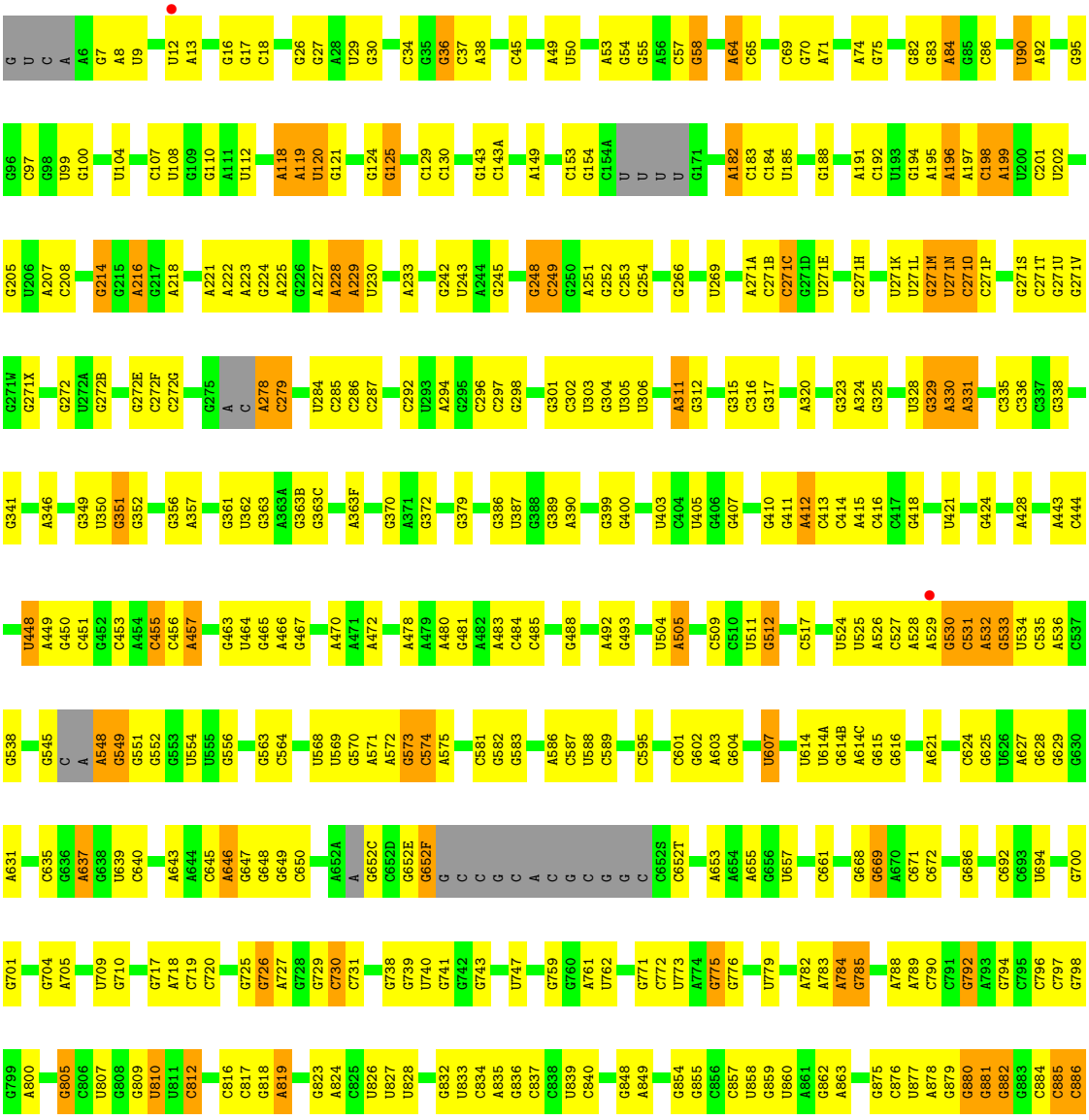
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	2U	2	Total O 2 2	0	0
60	2X	2	Total O 2 2	0	0
60	21	7	Total O 7 7	0	0
60	27	1	Total O 1 1	0	0
60	28	3	Total O 3 3	0	0
60	2a	286	Total O 286 286	0	0
60	2d	1	Total O 1 1	0	0
60	2e	3	Total O 3 3	0	0
60	2i	1	Total O 1 1	0	0
60	2l	2	Total O 2 2	0	0
60	2p	1	Total O 1 1	0	0
60	2r	1	Total O 1 1	0	0
60	2t	1	Total O 1 1	0	0
60	2v	2	Total O 2 2	0	0

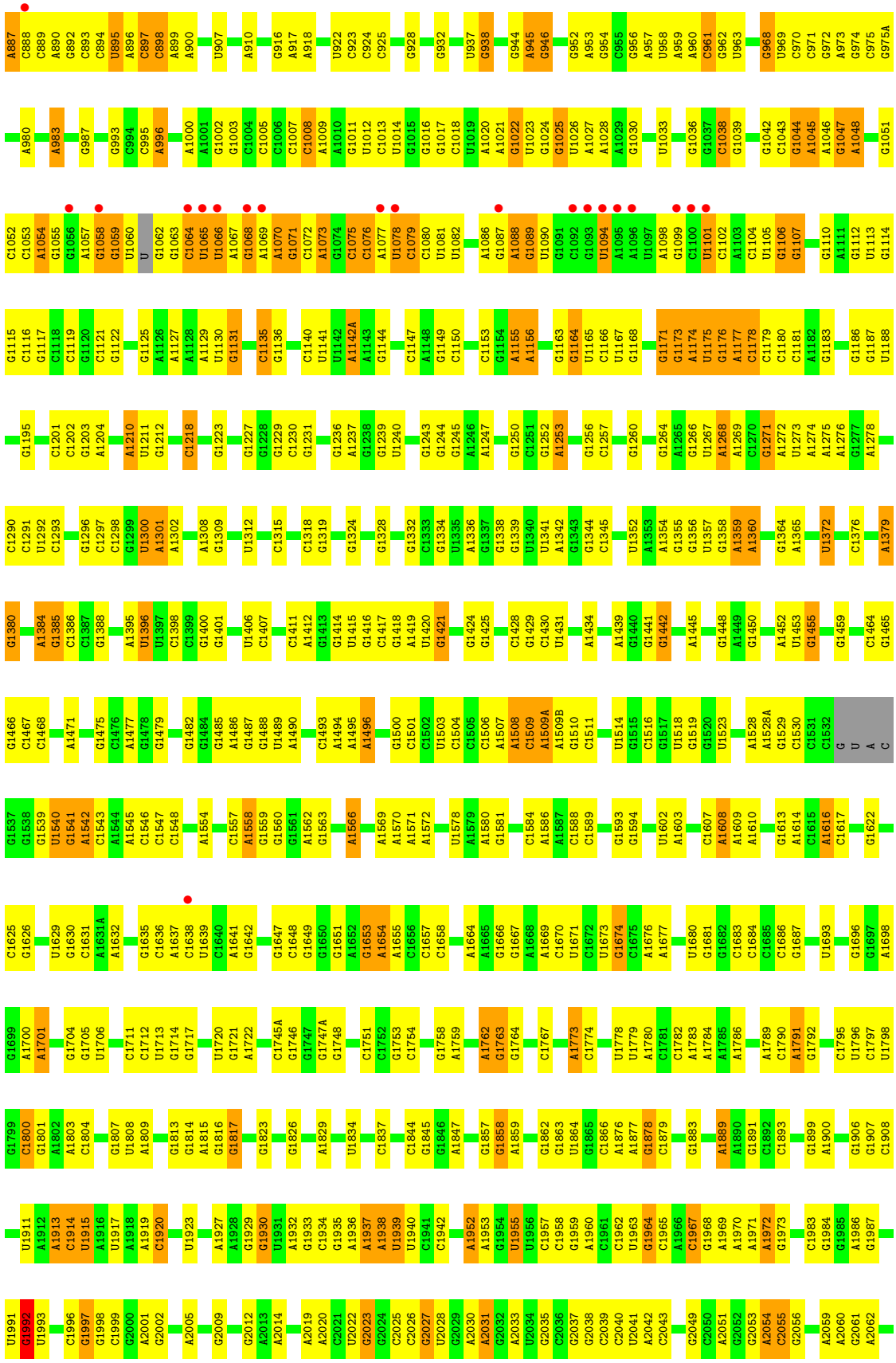
3 Residue-property plots (i)

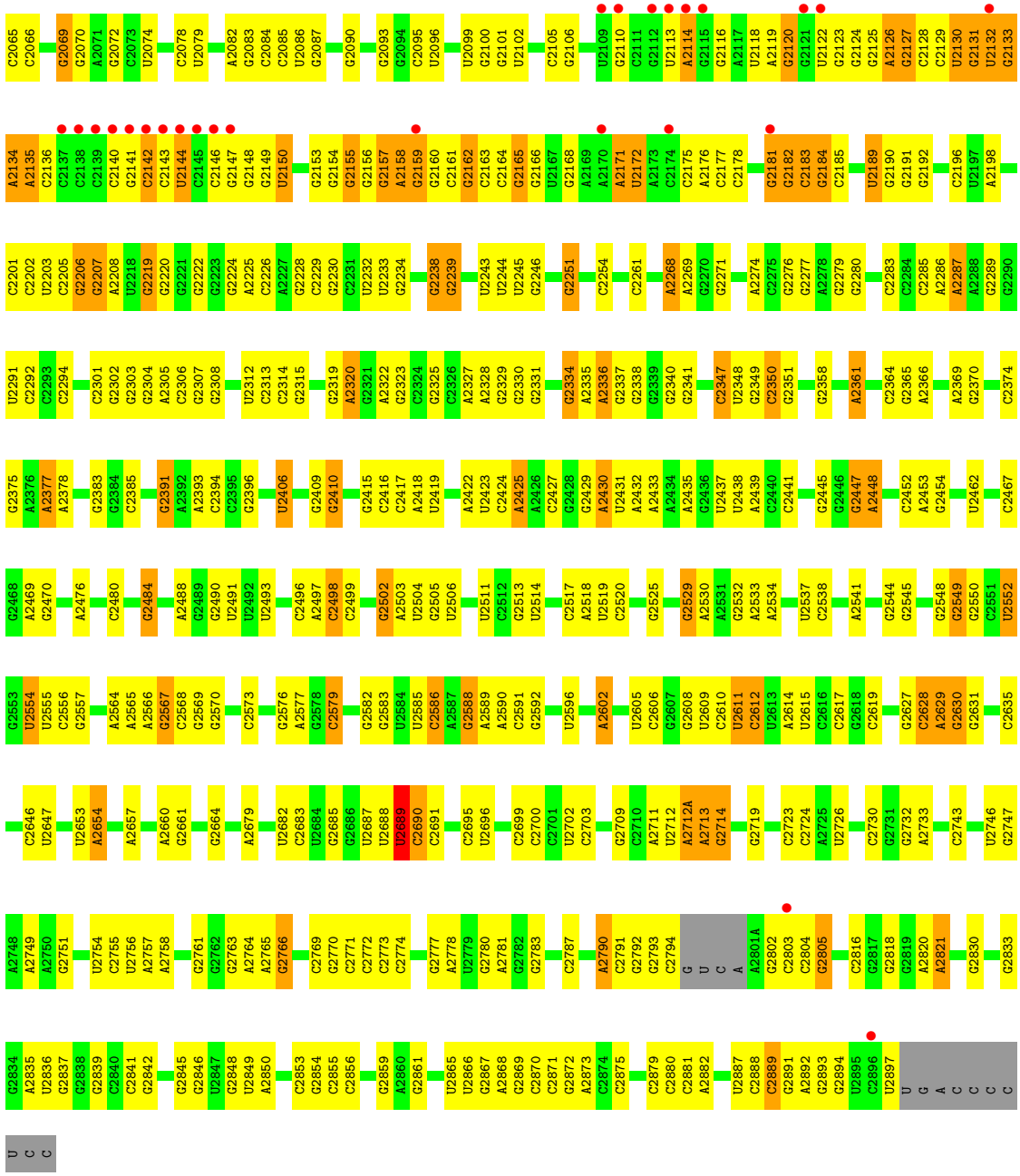
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: 23S Ribosomal RNA

Chain 1A:

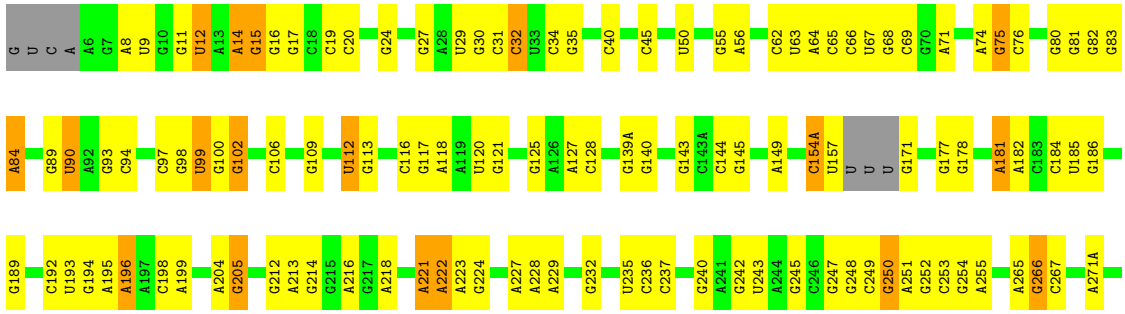


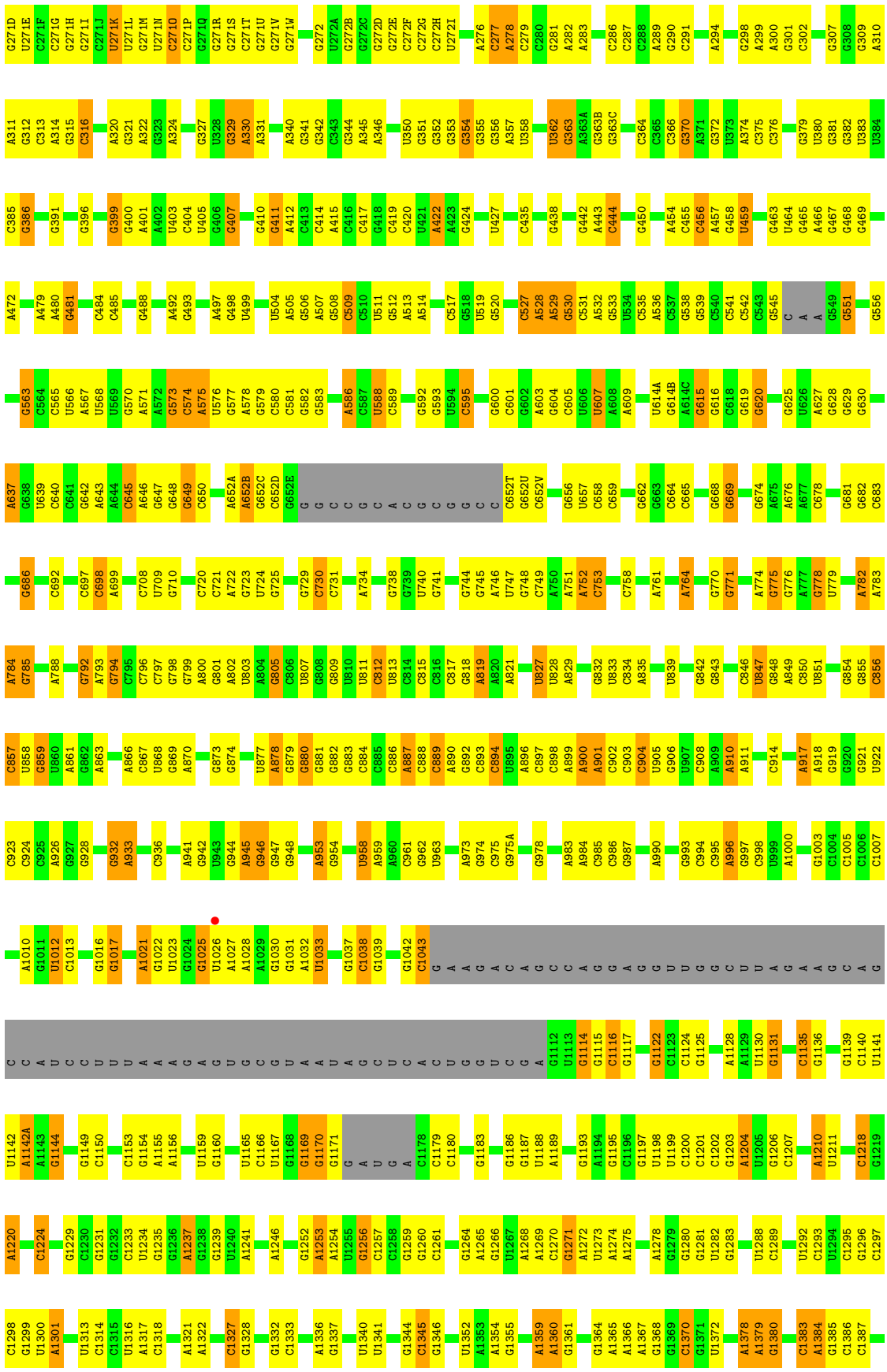

A887 C888 C889 A890 G892 C893 C894 U895 A896 C897 C898 A899 A900 U907 A910 G916 A917 A918 U922 C923 C924 C925 G928 G932 U937 G938 G944 A945 G946 G952 A953 G954 C955 G956 A957 U958 A959 A960 C961 G962 U963 G968 U969 C970 C971 G972 A973 G974 C975 G975A
A980 A983 G987 G993 C994 C995 A996 A1000 A1001 G1002 G1003 C1004 C1005 C1006 C1007 C1008 A1009 A1010 G1011 U1012 C1013 U1014 G1015 G1016 G1017 C1018 U1019 A1020 A1021 G1022 U1023 G1024 G1025 U1026 A1027 A1028 A1029 G1030 U1033 G1036 G1037 C1038 G1039 G1042 C1043 G1044 A1045 A1046 G1047 A1048 G1051
C1052 C1053 A1054 G1055 G1056 A1057 G1058 G1059 U1060 U G1062 G1063 C1064 U1065 U1066 A1067 G1068 A1069 A1070 G1071 C1072 A1073 G1074 A1075 C1076 A1077 U1078 C1079 C1080 U1081 U1082 A1086 G1087 A1088 G1089 U1090 G1091 C1092 G1093 U1094 A1095 A1096 U1097 A1098 G1099 C1100 U1101 C1102 A1103 C1104 U1105 G1106 G1107 G1110 A1111 G1112 U1113 G1114
G1115 C1116 G1117 C1118 C1119 G1120 C1121 G1122 G1125 A1126 A1127 A1128 A1129 U1130 G1131 C1135 G1136 C1140 U1141 U1142 A1142A A1143 G1144 C1147 A1148 G1149 C1150 C1153 G1154 A1155 A1156 G1163 G1164 U1165 C1166 U1167 G1168 G1171 G1173 A1174 U1175 G1176 A1177 C1178 C1179 C1180 C1181 A1182 G1183 G1186 G1187 U1188
G1195 C1201 C1202 G1203 A1204 A1210 U1211 G1212 C1218 G1223 G1227 G1228 G1229 C1230 G1231 G1236 A1237 G1238 G1239 U1240 G1243 G1244 G1245 A1246 A1247 G1250 C1251 A1252 A1253 G1256 C1257 G1260 G1264 A1265 G1266 U1267 A1268 A1269 C1270 G1271 A1272 U1273 A1274 A1275 A1276 G1277 A1278
C1290 C1291 U1292 C1293 G1296 C1297 C1298 G1299 U1300 A1301 A1302 A1308 G1309 U1312 C1315 C1318 G1319 G1324 G1328 G1332 C1333 G1334 U1335 A1336 G1337 G1338 G1339 U1340 U1341 A1342 G1343 G1344 C1345 U1352 A1353 A1354 G1355 G1356 U1357 G1358 A1359 A1360 G1364 A1365 U1372 C1376 A1379
G1380 A1384 G1385 C1386 C1387 G1388 A1395 U1396 U1397 C1398 C1399 G1400 G1401 U1406 C1407 C1411 A1412 G1413 G1414 U1415 G1416 C1417 G1418 A1419 U1420 G1421 G1424 G1425 C1428 G1429 C1430 U1431 A1434 A1439 G1440 G1441 G1442 A1445 G1448 A1449 G1450 A1452 U1453 G1455 G1459 C1464 G1465
G1466 C1467 C1468 A1471 G1475 C1476 A1477 G1478 G1479 G1482 G1484 G1485 A1486 G1487 G1488 U1489 A1490 C1493 A1494 A1495 A1496 G1500 C1501 C1502 U1503 C1504 C1505 C1506 A1507 A1508 C1509 A1509A A1509B G1510 C1511 U1514 G1515 C1516 G1517 U1518 G1519 G1520 U1523 A1528 A1528A G1529 C1530 C1531 C1532 G U A C
G1537 G1538 G1539 U1540 G1541 A1542 C1543 A1544 A1545 C1546 C1547 C1548 A1554 C1557 A1558 G1559 G1560 G1561 A1562 G1563 A1566 A1569 A1570 A1571 A1572 U1578 A1579 A1580 G1581 C1584 A1586 A1587 C1588 C1589 G1593 G1594 U1602 A1603 C1607 A1608 A1609 A1610 G1613 A1614 C1615 A1616 C1617 G1622
C1625 G1626 U1629 G1630 C1631 A1631A A1632 G1635 C1636 A1637 C1638 U1639 C1640 A1641 G1642 G1647 C1648 G1649 G1650 G1651 A1652 G1653 A1654 A1655 C1656 C1657 C1658 A1664 A1665 G1666 G1667 A1668 A1669 C1670 U1671 C1672 U1673 G1674 C1675 A1676 A1677 U1680 G1681 G1682 C1683 C1684 C1685 C1686 G1687 U1693 G1696 G1697 A1698
G1699 A1700 A1701 G1704 G1705 U1706 C1711 C1712 U1713 G1714 G1717 U1720 G1721 A1722 C1745A G1746 G1747 G1747A G1748 C1751 C1752 G1753 C1754 G1758 A1759 A1762 G1763 G1764 C1767 A1773 C1774 U1778 U1779 A1780 C1781 C1782 A1783 A1784 A1785 A1786 A1789 C1790 A1791 G1792 C1795 U1796 C1797 U1798
G1799 C1800 G1801 A1802 A1803 C1804 G1807 U1808 A1809 G1813 G1814 A1815 G1816 G1817 G1823 G1826 A1829 U1834 C1837 C1844 G1845 G1846 A1847 G1857 G1858 A1859 G1862 G1863 U1864 G1865 C1866 A1876 A1877 G1878 C1879 G1883 A1889 A1890 G1891 C1892 C1893 G1899 A1900 G1906 G1907 C1908
U1911 A1912 A1913 C1914 U1915 A1916 U1917 A1918 A1919 C1920 U1923 A1927 A1928 G1929 G1930 U1931 A1932 G1933 C1934 G1935 A1936 A1937 A1938 U1939 U1940 C1941 C1942 A1952 A1953 G1954 U1955 U1956 C1957 C1958 G1959 A1960 C1961 C1962 U1963 G1964 C1965 A1966 C1967 G1968 A1969 A1970 A1971 A1972 G1973 C1983 G1984 G1985 A1986 G1987
U1991 G1992 U1993 C1996 G1997 G1998 C1999 G2000 A2001 G2002 A2005 G2009 G2012 A2013 A2014 A2019 A2020 C2021 U2022 G2023 G2024 C2025 C2026 G2027 U2028 G2029 A2030 A2031 G2032 A2033 U2034 G2035 C2036 G2037 G2038 C2039 C2040 U2041 A2042 C2043 G2049 C2050 A2051 G2052 G2053 A2054 C2055 G2056 A2059 A2060 G2061 A2062

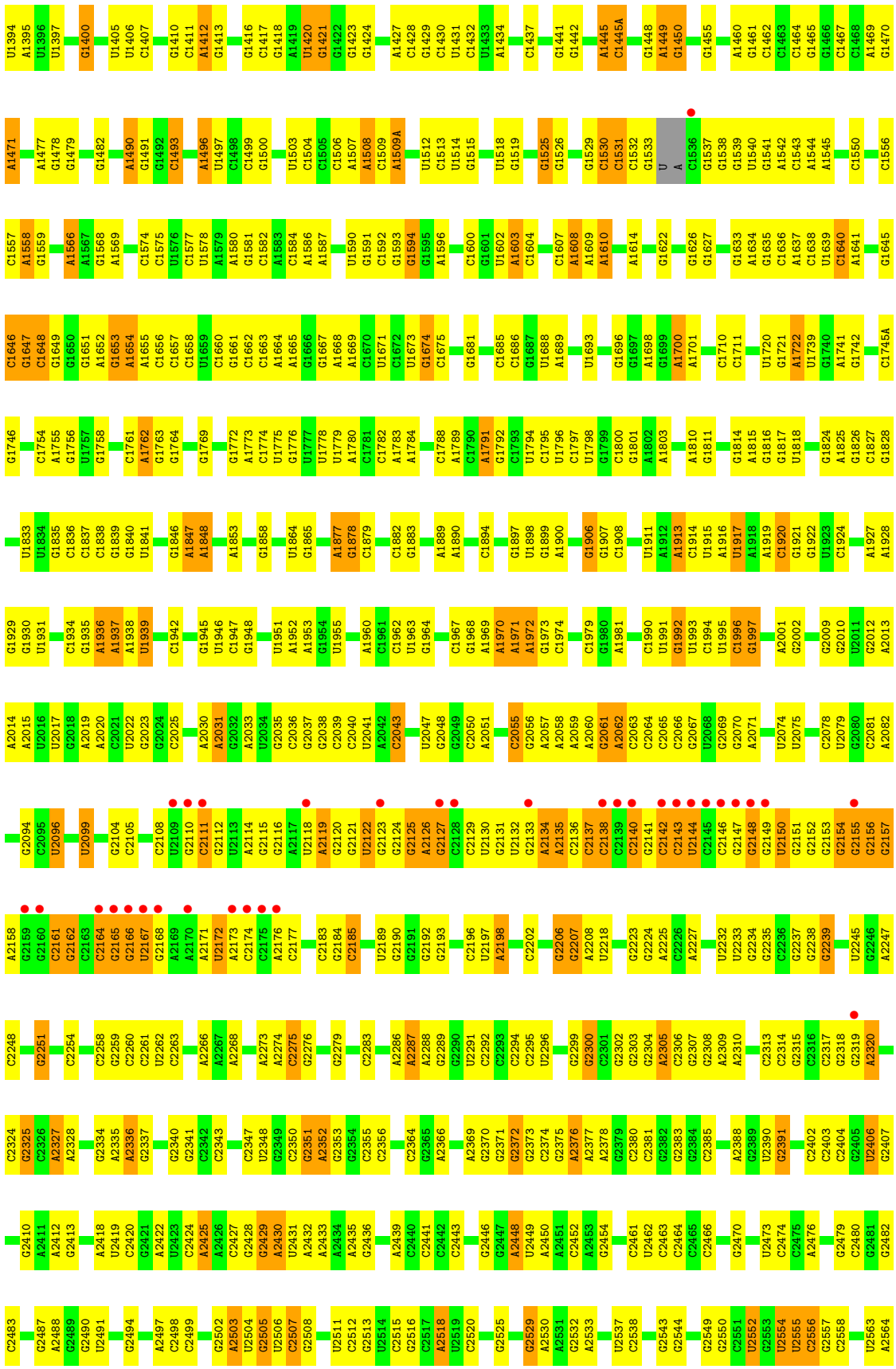


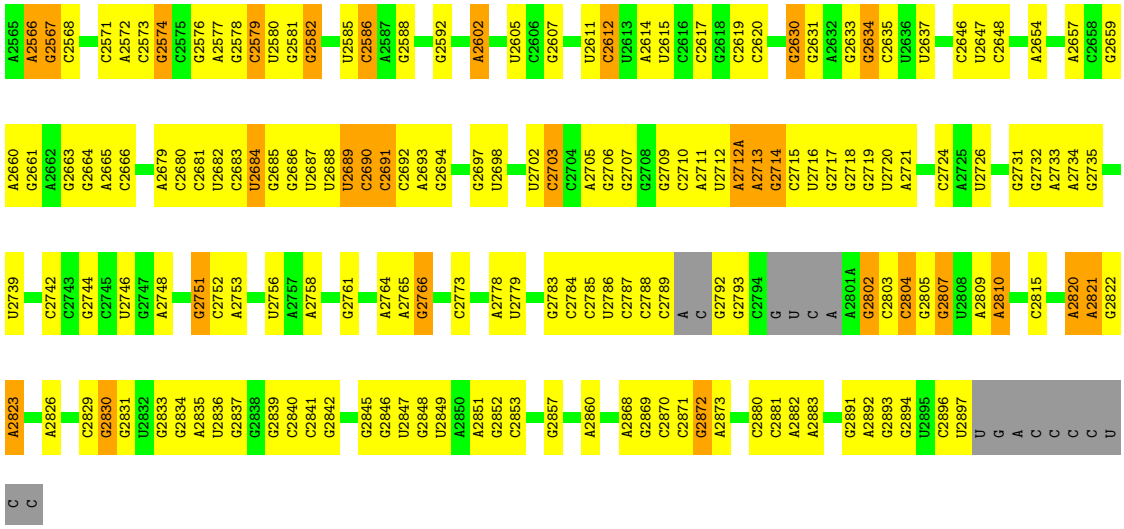
• Molecule 1: 23S Ribosomal RNA

Chain 2A:



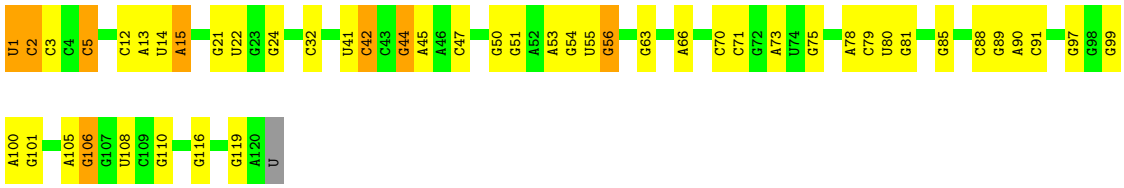

C1298 G1299 U1300 A1301 U1313 C1314 C1315 U1316 A1317 C1318 A1321 A1322 C1327 G1328 G1332 C1333 A1336 G1337 U1340 U1341 G1344 C1345 G1346 U1352 A1353 A1354 G1355 A1359 A1360 G1361 G1364 A1365 A1366 A1367 G1368 G1369 C1370 G1371 U1372 A1378 A1379 G1380 C1383 A1384 G1385 C1386 C1387
A1220 C1224 G1229 C1230 G1231 G1232 C1233 U1234 G1235 G1236 A1237 G1238 G1239 U1240 A1241 A1246 G1252 A1253 A1254 U1255 G1256 C1257 C1258 G1259 G1260 C1261 G1264 A1265 G1266 U1267 A1268 A1269 C1270 G1271 A1272 U1273 A1274 A1275 A1278 G1279 G1280 C1281 U1282 G1283 U1288 U1289 U1292 C1293 U1294 C1295 G1296 C1297
U1142 A1142A A1143 G1144 G1149 C1150 C1153 G1154 A1155 A1156 U1159 G1160 U1165 C1166 U1167 G1168 G1169 G1170 G1171 G A U G A C1178 C1179 C1180 G1183 G1186 G1187 U1188 A1189 G1193 A1194 G1195 C1196 G1197 U1198 U1199 C1200 C1201 C1202 G1203 A1204 U1205 G1206 C1207 A1210 U1211 C1218 G1219
A1010 G1011 U1012 C1013 G1016 G1017 A1021 G1022 U1023 G1024 G1025 U1026 A1027 A1028 A1029 G1030 G1031 A1032 U1033 G1037 C1038 G1039 G1042 C1043 G A A G A C C A G C C A G G G G C C U U U A G G G U C C G A C C U G G U A U G A G C C U U G G A G C U U G G A G G C C A A G G C C A G
C C A U C C U U U A A A G A G U A A U C C G A C C U G G U C C G A C C U G G A G C U U G G A G G C C A A G G C C A G
C385 G386 G391 G396 G399 G400 A401 A402 U403 C404 U405 G406 G407 G410 G411 A412 C413 C414 A415 C416 C417 G418 C419 C420 U421 A422 A423 G424 U427 C435 G438 G442 A443 C444 G450 A454 C455 C456 A457 G458 U459 G463 U464 G465 A466 G467 G468 G469
A311 G312 C313 A314 G315 C316 A320 G321 A322 G323 A324 G327 U328 G329 A330 A331 A340 G341 G342 C343 G344 A345 A346 U350 U351 G352 G353 G354 G355 G356 A357 U358 U362 G363 A363A G363B G363C C364 C365 C366 G370 A371 G372 U373 A374 C375 C376 G379 U380 G381 G382 U383 U384
A472 A479 A480 G481 C484 C485 G488 A492 G493 A497 G498 U499 U504 A505 G506 A507 G508 C509 C510 U511 G512 A513 A514 C517 G518 U519 G520 C527 A528 A529 G530 C531 A532 G533 U534 C535 A536 C537 G538 G539 C540 C541 C542 G543 G545 C A A G549 G551 G556
G563 C564 C565 U566 A567 U568 U569 C570 A571 A572 C573 C574 A575 U576 G577 A578 C579 C580 C581 C582 G583 A586 C587 U588 C589 G592 G593 U594 C595 G600 C601 G602 A603 G604 C605 U606 U607 A608 A609 U614A G614B A614C G615 G616 C618 G619 G620 G625 U626 A627 G628 G629 G630
A637 G638 U639 C640 C641 G642 A643 A644 C645 A646 G647 G648 G649 C650 A652A A652B G652C C652D G652E G G G C C C A C G G C G G C C C652T G652U C652V G656 U657 C658 C659 G662 G663 C664 C665 G668 G669 G674 A675 A676 A677 C678 G681 G682 C683
G686 C692 C697 C698 A699 C708 U709 G710 C720 C721 A722 G723 U724 G725 G729 C730 C731 A734 G738 G739 U740 G741 G744 G745 A746 U747 G748 C749 A750 A751 A752 C753 C758 A761 A764 G770 G771 A774 G775 G776 A777 G778 U779 A782 A783
A784 G785 A788 G792 A793 G794 C795 C796 C797 G798 G799 A800 G801 A802 U803 A804 G805 C806 U807 G808 G809 U810 U811 C812 U813 C814 C815 C816 C817 G818 A819 A820 A821 U827 U828 A829 G832 U833 C834 A835 U839 G842 G843 C846 U847 G848 A849 C850 U851 G854 G855 C856
C857 U858 G859 U860 A861 G862 A863 A866 C867 U868 G869 A870 G873 G874 U877 A878 G879 G880 G881 G882 G883 C884 C885 C886 A887 C888 C889 A890 G892 C893 C894 U895 A896 C897 C898 A899 A900 A901 C902 C903 C904 U905 G906 U907 C908 A909 A910 A911 C914 A917 A918 G919 G920 G921 U922
C923 C924 G925 A926 G927 G928 G932 A933 C936 A941 G942 U943 G944 A945 G946 G947 G948 A953 G954 U958 A959 A960 C961 G962 U963 A973 G974 C975 G975A G978 A983 A984 C985 C986 G987 A990 G993 C994 C995 A996 G997 C998 U999 A1000 G1003 C1004 C1005 C1006 C1007
G1112 U1113 G1114 G1115 C1116 G1117 G1122 C1123 C1124 G1125 A1128 A1129 U1130 G1131 C1135 G1136 G1139 C1140 U1141
G271D U271E C271F C271G G271H C271I C271J U271K U271L G271M U271N C271O C271P G271Q C271R G271S C271T C271U G271V G271W G272 U272A G272B G272C G272D G272E C272F C272G C272H U272I A276 C277 A278 C279 C280 G281 A282 A283 C286 C287 C288 A289 G290 C291 A294 G298 A299 A300 G301 C302 G307 G308 G309 A310


U1394 A1395 U1396 U1397 G1400 U1405 U1406 C1407 G1410 C1411 A1412 G1413 G1416 C1417 G1418 A1419 U1420 G1421 G1422 G1423 G1424 A1427 C1428 G1429 C1430 U1431 C1432 U1433 A1434 C1437 G1441 G1442 A1445 C1445A G1448 A1449 G1450 G1455 A1460 G1461 C1462 C1463 C1464 G1465 G1466 C1467 C1468 A1469 G1470
A1471 A1477 G1478 G1479 G1482 A1490 G1491 G1492 C1493 A1496 U1497 C1498 C1499 G1500 U1503 C1504 C1505 C1506 A1507 A1508 C1509 A1509A U1512 C1513 U1514 G1515 U1518 G1519 G1525 G1526 G1529 C1530 C1531 C1532 G1533 U A C1536 G1537 G1538 G1539 U1540 G1541 A1542 C1543 A1544 A1545 C1550 C1556
C1557 A1558 G1559 A1566 A1567 G1568 A1569 C1574 C1575 U1576 C1577 U1578 A1579 A1580 G1581 C1582 A1583 C1584 A1586 A1587 U1590 G1591 C1592 G1593 G1594 G1595 A1596 C1600 G1601 U1602 A1603 C1604 C1607 A1608 A1609 A1610 A1614 G1622 G1626 G1627 G1633 A1634 G1635 C1636 A1637 C1638 U1639 C1640 A1641 G1645
C1646 G1647 C1648 G1649 G1650 G1651 A1652 G1653 A1654 A1655 C1656 C1657 C1658 U1659 C1660 G1661 C1662 C1663 A1664 A1665 G1666 G1667 A1668 A1669 C1670 U1671 C1672 U1673 G1674 C1675 G1681 C1685 C1686 G1687 U1688 A1689 U1693 G1696 G1697 A1698 G1699 A1700 A1701 C1710 C1711 U1720 G1721 A1722 U1739 G1740 A1741 G1742 C1745A
G1746 C1754 A1755 G1756 U1757 G1758 C1761 A1762 G1763 G1764 G1769 G1772 A1773 C1774 U1775 G1776 U1777 U1778 U1779 A1780 C1781 C1782 A1783 A1784 C1788 A1789 C1790 A1791 G1792 C1793 U1794 C1795 U1796 C1797 U1798 G1799 C1800 G1801 A1802 A1803 A1810 G1811 G1814 A1815 G1816 G1817 U1818 G1824 A1825 G1826 C1827 G1828
U1833 U1834 G1835 C1836 C1837 C1838 G1839 G1840 U1841 G1846 A1847 A1848 A1853 G1858 U1864 G1865 A1877 G1878 C1879 C1882 G1883 A1889 A1890 C1894 G1897 U1898 G1899 A1900 G1906 G1907 C1908 U1911 A1912 A1913 C1914 U1915 A1916 U1917 A1918 A1919 C1920 G1921 G1922 U1923 C1924 A1927 A1928
G1929 G1930 U1931 C1934 G1935 A1936 A1937 A1938 U1939 C1942 G1945 U1946 C1947 G1948 U1951 A1952 A1953 G1954 U1955 A1960 C1961 C1962 U1963 G1964 C1967 G1968 A1969 A1970 A1971 A1972 G1973 C1974 C1979 G1980 A1981 C1990 U1991 G1992 U1993 C1994 U1995 C1996 G1997 A2001 G2002 G2009 G2010 U2011 G2012 A2013
A2014 A2015 U2016 U2017 G2018 A2019 A2020 C2021 U2022 G2023 G2024 C2025 A2030 A2031 G2032 A2033 U2034 G2035 C2036 G2037 G2038 C2039 C2040 U2041 A2042 C2043 U2047 G2048 G2049 C2050 A2051 C2055 G2056 A2057 A2058 A2059 A2060 G2061 A2062 C2063 C2064 C2065 C2066 G2067 U2068 G2069 G2070 A2071 U2074 U2075 C2078 U2079 G2080 C2081 A2082
G2094 C2095 U2096 U2099 G2104 C2105 C2108 U2109 G2110 C2111 G2112 U2113 A2114 G2115 G2116 A2117 U2118 A2119 G2120 G2121 U2122 G2123 G2124 G2125 A2126 G2127 C2128 C2129 U2130 G2131 U2132 G2133 A2134 A2135 C2136 C2137 C2138 C2139 C2140 G2141 C2142 C2143 U2144 C2145 C2146 G2147 G2148 G2149 U2150 G2151 G2152 G2153 G2154 G2155 G2156 G2157
A2158 G2159 G2160 C2161 G2162 C2163 C2164 G2165 G2166 U2167 G2168 A2169 A2170 A2171 U2172 A2173 A2174 C2175 A2176 C2177 C2183 G2184 C2185 U2189 G2190 G2191 G2192 G2193 C2196 U2197 A2198 C2202 G2206 G2207 A2208 U2218 G2223 G2224 A2225 C2226 A2227 U2232 U2233 G2234 G2235 C2236 G2237 G2238 G2239 U2245 G2246 A2247
C2248 G2251 C2254 C2258 G2259 C2260 C2261 U2262 C2263 A2266 A2267 A2268 A2273 A2274 C2275 G2276 G2279 C2283 A2286 A2287 A2288 G2289 G2290 U2291 C2292 C2293 C2294 C2295 U2296 G2299 G2300 C2301 G2302 G2303 G2304 A2305 C2306 G2307 G2308 A2309 A2310 C2313 C2314 G2315 C2316 C2317 G2318 G2319 A2320
C2324 G2325 C2326 A2327 A2328 G2334 A2335 A2336 G2337 G2340 G2341 C2342 C2343 C2347 U2348 G2349 U2350 G2351 A2352 G2353 G2354 C2355 C2356 C2364 G2365 A2366 A2369 G2370 G2371 G2372 C2373 C2374 A2376 A2377 A2378 G2379 C2380 C2381 G2382 G2383 G2384 C2385 A2388 G2389 U2390 G2391 C2402 C2403 C2404 G2405 U2406 G2407
G2410 A2411 A2412 G2413 A2418 U2419 C2420 G2421 A2422 U2423 C2424 A2425 A2426 C2427 G2428 G2429 A2430 U2431 A2432 A2433 A2434 A2435 G2436 A2439 C2440 C2441 C2442 C2443 G2446 G2447 A2448 U2449 A2450 A2451 C2452 A2453 G2454 C2461 U2462 C2463 C2464 C2465 C2466 G2470 U2473 C2474 C2475 A2476 G2479 C2480 G2481 G2482
C2483 G2487 A2488 G2489 G2490 U2491 G2494 A2497 C2498 C2499 G2502 A2503 U2504 G2505 U2506 C2507 G2508 U2511 C2512 G2513 U2514 C2515 G2516 C2517 A2518 U2519 C2520 G2525 G2529 A2530 A2531 C2532 A2533 U2537 C2538 G2543 C2544 G2549 G2550 C2551 U2552 G2553 U2554 U2555 C2556 G2557 C2558 U2563 A2564



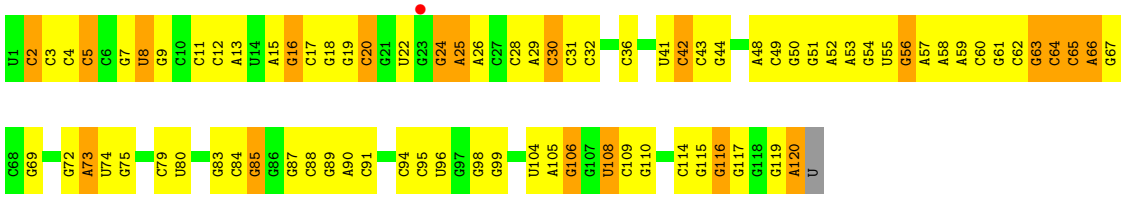
- Molecule 2: 5S Ribosomal RNA

Chain 1B:



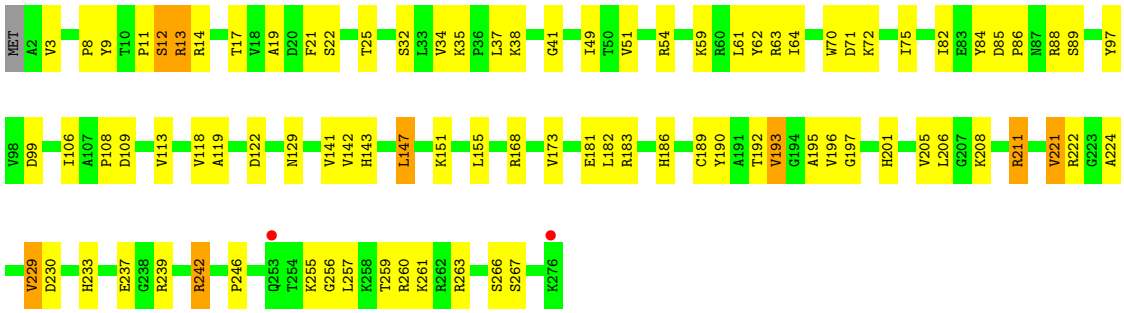
- Molecule 2: 5S Ribosomal RNA

Chain 2B:



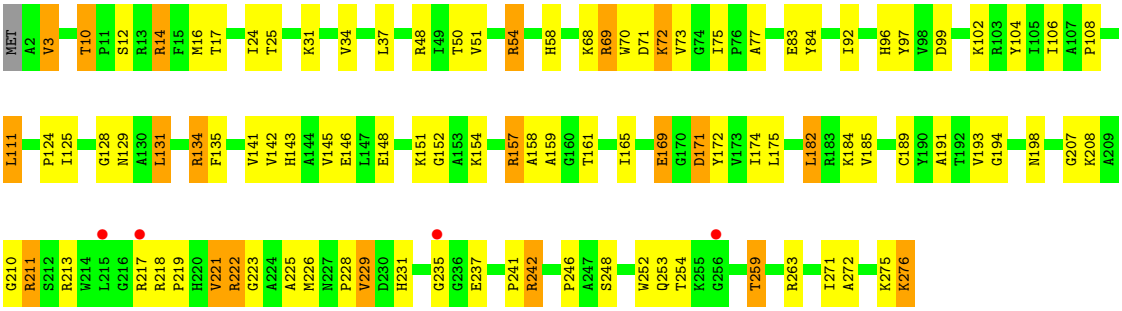
- Molecule 3: 50S ribosomal protein L2

Chain 1D:



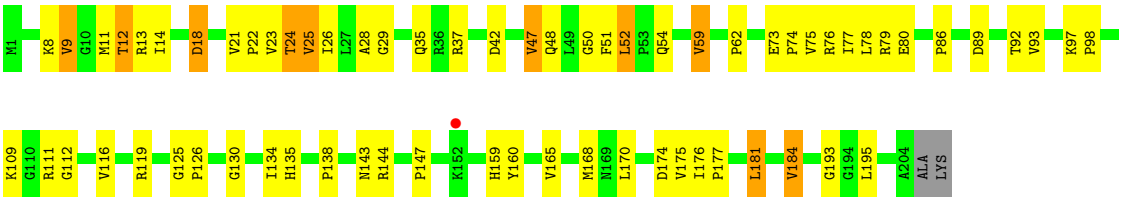
- Molecule 3: 50S ribosomal protein L2

Chain 2D:



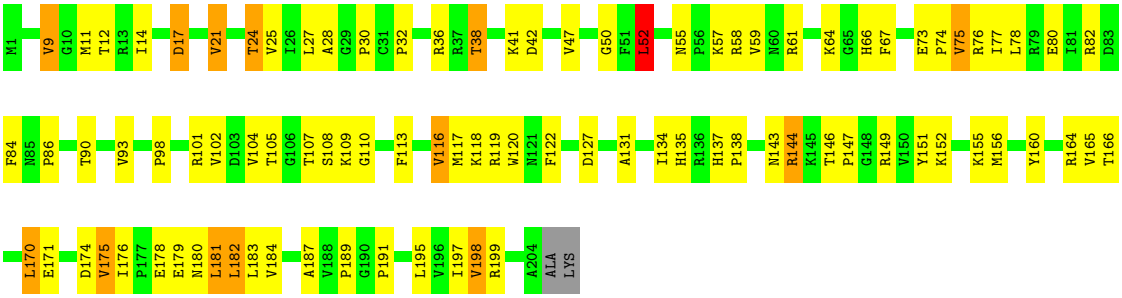
- Molecule 4: 50S ribosomal protein L3

Chain 1E:



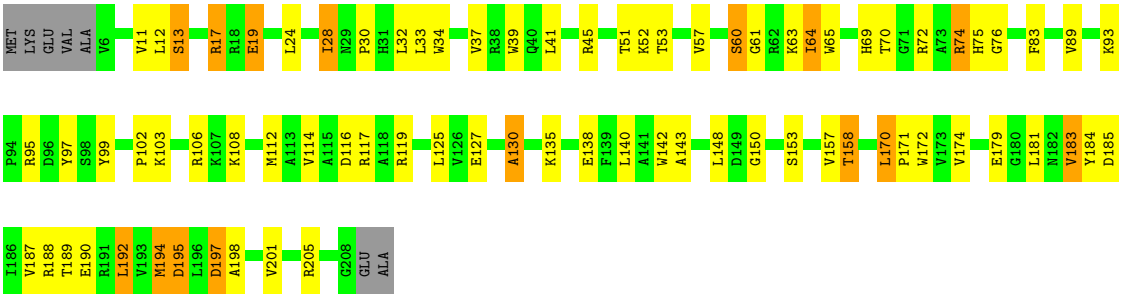
- Molecule 4: 50S ribosomal protein L3

Chain 2E:



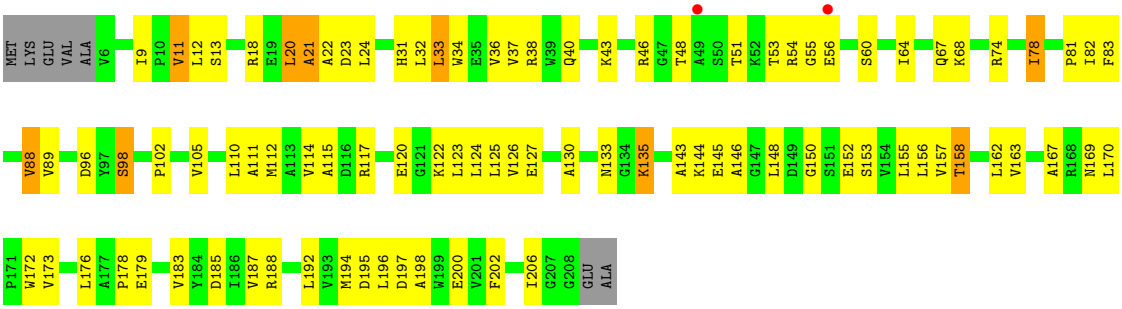
- Molecule 5: 50S ribosomal protein L4

Chain 1F:



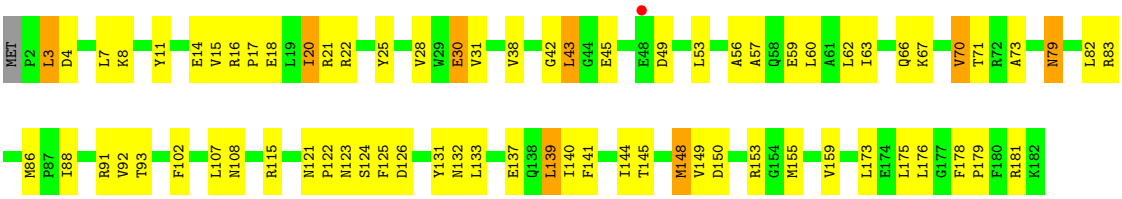
- Molecule 5: 50S ribosomal protein L4

Chain 2F:



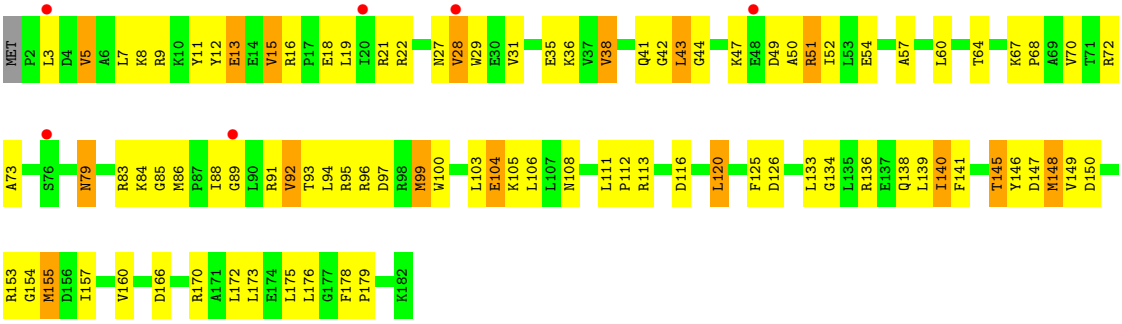
- Molecule 6: 50S ribosomal protein L5

Chain 1G:



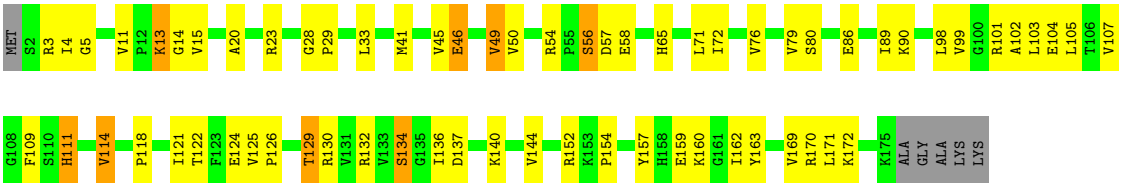
- Molecule 6: 50S ribosomal protein L5

Chain 2G:



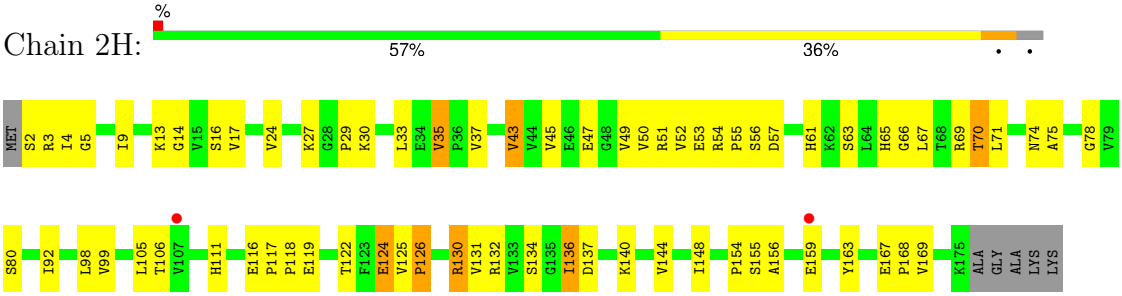
- Molecule 7: 50S ribosomal protein L6

Chain 1H:



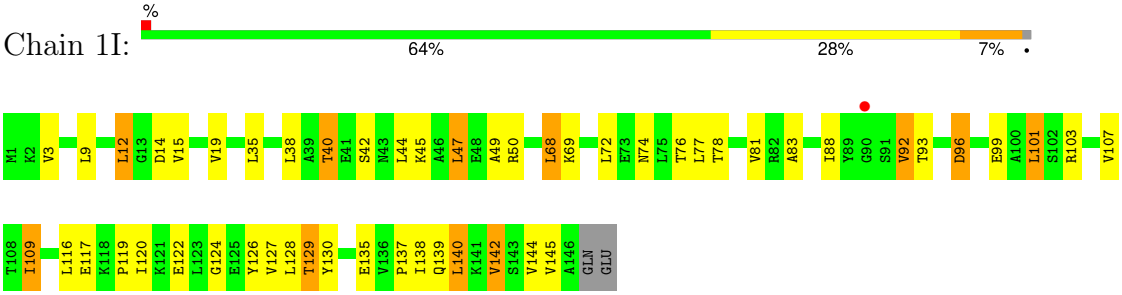
- Molecule 7: 50S ribosomal protein L6

Chain 2H:



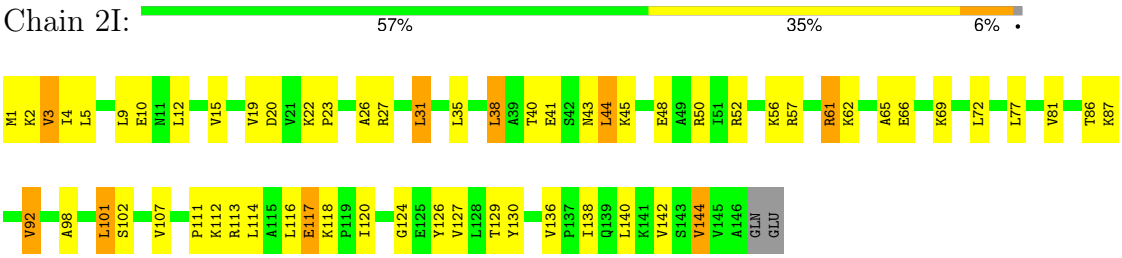
• Molecule 8: 50S ribosomal protein L9

Chain 1I:



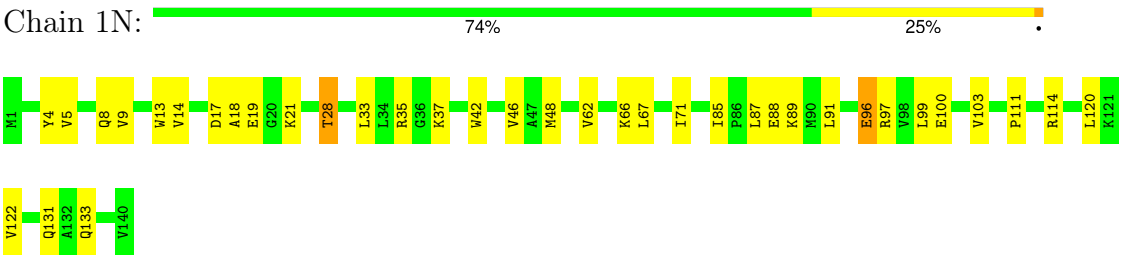
• Molecule 8: 50S ribosomal protein L9

Chain 2I:



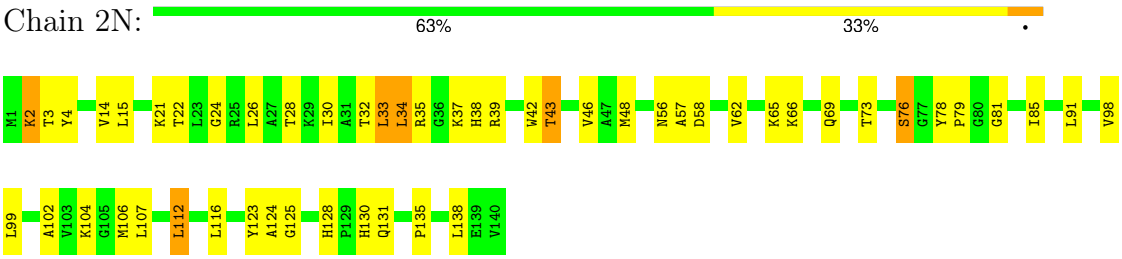
• Molecule 9: 50S ribosomal protein L13

Chain 1N:



• Molecule 9: 50S ribosomal protein L13

Chain 2N:



• Molecule 10: 50S ribosomal protein L14

Chain 1O: 69% 26% 5%

M1 I2 T6 V10 N13 A16 R17 C21 I22 R23 K31 V35 V38 P48 R64 T65 K66 K67 E68 I69 K70 S75 A76 I77 R78 F79 D80 I87 N88 E92 T96 R97 V98 F99 G100 P101 V102 A103 G110 F111 M112 K113 I114 V115 V121 L122

• Molecule 10: 50S ribosomal protein L14

Chain 2O: % 57% 38%

M1 I2 Q3 P4 Q5 E9 V10 G15 A16 R17 K18 I19 I22 L25 T34 V35 G36 D37 V40 A41 S42 V43 A46 I47 P48 R49 G50 K53 D56 K59 A60 V61 V62 V63 K67 E68 I69 K70 D73 G74 S75 A76 I77 R78 F79 D80 A83 A84 V85 I86 N89 E92 P93 R94 V98 V102 A103 R104 E105 L106 K109 G110 F111 I114 V115 V121 L122

• Molecule 11: 50S ribosomal protein L15

Chain 1P: 58% 35% 6%

M1 K2 L3 S4 D5 L6 R7 N13 R21 K29 T30 K36 R41 S42 G43 G44 L45 K46 R50 F51 E52 G53 G54 R55 S56 T57 T58 L59 M60 R61 L62 P63 K64 R65 G66 M67 Q68 G69 Q70 V71 P72 G73 K76 Q81 G82 V83 K86 E94 V95 T96 P97 E98 L99 L105 L106 K107 K108 K113 I114 L115 G116 E117 G118 K121 P122 L123 K124 V125 V126 A127 H128 A129 F130 L135 E136 K137 L138 K139 A140 L147 L148 E149 ALA

• Molecule 11: 50S ribosomal protein L15

Chain 2P: 2% 63% 30% 7%

M1 D5 L6 R7 P8 N9 R21 S25 G26 H27 G28 K29 T30 A31 T32 K36 G37 Q38 K39 S40 R41 S42 G43 G44 L45 K46 R50 S56 T57 T58 L59 M60 R61 L62 P63 Q68 G69 Q70 G73 E74 R77 P78 R79 Y80 Q81 G82 K86 V95 T96 P97 E98 L99 L100 V101 L106 K107 K108 G109 Y110 K113 I114 E117 K121 P122 L123 K124 V125 V126 S133 V146 L147 L148 E149 ALA

• Molecule 12: 50S ribosomal protein L16

Chain 1Q: % 72% 26%

M1 M7 R10 K11 R16 L17 K18 D25 Y26 V27 G33 L34 V35 P39 M54 V55 R56 H57 F58 R59 R60 G61 G62 K63 K76 L79 E80 V81 G84 K85 M103 F104 T110 E111 E112 Q113 A117 L118 K124 L125 P126 I127 K128 T129 K130

R133 A136 Y137 A140 Q141

- Molecule 12: 50S ribosomal protein L16

Chain 2Q:

M1 L2 M3 P4 R5 R6 M7 K8 Y9 Q12 Q13 R14 G15 R16 T21 K22 G23 G24 D25 Y26 V27 A28 F29 G30 D31 L34 V35 A36 L37 E38 P39 T43 V52 V55 R56 R60 F65 I66 R67 I68 F69 T75 L79 E80 K85 G86 K87 V90

V94 V97 K98 P99 G100 R101 V102 M103 F104 E105 V106 V109 T110 E111 E112 Q113 L118 R119 I120 K124 I127 K128 T129 K130 R133 R134 D135 Q141

- Molecule 13: 50S ribosomal protein L17

Chain 1R:

M1 R2 S6 N11 R12 H13 S14 S15 H16 R17 N23 S27 L28 R33 T36 T37 V38 L44 V48 D49 H53 L54 L65 V66 L67 D72 L75 V76 L79 Y94 V97 L98 K99 R103 D107 G108 A109 P110 L111 A112 L113 V114

E118

- Molecule 13: 50S ribosomal protein L17

Chain 2R:

M1 R2 S6 N11 R12 H13 S14 S15 H16 R17 L18 Y21 R22 N23 Q24 A25 K26 S27 L28 L29 T36 T37 L44 R45 G46 F47 V48 D49 H53 L54 A55 K56 R57 G58 D59 A62 L67 R68 D69 L70 Q71 D72 L75 V76 D81 Y87 R90

T95 L100 R103 R104 R105 G108 L111 V117 E118

- Molecule 14: 50S ribosomal protein L18

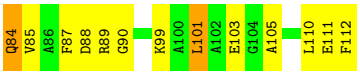
Chain 1S:

MET ALA R3 L4 R9 R10 K11 V14 R15 R25 L26 S27 Y36 A37 Q38 I39 D42 V46 V49 S50 L56 N61 K62 T63 E64 V65 V69 L73 F87 D88 R89 G90 P91 Y94 H95 V98 K99 A102 F112

- Molecule 14: 50S ribosomal protein L18

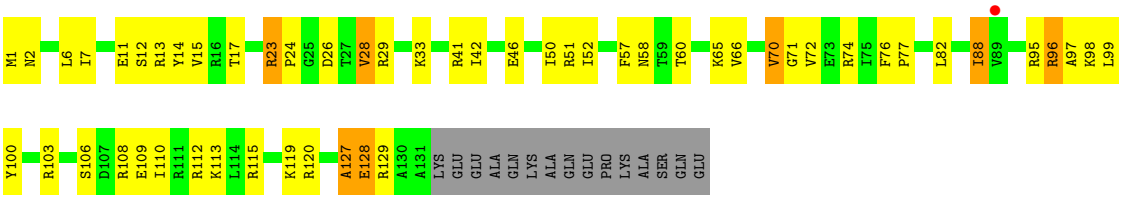
Chain 2S:

MET ALA R3 L4 T5 E8 R9 R13 V14 R15 N16 R17 I18 K19 R20 T21 L24 R25 L26 S27 V28 F29 R30 S31 Y36 A37 Q38 I39 T47 L48 V49 S50 A51 S52 S53 L56 K57 L58 N61 V65 A66 R67 Q68 V69 G70 R71 K76 A79 K83



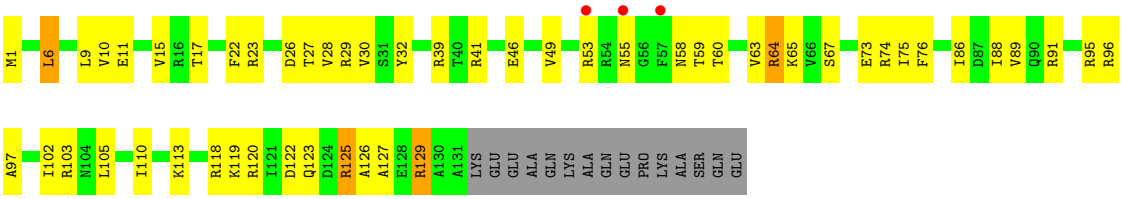
• Molecule 15: 50S ribosomal protein L19

Chain 1T:



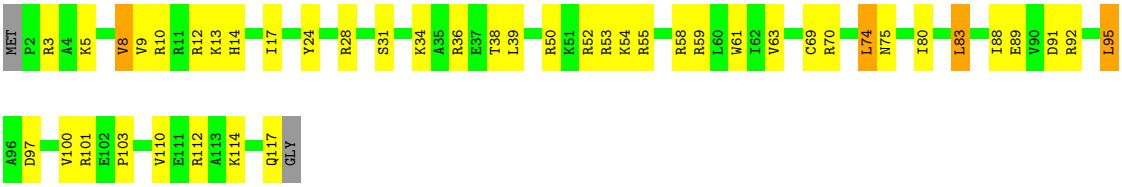
• Molecule 15: 50S ribosomal protein L19

Chain 2T:



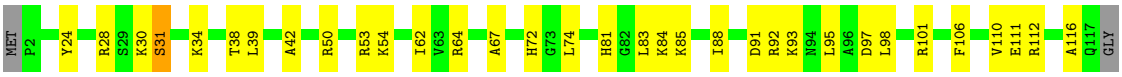
• Molecule 16: 50S ribosomal protein L20

Chain 1U:



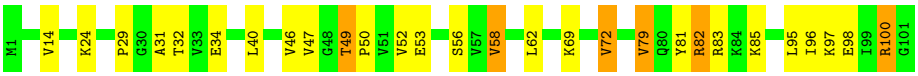
• Molecule 16: 50S ribosomal protein L20

Chain 2U:



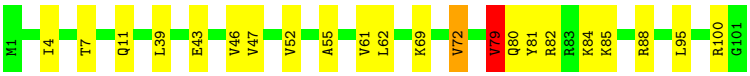
• Molecule 17: 50S ribosomal protein L21

Chain 1V:



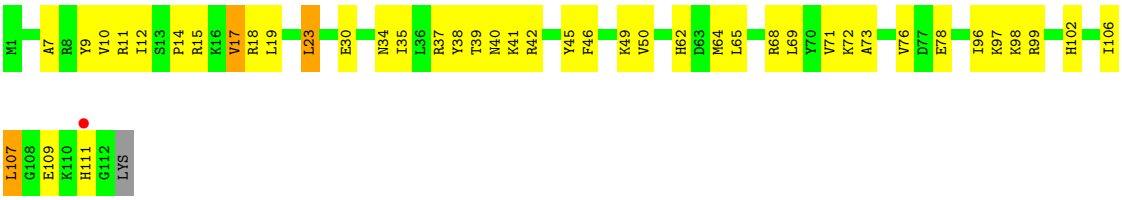
• Molecule 17: 50S ribosomal protein L21

Chain 2V:



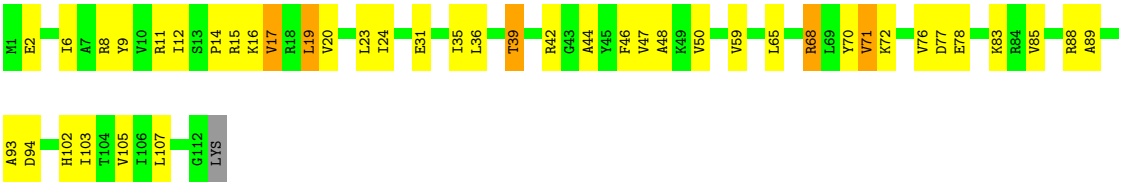
- Molecule 18: 50S ribosomal protein L22

Chain 1W:



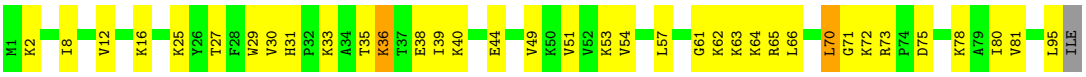
- Molecule 18: 50S ribosomal protein L22

Chain 2W:



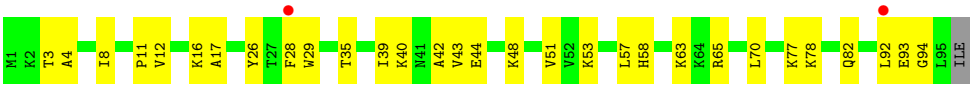
- Molecule 19: 50S ribosomal protein L23

Chain 1X:



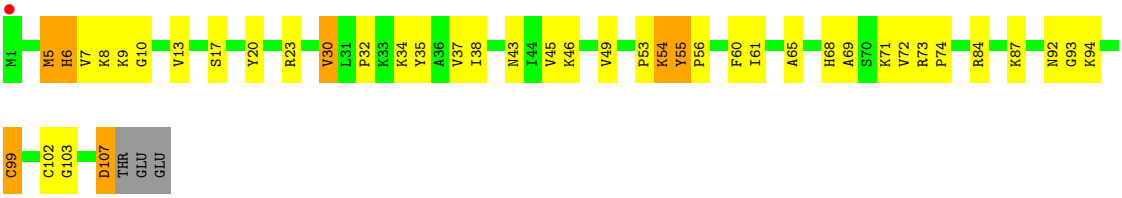
- Molecule 19: 50S ribosomal protein L23

Chain 2X:



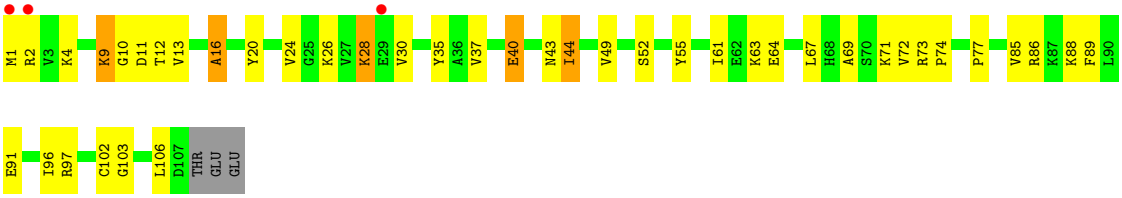
- Molecule 20: 50S ribosomal protein L24

Chain 1Y:



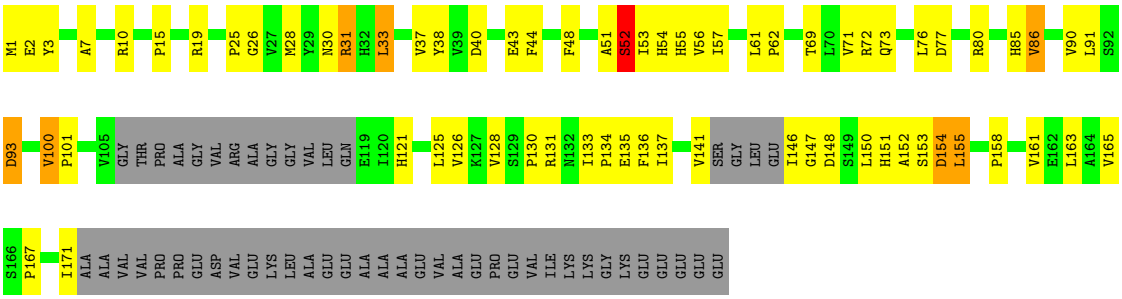
- Molecule 20: 50S ribosomal protein L24

Chain 2Y:



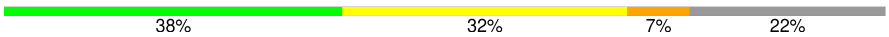
- Molecule 21: 50S ribosomal protein L25

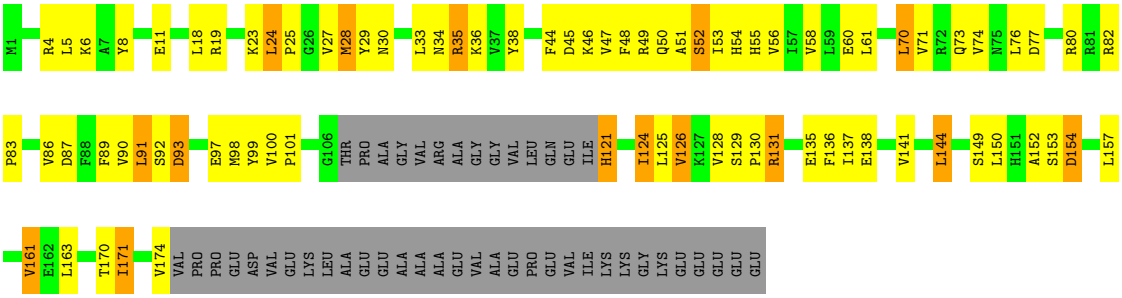
Chain 1Z:



- Molecule 21: 50S ribosomal protein L25

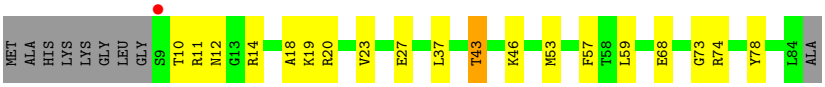
Chain 2Z:





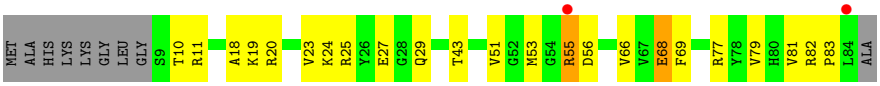
- Molecule 22: 50S ribosomal protein L27

Chain 10:



- Molecule 22: 50S ribosomal protein L27

Chain 20:

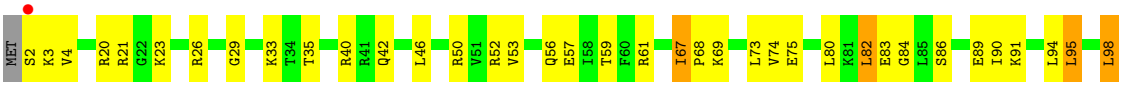


• Molecule 23: 50S ribosomal protein L28

Chain 11:

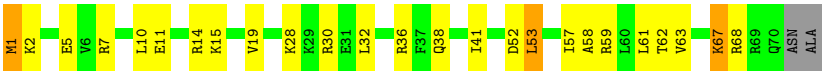
• Molecule 23: 50S ribosomal protein L28

Chain 21:



• Molecule 24: 50S ribosomal protein L29

Chain 12:



• Molecule 24: 50S ribosomal protein L29

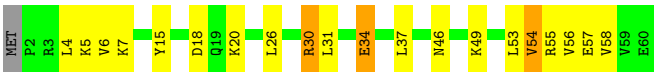
Chain 22:

• Molecule 25: 50S ribosomal protein L30

Chain 13:

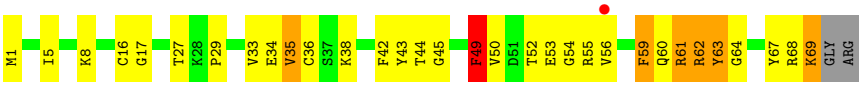
• Molecule 25: 50S ribosomal protein L30

Chain 23:



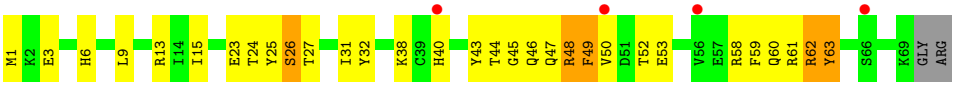
• Molecule 26: 50S ribosomal protein L31

Chain 14:



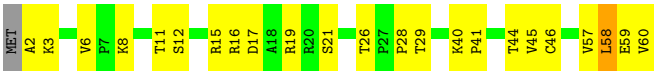
• Molecule 26: 50S ribosomal protein L31

Chain 24:



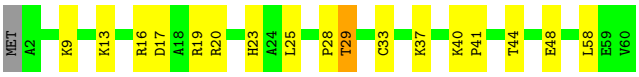
• Molecule 27: 50S ribosomal protein L32

Chain 15:



• Molecule 27: 50S ribosomal protein L32

Chain 25:



• Molecule 28: 50S ribosomal protein L33

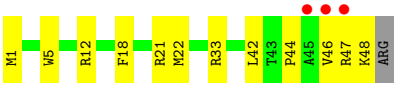
Chain 16:

• Molecule 28: 50S ribosomal protein L33

Chain 26:

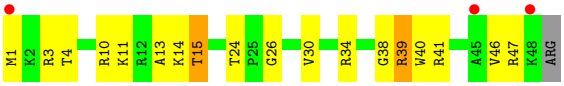
• Molecule 29: 50S ribosomal protein L34

Chain 17:



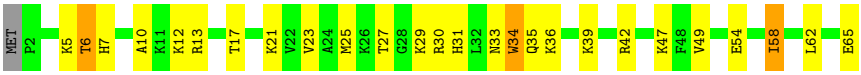
• Molecule 29: 50S ribosomal protein L34

Chain 27:



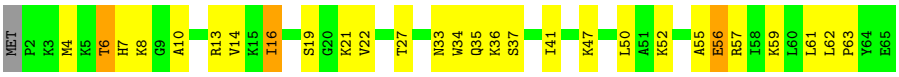
• Molecule 30: 50S ribosomal protein L35

Chain 18:



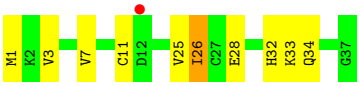
• Molecule 30: 50S ribosomal protein L35

Chain 28:



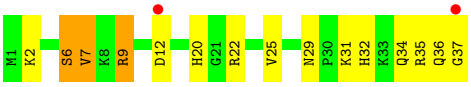
• Molecule 31: 50S ribosomal protein L36

Chain 19:



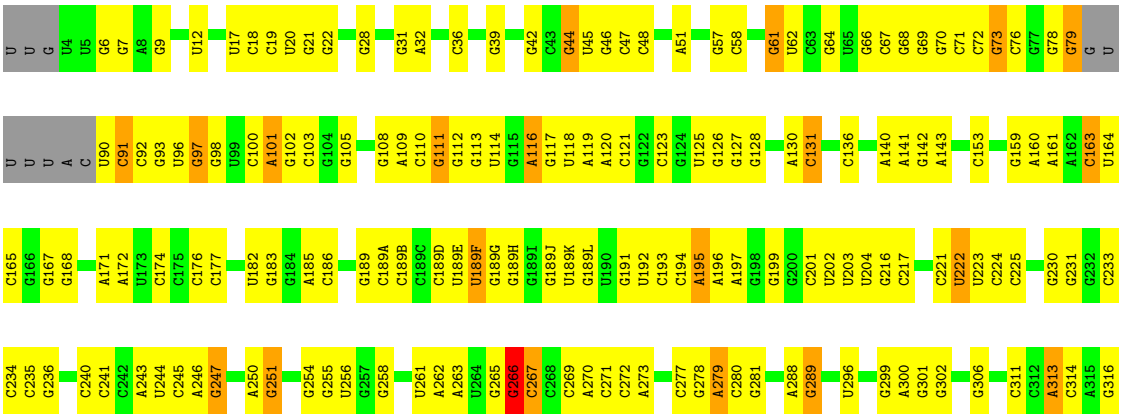
• Molecule 31: 50S ribosomal protein L36

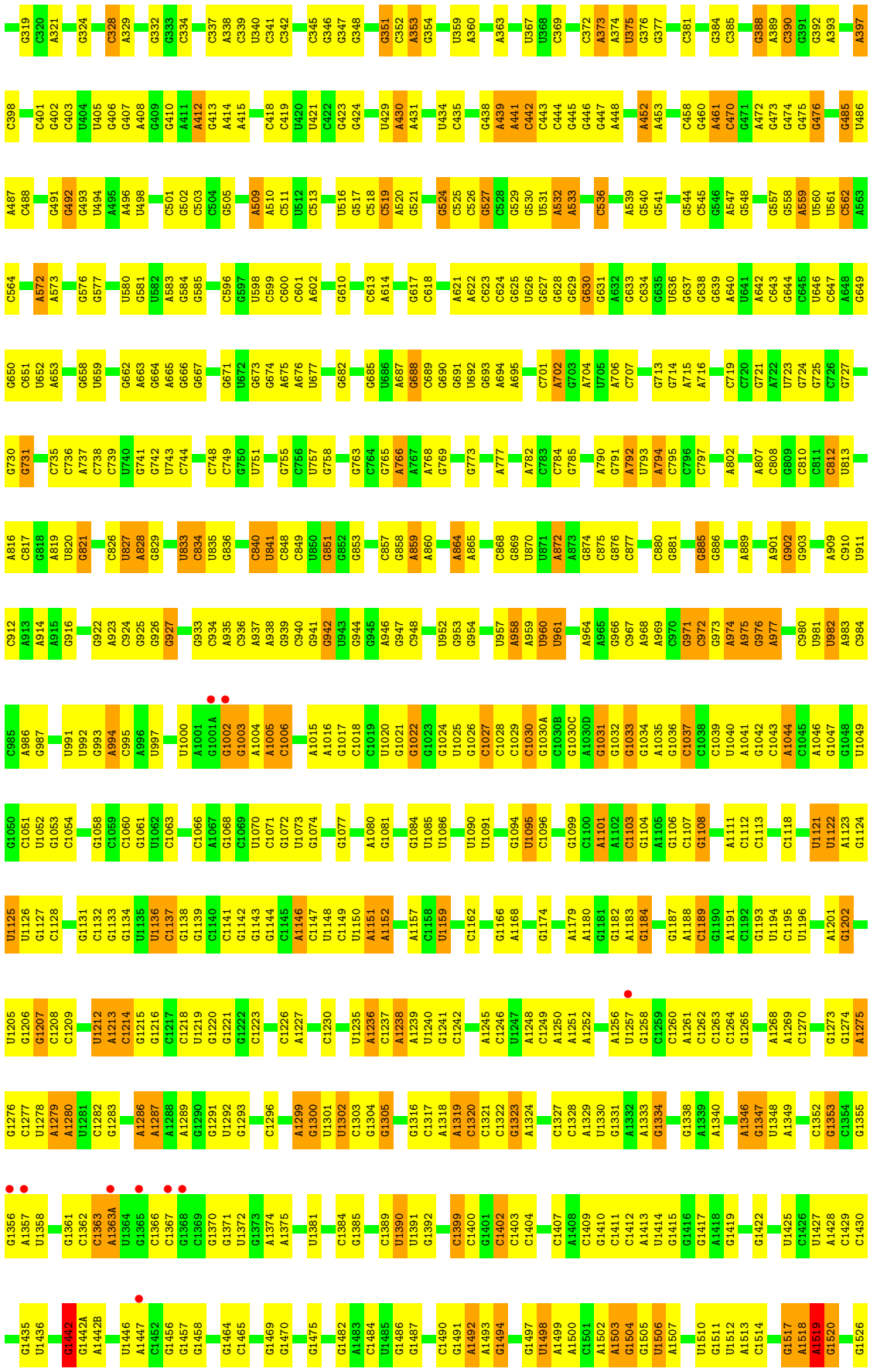
Chain 29:

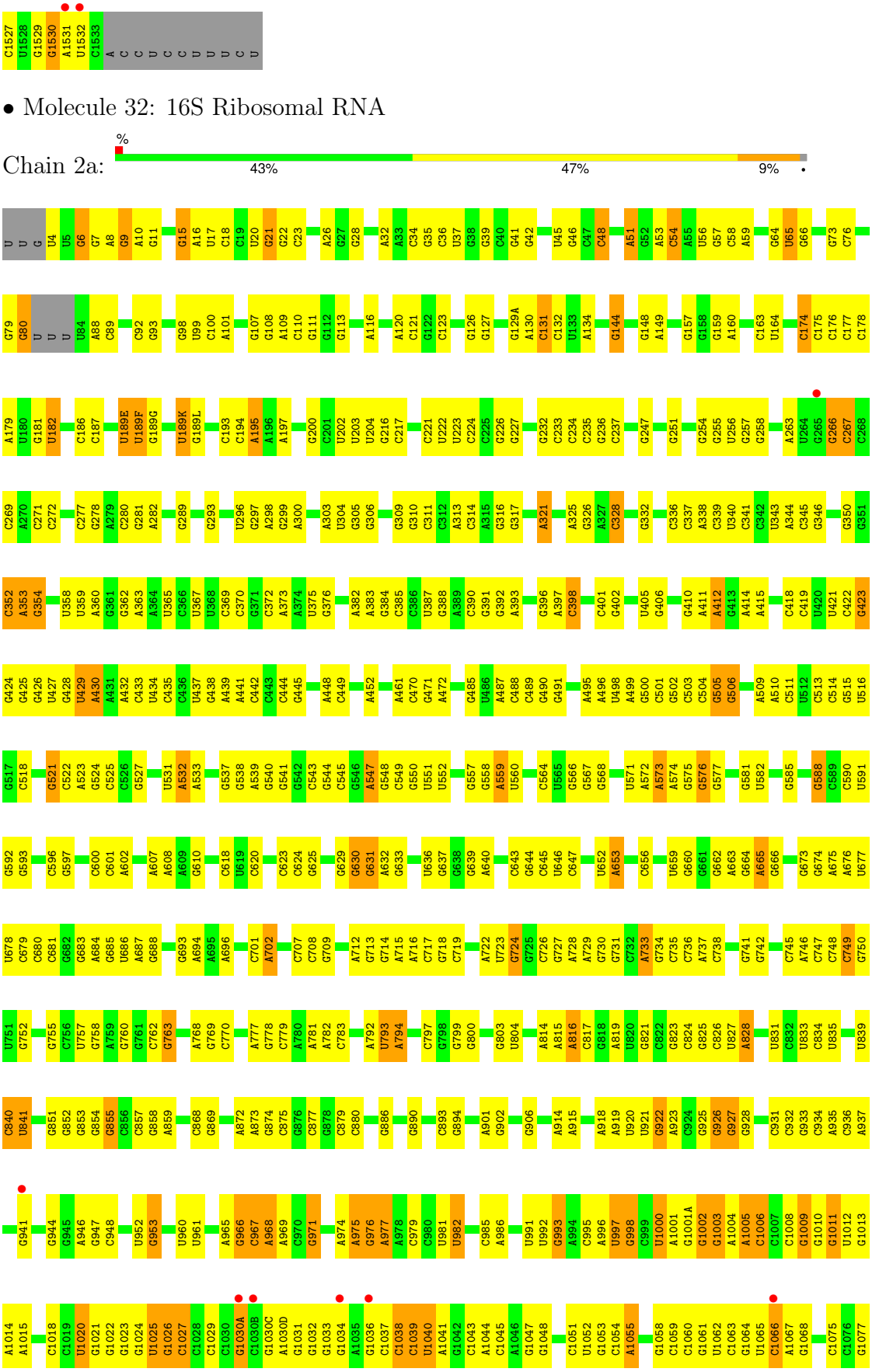


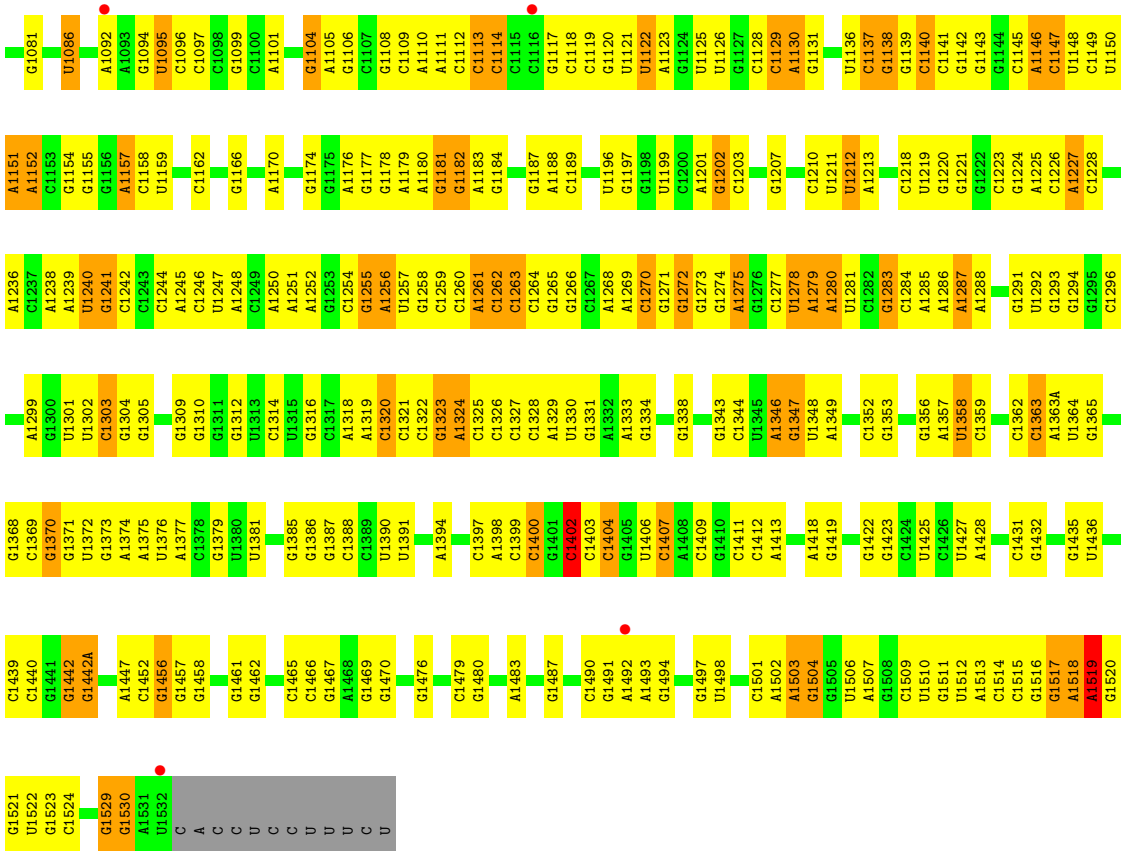
• Molecule 32: 16S Ribosomal RNA

Chain 1a:



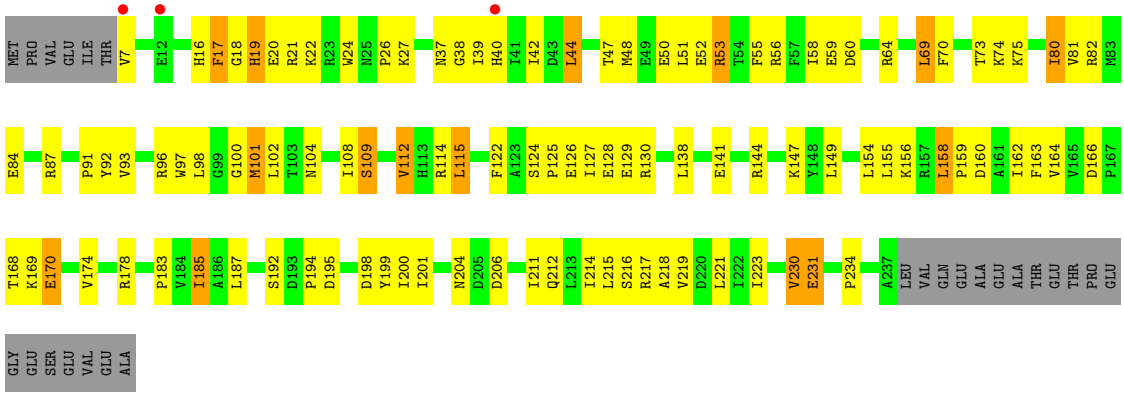

G319 C320 A321 G324 C328 A329 G332 G333 C334 C337 A338 C339 U340 C341 C342 C345 G346 G347 G348 G351 C352 A353 G354 U359 A360 A363 U367 U368 C369 C372 A373 A374 U375 G376 G377 C381 G384 C385 G388 A389 C390 G391 G392 A393 A397
C398 C401 G402 C403 U404 U405 G406 G407 A408 G409 G410 A411 A412 G413 A414 A415 C418 C419 U420 U421 C422 G423 G424 U429 A430 A431 U434 C435 G438 A439 A441 C442 C443 C444 G445 G446 G447 A448 A452 A453 C458 G460 A461 C470 G471 A472 G473 G474 G475 G476 G485 U486
A487 C488 G491 G492 G493 U494 A495 A496 U498 C501 G502 C503 C504 G505 A509 A510 C511 U512 C513 U516 G517 C518 C519 A520 G521 G524 C525 C526 G527 C528 G529 G530 U531 A532 A533 C536 A539 G540 G541 G544 C545 G546 A547 G548 G557 G558 A559 U560 U561 C562 A563
C564 A572 A573 G576 G577 U580 G581 U582 A583 G584 G585 C596 G597 U598 C599 C600 C601 A602 U610 C613 A614 G617 C618 A621 A622 C623 C624 G625 U626 G627 G628 G629 G630 G631 A632 G633 C634 G635 U636 G637 G638 G639 A640 U641 A642 C643 G644 C645 U646 C647 A648 G649
G650 C651 U652 A653 G658 U659 G662 A663 G664 A665 G666 G667 G671 U672 G673 G674 A675 A676 U677 G682 G685 U686 A687 G688 C689 G690 G691 U692 G693 A694 A695 C701 A702 G703 A704 U705 A706 C707 G713 G714 A715 A716 C719 C720 G721 A722 U723 G724 G725 C726 G727
G730 G731 C735 C736 A737 C738 C739 U740 G741 G742 U743 C744 C748 C749 G750 U751 G755 C756 U757 G758 G763 C764 G765 A766 A767 A768 G769 G773 A777 A782 C783 C784 G785 A790 G791 A792 U793 A794 C795 C796 C797 A802 A807 C808 G809 C810 C811 C812 U813
A816 C817 G818 A819 U820 G821 C826 U827 A828 G829 U833 C834 U835 G836 C840 U841 C848 G849 U850 G851 G852 G853 C857 G858 A859 A860 A864 A865 C868 G869 U870 U871 A872 A873 G874 C875 G876 C877 C880 G881 G885 G886 A889 A901 G902 G903 A909 C910 U911
C912 A913 A914 A915 G916 G922 A923 C924 G925 G926 G927 G933 C934 A935 C936 A937 A938 G939 C940 G941 G942 U943 G944 G945 A946 G947 C948 U952 G953 G954 U957 A958 A959 U960 U961 A964 A965 G966 C967 A968 A969 C970 G971 C972 G973 A974 A975 G976 A977 C980 U981 U982 A983 C984
C985 A986 G987 U991 U992 G993 A994 C995 A996 U997 U1000 A1001 G1001A G1002 G1003 A1004 A1005 C1006 A1015 A1016 G1017 C1018 C1019 U1020 G1021 G1022 G1023 G1024 U1025 G1026 C1027 C1028 C1029 C1030 G1030A C1030B G1030C A1030D G1031 G1032 G1033 G1034 A1035 G1036 C1037 C1038 C1039 U1040 A1041 G1042 C1043 A1044 C1045 A1046 G1047 G1048 U1049
G1050 C1051 U1052 G1053 C1054 G1058 C1059 C1060 G1061 U1062 C1063 C1066 A1067 G1068 C1069 U1070 C1071 G1072 U1073 G1074 G1077 A1080 G1081 G1084 U1085 U1086 U1090 U1091 G1094 U1095 C1096 G1099 C1100 A1101 A1102 C1103 G1104 A1105 G1106 C1107 G1108 A1111 C1112 C1113 C1118 U1121 U1122 A1123 G1124
U1125 U1126 G1127 C1128 G1131 C1132 G1133 G1134 U1135 U1136 C1137 G1138 G1139 C1140 C1141 G1142 G1143 G1144 C1145 A1146 C1147 U1148 C1149 U1150 A1151 A1152 A1157 C1158 U1159 C1162 G1166 A1168 G1174 A1179 A1180 G1181 G1182 A1183 G1184 G1187 A1188 C1189 G1190 A1191 C1192 G1193 U1194 C1195 U1196 A1201 G1202
U1205 G1206 G1207 C1208 C1209 U1212 A1213 C1214 G1215 G1216 C1217 C1218 U1219 G1220 G1221 G1222 G1223 C1226 A1227 C1230 U1235 A1236 C1237 A1238 A1239 U1240 G1241 C1242 A1245 C1246 U1247 A1248 C1249 A1250 A1251 A1252 A1256 U1257 G1258 C1259 C1260 A1261 C1262 C1263 C1264 G1265 A1268 A1269 C1270 G1273 G1274 A1275
G1276 C1277 U1278 A1279 A1280 U1281 C1282 G1283 A1286 A1287 A1288 A1289 G1290 G1291 U1292 G1293 C1296 A1299 G1300 U1301 U1302 C1303 A1304 G1305 G1316 C1317 A1318 A1319 C1320 C1321 C1322 G1323 A1324 C1327 C1328 A1329 U1330 G1331 A1332 A1333 G1334 G1338 A1339 A1340 A1346 G1347 U1348 A1349 C1352 G1353 C1354 G1355
G1356 A1357 U1358 G1361 C1362 C1363 A1363A U1364 G1365 C1366 C1367 G1368 C1369 G1370 G1371 U1372 G1373 A1374 A1375 U1381 C1384 G1385 C1389 U1390 U1391 G1392 C1399 C1400 G1401 C1402 C1403 C1404 C1407 A1408 C1409 C1410 C1411 C1412 A1413 U1414 G1415 G1416 G1417 A1418 G1419 G1422 U1425 C1426 U1427 A1428 C1429 C1430
G1435 U1436 G1442 G1442A A1442B U1446 A1447 C1452 G1456 G1457 G1458 G1464 C1465 G1469 G1470 G1475 G1482 A1483 C1484 U1485 G1486 G1487 C1490 G1491 A1492 A1493 G1494 G1497 U1498 A1499 A1500 C1501 A1502 A1503 G1504 G1505 U1506 A1507 U1510 G1511 U1512 A1513 C1514 G1517 A1518 A1519 G1520 G1526


C1527 U1528 G1529 G1530 A1531 U1532 C1533 A C C U C C U U U C U
• Molecule 32: 16S Ribosomal RNA
Chain 2a:
%
43%
47%
9%
•



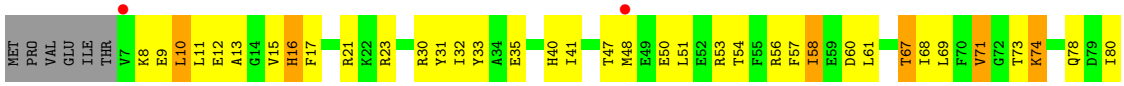
• Molecule 33: 30S ribosomal protein S2

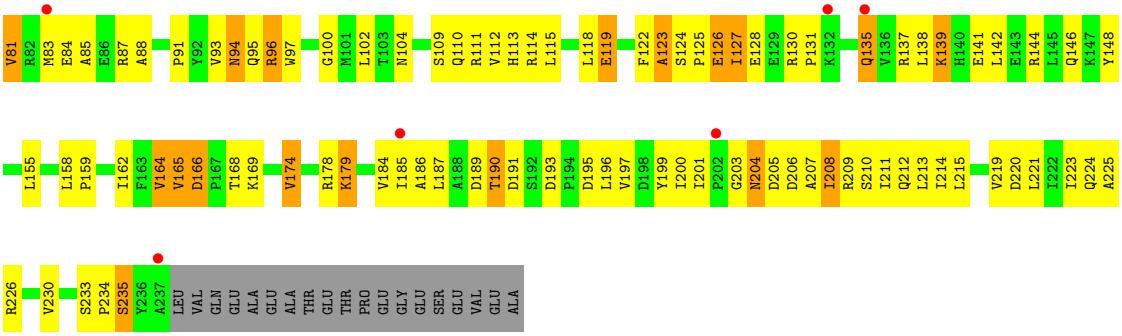
Chain 1b:



• Molecule 33: 30S ribosomal protein S2

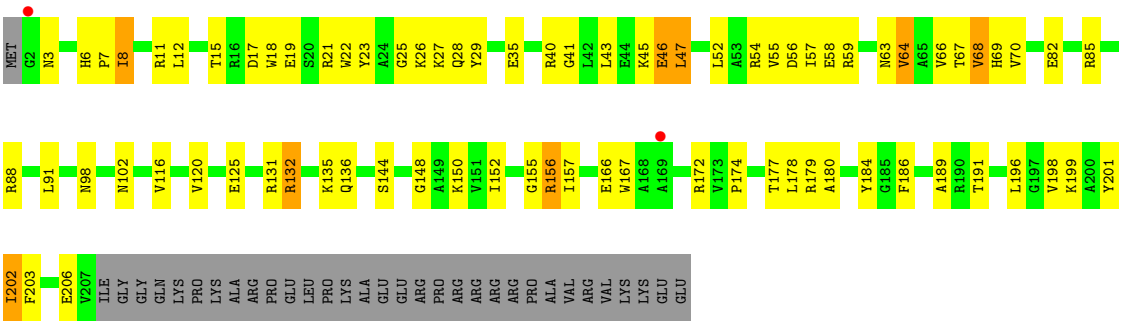
Chain 2b:





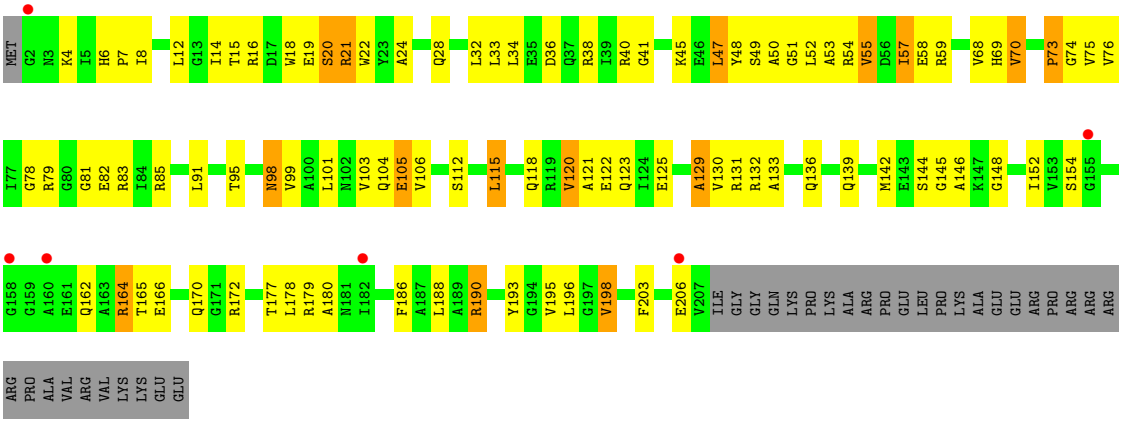
- Molecule 34: 30S ribosomal protein S3

Chain 1c:



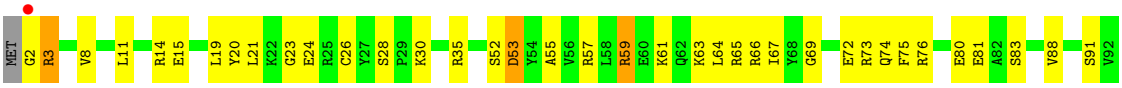
- Molecule 34: 30S ribosomal protein S3

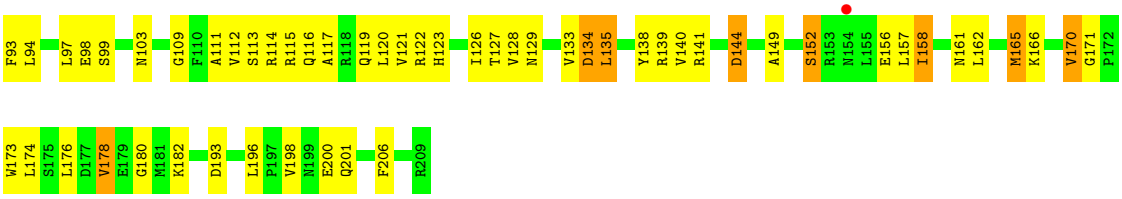
Chain 2c:



- Molecule 35: 30S ribosomal protein S4

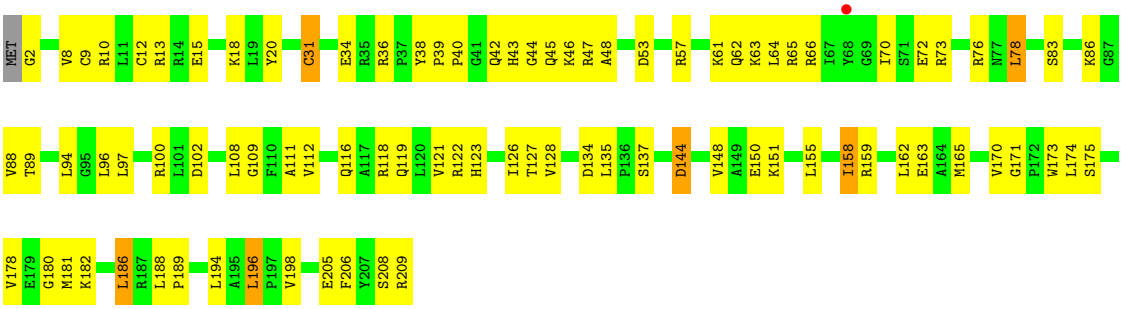
Chain 1d:





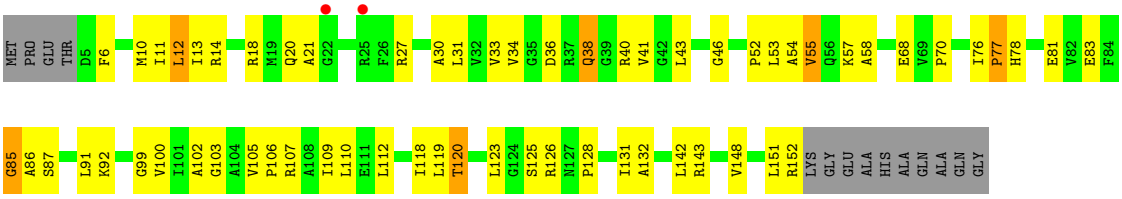
• Molecule 35: 30S ribosomal protein S4

Chain 2d:



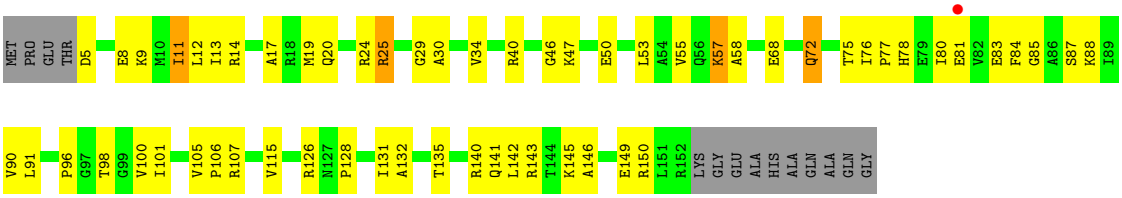
• Molecule 36: 30S ribosomal protein S5

Chain 1e:



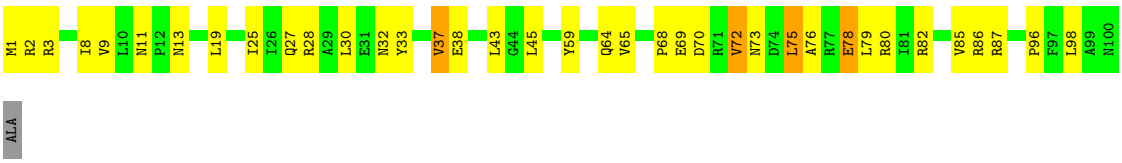
• Molecule 36: 30S ribosomal protein S5

Chain 2e:



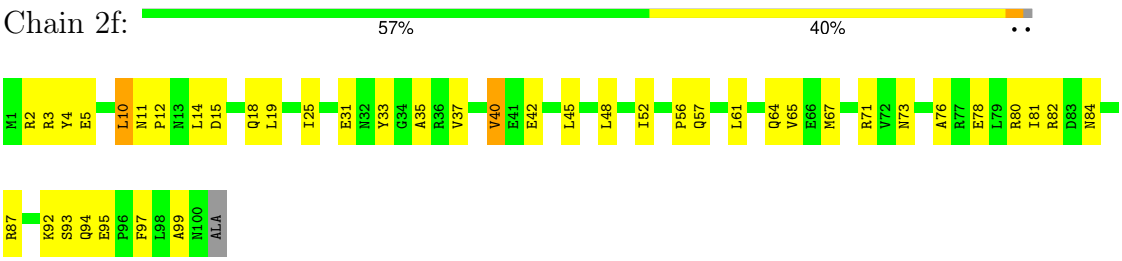
• Molecule 37: 30S ribosomal protein S6

Chain 1f:



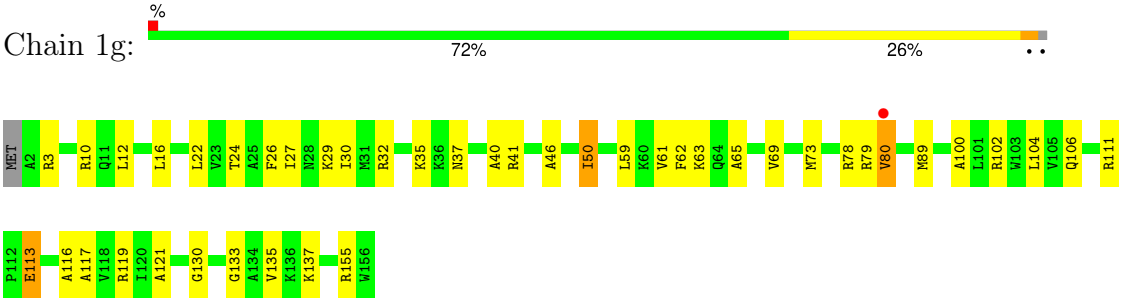
- Molecule 37: 30S ribosomal protein S6

Chain 2f:



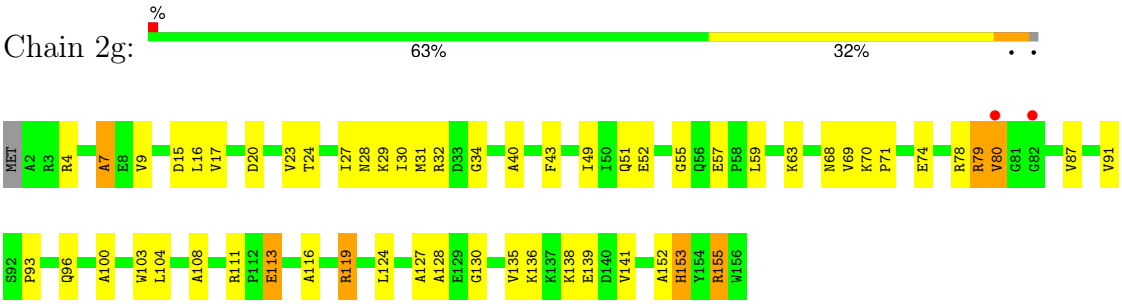
- Molecule 38: 30S ribosomal protein S7

Chain 1g:



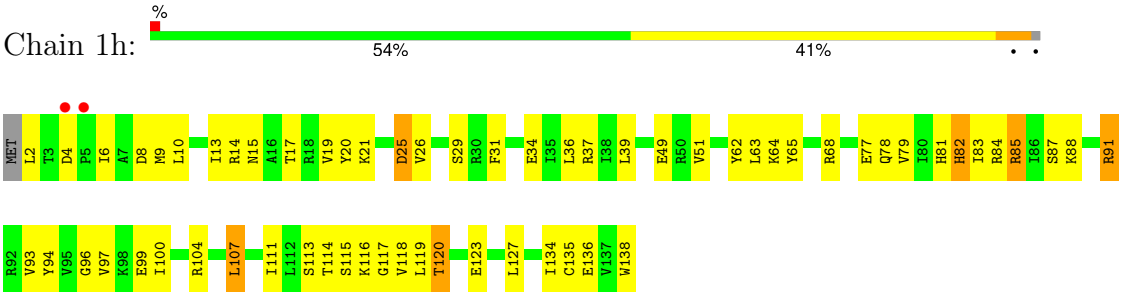
- Molecule 38: 30S ribosomal protein S7

Chain 2g:



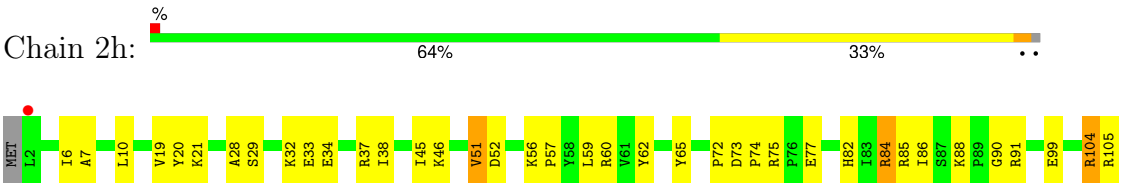
- Molecule 39: 30S ribosomal protein S8

Chain 1h:



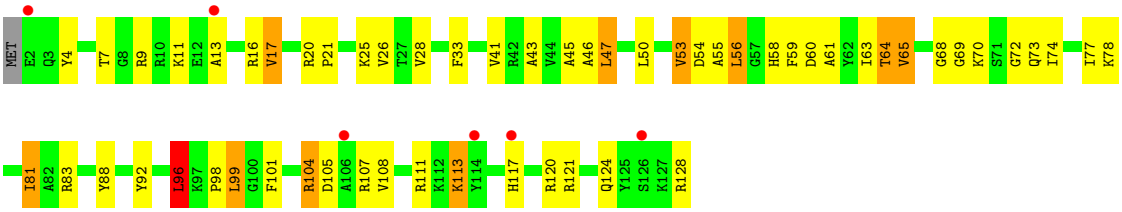
- Molecule 39: 30S ribosomal protein S8

Chain 2h:



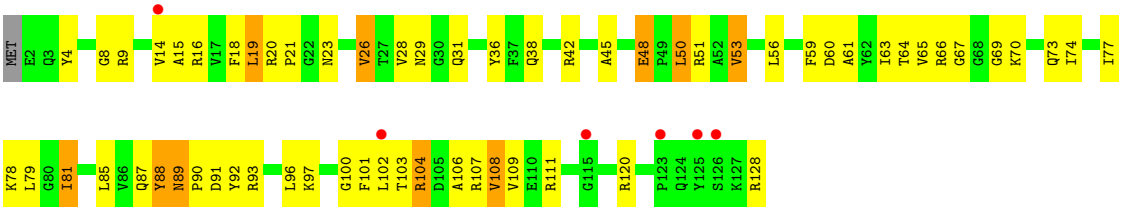
• Molecule 40: 30S ribosomal protein S9

Chain 1i:



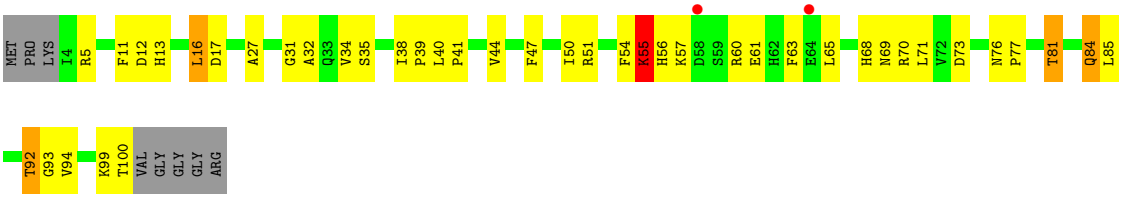
• Molecule 40: 30S ribosomal protein S9

Chain 2i:



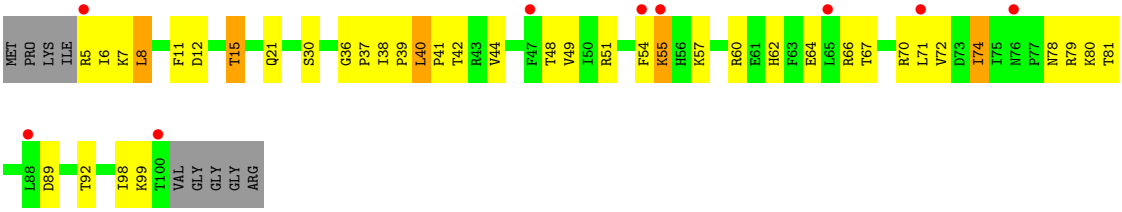
• Molecule 41: 30S ribosomal protein S10

Chain 1j:



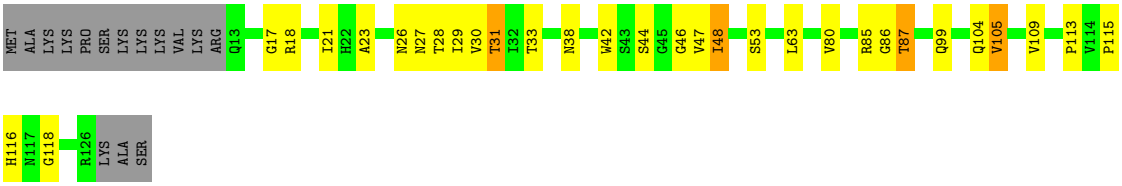
• Molecule 41: 30S ribosomal protein S10

Chain 2j:



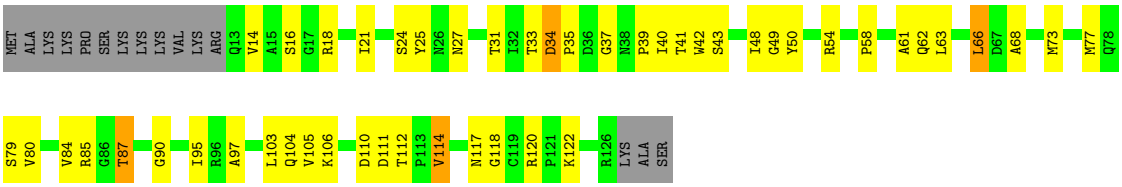
• Molecule 42: 30S ribosomal protein S11

Chain 1k:



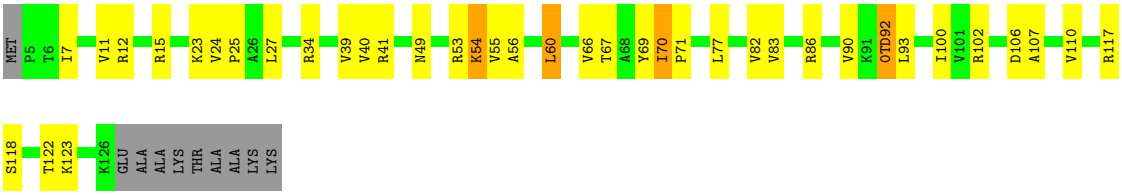
• Molecule 42: 30S ribosomal protein S11

Chain 2k:



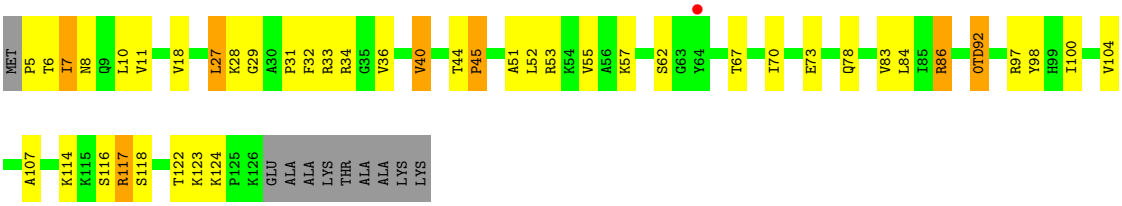
• Molecule 43: 30S ribosomal protein S12

Chain 1l:



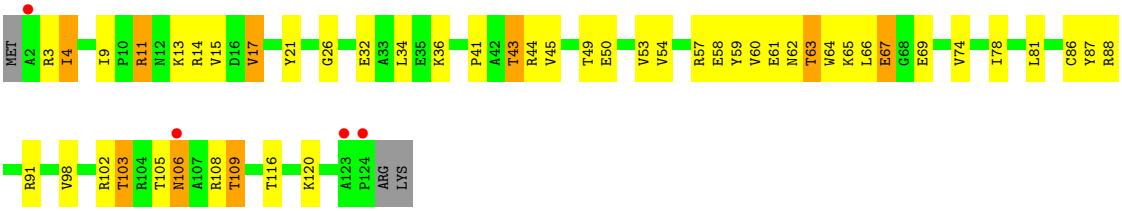
• Molecule 43: 30S ribosomal protein S12

Chain 2l:



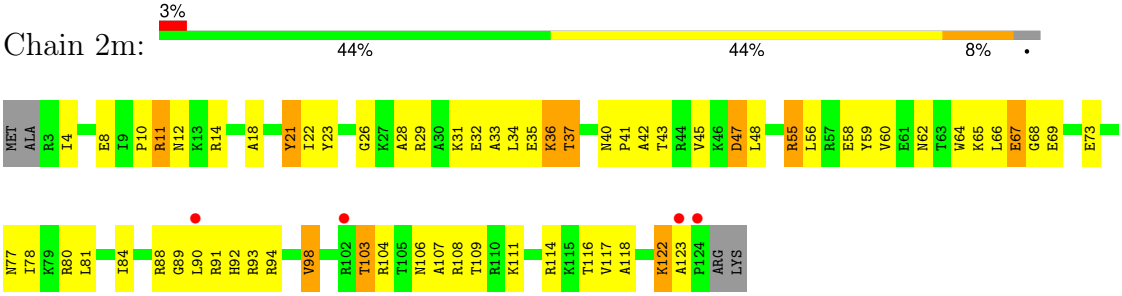
• Molecule 44: 30S ribosomal protein S13

Chain 1m:



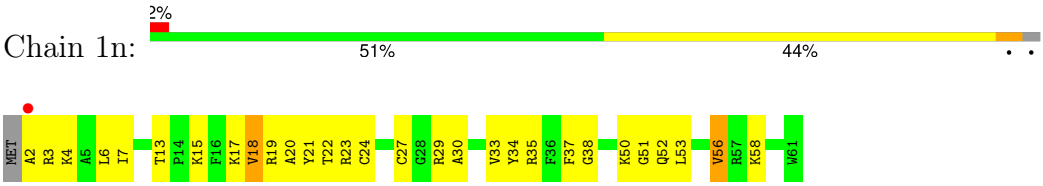
• Molecule 44: 30S ribosomal protein S13

Chain 2m:



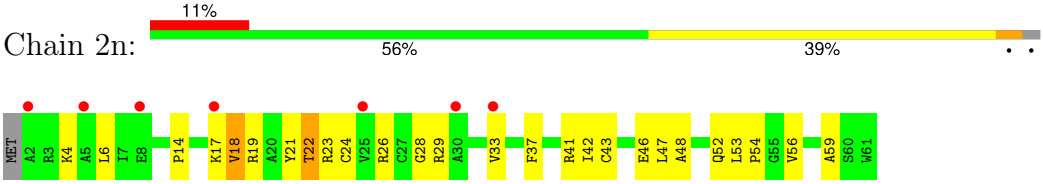
- Molecule 45: 30S ribosomal protein S14 type Z

Chain 1n:



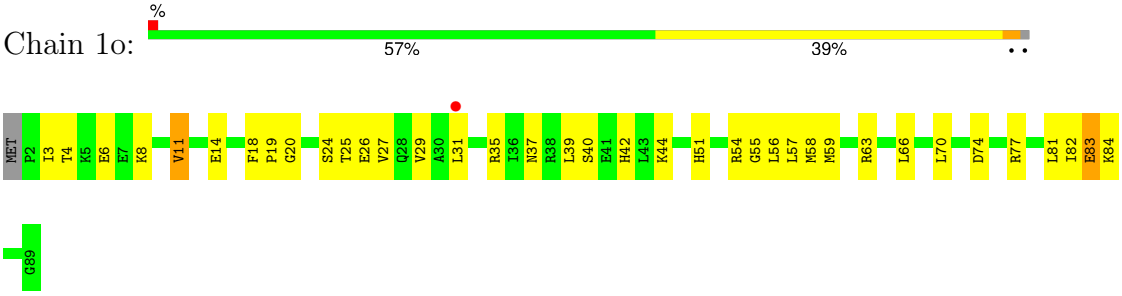
- Molecule 45: 30S ribosomal protein S14 type Z

Chain 2n:



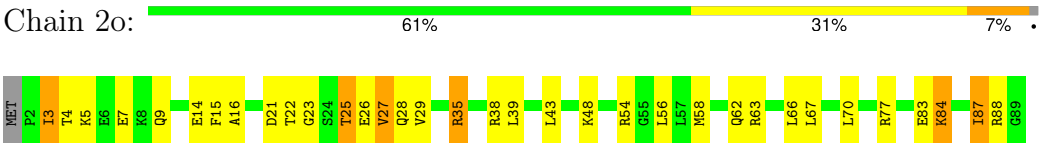
- Molecule 46: 30S ribosomal protein S15

Chain 1o:



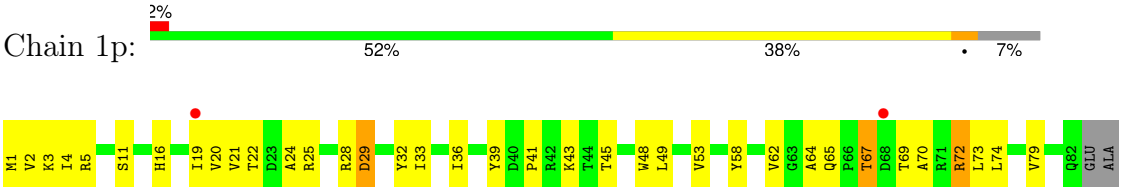
- Molecule 46: 30S ribosomal protein S15

Chain 2o:



- Molecule 47: 30S ribosomal protein S16

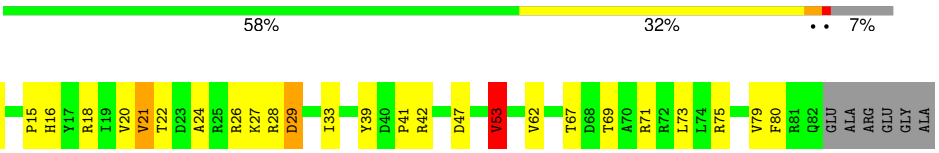
Chain 1p:



ARG GLU GLY ALA

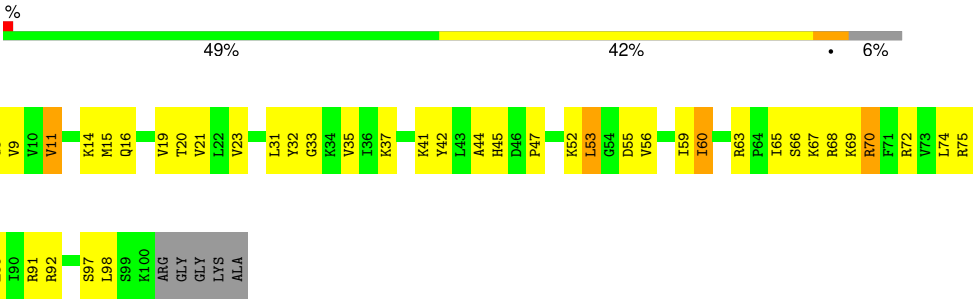
- Molecule 47: 30S ribosomal protein S16

Chain 2p:



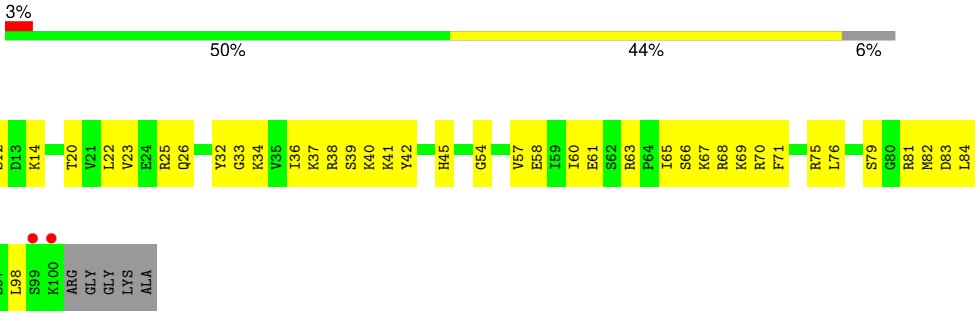
- Molecule 48: 30S ribosomal protein S17

Chain 1q:



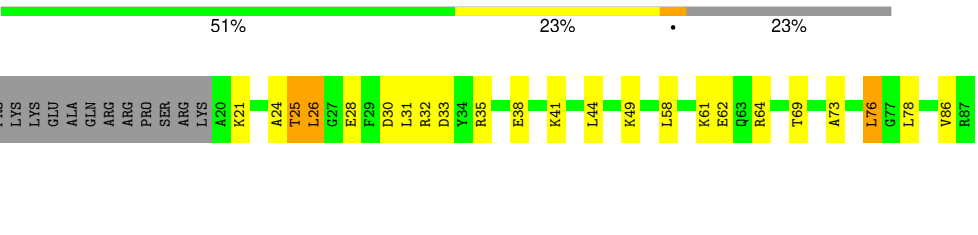
- Molecule 48: 30S ribosomal protein S17

Chain 2q:



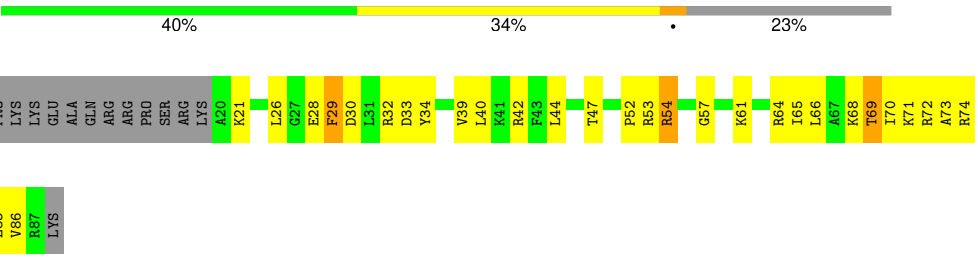
- Molecule 49: 30S ribosomal protein S18

Chain 1r:



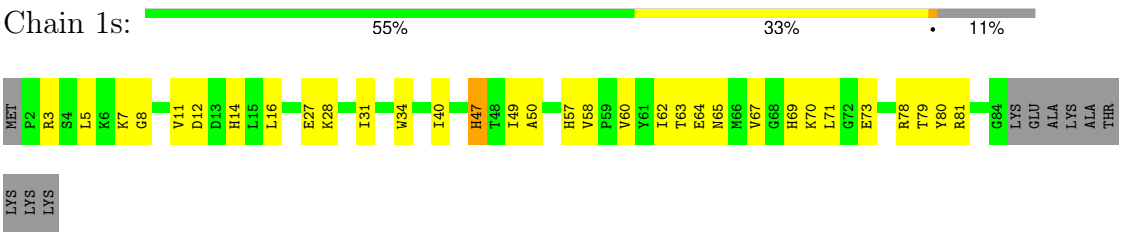
- Molecule 49: 30S ribosomal protein S18

Chain 2r:



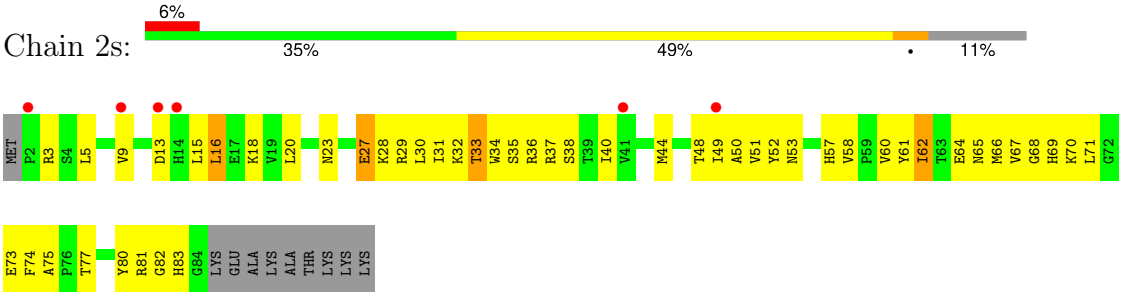
• Molecule 50: 30S ribosomal protein S19

Chain 1s:



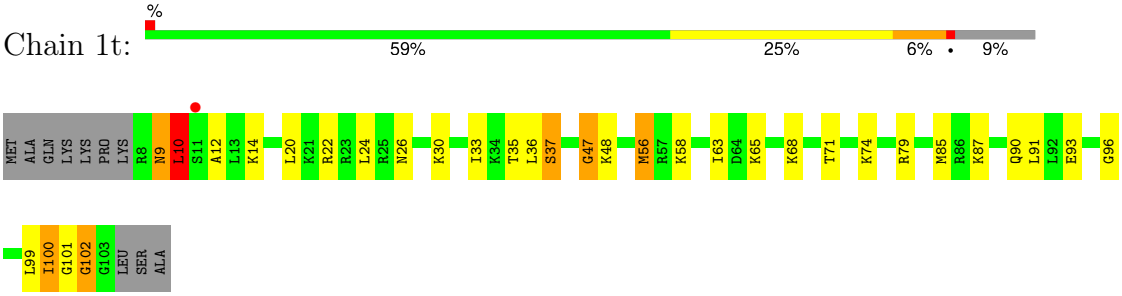
• Molecule 50: 30S ribosomal protein S19

Chain 2s:



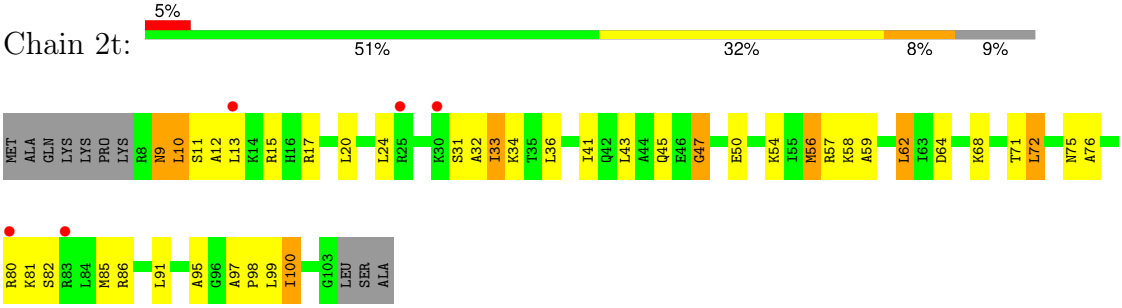
• Molecule 51: 30S ribosomal protein S20

Chain 1t:



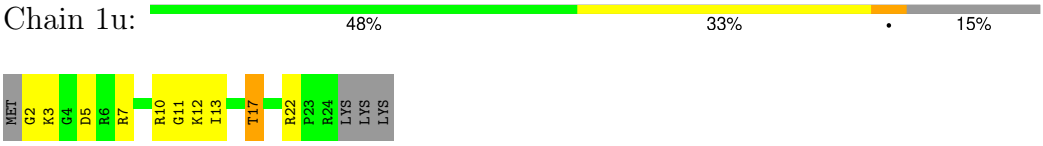
• Molecule 51: 30S ribosomal protein S20

Chain 2t:



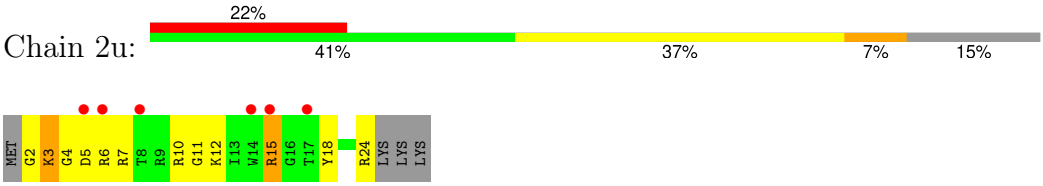
• Molecule 52: 30S ribosomal protein Thx

Chain 1u:



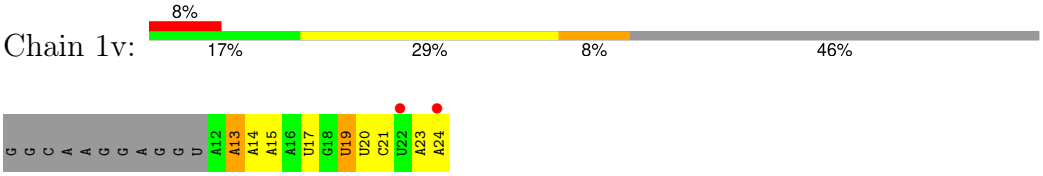
• Molecule 52: 30S ribosomal protein Thx

Chain 2u:



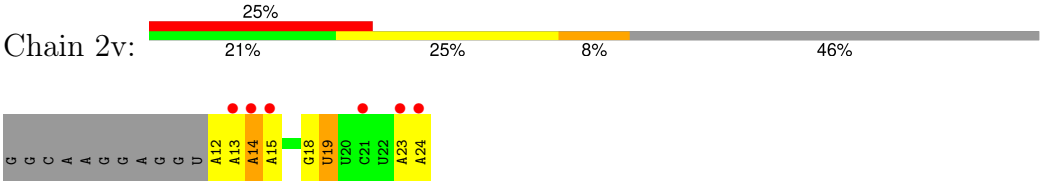
• Molecule 53: mRNA

Chain 1v:



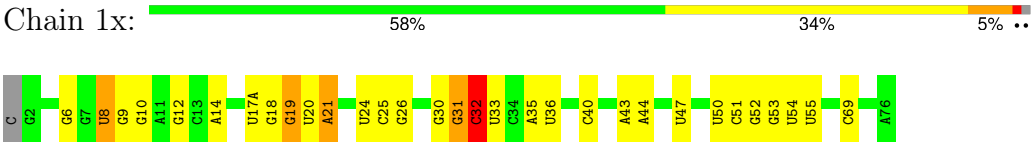
• Molecule 53: mRNA

Chain 2v:



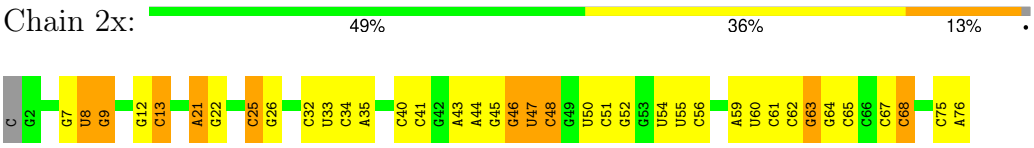
• Molecule 54: P-site tRNA

Chain 1x:



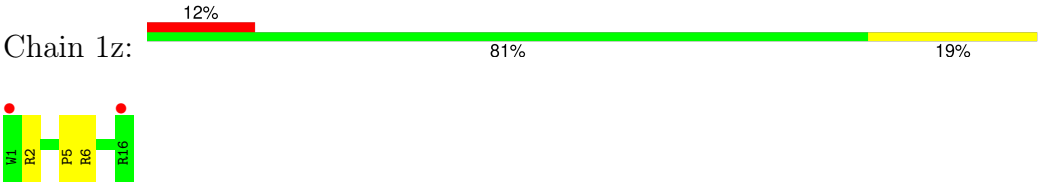
• Molecule 54: P-site tRNA

Chain 2x:



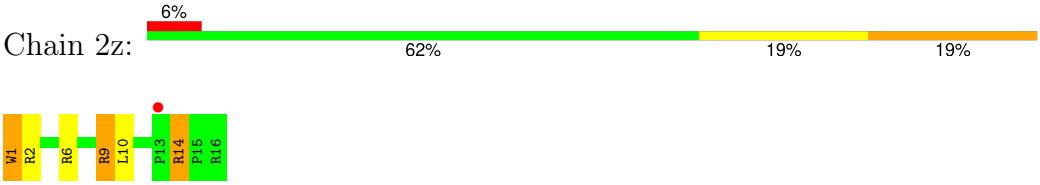
• Molecule 55: Bac7-001

Chain 1z:



• Molecule 55: Bac7-001

Chain 2z:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	209.09Å 449.88Å 621.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	76.76 – 3.00 76.76 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.4 (76.76-3.00) 99.4 (76.76-3.00)	Depositor EDS
R_{merge}	0.26	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.28 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.226 , 0.285 0.227 , 0.286	Depositor DCC
R_{free} test set	57578 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	68.0	Xtriage
Anisotropy	0.305	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 46.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.38$, $< L^2 > = 0.20$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	293228	wwPDB-VP
Average B, all atoms (Å^2)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.47% 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: UR3, ZN, PSU, 4OC, MG, 2MU, M2G, 2MA, MA6, OMG, 4SU, 5MU, 0TD, K, 7MG, 2MG, SF4, 5MC

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	1A	0.28	0/69009	0.45	2/107712 (0.0%)
1	2A	0.23	0/67293	0.41	0/105034
2	1B	0.23	0/2882	0.42	0/4494
2	2B	0.22	0/2879	0.42	0/4487
3	1D	0.28	0/2186	0.52	1/2944 (0.0%)
3	2D	0.23	0/2186	0.49	0/2944
4	1E	0.26	0/1592	0.48	0/2149
4	2E	0.21	0/1592	0.46	0/2149
5	1F	0.26	0/1619	0.50	0/2193
5	2F	0.22	0/1615	0.49	2/2188 (0.1%)
6	1G	0.23	0/1448	0.48	0/1957
6	2G	0.23	0/1453	0.51	1/1963 (0.1%)
7	1H	0.24	0/1356	0.46	0/1834
7	2H	0.19	0/1356	0.37	0/1834
8	1I	0.21	0/1112	0.44	0/1514
8	2I	0.21	0/1079	0.45	0/1475
9	1N	0.25	0/1144	0.44	0/1543
9	2N	0.21	0/1144	0.42	0/1543
10	1O	0.24	0/943	0.45	0/1269
10	2O	0.22	0/943	0.49	0/1269
11	1P	0.26	0/1152	0.55	0/1533
11	2P	0.22	0/1152	0.53	0/1533
12	1Q	0.27	0/1143	0.50	0/1527
12	2Q	0.23	0/1143	0.50	0/1527
13	1R	0.24	0/982	0.47	0/1312
13	2R	0.21	0/982	0.47	0/1312
14	1S	0.22	0/883	0.46	0/1176
14	2S	0.22	0/880	0.46	0/1172
15	1T	0.25	0/1105	0.50	0/1477
15	2T	0.20	0/1097	0.41	0/1468
16	1U	0.27	0/977	0.48	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
16	2U	0.20	0/977	0.44	0/1301
17	1V	0.25	0/782	0.47	0/1049
17	2V	0.19	0/782	0.42	0/1049
18	1W	0.27	0/897	0.46	0/1205
18	2W	0.21	0/897	0.43	0/1205
19	1X	0.28	0/764	0.50	0/1025
19	2X	0.21	0/764	0.43	0/1025
20	1Y	0.22	0/819	0.45	0/1095
20	2Y	0.21	0/819	0.44	0/1095
21	1Z	0.24	0/1267	0.48	0/1717
21	2Z	0.23	0/1299	0.46	0/1763
22	10	0.27	0/612	0.49	0/816
22	20	0.24	0/612	0.50	0/816
23	11	0.25	0/762	0.44	0/1014
23	21	0.21	0/762	0.43	0/1014
24	12	0.26	0/590	0.46	0/781
24	22	0.21	0/590	0.40	0/781
25	13	0.26	0/474	0.48	0/635
25	23	0.21	0/469	0.42	0/630
26	14	0.27	0/565	0.63	1/761 (0.1%)
26	24	0.27	0/545	0.60	0/737
27	15	0.27	0/469	0.49	0/635
27	25	0.26	0/469	0.51	0/635
28	16	0.26	0/460	0.51	0/613
28	26	0.23	0/456	0.44	0/608
29	17	0.29	0/426	0.51	0/561
29	27	0.23	0/426	0.49	0/561
30	18	0.28	0/525	0.49	0/691
30	28	0.23	0/525	0.44	0/691
31	19	0.25	0/310	0.46	0/407
31	29	0.23	0/310	0.48	0/407
32	1a	0.21	0/35795	0.40	3/55864 (0.0%)
32	2a	0.21	0/35886	0.39	0/56005
33	1b	0.23	0/1881	0.52	1/2542 (0.0%)
33	2b	0.23	0/1860	0.49	0/2518
34	1c	0.22	0/1572	0.45	0/2126
34	2c	0.21	0/1566	0.49	0/2119
35	1d	0.22	0/1685	0.44	0/2262
35	2d	0.21	0/1704	0.46	0/2284
36	1e	0.21	0/1145	0.50	0/1543
36	2e	0.24	0/1149	0.48	0/1548
37	1f	0.19	0/823	0.43	0/1115
37	2f	0.21	0/829	0.42	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
38	1g	0.20	0/1250	0.44	0/1679
38	2g	0.21	0/1254	0.44	0/1683
39	1h	0.19	0/1108	0.43	0/1494
39	2h	0.19	0/1108	0.42	0/1494
40	1i	0.24	0/1002	0.56	1/1346 (0.1%)
40	2i	0.23	0/997	0.50	0/1343
41	1j	0.23	0/722	0.51	0/982
41	2j	0.25	0/727	0.46	0/988
42	1k	0.20	0/844	0.43	0/1145
42	2k	0.26	0/848	0.46	0/1149
43	1l	0.23	0/937	0.44	0/1260
43	2l	0.22	0/937	0.45	0/1260
44	1m	0.23	0/969	0.50	0/1302
44	2m	0.24	0/961	0.50	0/1291
45	1n	0.23	0/501	0.45	0/664
45	2n	0.20	0/501	0.45	0/664
46	1o	0.20	0/739	0.41	0/985
46	2o	0.18	0/739	0.39	0/985
47	1p	0.21	0/697	0.50	0/939
47	2p	0.20	0/693	0.45	0/935
48	1q	0.22	0/836	0.49	0/1117
48	2q	0.21	0/836	0.42	0/1117
49	1r	0.22	0/560	0.48	0/746
49	2r	0.23	0/560	0.41	0/746
50	1s	0.21	0/667	0.54	0/900
50	2s	0.24	0/661	0.56	0/893
51	1t	0.22	0/730	0.47	0/965
51	2t	0.22	0/729	0.51	0/965
52	1u	0.21	0/203	0.48	0/266
52	2u	0.22	0/203	0.47	0/266
53	1v	0.25	0/310	0.36	0/480
53	2v	0.32	0/310	0.42	0/480
54	1x	0.26	0/1725	0.42	0/2689
54	2x	0.26	0/1725	0.42	0/2689
55	1z	0.28	0/150	0.53	0/205
55	2z	0.25	0/150	0.56	0/205
All	All	0.24	0/310535	0.43	12/464522 (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
33	1b	0	1
51	2t	0	1
All	All	0	2

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	1i	96	LEU	N-CA-C	-8.07	105.42	114.62
33	1b	38	GLY	N-CA-C	-6.12	107.22	115.36
32	1a	266	G	P-O3'-C3'	5.63	128.65	120.20
6	2G	148	MET	N-CA-C	-5.45	106.94	113.21
32	1a	266	G	C2'-C3'-O3'	5.37	117.55	109.50

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
33	1b	122	PHE	Peptide
51	2t	9	ASN	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	1A	61852	0	31188	1013	0
1	2A	60322	0	30421	1082	0
2	1B	2577	0	1304	37	0
2	2B	2575	0	1303	72	0
3	1D	2136	0	2218	65	0
3	2D	2136	0	2218	70	0
4	1E	1559	0	1618	53	0
4	2E	1559	0	1618	79	0
5	1F	1584	0	1625	56	0
5	2F	1580	0	1619	73	0
6	1G	1423	0	1436	47	0
6	2G	1428	0	1438	69	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	1H	1330	0	1407	44	0
7	2H	1330	0	1407	41	0
8	1I	1097	0	1140	33	0
8	2I	1064	0	1082	36	0
9	1N	1117	0	1184	17	0
9	2N	1117	0	1184	37	0
10	1O	933	0	996	30	0
10	2O	933	0	996	40	0
11	1P	1135	0	1212	56	0
11	2P	1135	0	1212	48	0
12	1Q	1122	0	1179	25	0
12	2Q	1122	0	1179	37	0
13	1R	968	0	1033	23	1
13	2R	968	0	1033	33	0
14	1S	873	0	927	16	0
14	2S	870	0	923	40	0
15	1T	1091	0	1150	41	0
15	2T	1083	0	1136	44	0
16	1U	959	0	1018	36	0
16	2U	959	0	1019	26	0
17	1V	771	0	829	17	1
17	2V	771	0	830	12	0
18	1W	886	0	940	23	0
18	2W	886	0	940	29	0
19	1X	750	0	814	24	0
19	2X	750	0	814	19	0
20	1Y	806	0	881	33	0
20	2Y	806	0	881	24	0
21	1Z	1240	0	1240	45	0
21	2Z	1271	0	1273	51	0
22	10	604	0	619	17	0
22	20	604	0	619	18	0
23	11	755	0	826	27	0
23	21	755	0	826	25	0
24	12	588	0	643	14	0
24	22	588	0	643	20	0
25	13	469	0	518	19	0
25	23	464	0	514	15	0
26	14	552	0	533	19	0
26	24	532	0	503	28	0
27	15	455	0	465	15	0
27	25	455	0	465	15	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	16	453	0	473	8	0
28	26	449	0	469	15	0
29	17	418	0	467	11	0
29	27	418	0	467	15	0
30	18	517	0	582	27	0
30	28	517	0	582	27	0
31	19	307	0	335	6	0
31	29	307	0	335	15	0
32	1a	32246	0	16296	631	0
32	2a	32327	0	16338	681	0
33	1b	1846	0	1867	66	0
33	2b	1825	0	1828	87	0
34	1c	1548	0	1535	56	0
34	2c	1542	0	1517	62	0
35	1d	1655	0	1672	61	0
35	2d	1674	0	1714	66	0
36	1e	1129	0	1185	46	0
36	2e	1133	0	1191	43	0
37	1f	810	0	804	25	0
37	2f	816	0	808	24	0
38	1g	1231	0	1238	28	0
38	2g	1235	0	1249	42	0
39	1h	1088	0	1126	40	0
39	2h	1088	0	1126	33	0
40	1i	983	0	986	41	0
40	2i	978	0	966	59	0
41	1j	709	0	650	36	0
41	2j	714	0	672	30	0
42	1k	829	0	825	17	0
42	2k	833	0	836	34	0
43	1l	932	0	981	25	0
43	2l	932	0	978	38	0
44	1m	958	0	1002	34	0
44	2m	950	0	988	62	0
45	1n	492	0	529	23	0
45	2n	492	0	529	22	0
46	1o	728	0	760	24	0
46	2o	728	0	760	23	0
47	1p	681	0	697	23	0
47	2p	677	0	686	18	0
48	1q	823	0	891	40	0
48	2q	823	0	891	34	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
49	1r	555	0	618	14	0
49	2r	555	0	618	21	0
50	1s	652	0	662	25	0
50	2s	646	0	644	45	0
51	1t	728	0	798	22	0
51	2t	727	0	796	28	0
52	1u	199	0	208	9	0
52	2u	199	0	208	10	0
53	1v	277	0	140	6	0
53	2v	277	0	140	6	0
54	1x	1625	0	829	18	0
54	2x	1625	0	829	27	0
55	1z	143	0	156	6	0
55	2z	143	0	156	8	0
56	10	8	0	0	0	0
56	11	1	0	0	0	0
56	13	4	0	0	0	0
56	15	7	0	0	0	0
56	16	2	0	0	0	0
56	17	7	0	0	0	0
56	18	3	0	0	0	0
56	19	2	0	0	0	0
56	1A	1041	0	0	0	0
56	1B	31	0	0	0	0
56	1D	10	0	0	0	0
56	1E	9	0	0	0	0
56	1F	9	0	0	0	0
56	1G	4	0	0	0	0
56	1N	2	0	0	0	0
56	1O	2	0	0	0	0
56	1P	4	0	0	0	0
56	1Q	5	0	0	0	0
56	1R	3	0	0	0	0
56	1S	2	0	0	0	0
56	1T	5	0	0	0	0
56	1U	10	0	0	0	0
56	1V	6	0	0	0	0
56	1W	5	0	0	0	0
56	1X	5	0	0	0	0
56	1Y	1	0	0	0	0
56	1Z	2	0	0	0	0
56	1a	221	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	1b	1	0	0	0	0
56	1e	1	0	0	0	0
56	1f	2	0	0	0	0
56	1h	1	0	0	0	0
56	1l	3	0	0	0	0
56	1m	1	0	0	0	0
56	1n	2	0	0	0	0
56	1s	1	0	0	0	0
56	1t	1	0	0	0	0
56	1v	1	0	0	0	0
56	1x	15	0	0	0	0
56	20	3	0	0	0	0
56	23	1	0	0	0	0
56	25	4	0	0	0	0
56	26	1	0	0	0	0
56	27	1	0	0	0	0
56	28	1	0	0	0	0
56	2A	810	0	0	0	0
56	2B	15	0	0	0	0
56	2D	4	0	0	0	0
56	2E	9	0	0	0	0
56	2F	2	0	0	0	0
56	2G	1	0	0	0	0
56	2O	2	0	0	0	0
56	2P	2	0	0	0	0
56	2Q	2	0	0	0	0
56	2R	4	0	0	0	0
56	2T	4	0	0	0	0
56	2U	2	0	0	0	0
56	2V	2	0	0	0	0
56	2W	2	0	0	0	0
56	2X	2	0	0	0	0
56	2Y	1	0	0	0	0
56	2a	217	0	0	0	0
56	2d	1	0	0	0	0
56	2e	1	0	0	0	0
56	2f	1	0	0	0	0
56	2i	1	0	0	0	0
56	2k	1	0	0	0	0
56	2l	1	0	0	0	0
56	2n	1	0	0	0	0
56	2q	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	2r	1	0	0	0	0
56	2t	1	0	0	0	0
56	2v	1	0	0	0	0
56	2x	5	0	0	0	0
57	14	1	0	0	0	0
57	15	1	0	0	0	0
57	16	1	0	0	0	0
57	19	1	0	0	0	0
57	1Y	1	0	0	0	0
57	1n	1	0	0	0	0
57	24	1	0	0	0	0
57	25	1	0	0	0	0
57	26	1	0	0	0	0
57	29	1	0	0	0	0
57	2Y	1	0	0	0	0
57	2n	1	0	0	0	0
58	1d	8	0	0	0	0
58	2d	8	0	0	0	0
59	2A	1	0	0	0	0
60	10	5	0	0	1	0
60	11	6	0	0	0	0
60	13	5	0	0	0	0
60	14	1	0	0	0	0
60	15	5	0	0	3	0
60	16	1	0	0	0	0
60	17	7	0	0	2	0
60	18	12	0	0	2	0
60	19	1	0	0	0	0
60	1A	1949	0	0	178	0
60	1B	50	0	0	5	0
60	1D	21	0	0	2	0
60	1E	14	0	0	1	0
60	1F	9	0	0	0	0
60	1G	1	0	0	0	0
60	1N	3	0	0	0	0
60	1O	4	0	0	0	0
60	1P	17	0	0	2	0
60	1Q	3	0	0	0	0
60	1R	8	0	0	2	0
60	1S	1	0	0	0	0
60	1T	3	0	0	0	0
60	1U	5	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	1V	2	0	0	0	0
60	1W	5	0	0	0	0
60	1X	3	0	0	0	0
60	1Y	1	0	0	1	0
60	1a	301	0	0	20	0
60	1b	1	0	0	0	0
60	1e	1	0	0	0	0
60	1i	1	0	0	0	0
60	1l	4	0	0	1	0
60	1o	1	0	0	0	0
60	1q	3	0	0	0	0
60	1v	5	0	0	0	0
60	1x	16	0	0	0	0
60	1z	3	0	0	0	0
60	21	7	0	0	0	0
60	27	1	0	0	0	0
60	28	3	0	0	0	0
60	2A	917	0	0	122	0
60	2B	4	0	0	1	0
60	2D	14	0	0	2	0
60	2E	10	0	0	3	0
60	2F	12	0	0	0	0
60	2N	1	0	0	0	0
60	2O	2	0	0	0	0
60	2P	8	0	0	0	0
60	2Q	1	0	0	0	0
60	2R	2	0	0	1	0
60	2T	2	0	0	0	0
60	2U	2	0	0	0	0
60	2X	2	0	0	0	0
60	2a	286	0	0	25	0
60	2d	1	0	0	0	0
60	2e	3	0	0	1	0
60	2i	1	0	0	0	0
60	2l	2	0	0	1	0
60	2p	1	0	0	0	0
60	2r	1	0	0	0	0
60	2t	1	0	0	0	0
60	2v	2	0	0	0	0
All	All	293228	0	193672	5977	1

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

The worst 5 of 5977 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)
1:1A:1082:U:H3	1:1A:1086:A:N6	1.42	1.17
32:1a:987:G:H1	32:1a:1218:C:H42	1.09	1.00
9:2N:123:TYR:HH	9:2N:130:HIS:HE2	1.04	1.00
32:2a:1029:C:N4	32:2a:1032:G:H1	1.60	0.98
32:1a:559:A:H4'	32:1a:560:U:H3'	1.47	0.96

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1R:33:ARG:NH2	17:1V:53:GLU:OE2[4_445]	2.18	0.02

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	
3	1D	273/276 (99%)	251 (92%)	21 (8%)	1 (0%)	30	65
3	2D	273/276 (99%)	245 (90%)	27 (10%)	1 (0%)	30	65
4	1E	202/206 (98%)	189 (94%)	12 (6%)	1 (0%)	24	60
4	2E	202/206 (98%)	184 (91%)	15 (7%)	3 (2%)	8	35
5	1F	201/210 (96%)	184 (92%)	16 (8%)	1 (0%)	24	60
5	2F	201/210 (96%)	190 (94%)	10 (5%)	1 (0%)	24	60
6	1G	179/182 (98%)	165 (92%)	10 (6%)	4 (2%)	5	26
6	2G	179/182 (98%)	151 (84%)	26 (14%)	2 (1%)	11	43
7	1H	172/180 (96%)	149 (87%)	20 (12%)	3 (2%)	7	32
7	2H	172/180 (96%)	156 (91%)	12 (7%)	4 (2%)	5	25
8	1I	144/148 (97%)	129 (90%)	15 (10%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	2I	144/148 (97%)	115 (80%)	25 (17%)	4 (3%)	4	21
9	1N	138/140 (99%)	128 (93%)	8 (6%)	2 (1%)	9	36
9	2N	138/140 (99%)	126 (91%)	11 (8%)	1 (1%)	18	53
10	1O	120/122 (98%)	109 (91%)	11 (9%)	0	100	100
10	2O	120/122 (98%)	107 (89%)	12 (10%)	1 (1%)	16	50
11	1P	147/150 (98%)	135 (92%)	10 (7%)	2 (1%)	9	36
11	2P	147/150 (98%)	129 (88%)	18 (12%)	0	100	100
12	1Q	139/141 (99%)	123 (88%)	15 (11%)	1 (1%)	18	53
12	2Q	139/141 (99%)	126 (91%)	12 (9%)	1 (1%)	18	53
13	1R	116/118 (98%)	109 (94%)	5 (4%)	2 (2%)	7	32
13	2R	116/118 (98%)	105 (90%)	10 (9%)	1 (1%)	14	48
14	1S	108/112 (96%)	97 (90%)	10 (9%)	1 (1%)	14	48
14	2S	108/112 (96%)	98 (91%)	8 (7%)	2 (2%)	6	30
15	1T	129/146 (88%)	115 (89%)	11 (8%)	3 (2%)	5	25
15	2T	129/146 (88%)	118 (92%)	10 (8%)	1 (1%)	16	50
16	1U	114/118 (97%)	107 (94%)	7 (6%)	0	100	100
16	2U	114/118 (97%)	108 (95%)	6 (5%)	0	100	100
17	1V	99/101 (98%)	89 (90%)	10 (10%)	0	100	100
17	2V	99/101 (98%)	89 (90%)	9 (9%)	1 (1%)	12	45
18	1W	110/113 (97%)	105 (96%)	3 (3%)	2 (2%)	6	31
18	2W	110/113 (97%)	101 (92%)	9 (8%)	0	100	100
19	1X	93/96 (97%)	85 (91%)	8 (9%)	0	100	100
19	2X	93/96 (97%)	79 (85%)	13 (14%)	1 (1%)	11	43
20	1Y	105/110 (96%)	94 (90%)	9 (9%)	2 (2%)	6	30
20	2Y	105/110 (96%)	90 (86%)	14 (13%)	1 (1%)	12	45
21	1Z	148/206 (72%)	127 (86%)	20 (14%)	1 (1%)	18	53
21	2Z	156/206 (76%)	130 (83%)	24 (15%)	2 (1%)	9	38
22	10	74/85 (87%)	69 (93%)	5 (7%)	0	100	100
22	20	74/85 (87%)	65 (88%)	8 (11%)	1 (1%)	9	36
23	11	95/98 (97%)	92 (97%)	3 (3%)	0	100	100
23	21	95/98 (97%)	90 (95%)	5 (5%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
24	12	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
24	22	68/72 (94%)	65 (96%)	2 (3%)	1 (2%)	8	35
25	13	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
25	23	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
26	14	67/71 (94%)	50 (75%)	12 (18%)	5 (8%)	1	4
26	24	67/71 (94%)	48 (72%)	15 (22%)	4 (6%)	1	7
27	15	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
27	25	57/60 (95%)	57 (100%)	0	0	100	100
28	16	51/54 (94%)	50 (98%)	1 (2%)	0	100	100
28	26	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
29	17	46/49 (94%)	44 (96%)	2 (4%)	0	100	100
29	27	46/49 (94%)	44 (96%)	2 (4%)	0	100	100
30	18	62/65 (95%)	59 (95%)	3 (5%)	0	100	100
30	28	62/65 (95%)	58 (94%)	4 (6%)	0	100	100
31	19	35/37 (95%)	35 (100%)	0	0	100	100
31	29	35/37 (95%)	31 (89%)	4 (11%)	0	100	100
33	1b	229/256 (90%)	198 (86%)	24 (10%)	7 (3%)	3	19
33	2b	229/256 (90%)	182 (80%)	38 (17%)	9 (4%)	2	14
34	1c	204/239 (85%)	179 (88%)	23 (11%)	2 (1%)	12	45
34	2c	204/239 (85%)	165 (81%)	33 (16%)	6 (3%)	3	20
35	1d	206/209 (99%)	191 (93%)	15 (7%)	0	100	100
35	2d	206/209 (99%)	183 (89%)	21 (10%)	2 (1%)	12	45
36	1e	146/162 (90%)	130 (89%)	12 (8%)	4 (3%)	4	22
36	2e	146/162 (90%)	130 (89%)	15 (10%)	1 (1%)	18	53
37	1f	98/101 (97%)	85 (87%)	13 (13%)	0	100	100
37	2f	98/101 (97%)	93 (95%)	4 (4%)	1 (1%)	12	45
38	1g	153/156 (98%)	130 (85%)	21 (14%)	2 (1%)	9	38
38	2g	153/156 (98%)	132 (86%)	17 (11%)	4 (3%)	4	23
39	1h	135/138 (98%)	121 (90%)	14 (10%)	0	100	100
39	2h	135/138 (98%)	121 (90%)	14 (10%)	0	100	100
40	1i	125/128 (98%)	109 (87%)	13 (10%)	3 (2%)	4	24

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	2i	125/128 (98%)	104 (83%)	20 (16%)	1 (1%)	16	50
41	1j	95/105 (90%)	78 (82%)	13 (14%)	4 (4%)	2	13
41	2j	94/105 (90%)	79 (84%)	13 (14%)	2 (2%)	5	27
42	1k	112/129 (87%)	100 (89%)	12 (11%)	0	100	100
42	2k	112/129 (87%)	88 (79%)	19 (17%)	5 (4%)	2	12
43	1l	119/132 (90%)	104 (87%)	15 (13%)	0	100	100
43	2l	119/132 (90%)	103 (87%)	15 (13%)	1 (1%)	16	50
44	1m	121/126 (96%)	106 (88%)	12 (10%)	3 (2%)	4	23
44	2m	120/126 (95%)	96 (80%)	20 (17%)	4 (3%)	3	17
45	1n	58/61 (95%)	49 (84%)	9 (16%)	0	100	100
45	2n	58/61 (95%)	49 (84%)	8 (14%)	1 (2%)	7	32
46	1o	86/89 (97%)	79 (92%)	6 (7%)	1 (1%)	10	40
46	2o	86/89 (97%)	76 (88%)	10 (12%)	0	100	100
47	1p	80/88 (91%)	70 (88%)	9 (11%)	1 (1%)	9	38
47	2p	80/88 (91%)	69 (86%)	10 (12%)	1 (1%)	9	38
48	1q	97/105 (92%)	79 (81%)	18 (19%)	0	100	100
48	2q	97/105 (92%)	85 (88%)	12 (12%)	0	100	100
49	1r	66/88 (75%)	59 (89%)	5 (8%)	2 (3%)	3	19
49	2r	66/88 (75%)	64 (97%)	2 (3%)	0	100	100
50	1s	81/93 (87%)	68 (84%)	13 (16%)	0	100	100
50	2s	81/93 (87%)	63 (78%)	17 (21%)	1 (1%)	10	40
51	1t	94/106 (89%)	79 (84%)	10 (11%)	5 (5%)	1	9
51	2t	94/106 (89%)	82 (87%)	8 (8%)	4 (4%)	2	12
52	1u	21/27 (78%)	19 (90%)	2 (10%)	0	100	100
52	2u	21/27 (78%)	17 (81%)	3 (14%)	1 (5%)	2	11
55	1z	14/16 (88%)	14 (100%)	0	0	100	100
55	2z	14/16 (88%)	14 (100%)	0	0	100	100
All	All	11384/12160 (94%)	10116 (89%)	1126 (10%)	142 (1%)	10	40

5 of 142 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	1F	130	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	1H	126	PRO
11	1P	53	GLY
12	1Q	60	ARG
21	1Z	52	SER

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
3	1D	215/218 (99%)	192 (89%)	23 (11%)	6 26
3	2D	215/218 (99%)	183 (85%)	32 (15%)	3 15
4	1E	164/166 (99%)	148 (90%)	16 (10%)	7 30
4	2E	164/166 (99%)	147 (90%)	17 (10%)	7 28
5	1F	160/166 (96%)	138 (86%)	22 (14%)	3 17
5	2F	159/166 (96%)	145 (91%)	14 (9%)	9 35
6	1G	143/156 (92%)	122 (85%)	21 (15%)	3 15
6	2G	143/156 (92%)	125 (87%)	18 (13%)	4 20
7	1H	144/148 (97%)	132 (92%)	12 (8%)	10 37
7	2H	144/148 (97%)	128 (89%)	16 (11%)	6 25
8	1I	113/124 (91%)	96 (85%)	17 (15%)	3 14
8	2I	105/124 (85%)	88 (84%)	17 (16%)	2 12
9	1N	118/119 (99%)	104 (88%)	14 (12%)	5 22
9	2N	118/119 (99%)	104 (88%)	14 (12%)	5 22
10	1O	100/100 (100%)	91 (91%)	9 (9%)	9 34
10	2O	100/100 (100%)	91 (91%)	9 (9%)	9 34
11	1P	115/116 (99%)	102 (89%)	13 (11%)	5 24
11	2P	115/116 (99%)	99 (86%)	16 (14%)	3 17
12	1Q	111/111 (100%)	102 (92%)	9 (8%)	11 38
12	2Q	111/111 (100%)	91 (82%)	20 (18%)	2 10

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	1R	101/101 (100%)	87 (86%)	14 (14%)	3	17
13	2R	101/101 (100%)	91 (90%)	10 (10%)	7	30
14	1S	86/88 (98%)	74 (86%)	12 (14%)	3	16
14	2S	85/88 (97%)	78 (92%)	7 (8%)	10	37
15	1T	115/127 (91%)	107 (93%)	8 (7%)	14	44
15	2T	113/127 (89%)	106 (94%)	7 (6%)	16	49
16	1U	93/94 (99%)	85 (91%)	8 (9%)	10	36
16	2U	93/94 (99%)	87 (94%)	6 (6%)	15	47
17	1V	80/82 (98%)	71 (89%)	9 (11%)	5	24
17	2V	80/82 (98%)	72 (90%)	8 (10%)	7	29
18	1W	90/92 (98%)	83 (92%)	7 (8%)	11	39
18	2W	90/92 (98%)	80 (89%)	10 (11%)	6	25
19	1X	77/78 (99%)	72 (94%)	5 (6%)	15	47
19	2X	77/78 (99%)	73 (95%)	4 (5%)	21	55
20	1Y	85/91 (93%)	74 (87%)	11 (13%)	4	19
20	2Y	85/91 (93%)	73 (86%)	12 (14%)	3	16
21	1Z	135/179 (75%)	120 (89%)	15 (11%)	6	25
21	2Z	137/179 (76%)	109 (80%)	28 (20%)	1	7
22	10	61/67 (91%)	59 (97%)	2 (3%)	33	67
22	20	61/67 (91%)	56 (92%)	5 (8%)	10	37
23	11	80/83 (96%)	75 (94%)	5 (6%)	16	48
23	21	80/83 (96%)	73 (91%)	7 (9%)	9	35
24	12	65/67 (97%)	57 (88%)	8 (12%)	4	21
24	22	65/67 (97%)	59 (91%)	6 (9%)	8	33
25	13	51/52 (98%)	44 (86%)	7 (14%)	3	17
25	23	50/52 (96%)	44 (88%)	6 (12%)	5	22
26	14	59/63 (94%)	48 (81%)	11 (19%)	1	9
26	24	53/63 (84%)	48 (91%)	5 (9%)	8	32
27	15	50/52 (96%)	43 (86%)	7 (14%)	3	16
27	25	50/52 (96%)	47 (94%)	3 (6%)	17	50
28	16	51/52 (98%)	44 (86%)	7 (14%)	3	17

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	26	50/52 (96%)	40 (80%)	10 (20%)	1	7
29	17	41/42 (98%)	38 (93%)	3 (7%)	13	42
29	27	41/42 (98%)	34 (83%)	7 (17%)	2	11
30	18	54/55 (98%)	49 (91%)	5 (9%)	8	32
30	28	54/55 (98%)	49 (91%)	5 (9%)	8	32
31	19	34/34 (100%)	30 (88%)	4 (12%)	5	22
31	29	34/34 (100%)	30 (88%)	4 (12%)	5	22
33	1b	192/220 (87%)	165 (86%)	27 (14%)	3	16
33	2b	187/220 (85%)	159 (85%)	28 (15%)	3	14
34	1c	142/188 (76%)	128 (90%)	14 (10%)	7	30
34	2c	140/188 (74%)	115 (82%)	25 (18%)	2	10
35	1d	169/181 (93%)	144 (85%)	25 (15%)	3	15
35	2d	173/181 (96%)	159 (92%)	14 (8%)	11	38
36	1e	113/123 (92%)	103 (91%)	10 (9%)	9	35
36	2e	114/123 (93%)	100 (88%)	14 (12%)	4	21
37	1f	84/90 (93%)	76 (90%)	8 (10%)	8	31
37	2f	85/90 (94%)	74 (87%)	11 (13%)	4	19
38	1g	119/127 (94%)	113 (95%)	6 (5%)	22	56
38	2g	120/127 (94%)	111 (92%)	9 (8%)	12	41
39	1h	114/119 (96%)	102 (90%)	12 (10%)	6	27
39	2h	114/119 (96%)	105 (92%)	9 (8%)	11	39
40	1i	90/99 (91%)	74 (82%)	16 (18%)	2	10
40	2i	89/99 (90%)	77 (86%)	12 (14%)	4	18
41	1j	66/92 (72%)	57 (86%)	9 (14%)	3	17
41	2j	69/92 (75%)	61 (88%)	8 (12%)	5	23
42	1k	82/99 (83%)	73 (89%)	9 (11%)	6	25
42	2k	83/99 (84%)	72 (87%)	11 (13%)	4	18
43	1l	96/108 (89%)	86 (90%)	10 (10%)	7	28
43	2l	96/108 (89%)	85 (88%)	11 (12%)	5	24
44	1m	93/101 (92%)	83 (89%)	10 (11%)	6	26
44	2m	92/101 (91%)	81 (88%)	11 (12%)	5	22

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
45	1n	49/50 (98%)	43 (88%)	6 (12%)	5	21
45	2n	49/50 (98%)	44 (90%)	5 (10%)	7	29
46	1o	78/80 (98%)	70 (90%)	8 (10%)	7	28
46	2o	78/80 (98%)	68 (87%)	10 (13%)	4	19
47	1p	69/74 (93%)	60 (87%)	9 (13%)	4	19
47	2p	68/74 (92%)	59 (87%)	9 (13%)	4	18
48	1q	94/97 (97%)	85 (90%)	9 (10%)	8	31
48	2q	94/97 (97%)	88 (94%)	6 (6%)	16	48
49	1r	59/77 (77%)	53 (90%)	6 (10%)	7	29
49	2r	59/77 (77%)	49 (83%)	10 (17%)	2	11
50	1s	69/80 (86%)	65 (94%)	4 (6%)	18	51
50	2s	67/80 (84%)	59 (88%)	8 (12%)	5	22
51	1t	70/82 (85%)	62 (89%)	8 (11%)	5	24
51	2t	70/82 (85%)	61 (87%)	9 (13%)	4	19
52	1u	18/22 (82%)	17 (94%)	1 (6%)	19	52
52	2u	18/22 (82%)	16 (89%)	2 (11%)	6	25
55	1z	15/16 (94%)	15 (100%)	0	100	100
55	2z	15/16 (94%)	12 (80%)	3 (20%)	1	7
All	All	9325/10096 (92%)	8266 (89%)	1059 (11%)	5	24

5 of 1059 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
38	2g	9	VAL
40	2i	89	ASN
37	2f	95	GLU
50	2s	31	ILE
38	1g	24	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 135 such sidechains are listed below:

Mol	Chain	Res	Type
38	2g	106	GLN
40	2i	29	ASN
50	2s	57	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
37	1f	73	ASN
36	1e	78	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2864/2915 (98%)	499 (17%)	29 (1%)
1	2A	2791/2915 (95%)	526 (18%)	21 (0%)
2	1B	120/121 (99%)	14 (11%)	1 (0%)
2	2B	118/121 (97%)	31 (26%)	0
32	1a	1497/1521 (98%)	278 (18%)	0
32	2a	1501/1521 (98%)	272 (18%)	0
53	1v	12/24 (50%)	6 (50%)	0
53	2v	12/24 (50%)	4 (33%)	0
54	1x	75/77 (97%)	11 (14%)	0
54	2x	75/77 (97%)	13 (17%)	0
All	All	9065/9316 (97%)	1654 (18%)	51 (0%)

5 of 1654 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	12	U
1	1A	13	A
1	1A	34	C
1	1A	36	G
1	1A	45	C

5 of 51 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	2756	U
1	2A	752	A
1	2A	2351	G
2	1B	1	U
1	2A	271(M)	G

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

56 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	$\#\|Z\| > 2$
32	MA6	2a	1519	32	23,26,27	1.52	5 (21%)	33,38,41	2.23	11 (33%)
1	2MU	1A	2552	56,1	19,22,24	1.21	2 (10%)	25,31,36	2.03	6 (24%)
1	5MU	1A	1915	1	19,22,23	1.47	4 (21%)	27,32,35	2.12	7 (25%)
43	0TD	1l	92	43	8,9,10	4.46	1 (12%)	6,11,13	3.45	2 (33%)
32	5MC	2a	1407	32	19,22,23	1.48	3 (15%)	26,32,35	1.15	3 (11%)
32	MA6	1a	1518	32	23,26,27	1.52	5 (21%)	33,38,41	2.30	14 (42%)
54	4SU	1x	8	54	18,21,22	2.09	4 (22%)	25,30,33	1.54	2 (8%)
1	5MC	1A	1962	56,1	19,22,23	1.64	3 (15%)	26,32,35	1.09	2 (7%)
1	PSU	2A	1917	1	18,21,22	1.39	2 (11%)	21,30,33	2.09	3 (14%)
1	2MU	2A	2552	56,1	19,22,24	1.29	3 (15%)	25,31,36	1.92	6 (24%)
32	4OC	1a	1402	32	20,23,24	0.74	0	25,32,35	0.91	1 (4%)
1	PSU	1A	1917	1	18,21,22	1.36	2 (11%)	21,30,33	1.97	3 (14%)
32	7MG	1a	527	56,32	23,26,27	1.38	4 (17%)	27,39,42	2.54	7 (25%)
1	PSU	1A	2605	1	18,21,22	1.39	3 (16%)	21,30,33	1.86	4 (19%)
32	M2G	1a	966	32	24,27,28	1.27	4 (16%)	33,40,43	1.89	6 (18%)
1	5MU	2A	1915	56,1	19,22,23	1.44	6 (31%)	27,32,35	2.09	7 (25%)
54	4SU	2x	8	54	18,21,22	2.04	6 (33%)	25,30,33	1.64	6 (24%)
1	4OC	1A	1920	1	19,22,24	0.84	0	25,31,35	0.98	1 (4%)
1	OMG	1A	2251	56,54,1	23,26,27	1.26	3 (13%)	32,38,41	2.05	6 (18%)
1	5MC	2A	1962	56,1	19,22,23	1.56	3 (15%)	26,32,35	1.25	3 (11%)
32	5MC	1a	967	32	19,22,23	1.68	3 (15%)	26,32,35	1.05	3 (11%)
32	7MG	2a	527	32	23,26,27	1.35	4 (17%)	27,39,42	2.54	7 (25%)
1	5MU	2A	1939	1	19,22,23	1.50	5 (26%)	27,32,35	2.33	8 (29%)
32	5MC	2a	1404	32	19,22,23	1.55	3 (15%)	26,32,35	1.08	2 (7%)
32	PSU	2a	516	32	18,21,22	1.37	2 (11%)	21,30,33	1.98	4 (19%)
32	5MC	1a	1407	32	19,22,23	1.47	2 (10%)	26,32,35	1.11	2 (7%)
32	4OC	2a	1402	56,32	20,23,24	0.77	0	25,32,35	0.99	2 (8%)
1	OMG	2A	2251	56,54,1	23,26,27	1.23	3 (13%)	32,38,41	1.98	5 (15%)
1	PSU	2A	2605	1	18,21,22	1.39	3 (16%)	21,30,33	2.00	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
32	PSU	1a	516	56,32	18,21,22	1.39	2 (11%)	21,30,33	1.96	4 (19%)
32	UR3	1a	1498	32	19,22,23	1.03	1 (5%)	26,32,35	1.82	4 (15%)
54	PSU	1x	55	56,54	18,21,22	1.32	2 (11%)	21,30,33	2.09	4 (19%)
32	2MG	2a	1207	32	23,26,27	1.24	3 (13%)	33,38,41	2.10	8 (24%)
54	5MC	2x	32	54	19,22,23	1.45	3 (15%)	26,32,35	1.16	2 (7%)
1	5MC	1A	1942	56,1	19,22,23	1.57	3 (15%)	26,32,35	1.08	2 (7%)
32	5MC	2a	967	32	19,22,23	1.72	2 (10%)	26,32,35	1.11	3 (11%)
1	PSU	1A	1911	1	18,21,22	1.39	3 (16%)	21,30,33	2.00	3 (14%)
32	MA6	1a	1519	32	23,26,27	1.54	5 (21%)	33,38,41	2.24	11 (33%)
1	4OC	2A	1920	1	19,22,24	0.77	0	25,31,35	1.11	2 (8%)
1	5MC	2A	1942	1	19,22,23	1.65	3 (15%)	26,32,35	1.18	2 (7%)
32	MA6	2a	1518	32	23,26,27	1.57	5 (21%)	33,38,41	2.26	13 (39%)
32	5MC	2a	1400	32	19,22,23	1.76	3 (15%)	26,32,35	1.16	3 (11%)
54	5MC	1x	32	54	19,22,23	1.77	3 (15%)	26,32,35	1.39	4 (15%)
1	2MA	1A	2503	56,1	22,25,26	1.43	5 (22%)	32,37,40	2.31	9 (28%)
54	5MU	2x	54	54	19,22,23	1.44	4 (21%)	27,32,35	2.01	6 (22%)
32	2MG	1a	1207	32	23,26,27	1.27	4 (17%)	33,38,41	2.23	8 (24%)
1	5MU	1A	1939	1	19,22,23	1.46	6 (31%)	27,32,35	2.03	5 (18%)
1	2MA	2A	2503	56,1	22,25,26	1.48	5 (22%)	32,37,40	2.19	9 (28%)
43	0TD	2l	92	43	8,9,10	4.62	2 (25%)	6,11,13	9.45	1 (16%)
32	M2G	2a	966	32	24,27,28	1.36	4 (16%)	33,40,43	1.89	5 (15%)
54	PSU	2x	55	54	18,21,22	1.36	2 (11%)	21,30,33	1.94	4 (19%)
32	UR3	2a	1498	32	19,22,23	0.96	0	26,32,35	1.83	3 (11%)
1	PSU	2A	1911	1	18,21,22	1.37	3 (16%)	21,30,33	1.98	3 (14%)
32	5MC	1a	1400	32	19,22,23	1.94	3 (15%)	26,32,35	1.21	4 (15%)
32	5MC	1a	1404	32	19,22,23	1.80	3 (15%)	26,32,35	1.22	5 (19%)
54	5MU	1x	54	54	19,22,23	1.39	5 (26%)	27,32,35	1.91	6 (22%)

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
32	MA6	2a	1519	32	-	5/11/29/30	0/3/3/3
1	2MU	1A	2552	56,1	-	0/9/27/28	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5MU	1A	1915	1	-	2/7/25/26	0/2/2/2
43	0TD	1l	92	43	-	2/7/12/14	-
32	5MC	2a	1407	32	-	0/7/25/26	0/2/2/2
32	MA6	1a	1518	32	-	3/11/29/30	0/3/3/3
54	4SU	1x	8	54	-	0/7/25/26	0/2/2/2
1	5MC	1A	1962	56,1	-	0/7/25/26	0/2/2/2
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
1	2MU	2A	2552	56,1	-	1/9/27/28	0/2/2/2
32	4OC	1a	1402	32	-	3/9/29/30	0/2/2/2
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
32	7MG	1a	527	56,32	-	2/7/37/38	0/3/3/3
1	PSU	1A	2605	1	-	0/7/25/26	0/2/2/2
32	M2G	1a	966	32	-	0/11/29/30	0/3/3/3
1	5MU	2A	1915	56,1	-	0/7/25/26	0/2/2/2
54	4SU	2x	8	54	-	0/7/25/26	0/2/2/2
1	4OC	1A	1920	1	-	0/9/27/30	0/2/2/2
1	OMG	1A	2251	56,54,1	-	0/9/27/28	0/3/3/3
1	5MC	2A	1962	56,1	-	2/7/25/26	0/2/2/2
32	5MC	1a	967	32	-	1/7/25/26	0/2/2/2
32	7MG	2a	527	32	-	2/7/37/38	0/3/3/3
1	5MU	2A	1939	1	-	0/7/25/26	0/2/2/2
32	5MC	2a	1404	32	-	0/7/25/26	0/2/2/2
32	PSU	2a	516	32	-	0/7/25/26	0/2/2/2
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
32	4OC	2a	1402	56,32	-	3/9/29/30	0/2/2/2
1	OMG	2A	2251	56,54,1	-	1/9/27/28	0/3/3/3
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
32	PSU	1a	516	56,32	-	0/7/25/26	0/2/2/2
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
54	PSU	1x	55	56,54	-	0/7/25/26	0/2/2/2
32	2MG	2a	1207	32	-	0/9/27/28	0/3/3/3
54	5MC	2x	32	54	-	0/7/25/26	0/2/2/2
1	5MC	1A	1942	56,1	-	0/7/25/26	0/2/2/2
32	5MC	2a	967	32	-	0/7/25/26	0/2/2/2
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
32	MA6	1a	1519	32	-	4/11/29/30	0/3/3/3
1	4OC	2A	1920	1	-	2/9/27/30	0/2/2/2
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
32	MA6	2a	1518	32	-	3/11/29/30	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	5MC	2a	1400	32	-	2/7/25/26	0/2/2/2
54	5MC	1x	32	54	-	0/7/25/26	0/2/2/2
1	2MA	1A	2503	56,1	-	2/7/25/26	0/3/3/3
54	5MU	2x	54	54	-	0/7/25/26	0/2/2/2
32	2MG	1a	1207	32	-	0/9/27/28	0/3/3/3
1	5MU	1A	1939	1	-	0/7/25/26	0/2/2/2
1	2MA	2A	2503	56,1	-	0/7/25/26	0/3/3/3
43	0TD	2l	92	43	-	3/7/12/14	-
32	M2G	2a	966	32	-	4/11/29/30	0/3/3/3
54	PSU	2x	55	54	-	0/7/25/26	0/2/2/2
32	UR3	2a	1498	32	-	0/7/25/26	0/2/2/2
1	PSU	2A	1911	1	-	1/7/25/26	0/2/2/2
32	5MC	1a	1400	32	-	0/7/25/26	0/2/2/2
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
54	5MU	1x	54	54	-	0/7/25/26	0/2/2/2

The worst 5 of 172 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	2l	92	0TD	CB-SB	-12.38	1.69	1.82
43	1l	92	0TD	CB-SB	-12.16	1.70	1.82
32	1a	1400	5MC	C5-C4	7.33	1.49	1.44
32	1a	1404	5MC	C5-C4	6.66	1.49	1.44
32	2a	1400	5MC	C5-C4	6.48	1.49	1.44

The worst 5 of 270 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	2l	92	0TD	CSB-SB-CB	-23.03	60.97	102.36
32	1a	527	7MG	N9-C4-N3	8.81	138.37	125.46
32	2a	527	7MG	N9-C4-N3	8.48	137.89	125.46
1	1A	2503	2MA	C5-C4-N3	-8.09	118.65	127.18
1	2A	2503	2MA	C5-C4-N3	-7.88	118.88	127.18

There are no chirality outliers.

5 of 48 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	1a	1518	MA6	C5-C6-N6-C9
32	1a	1519	MA6	O4'-C4'-C5'-O5'
1	2A	2251	OMG	C1'-C2'-O2'-CM2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
32	2a	966	M2G	N1-C2-N2-CM2
32	2a	966	M2G	N3-C2-N2-CM1

There are no ring outliers.

27 monomers are involved in 40 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	2a	1519	MA6	4	0
1	1A	2552	2MU	2	0
43	1l	92	0TD	1	0
32	2a	1407	5MC	1	0
32	1a	1518	MA6	2	0
54	1x	8	4SU	2	0
1	2A	1917	PSU	1	0
1	2A	2552	2MU	2	0
32	1a	1402	4OC	2	0
54	2x	8	4SU	2	0
1	1A	1920	4OC	1	0
1	1A	2251	OMG	1	0
1	2A	1939	5MU	1	0
32	2a	1404	5MC	1	0
32	2a	1402	4OC	1	0
1	2A	2251	OMG	1	0
32	1a	1498	UR3	1	0
32	2a	967	5MC	3	0
32	1a	1519	MA6	2	0
1	2A	1920	4OC	1	0
32	2a	1518	MA6	4	0
54	1x	32	5MC	1	0
32	1a	1207	2MG	2	0
1	1A	1939	5MU	1	0
1	2A	2503	2MA	4	0
43	2l	92	0TD	1	0
32	2a	966	M2G	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2563 ligands modelled in this entry, 2561 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
58	SF4	2d	302	35	0,12,12	-	-	-		
58	SF4	1d	501	35	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
58	SF4	2d	302	35	-	-	0/6/5/5
58	SF4	1d	501	35	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	1A	2860/2915 (98%)	-0.48	48 (1%)	69	45	28, 46, 94, 110	0
1	2A	2789/2915 (95%)	-0.31	35 (1%)	75	53	39, 62, 93, 108	0
2	1B	120/121 (99%)	-0.65	0	100	100	37, 56, 68, 89	0
2	2B	120/121 (99%)	0.09	1 (0%)	82	64	62, 80, 90, 95	0
3	1D	275/276 (99%)	-0.03	2 (0%)	84	66	30, 47, 59, 71	0
3	2D	275/276 (99%)	0.11	4 (1%)	72	49	40, 56, 69, 75	0
4	1E	204/206 (99%)	-0.23	1 (0%)	87	72	33, 47, 62, 76	0
4	2E	204/206 (99%)	-0.06	0	100	100	41, 62, 71, 78	0
5	1F	203/210 (96%)	-0.24	0	100	100	31, 49, 67, 83	0
5	2F	203/210 (96%)	-0.04	2 (0%)	79	59	46, 66, 79, 85	0
6	1G	181/182 (99%)	-0.18	1 (0%)	85	69	44, 60, 71, 85	0
6	2G	181/182 (99%)	0.58	6 (3%)	49	28	69, 80, 87, 93	0
7	1H	174/180 (96%)	-0.14	0	100	100	43, 58, 69, 75	0
7	2H	174/180 (96%)	0.21	2 (1%)	78	57	66, 79, 88, 95	0
8	1I	146/148 (98%)	-0.12	1 (0%)	84	66	48, 70, 78, 85	0
8	2I	146/148 (98%)	0.21	0	100	100	59, 75, 84, 89	0
9	1N	140/140 (100%)	-0.16	0	100	100	35, 48, 62, 70	0
9	2N	140/140 (100%)	0.13	0	100	100	51, 66, 80, 87	0
10	1O	122/122 (100%)	-0.21	0	100	100	36, 50, 62, 68	0
10	2O	122/122 (100%)	-0.08	1 (0%)	82	64	48, 58, 68, 73	0
11	1P	149/150 (99%)	-0.09	0	100	100	33, 52, 68, 74	0
11	2P	149/150 (99%)	0.08	3 (2%)	65	41	42, 66, 79, 84	0
12	1Q	141/141 (100%)	-0.09	1 (0%)	84	66	38, 50, 60, 66	0
12	2Q	141/141 (100%)	0.28	3 (2%)	63	40	51, 65, 75, 83	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
13	1R	118/118 (100%)	-0.21	1 (0%)	82	64	35, 44, 56, 67	0
13	2R	118/118 (100%)	0.02	1 (0%)	82	64	48, 58, 67, 77	0
14	1S	110/112 (98%)	-0.13	0	100	100	44, 53, 62, 66	0
14	2S	110/112 (98%)	0.36	0	100	100	62, 74, 82, 87	0
15	1T	131/146 (89%)	-0.14	1 (0%)	82	64	41, 53, 69, 82	0
15	2T	131/146 (89%)	0.01	3 (2%)	61	38	52, 62, 75, 83	0
16	1U	116/118 (98%)	-0.27	0	100	100	33, 42, 54, 69	0
16	2U	116/118 (98%)	-0.05	0	100	100	48, 64, 74, 82	0
17	1V	101/101 (100%)	-0.43	0	100	100	33, 47, 63, 74	0
17	2V	101/101 (100%)	-0.10	0	100	100	54, 68, 78, 86	0
18	1W	112/113 (99%)	-0.27	1 (0%)	81	61	34, 42, 56, 77	0
18	2W	112/113 (99%)	-0.10	0	100	100	43, 55, 68, 76	0
19	1X	95/96 (98%)	-0.10	0	100	100	34, 46, 61, 78	0
19	2X	95/96 (98%)	0.26	2 (2%)	63	40	48, 66, 77, 80	0
20	1Y	107/110 (97%)	-0.17	1 (0%)	81	61	41, 54, 70, 77	0
20	2Y	107/110 (97%)	0.45	3 (2%)	55	32	61, 72, 79, 87	0
21	1Z	154/206 (74%)	-0.04	0	100	100	45, 62, 74, 83	0
21	2Z	160/206 (77%)	0.28	0	100	100	64, 75, 83, 87	0
22	10	76/85 (89%)	-0.15	1 (1%)	75	53	37, 47, 56, 61	0
22	20	76/85 (89%)	0.28	2 (2%)	57	34	55, 64, 71, 79	0
23	11	97/98 (98%)	0.07	2 (2%)	63	40	36, 51, 70, 80	0
23	21	97/98 (98%)	0.17	1 (1%)	79	59	48, 62, 75, 77	0
24	12	70/72 (97%)	-0.08	0	100	100	40, 54, 63, 72	0
24	22	70/72 (97%)	-0.05	1 (1%)	73	51	60, 71, 77, 79	0
25	13	59/60 (98%)	-0.35	0	100	100	37, 45, 62, 71	0
25	23	59/60 (98%)	-0.05	0	100	100	53, 66, 79, 88	0
26	14	69/71 (97%)	-0.02	1 (1%)	73	51	57, 73, 84, 94	0
26	24	69/71 (97%)	0.43	4 (5%)	29	15	70, 83, 91, 95	0
27	15	59/60 (98%)	-0.24	0	100	100	33, 42, 57, 71	0
27	25	59/60 (98%)	-0.02	0	100	100	48, 56, 67, 71	0
28	16	53/54 (98%)	-0.49	0	100	100	40, 47, 57, 63	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
28	26	53/54 (98%)	0.11	0	100	100	55, 62, 72, 79	0
29	17	48/49 (97%)	0.09	3 (6%)	26	13	32, 41, 60, 69	0
29	27	48/49 (97%)	0.28	3 (6%)	26	13	45, 51, 73, 80	0
30	18	64/65 (98%)	-0.26	0	100	100	34, 43, 52, 64	0
30	28	64/65 (98%)	0.06	0	100	100	49, 59, 67, 73	0
31	19	37/37 (100%)	0.15	1 (2%)	56	33	39, 50, 66, 73	0
31	29	37/37 (100%)	0.37	2 (5%)	31	16	61, 68, 78, 80	0
32	1a	1488/1521 (97%)	-0.16	12 (0%)	82	64	44, 72, 92, 106	0
32	2a	1491/1521 (98%)	-0.07	11 (0%)	84	66	56, 77, 95, 106	0
33	1b	231/256 (90%)	0.23	3 (1%)	75	53	65, 77, 87, 92	0
33	2b	231/256 (90%)	0.49	8 (3%)	47	27	67, 83, 89, 95	0
34	1c	206/239 (86%)	0.12	2 (0%)	79	59	63, 74, 82, 90	0
34	2c	206/239 (86%)	0.35	6 (2%)	53	31	66, 81, 89, 92	0
35	1d	208/209 (99%)	0.27	2 (0%)	79	59	62, 73, 81, 91	0
35	2d	208/209 (99%)	0.25	1 (0%)	87	72	62, 74, 80, 86	0
36	1e	148/162 (91%)	0.04	2 (1%)	73	51	56, 68, 77, 80	0
36	2e	148/162 (91%)	0.07	1 (0%)	84	66	63, 74, 81, 88	0
37	1f	100/101 (99%)	0.04	0	100	100	58, 70, 78, 79	0
37	2f	100/101 (99%)	-0.09	0	100	100	56, 70, 80, 82	0
38	1g	155/156 (99%)	-0.06	1 (0%)	85	69	64, 72, 83, 88	0
38	2g	155/156 (99%)	0.19	2 (1%)	75	53	70, 79, 90, 104	0
39	1h	137/138 (99%)	0.14	2 (1%)	72	49	61, 69, 76, 81	0
39	2h	137/138 (99%)	0.21	1 (0%)	84	66	65, 75, 82, 86	0
40	1i	127/128 (99%)	0.52	6 (4%)	36	19	60, 76, 82, 86	0
40	2i	127/128 (99%)	0.68	6 (4%)	36	19	69, 83, 90, 92	0
41	1j	97/105 (92%)	0.50	2 (2%)	63	40	64, 78, 86, 93	0
41	2j	96/105 (91%)	0.87	9 (9%)	14	7	71, 84, 90, 92	0
42	1k	114/129 (88%)	0.01	0	100	100	53, 69, 80, 82	0
42	2k	114/129 (88%)	0.07	0	100	100	64, 73, 79, 84	0
43	1l	121/132 (91%)	0.17	0	100	100	53, 64, 73, 77	0
43	2l	121/132 (91%)	0.22	1 (0%)	82	64	58, 67, 76, 84	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
44	1m	123/126 (97%)	0.22	4 (3%) 49 28	62, 72, 80, 94	0
44	2m	122/126 (96%)	0.56	4 (3%) 49 28	71, 80, 86, 102	0
45	1n	60/61 (98%)	0.47	1 (1%) 69 45	65, 72, 78, 81	0
45	2n	60/61 (98%)	1.10	7 (11%) 9 5	72, 82, 88, 91	0
46	1o	88/89 (98%)	0.15	1 (1%) 78 57	55, 66, 79, 84	0
46	2o	88/89 (98%)	0.02	0 100 100	62, 71, 79, 84	0
47	1p	82/88 (93%)	0.68	2 (2%) 59 36	59, 75, 83, 87	0
47	2p	82/88 (93%)	0.35	0 100 100	60, 70, 79, 83	0
48	1q	99/105 (94%)	0.15	1 (1%) 79 59	58, 68, 78, 82	0
48	2q	99/105 (94%)	0.28	3 (3%) 52 30	57, 71, 77, 80	0
49	1r	68/88 (77%)	0.04	0 100 100	62, 71, 78, 83	0
49	2r	68/88 (77%)	-0.19	0 100 100	64, 71, 76, 82	0
50	1s	83/93 (89%)	0.05	0 100 100	64, 75, 82, 84	0
50	2s	83/93 (89%)	0.69	6 (7%) 21 11	75, 84, 90, 95	0
51	1t	96/106 (90%)	0.29	1 (1%) 79 59	61, 70, 78, 82	0
51	2t	96/106 (90%)	0.34	5 (5%) 33 17	56, 71, 79, 81	0
52	1u	23/27 (85%)	0.41	0 100 100	64, 70, 73, 76	0
52	2u	23/27 (85%)	1.41	6 (26%) 1 1	73, 79, 84, 86	0
53	1v	13/24 (54%)	1.13	2 (15%) 5 3	53, 92, 100, 103	0
53	2v	13/24 (54%)	1.90	6 (46%) 0 0	72, 97, 102, 103	0
54	1x	72/77 (93%)	-0.37	0 100 100	46, 66, 82, 88	0
54	2x	72/77 (93%)	-0.33	0 100 100	56, 77, 89, 94	0
55	1z	16/16 (100%)	0.53	2 (12%) 8 5	38, 47, 62, 71	0
55	2z	16/16 (100%)	0.53	1 (6%) 26 13	52, 58, 66, 72	0
All	All	20628/21476 (96%)	-0.07	275 (1%) 75 53	28, 66, 87, 110	0

The worst 5 of 275 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
23	21	2	SER	7.1
44	2m	124	PRO	6.9
1	2A	2145	C	5.6
1	2A	2144	U	5.4
1	2A	2146	C	5.2

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
32	2MG	2a	1207	24/25	0.83	0.11	69,82,87,90	0
54	5MU	2x	54	21/22	0.84	0.10	73,80,87,94	0
1	5MU	2A	1915	21/22	0.85	0.09	64,79,83,84	0
54	PSU	2x	55	20/21	0.85	0.09	75,83,87,87	0
54	4SU	2x	8	20/21	0.88	0.08	69,83,95,100	0
32	PSU	2a	516	20/21	0.88	0.08	72,79,81,87	0
1	5MU	1A	1915	21/22	0.88	0.08	64,75,82,97	0
1	PSU	1A	1917	20/21	0.91	0.10	52,67,74,75	0
32	PSU	1a	516	20/21	0.91	0.10	68,73,77,78	0
32	5MC	2a	967	21/22	0.91	0.14	62,73,80,86	0
32	2MG	1a	1207	24/25	0.91	0.12	65,71,79,86	0
32	4OC	2a	1402	22/23	0.91	0.13	61,67,72,77	0
43	0TD	1l	92	10/11	0.91	0.11	54,61,67,68	0
54	5MC	2x	32	21/22	0.91	0.12	65,74,78,80	0
54	PSU	1x	55	20/21	0.91	0.09	56,67,76,82	0
1	PSU	2A	1911	20/21	0.91	0.08	54,67,70,74	0
54	5MC	1x	32	21/22	0.92	0.11	50,61,69,75	0
32	M2G	2a	966	25/26	0.92	0.13	64,70,82,85	0
54	4SU	1x	8	20/21	0.92	0.08	65,70,77,81	0
54	5MU	1x	54	21/22	0.93	0.08	64,67,72,78	0
32	5MC	2a	1400	21/22	0.93	0.10	63,66,71,77	0
32	7MG	2a	527	24/25	0.93	0.09	63,67,75,77	0
43	0TD	2l	92	10/11	0.93	0.09	63,69,73,80	0
1	4OC	2A	1920	21/23	0.94	0.09	61,68,73,80	0
1	PSU	1A	1911	20/21	0.94	0.08	58,66,67,69	0
32	5MC	2a	1404	21/22	0.94	0.09	58,65,70,73	0
32	7MG	1a	527	24/25	0.94	0.10	51,57,66,73	0
1	4OC	1A	1920	21/23	0.95	0.11	34,57,65,66	0
1	PSU	2A	1917	20/21	0.95	0.06	67,75,82,84	0
32	5MC	1a	1400	21/22	0.95	0.08	57,61,66,70	0
1	5MC	2A	1942	21/22	0.95	0.08	52,63,73,76	0
1	5MC	2A	1962	21/22	0.95	0.10	46,59,63,72	0
32	5MC	2a	1407	21/22	0.95	0.07	60,64,68,71	0
32	UR3	2a	1498	21/22	0.95	0.09	53,59,64,72	0
1	OMG	2A	2251	24/25	0.95	0.10	44,49,54,59	0
1	2MA	2A	2503	23/24	0.95	0.12	37,43,51,56	0
32	5MC	1a	1404	21/22	0.95	0.10	37,56,62,65	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
32	MA6	1a	1519	24/25	0.95	0.13	48,56,60,69	0
32	5MC	1a	967	21/22	0.95	0.09	59,67,72,76	0
1	5MU	2A	1939	21/22	0.96	0.08	41,54,59,64	0
1	5MC	1A	1942	21/22	0.96	0.08	47,52,59,64	0
32	MA6	2a	1518	24/25	0.96	0.09	56,64,68,70	0
32	4OC	1a	1402	22/23	0.96	0.08	58,61,65,74	0
32	M2G	1a	966	25/26	0.96	0.08	55,63,68,73	0
32	5MC	1a	1407	21/22	0.96	0.09	44,53,61,61	0
1	PSU	2A	2605	20/21	0.96	0.10	41,48,51,52	0
32	MA6	1a	1518	24/25	0.96	0.10	46,55,61,63	0
1	5MU	1A	1939	21/22	0.97	0.07	37,43,47,52	0
1	5MC	1A	1962	21/22	0.97	0.09	39,51,59,68	0
32	MA6	2a	1519	24/25	0.97	0.09	54,65,68,69	0
1	OMG	1A	2251	24/25	0.97	0.08	27,39,44,45	0
1	2MU	2A	2552	21/23	0.97	0.07	43,49,56,59	0
1	2MU	1A	2552	21/23	0.97	0.08	40,43,50,51	0
32	UR3	1a	1498	21/22	0.97	0.07	41,50,53,56	0
1	PSU	1A	2605	20/21	0.97	0.08	35,40,44,48	0
1	2MA	1A	2503	23/24	0.98	0.08	22,35,40,45	0

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1B	227	1/1	0.55	0.21	77,77,77,77	0
56	MG	1a	1733	1/1	0.58	0.31	81,81,81,81	0
56	MG	1x	110	1/1	0.58	0.30	76,76,76,76	0
56	MG	2A	3455	1/1	0.59	0.24	61,61,61,61	0
56	MG	2A	3263	1/1	0.64	0.11	58,58,58,58	0
56	MG	2A	3668	1/1	0.65	0.14	64,64,64,64	0
56	MG	2A	3717	1/1	0.65	0.20	73,73,73,73	0
56	MG	2a	3209	1/1	0.65	0.27	76,76,76,76	0
56	MG	1A	3237	1/1	0.67	0.19	57,57,57,57	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3936	1/1	0.67	0.26	97,97,97,97	0
56	MG	2A	3099	1/1	0.68	0.25	64,64,64,64	0
56	MG	2a	3095	1/1	0.68	0.23	70,70,70,70	0
56	MG	2a	3119	1/1	0.68	0.25	85,85,85,85	0
56	MG	2A	3069	1/1	0.68	0.19	63,63,63,63	0
56	MG	2B	214	1/1	0.70	0.17	65,65,65,65	0
56	MG	2A	3634	1/1	0.70	0.17	58,58,58,58	0
56	MG	1A	3599	1/1	0.71	0.16	64,64,64,64	0
56	MG	2A	3319	1/1	0.71	0.23	83,83,83,83	0
56	MG	2a	3217	1/1	0.71	0.08	76,76,76,76	0
56	MG	1a	1679	1/1	0.72	0.19	78,78,78,78	0
56	MG	2A	3304	1/1	0.72	0.23	78,78,78,78	0
56	MG	2A	3512	1/1	0.72	0.17	69,69,69,69	0
56	MG	2A	3555	1/1	0.72	0.17	71,71,71,71	0
59	K	2A	3421	1/1	0.72	0.27	91,91,91,91	0
56	MG	2v	101	1/1	0.73	0.14	77,77,77,77	0
56	MG	2A	3593	1/1	0.73	0.20	73,73,73,73	0
56	MG	2a	3081	1/1	0.74	0.18	75,75,75,75	0
56	MG	2a	3184	1/1	0.74	0.20	69,69,69,69	0
56	MG	2A	3678	1/1	0.74	0.20	63,63,63,63	0
56	MG	2A	3301	1/1	0.75	0.12	57,57,57,57	0
56	MG	2A	3787	1/1	0.75	0.23	69,69,69,69	0
56	MG	2A	3225	1/1	0.75	0.26	63,63,63,63	0
56	MG	2A	3513	1/1	0.75	0.24	70,70,70,70	0
56	MG	1A	3167	1/1	0.75	0.24	60,60,60,60	0
56	MG	2a	3100	1/1	0.75	0.25	76,76,76,76	0
56	MG	1A	3739	1/1	0.76	0.16	74,74,74,74	0
56	MG	2A	3793	1/1	0.76	0.12	55,55,55,55	0
56	MG	1A	3338	1/1	0.76	0.12	70,70,70,70	0
56	MG	1x	114	1/1	0.76	0.20	71,71,71,71	0
56	MG	2A	3058	1/1	0.76	0.17	56,56,56,56	0
56	MG	1a	1691	1/1	0.76	0.20	62,62,62,62	0
56	MG	2a	3114	1/1	0.77	0.17	60,60,60,60	0
56	MG	2a	3020	1/1	0.77	0.30	63,63,63,63	0
56	MG	2a	3152	1/1	0.77	0.13	79,79,79,79	0
56	MG	2a	3013	1/1	0.77	0.29	68,68,68,68	0
56	MG	1a	1777	1/1	0.78	0.14	69,69,69,69	0
56	MG	1A	3515	1/1	0.78	0.08	54,54,54,54	0
56	MG	2A	3699	1/1	0.78	0.15	69,69,69,69	0
56	MG	1A	3330	1/1	0.78	0.18	52,52,52,52	0
56	MG	2A	3005	1/1	0.78	0.36	71,71,71,71	0
56	MG	2A	3284	1/1	0.78	0.11	53,53,53,53	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3592	1/1	0.78	0.14	61,61,61,61	0
56	MG	2A	3042	1/1	0.78	0.20	78,78,78,78	0
56	MG	1a	1774	1/1	0.78	0.16	67,67,67,67	0
56	MG	2A	3640	1/1	0.78	0.18	75,75,75,75	0
56	MG	1a	1731	1/1	0.79	0.10	62,62,62,62	0
56	MG	2A	3320	1/1	0.79	0.26	62,62,62,62	0
56	MG	2A	3321	1/1	0.79	0.26	54,54,54,54	0
56	MG	2a	3120	1/1	0.79	0.24	67,67,67,67	0
56	MG	2A	3407	1/1	0.79	0.20	49,49,49,49	0
56	MG	2A	3422	1/1	0.79	0.30	65,65,65,65	0
56	MG	1A	3857	1/1	0.79	0.35	72,72,72,72	0
56	MG	2a	3031	1/1	0.79	0.21	81,81,81,81	0
56	MG	2A	3195	1/1	0.79	0.26	76,76,76,76	0
56	MG	2x	102	1/1	0.79	0.10	69,69,69,69	0
56	MG	1a	1666	1/1	0.79	0.23	66,66,66,66	0
56	MG	2a	3003	1/1	0.80	0.17	77,77,77,77	0
56	MG	2a	3006	1/1	0.80	0.20	59,59,59,59	0
56	MG	2A	3526	1/1	0.80	0.21	75,75,75,75	0
56	MG	1A	4026	1/1	0.80	0.12	66,66,66,66	0
56	MG	2A	3570	1/1	0.80	0.13	51,51,51,51	0
56	MG	1A	4028	1/1	0.80	0.16	52,52,52,52	0
56	MG	1A	3750	1/1	0.80	0.11	54,54,54,54	0
56	MG	19	102	1/1	0.80	0.21	45,45,45,45	0
56	MG	2A	3082	1/1	0.80	0.35	77,77,77,77	0
56	MG	1a	1663	1/1	0.80	0.30	70,70,70,70	0
56	MG	2A	3677	1/1	0.80	0.23	66,66,66,66	0
56	MG	2A	3340	1/1	0.80	0.17	69,69,69,69	0
56	MG	1x	108	1/1	0.80	0.10	64,64,64,64	0
56	MG	2a	3198	1/1	0.80	0.17	62,62,62,62	0
56	MG	2a	3200	1/1	0.80	0.23	73,73,73,73	0
56	MG	2A	3209	1/1	0.80	0.19	64,64,64,64	0
56	MG	2a	3214	1/1	0.80	0.14	64,64,64,64	0
56	MG	2A	3786	1/1	0.80	0.20	79,79,79,79	0
56	MG	1A	3438	1/1	0.80	0.08	54,54,54,54	0
56	MG	2A	3244	1/1	0.80	0.21	64,64,64,64	0
56	MG	1A	3068	1/1	0.80	0.16	32,32,32,32	0
56	MG	2a	3008	1/1	0.81	0.22	61,61,61,61	0
56	MG	1A	3365	1/1	0.81	0.16	44,44,44,44	0
56	MG	1x	109	1/1	0.81	0.16	60,60,60,60	0
56	MG	2A	3285	1/1	0.81	0.09	54,54,54,54	0
56	MG	2a	3056	1/1	0.81	0.18	75,75,75,75	0
56	MG	1A	3825	1/1	0.81	0.16	65,65,65,65	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3382	1/1	0.81	0.23	55,55,55,55	0
56	MG	1B	228	1/1	0.81	0.13	51,51,51,51	0
56	MG	1a	1718	1/1	0.81	0.11	46,46,46,46	0
56	MG	2A	3674	1/1	0.81	0.18	63,63,63,63	0
56	MG	1a	1720	1/1	0.81	0.19	69,69,69,69	0
56	MG	2a	3130	1/1	0.81	0.08	100,100,100,100	0
56	MG	1A	3313	1/1	0.81	0.23	53,53,53,53	0
56	MG	2A	3378	1/1	0.81	0.21	47,47,47,47	0
56	MG	1a	1602	1/1	0.81	0.23	74,74,74,74	0
56	MG	2A	3782	1/1	0.81	0.29	56,56,56,56	0
56	MG	2a	3203	1/1	0.81	0.14	64,64,64,64	0
56	MG	1a	1617	1/1	0.81	0.08	51,51,51,51	0
56	MG	1a	1637	1/1	0.81	0.15	48,48,48,48	0
56	MG	2a	3216	1/1	0.81	0.17	67,67,67,67	0
56	MG	1a	1780	1/1	0.81	0.17	74,74,74,74	0
56	MG	1b	301	1/1	0.81	0.09	77,77,77,77	0
56	MG	2A	3516	1/1	0.81	0.24	65,65,65,65	0
56	MG	1x	104	1/1	0.81	0.23	64,64,64,64	0
56	MG	1a	1730	1/1	0.82	0.20	80,80,80,80	0
56	MG	2A	3242	1/1	0.82	0.10	56,56,56,56	0
56	MG	2a	3016	1/1	0.82	0.18	61,61,61,61	0
56	MG	1A	3304	1/1	0.82	0.12	62,62,62,62	0
56	MG	1A	3464	1/1	0.82	0.10	57,57,57,57	0
56	MG	2a	3036	1/1	0.82	0.14	70,70,70,70	0
56	MG	2A	3034	1/1	0.82	0.26	51,51,51,51	0
56	MG	1A	3056	1/1	0.82	0.10	32,32,32,32	0
56	MG	2A	3626	1/1	0.82	0.17	75,75,75,75	0
56	MG	1A	3583	1/1	0.82	0.22	64,64,64,64	0
56	MG	2a	3108	1/1	0.82	0.16	73,73,73,73	0
56	MG	2A	3636	1/1	0.82	0.27	50,50,50,50	0
56	MG	1a	1673	1/1	0.82	0.13	43,43,43,43	0
56	MG	2A	3645	1/1	0.82	0.15	64,64,64,64	0
56	MG	2A	3307	1/1	0.82	0.08	61,61,61,61	0
56	MG	13	104	1/1	0.82	0.12	62,62,62,62	0
56	MG	17	106	1/1	0.82	0.22	41,41,41,41	0
56	MG	2A	3111	1/1	0.82	0.19	69,69,69,69	0
56	MG	2A	3327	1/1	0.82	0.16	70,70,70,70	0
56	MG	2A	3139	1/1	0.82	0.14	53,53,53,53	0
56	MG	2a	3208	1/1	0.82	0.13	66,66,66,66	0
56	MG	2A	3359	1/1	0.82	0.21	67,67,67,67	0
56	MG	2A	3143	1/1	0.82	0.13	59,59,59,59	0
56	MG	2a	3215	1/1	0.82	0.16	75,75,75,75	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3156	1/1	0.82	0.13	70,70,70,70	0
56	MG	2A	3184	1/1	0.82	0.18	59,59,59,59	0
56	MG	1A	3257	1/1	0.82	0.15	70,70,70,70	0
56	MG	2A	3198	1/1	0.82	0.14	47,47,47,47	0
56	MG	1A	3962	1/1	0.82	0.22	81,81,81,81	0
56	MG	2A	3228	1/1	0.83	0.10	49,49,49,49	0
56	MG	2A	3063	1/1	0.83	0.12	46,46,46,46	0
56	MG	1A	3050	1/1	0.83	0.28	56,56,56,56	0
56	MG	2A	3247	1/1	0.83	0.10	61,61,61,61	0
56	MG	2A	3080	1/1	0.83	0.13	53,53,53,53	0
56	MG	2a	3035	1/1	0.83	0.25	62,62,62,62	0
56	MG	1A	3592	1/1	0.83	0.09	79,79,79,79	0
56	MG	2a	3042	1/1	0.83	0.18	51,51,51,51	0
56	MG	1A	3320	1/1	0.83	0.16	51,51,51,51	0
56	MG	2a	3067	1/1	0.83	0.24	49,49,49,49	0
56	MG	1A	3659	1/1	0.83	0.15	53,53,53,53	0
56	MG	2A	3123	1/1	0.83	0.28	51,51,51,51	0
56	MG	2A	3635	1/1	0.83	0.13	76,76,76,76	0
56	MG	2a	3102	1/1	0.83	0.16	62,62,62,62	0
56	MG	2A	3133	1/1	0.83	0.10	52,52,52,52	0
56	MG	1a	1695	1/1	0.83	0.20	69,69,69,69	0
56	MG	1A	3664	1/1	0.83	0.17	69,69,69,69	0
56	MG	1A	3468	1/1	0.83	0.14	37,37,37,37	0
56	MG	2A	3158	1/1	0.83	0.29	72,72,72,72	0
56	MG	2A	3183	1/1	0.83	0.24	66,66,66,66	0
56	MG	2a	3171	1/1	0.83	0.17	70,70,70,70	0
56	MG	2A	3357	1/1	0.83	0.24	67,67,67,67	0
56	MG	1a	1624	1/1	0.83	0.18	68,68,68,68	0
56	MG	2A	3709	1/1	0.83	0.13	69,69,69,69	0
56	MG	2A	3360	1/1	0.83	0.13	71,71,71,71	0
56	MG	1A	4036	1/1	0.83	0.19	40,40,40,40	0
56	MG	2A	3404	1/1	0.83	0.28	51,51,51,51	0
56	MG	1a	1653	1/1	0.83	0.37	61,61,61,61	0
56	MG	2A	3203	1/1	0.83	0.09	45,45,45,45	0
56	MG	2A	3807	1/1	0.83	0.11	51,51,51,51	0
56	MG	1a	1751	1/1	0.83	0.16	73,73,73,73	0
56	MG	2T	201	1/1	0.83	0.15	63,63,63,63	0
56	MG	2A	3464	1/1	0.83	0.11	75,75,75,75	0
56	MG	1A	3397	1/1	0.83	0.14	58,58,58,58	0
56	MG	1A	3409	1/1	0.84	0.15	46,46,46,46	0
56	MG	1A	3533	1/1	0.84	0.27	63,63,63,63	0
56	MG	2A	3350	1/1	0.84	0.08	71,71,71,71	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3222	1/1	0.84	0.17	69,69,69,69	0
56	MG	2A	3646	1/1	0.84	0.06	71,71,71,71	0
56	MG	1A	3826	1/1	0.84	0.16	45,45,45,45	0
56	MG	1A	3426	1/1	0.84	0.17	51,51,51,51	0
56	MG	2A	3366	1/1	0.84	0.14	64,64,64,64	0
56	MG	2A	3229	1/1	0.84	0.06	39,39,39,39	0
56	MG	1A	3428	1/1	0.84	0.07	62,62,62,62	0
56	MG	2a	3109	1/1	0.84	0.11	60,60,60,60	0
56	MG	1A	3321	1/1	0.84	0.14	63,63,63,63	0
56	MG	2A	3420	1/1	0.84	0.09	52,52,52,52	0
56	MG	2A	3773	1/1	0.84	0.10	67,67,67,67	0
56	MG	1a	1608	1/1	0.84	0.10	60,60,60,60	0
56	MG	2A	3261	1/1	0.84	0.07	46,46,46,46	0
56	MG	1x	112	1/1	0.84	0.21	68,68,68,68	0
56	MG	1A	4025	1/1	0.84	0.20	74,74,74,74	0
56	MG	1x	115	1/1	0.84	0.09	71,71,71,71	0
56	MG	2B	212	1/1	0.84	0.12	61,61,61,61	0
56	MG	2A	3294	1/1	0.84	0.12	55,55,55,55	0
56	MG	2E	301	1/1	0.84	0.25	62,62,62,62	0
56	MG	1A	3458	1/1	0.84	0.09	63,63,63,63	0
56	MG	1a	1632	1/1	0.84	0.14	47,47,47,47	0
56	MG	1A	3390	1/1	0.84	0.23	56,56,56,56	0
56	MG	2A	3193	1/1	0.84	0.13	63,63,63,63	0
56	MG	1A	3182	1/1	0.84	0.15	53,53,53,53	0
56	MG	2i	201	1/1	0.84	0.06	54,54,54,54	0
56	MG	2A	3616	1/1	0.84	0.21	69,69,69,69	0
56	MG	1a	1659	1/1	0.84	0.13	62,62,62,62	0
56	MG	2A	3324	1/1	0.84	0.26	67,67,67,67	0
56	MG	1A	3405	1/1	0.85	0.11	40,40,40,40	0
56	MG	2A	3380	1/1	0.85	0.23	44,44,44,44	0
56	MG	2a	3054	1/1	0.85	0.24	58,58,58,58	0
56	MG	2A	3168	1/1	0.85	0.11	44,44,44,44	0
56	MG	2A	3271	1/1	0.85	0.11	59,59,59,59	0
56	MG	2A	3172	1/1	0.85	0.11	64,64,64,64	0
56	MG	2a	3091	1/1	0.85	0.16	61,61,61,61	0
56	MG	2A	3052	1/1	0.85	0.14	61,61,61,61	0
56	MG	2a	3096	1/1	0.85	0.25	64,64,64,64	0
56	MG	2A	3445	1/1	0.85	0.08	58,58,58,58	0
56	MG	1B	219	1/1	0.85	0.16	53,53,53,53	0
56	MG	2A	3459	1/1	0.85	0.33	59,59,59,59	0
56	MG	1a	1692	1/1	0.85	0.10	70,70,70,70	0
56	MG	2A	3481	1/1	0.85	0.31	54,54,54,54	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3350	1/1	0.85	0.27	50,50,50,50	0
56	MG	2A	3791	1/1	0.85	0.14	56,56,56,56	0
56	MG	1A	3471	1/1	0.85	0.15	50,50,50,50	0
56	MG	2A	3798	1/1	0.85	0.26	59,59,59,59	0
56	MG	2a	3156	1/1	0.85	0.09	76,76,76,76	0
56	MG	2A	3313	1/1	0.85	0.22	52,52,52,52	0
56	MG	1a	1638	1/1	0.85	0.22	58,58,58,58	0
56	MG	2a	3185	1/1	0.85	0.12	55,55,55,55	0
56	MG	2A	3085	1/1	0.85	0.10	55,55,55,55	0
56	MG	1A	3445	1/1	0.85	0.15	57,57,57,57	0
56	MG	1A	3713	1/1	0.85	0.16	36,36,36,36	0
56	MG	1A	3447	1/1	0.85	0.09	50,50,50,50	0
56	MG	1A	3386	1/1	0.85	0.10	37,37,37,37	0
56	MG	2A	3239	1/1	0.85	0.24	66,66,66,66	0
56	MG	2A	3355	1/1	0.85	0.22	51,51,51,51	0
56	MG	1a	1766	1/1	0.85	0.15	83,83,83,83	0
56	MG	2a	3019	1/1	0.85	0.09	59,59,59,59	0
56	MG	1A	3795	1/1	0.85	0.10	51,51,51,51	0
56	MG	2a	3022	1/1	0.85	0.26	60,60,60,60	0
56	MG	2A	3035	1/1	0.85	0.19	67,67,67,67	0
56	MG	2A	3251	1/1	0.85	0.08	63,63,63,63	0
56	MG	2A	3028	1/1	0.86	0.16	50,50,50,50	0
56	MG	1A	3785	1/1	0.86	0.20	68,68,68,68	0
56	MG	1A	3423	1/1	0.86	0.15	55,55,55,55	0
56	MG	1A	3820	1/1	0.86	0.21	45,45,45,45	0
56	MG	1a	1701	1/1	0.86	0.19	55,55,55,55	0
56	MG	2A	3461	1/1	0.86	0.38	47,47,47,47	0
56	MG	2a	3010	1/1	0.86	0.19	70,70,70,70	0
56	MG	1a	1706	1/1	0.86	0.19	62,62,62,62	0
56	MG	2A	3468	1/1	0.86	0.13	59,59,59,59	0
56	MG	1a	1708	1/1	0.86	0.26	63,63,63,63	0
56	MG	1A	3375	1/1	0.86	0.08	57,57,57,57	0
56	MG	1A	3086	1/1	0.86	0.23	51,51,51,51	0
56	MG	1A	3841	1/1	0.86	0.15	48,48,48,48	0
56	MG	1A	3403	1/1	0.86	0.16	64,64,64,64	0
56	MG	2A	3089	1/1	0.86	0.22	61,61,61,61	0
56	MG	1A	3907	1/1	0.86	0.11	39,39,39,39	0
56	MG	2A	3580	1/1	0.86	0.20	54,54,54,54	0
56	MG	2A	3586	1/1	0.86	0.11	66,66,66,66	0
56	MG	1a	1623	1/1	0.86	0.08	65,65,65,65	0
56	MG	2a	3075	1/1	0.86	0.17	56,56,56,56	0
56	MG	2a	3076	1/1	0.86	0.14	56,56,56,56	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3113	1/1	0.86	0.12	66,66,66,66	0
56	MG	2A	3608	1/1	0.86	0.18	64,64,64,64	0
56	MG	1A	3662	1/1	0.86	0.15	68,68,68,68	0
56	MG	2A	3124	1/1	0.86	0.19	50,50,50,50	0
56	MG	2A	3127	1/1	0.86	0.16	70,70,70,70	0
56	MG	2A	3309	1/1	0.86	0.12	66,66,66,66	0
56	MG	1A	3496	1/1	0.86	0.14	60,60,60,60	0
56	MG	1A	3997	1/1	0.86	0.22	63,63,63,63	0
56	MG	1A	4015	1/1	0.86	0.11	61,61,61,61	0
56	MG	2a	3116	1/1	0.86	0.15	74,74,74,74	0
56	MG	1a	1644	1/1	0.86	0.20	66,66,66,66	0
56	MG	1f	201	1/1	0.86	0.19	53,53,53,53	0
56	MG	1A	3682	1/1	0.86	0.13	64,64,64,64	0
56	MG	2a	3133	1/1	0.86	0.10	78,78,78,78	0
56	MG	2A	3170	1/1	0.86	0.17	66,66,66,66	0
56	MG	1a	1654	1/1	0.86	0.17	48,48,48,48	0
56	MG	2A	3691	1/1	0.86	0.15	68,68,68,68	0
56	MG	2A	3697	1/1	0.86	0.12	62,62,62,62	0
56	MG	2A	3352	1/1	0.86	0.08	47,47,47,47	0
56	MG	2a	3191	1/1	0.86	0.10	67,67,67,67	0
56	MG	1A	3508	1/1	0.86	0.07	42,42,42,42	0
56	MG	2A	3715	1/1	0.86	0.11	63,63,63,63	0
56	MG	1A	3715	1/1	0.86	0.16	51,51,51,51	0
56	MG	2A	3185	1/1	0.86	0.09	46,46,46,46	0
56	MG	2A	3775	1/1	0.86	0.20	51,51,51,51	0
56	MG	1A	4029	1/1	0.86	0.09	54,54,54,54	0
56	MG	1A	3316	1/1	0.86	0.07	42,42,42,42	0
56	MG	1a	1677	1/1	0.86	0.20	66,66,66,66	0
56	MG	1A	3387	1/1	0.86	0.08	46,46,46,46	0
56	MG	2A	3392	1/1	0.86	0.15	56,56,56,56	0
56	MG	2A	3393	1/1	0.86	0.23	50,50,50,50	0
56	MG	2A	3018	1/1	0.86	0.09	56,56,56,56	0
56	MG	2A	3220	1/1	0.86	0.08	58,58,58,58	0
56	MG	1A	3570	1/1	0.87	0.16	40,40,40,40	0
56	MG	1A	3775	1/1	0.87	0.17	51,51,51,51	0
56	MG	1A	3783	1/1	0.87	0.12	57,57,57,57	0
56	MG	1A	3287	1/1	0.87	0.10	36,36,36,36	0
56	MG	2A	3810	1/1	0.87	0.17	51,51,51,51	0
56	MG	2B	204	1/1	0.87	0.10	61,61,61,61	0
56	MG	2B	205	1/1	0.87	0.15	62,62,62,62	0
56	MG	1A	3323	1/1	0.87	0.09	31,31,31,31	0
56	MG	1A	3806	1/1	0.87	0.60	45,45,45,45	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3812	1/1	0.87	0.11	49,49,49,49	0
56	MG	2A	3027	1/1	0.87	0.10	61,61,61,61	0
56	MG	20	101	1/1	0.87	0.30	47,47,47,47	0
56	MG	20	102	1/1	0.87	0.20	53,53,53,53	0
56	MG	2A	3439	1/1	0.87	0.27	62,62,62,62	0
56	MG	2a	3005	1/1	0.87	0.13	60,60,60,60	0
56	MG	1a	1682	1/1	0.87	0.11	57,57,57,57	0
56	MG	2A	3452	1/1	0.87	0.18	45,45,45,45	0
56	MG	1B	226	1/1	0.87	0.07	51,51,51,51	0
56	MG	1A	3814	1/1	0.87	0.12	38,38,38,38	0
56	MG	2a	3014	1/1	0.87	0.32	66,66,66,66	0
56	MG	2A	3237	1/1	0.87	0.25	56,56,56,56	0
56	MG	1a	1693	1/1	0.87	0.09	58,58,58,58	0
56	MG	2A	3241	1/1	0.87	0.07	40,40,40,40	0
56	MG	1a	1694	1/1	0.87	0.13	51,51,51,51	0
56	MG	2a	3026	1/1	0.87	0.17	48,48,48,48	0
56	MG	2A	3499	1/1	0.87	0.10	64,64,64,64	0
56	MG	2A	3056	1/1	0.87	0.13	67,67,67,67	0
56	MG	1A	3303	1/1	0.87	0.14	38,38,38,38	0
56	MG	2A	3250	1/1	0.87	0.36	61,61,61,61	0
56	MG	1a	1696	1/1	0.87	0.17	61,61,61,61	0
56	MG	2A	3258	1/1	0.87	0.17	62,62,62,62	0
56	MG	2a	3062	1/1	0.87	0.19	59,59,59,59	0
56	MG	2A	3559	1/1	0.87	0.08	51,51,51,51	0
56	MG	2a	3074	1/1	0.87	0.20	55,55,55,55	0
56	MG	2A	3565	1/1	0.87	0.18	47,47,47,47	0
56	MG	1G	204	1/1	0.87	0.08	53,53,53,53	0
56	MG	1Y	201	1/1	0.87	0.10	49,49,49,49	0
56	MG	2a	3089	1/1	0.87	0.12	53,53,53,53	0
56	MG	1A	3038	1/1	0.87	0.17	55,55,55,55	0
56	MG	1A	3119	1/1	0.87	0.08	61,61,61,61	0
56	MG	1A	3828	1/1	0.87	0.22	64,64,64,64	0
56	MG	2A	3290	1/1	0.87	0.14	54,54,54,54	0
56	MG	1A	3243	1/1	0.87	0.23	63,63,63,63	0
56	MG	2A	3300	1/1	0.87	0.13	57,57,57,57	0
56	MG	1A	3842	1/1	0.87	0.13	40,40,40,40	0
56	MG	1A	3081	1/1	0.87	0.11	41,41,41,41	0
56	MG	2a	3115	1/1	0.87	0.29	64,64,64,64	0
56	MG	1a	1747	1/1	0.87	0.33	59,59,59,59	0
56	MG	1a	1749	1/1	0.87	0.21	63,63,63,63	0
56	MG	2A	3643	1/1	0.87	0.19	61,61,61,61	0
56	MG	2a	3123	1/1	0.87	0.15	72,72,72,72	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2a	3124	1/1	0.87	0.24	60,60,60,60	0
56	MG	1A	3519	1/1	0.87	0.11	44,44,44,44	0
56	MG	1a	1756	1/1	0.87	0.20	70,70,70,70	0
56	MG	2A	3661	1/1	0.87	0.14	62,62,62,62	0
56	MG	2a	3155	1/1	0.87	0.12	72,72,72,72	0
56	MG	2A	3134	1/1	0.87	0.26	61,61,61,61	0
56	MG	1A	3925	1/1	0.87	0.20	82,82,82,82	0
56	MG	1a	1626	1/1	0.87	0.11	66,66,66,66	0
56	MG	2A	3145	1/1	0.87	0.10	49,49,49,49	0
56	MG	2A	3339	1/1	0.87	0.25	47,47,47,47	0
56	MG	2A	3151	1/1	0.87	0.21	50,50,50,50	0
56	MG	2A	3344	1/1	0.87	0.07	54,54,54,54	0
56	MG	1a	1627	1/1	0.87	0.21	60,60,60,60	0
56	MG	1A	3457	1/1	0.87	0.08	52,52,52,52	0
56	MG	1A	3947	1/1	0.87	0.18	60,60,60,60	0
56	MG	2A	3728	1/1	0.87	0.14	64,64,64,64	0
56	MG	2A	3729	1/1	0.87	0.08	66,66,66,66	0
56	MG	1A	3732	1/1	0.87	0.17	49,49,49,49	0
56	MG	1s	101	1/1	0.87	0.17	61,61,61,61	0
56	MG	2A	3776	1/1	0.87	0.12	62,62,62,62	0
56	MG	2k	201	1/1	0.87	0.16	59,59,59,59	0
56	MG	1A	3985	1/1	0.87	0.17	45,45,45,45	0
56	MG	1A	3561	1/1	0.87	0.09	41,41,41,41	0
56	MG	2x	105	1/1	0.87	0.30	59,59,59,59	0
56	MG	2A	3372	1/1	0.87	0.10	63,63,63,63	0
56	MG	1A	3660	1/1	0.88	0.12	52,52,52,52	0
56	MG	2A	3426	1/1	0.88	0.21	40,40,40,40	0
56	MG	2A	3430	1/1	0.88	0.16	42,42,42,42	0
56	MG	1U	208	1/1	0.88	0.42	40,40,40,40	0
56	MG	2A	3442	1/1	0.88	0.23	63,63,63,63	0
56	MG	1A	3401	1/1	0.88	0.15	48,48,48,48	0
56	MG	2F	301	1/1	0.88	0.16	50,50,50,50	0
56	MG	2O	201	1/1	0.88	0.15	61,61,61,61	0
56	MG	1O	102	1/1	0.88	0.24	68,68,68,68	0
56	MG	1A	3470	1/1	0.88	0.37	32,32,32,32	0
56	MG	1A	3255	1/1	0.88	0.17	38,38,38,38	0
56	MG	2a	3001	1/1	0.88	0.13	52,52,52,52	0
56	MG	1A	3312	1/1	0.88	0.20	64,64,64,64	0
56	MG	1A	3916	1/1	0.88	0.19	80,80,80,80	0
56	MG	2A	3467	1/1	0.88	0.20	61,61,61,61	0
56	MG	2a	3007	1/1	0.88	0.26	55,55,55,55	0
56	MG	1a	1603	1/1	0.88	0.08	54,54,54,54	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3475	1/1	0.88	0.17	50,50,50,50	0
56	MG	1a	1606	1/1	0.88	0.16	69,69,69,69	0
56	MG	1A	3355	1/1	0.88	0.06	41,41,41,41	0
56	MG	1a	1613	1/1	0.88	0.10	71,71,71,71	0
56	MG	2A	3091	1/1	0.88	0.24	54,54,54,54	0
56	MG	2A	3094	1/1	0.88	0.17	52,52,52,52	0
56	MG	2A	3268	1/1	0.88	0.17	57,57,57,57	0
56	MG	2A	3528	1/1	0.88	0.18	54,54,54,54	0
56	MG	2A	3530	1/1	0.88	0.14	46,46,46,46	0
56	MG	2a	3034	1/1	0.88	0.37	55,55,55,55	0
56	MG	2A	3533	1/1	0.88	0.21	65,65,65,65	0
56	MG	1a	1732	1/1	0.88	0.37	53,53,53,53	0
56	MG	2A	3281	1/1	0.88	0.19	59,59,59,59	0
56	MG	2A	3109	1/1	0.88	0.20	75,75,75,75	0
56	MG	2A	3566	1/1	0.88	0.20	66,66,66,66	0
56	MG	1A	3718	1/1	0.88	0.13	39,39,39,39	0
56	MG	2A	3579	1/1	0.88	0.14	67,67,67,67	0
56	MG	2a	3072	1/1	0.88	0.22	56,56,56,56	0
56	MG	1a	1618	1/1	0.88	0.13	53,53,53,53	0
56	MG	1A	3514	1/1	0.88	0.08	61,61,61,61	0
56	MG	1A	3256	1/1	0.88	0.10	36,36,36,36	0
56	MG	2a	3080	1/1	0.88	0.17	54,54,54,54	0
56	MG	1A	3149	1/1	0.88	0.75	40,40,40,40	0
56	MG	2a	3082	1/1	0.88	0.13	53,53,53,53	0
56	MG	2A	3595	1/1	0.88	0.24	57,57,57,57	0
56	MG	2a	3090	1/1	0.88	0.09	73,73,73,73	0
56	MG	1a	1764	1/1	0.88	0.15	60,60,60,60	0
56	MG	2A	3614	1/1	0.88	0.12	66,66,66,66	0
56	MG	1A	3380	1/1	0.88	0.11	42,42,42,42	0
56	MG	2A	3623	1/1	0.88	0.12	55,55,55,55	0
56	MG	2A	3308	1/1	0.88	0.15	74,74,74,74	0
56	MG	1A	3546	1/1	0.88	0.11	49,49,49,49	0
56	MG	2A	3310	1/1	0.88	0.07	55,55,55,55	0
56	MG	1A	3273	1/1	0.88	0.17	43,43,43,43	0
56	MG	2A	3315	1/1	0.88	0.23	67,67,67,67	0
56	MG	1A	3383	1/1	0.88	0.23	56,56,56,56	0
56	MG	1A	3797	1/1	0.88	0.16	52,52,52,52	0
56	MG	1a	1648	1/1	0.88	0.10	50,50,50,50	0
56	MG	1A	3159	1/1	0.88	0.10	60,60,60,60	0
56	MG	2A	3163	1/1	0.88	0.21	63,63,63,63	0
56	MG	2A	3329	1/1	0.88	0.10	55,55,55,55	0
56	MG	1A	3322	1/1	0.88	0.18	60,60,60,60	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	4041	1/1	0.88	0.25	69,69,69,69	0
56	MG	2A	3681	1/1	0.88	0.15	63,63,63,63	0
56	MG	1a	1661	1/1	0.88	0.10	70,70,70,70	0
56	MG	2a	3161	1/1	0.88	0.20	58,58,58,58	0
56	MG	2A	3176	1/1	0.88	0.28	65,65,65,65	0
56	MG	2a	3177	1/1	0.88	0.22	71,71,71,71	0
56	MG	2A	3698	1/1	0.88	0.09	54,54,54,54	0
56	MG	2A	3180	1/1	0.88	0.20	56,56,56,56	0
56	MG	2A	3354	1/1	0.88	0.13	51,51,51,51	0
56	MG	1B	204	1/1	0.88	0.18	49,49,49,49	0
56	MG	2a	3199	1/1	0.88	0.17	59,59,59,59	0
56	MG	1A	3594	1/1	0.88	0.20	36,36,36,36	0
56	MG	1a	1669	1/1	0.88	0.12	50,50,50,50	0
56	MG	2A	3190	1/1	0.88	0.11	49,49,49,49	0
56	MG	1B	220	1/1	0.88	0.17	56,56,56,56	0
56	MG	2a	3210	1/1	0.88	0.19	58,58,58,58	0
56	MG	2a	3213	1/1	0.88	0.18	70,70,70,70	0
56	MG	2A	3774	1/1	0.88	0.20	73,73,73,73	0
56	MG	1A	3298	1/1	0.88	0.08	43,43,43,43	0
56	MG	2A	3013	1/1	0.88	0.24	44,44,44,44	0
56	MG	2A	3014	1/1	0.88	0.28	66,66,66,66	0
56	MG	1A	3647	1/1	0.88	0.18	44,44,44,44	0
56	MG	2A	3218	1/1	0.88	0.36	64,64,64,64	0
56	MG	2n	101	1/1	0.88	0.46	60,60,60,60	0
56	MG	1A	3026	1/1	0.88	0.26	61,61,61,61	0
56	MG	1E	307	1/1	0.88	0.11	38,38,38,38	0
56	MG	2A	3414	1/1	0.88	0.24	73,73,73,73	0
56	MG	2A	3224	1/1	0.88	0.20	53,53,53,53	0
56	MG	1a	1630	1/1	0.89	0.12	57,57,57,57	0
56	MG	1a	1631	1/1	0.89	0.12	57,57,57,57	0
56	MG	2A	3395	1/1	0.89	0.31	64,64,64,64	0
56	MG	2B	203	1/1	0.89	0.09	66,66,66,66	0
56	MG	2A	3403	1/1	0.89	0.20	57,57,57,57	0
56	MG	1h	201	1/1	0.89	0.12	55,55,55,55	0
56	MG	2A	3406	1/1	0.89	0.07	64,64,64,64	0
56	MG	2A	3192	1/1	0.89	0.15	48,48,48,48	0
56	MG	2A	3409	1/1	0.89	0.09	56,56,56,56	0
56	MG	1A	3160	1/1	0.89	0.11	53,53,53,53	0
56	MG	1a	1633	1/1	0.89	0.15	49,49,49,49	0
56	MG	1a	1636	1/1	0.89	0.12	49,49,49,49	0
56	MG	1A	3744	1/1	0.89	0.11	27,27,27,27	0
56	MG	1A	4007	1/1	0.89	0.10	55,55,55,55	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	23	101	1/1	0.89	0.20	37,37,37,37	0
56	MG	1A	3051	1/1	0.89	0.27	67,67,67,67	0
56	MG	2a	3002	1/1	0.89	0.17	74,74,74,74	0
56	MG	1x	113	1/1	0.89	0.20	63,63,63,63	0
56	MG	1A	3754	1/1	0.89	0.28	54,54,54,54	0
56	MG	2A	3447	1/1	0.89	0.08	44,44,44,44	0
56	MG	1A	3773	1/1	0.89	0.13	51,51,51,51	0
56	MG	2A	3001	1/1	0.89	0.20	43,43,43,43	0
56	MG	2A	3456	1/1	0.89	0.13	59,59,59,59	0
56	MG	1A	4027	1/1	0.89	0.16	56,56,56,56	0
56	MG	2A	3012	1/1	0.89	0.11	64,64,64,64	0
56	MG	2a	3015	1/1	0.89	0.21	65,65,65,65	0
56	MG	2A	3463	1/1	0.89	0.23	61,61,61,61	0
56	MG	2a	3017	1/1	0.89	0.10	53,53,53,53	0
56	MG	1A	3176	1/1	0.89	0.11	44,44,44,44	0
56	MG	2A	3238	1/1	0.89	0.13	68,68,68,68	0
56	MG	1A	3542	1/1	0.89	0.51	46,46,46,46	0
56	MG	2a	3025	1/1	0.89	0.11	63,63,63,63	0
56	MG	1A	3359	1/1	0.89	0.18	42,42,42,42	0
56	MG	2A	3476	1/1	0.89	0.10	55,55,55,55	0
56	MG	1A	3789	1/1	0.89	0.09	48,48,48,48	0
56	MG	1A	3431	1/1	0.89	0.18	66,66,66,66	0
56	MG	1A	3435	1/1	0.89	0.17	61,61,61,61	0
56	MG	1a	1675	1/1	0.89	0.07	41,41,41,41	0
56	MG	1A	3801	1/1	0.89	0.10	83,83,83,83	0
56	MG	2A	3524	1/1	0.89	0.15	61,61,61,61	0
56	MG	2A	3255	1/1	0.89	0.20	50,50,50,50	0
56	MG	1A	3088	1/1	0.89	0.08	55,55,55,55	0
56	MG	2A	3260	1/1	0.89	0.10	62,62,62,62	0
56	MG	2A	3055	1/1	0.89	0.17	59,59,59,59	0
56	MG	2A	3535	1/1	0.89	0.18	59,59,59,59	0
56	MG	2A	3542	1/1	0.89	0.14	69,69,69,69	0
56	MG	1A	3585	1/1	0.89	0.08	23,23,23,23	0
56	MG	1A	3591	1/1	0.89	0.09	29,29,29,29	0
56	MG	1D	310	1/1	0.89	0.13	36,36,36,36	0
56	MG	2A	3277	1/1	0.89	0.11	74,74,74,74	0
56	MG	2A	3279	1/1	0.89	0.14	54,54,54,54	0
56	MG	2A	3574	1/1	0.89	0.13	61,61,61,61	0
56	MG	1A	3819	1/1	0.89	0.11	52,52,52,52	0
56	MG	2A	3074	1/1	0.89	0.14	65,65,65,65	0
56	MG	1F	304	1/1	0.89	0.12	47,47,47,47	0
56	MG	1A	3308	1/1	0.89	0.09	46,46,46,46	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2a	3106	1/1	0.89	0.13	63,63,63,63	0
56	MG	1A	3199	1/1	0.89	0.16	58,58,58,58	0
56	MG	1A	3448	1/1	0.89	0.18	44,44,44,44	0
56	MG	1A	3827	1/1	0.89	0.10	75,75,75,75	0
56	MG	1A	3231	1/1	0.89	0.09	42,42,42,42	0
56	MG	2A	3305	1/1	0.89	0.16	60,60,60,60	0
56	MG	1a	1712	1/1	0.89	0.25	64,64,64,64	0
56	MG	1a	1717	1/1	0.89	0.11	62,62,62,62	0
56	MG	1A	3116	1/1	0.89	0.10	43,43,43,43	0
56	MG	2A	3112	1/1	0.89	0.16	63,63,63,63	0
56	MG	2a	3127	1/1	0.89	0.08	71,71,71,71	0
56	MG	18	102	1/1	0.89	0.21	42,42,42,42	0
56	MG	2A	3118	1/1	0.89	0.19	58,58,58,58	0
56	MG	2a	3138	1/1	0.89	0.11	70,70,70,70	0
56	MG	1a	1723	1/1	0.89	0.14	50,50,50,50	0
56	MG	1A	3318	1/1	0.89	0.10	58,58,58,58	0
56	MG	1a	1601	1/1	0.89	0.08	65,65,65,65	0
56	MG	1A	3465	1/1	0.89	0.16	56,56,56,56	0
56	MG	2a	3167	1/1	0.89	0.12	54,54,54,54	0
56	MG	2a	3168	1/1	0.89	0.10	74,74,74,74	0
56	MG	1A	3860	1/1	0.89	0.12	37,37,37,37	0
56	MG	2a	3175	1/1	0.89	0.11	49,49,49,49	0
56	MG	1a	1742	1/1	0.89	0.29	52,52,52,52	0
56	MG	2a	3178	1/1	0.89	0.13	69,69,69,69	0
56	MG	2A	3331	1/1	0.89	0.21	43,43,43,43	0
56	MG	2A	3335	1/1	0.89	0.13	52,52,52,52	0
56	MG	2A	3337	1/1	0.89	0.12	56,56,56,56	0
56	MG	1A	3900	1/1	0.89	0.21	84,84,84,84	0
56	MG	2A	3144	1/1	0.89	0.17	48,48,48,48	0
56	MG	2A	3342	1/1	0.89	0.15	55,55,55,55	0
56	MG	1A	3903	1/1	0.89	0.18	76,76,76,76	0
56	MG	2A	3705	1/1	0.89	0.09	65,65,65,65	0
56	MG	2A	3348	1/1	0.89	0.18	57,57,57,57	0
56	MG	1A	3018	1/1	0.89	0.18	53,53,53,53	0
56	MG	1a	1755	1/1	0.89	0.12	55,55,55,55	0
56	MG	1A	3124	1/1	0.89	0.11	60,60,60,60	0
56	MG	1A	3040	1/1	0.89	0.10	37,37,37,37	0
56	MG	1A	3155	1/1	0.89	0.14	41,41,41,41	0
56	MG	1A	3027	1/1	0.89	0.20	69,69,69,69	0
56	MG	2d	301	1/1	0.89	0.24	59,59,59,59	0
56	MG	1A	3954	1/1	0.89	0.10	39,39,39,39	0
56	MG	1A	3335	1/1	0.89	0.07	47,47,47,47	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3177	1/1	0.89	0.11	46,46,46,46	0
56	MG	2t	201	1/1	0.89	0.24	53,53,53,53	0
56	MG	1a	1786	1/1	0.89	0.07	75,75,75,75	0
56	MG	2x	101	1/1	0.89	0.11	61,61,61,61	0
56	MG	1a	1819	1/1	0.89	0.26	56,56,56,56	0
56	MG	2A	3385	1/1	0.89	0.18	51,51,51,51	0
56	MG	2A	3387	1/1	0.89	0.10	49,49,49,49	0
56	MG	1A	3413	1/1	0.90	0.42	42,42,42,42	0
56	MG	1A	3276	1/1	0.90	0.10	51,51,51,51	0
56	MG	2A	3240	1/1	0.90	0.12	49,49,49,49	0
56	MG	2E	307	1/1	0.90	0.09	36,36,36,36	0
56	MG	16	101	1/1	0.90	0.24	44,44,44,44	0
56	MG	1A	3478	1/1	0.90	0.08	48,48,48,48	0
56	MG	2P	202	1/1	0.90	0.16	64,64,64,64	0
56	MG	2R	202	1/1	0.90	0.18	61,61,61,61	0
56	MG	1a	1697	1/1	0.90	0.12	67,67,67,67	0
56	MG	2W	202	1/1	0.90	0.06	47,47,47,47	0
56	MG	1A	3490	1/1	0.90	0.11	69,69,69,69	0
56	MG	1A	3872	1/1	0.90	0.07	50,50,50,50	0
56	MG	1A	3890	1/1	0.90	0.14	49,49,49,49	0
56	MG	2A	3253	1/1	0.90	0.09	49,49,49,49	0
56	MG	1A	3493	1/1	0.90	0.14	32,32,32,32	0
56	MG	1a	1714	1/1	0.90	0.08	54,54,54,54	0
56	MG	2A	3071	1/1	0.90	0.26	64,64,64,64	0
56	MG	2A	3072	1/1	0.90	0.21	51,51,51,51	0
56	MG	2A	3073	1/1	0.90	0.19	55,55,55,55	0
56	MG	1a	1715	1/1	0.90	0.12	55,55,55,55	0
56	MG	1A	3424	1/1	0.90	0.07	31,31,31,31	0
56	MG	2a	3011	1/1	0.90	0.14	60,60,60,60	0
56	MG	2A	3275	1/1	0.90	0.13	58,58,58,58	0
56	MG	2A	3483	1/1	0.90	0.28	56,56,56,56	0
56	MG	2A	3276	1/1	0.90	0.11	46,46,46,46	0
56	MG	2A	3500	1/1	0.90	0.16	54,54,54,54	0
56	MG	1A	3229	1/1	0.90	0.17	46,46,46,46	0
56	MG	1A	3513	1/1	0.90	0.13	38,38,38,38	0
56	MG	1A	3057	1/1	0.90	0.25	59,59,59,59	0
56	MG	1a	1615	1/1	0.90	0.13	48,48,48,48	0
56	MG	2a	3023	1/1	0.90	0.20	55,55,55,55	0
56	MG	1A	3430	1/1	0.90	0.17	59,59,59,59	0
56	MG	1A	3942	1/1	0.90	0.08	53,53,53,53	0
56	MG	2a	3027	1/1	0.90	0.27	52,52,52,52	0
56	MG	2A	3293	1/1	0.90	0.09	57,57,57,57	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1a	1621	1/1	0.90	0.11	53,53,53,53	0
56	MG	1a	1737	1/1	0.90	0.15	56,56,56,56	0
56	MG	1a	1741	1/1	0.90	0.24	54,54,54,54	0
56	MG	2a	3040	1/1	0.90	0.10	65,65,65,65	0
56	MG	1A	3945	1/1	0.90	0.09	35,35,35,35	0
56	MG	2a	3048	1/1	0.90	0.22	74,74,74,74	0
56	MG	1a	1746	1/1	0.90	0.23	44,44,44,44	0
56	MG	1A	3022	1/1	0.90	0.12	35,35,35,35	0
56	MG	2a	3058	1/1	0.90	0.18	76,76,76,76	0
56	MG	1A	3525	1/1	0.90	0.26	42,42,42,42	0
56	MG	2A	3126	1/1	0.90	0.13	56,56,56,56	0
56	MG	1A	3326	1/1	0.90	0.07	50,50,50,50	0
56	MG	2A	3577	1/1	0.90	0.13	70,70,70,70	0
56	MG	1a	1752	1/1	0.90	0.09	65,65,65,65	0
56	MG	2A	3314	1/1	0.90	0.09	52,52,52,52	0
56	MG	2A	3585	1/1	0.90	0.12	60,60,60,60	0
56	MG	1A	3756	1/1	0.90	0.13	39,39,39,39	0
56	MG	2A	3587	1/1	0.90	0.13	36,36,36,36	0
56	MG	2a	3083	1/1	0.90	0.08	57,57,57,57	0
56	MG	1A	3766	1/1	0.90	0.08	48,48,48,48	0
56	MG	1A	3769	1/1	0.90	0.12	47,47,47,47	0
56	MG	1A	3540	1/1	0.90	0.13	42,42,42,42	0
56	MG	2a	3093	1/1	0.90	0.17	53,53,53,53	0
56	MG	2A	3322	1/1	0.90	0.14	51,51,51,51	0
56	MG	1a	1767	1/1	0.90	0.13	54,54,54,54	0
56	MG	1a	1770	1/1	0.90	0.09	55,55,55,55	0
56	MG	2A	3152	1/1	0.90	0.12	47,47,47,47	0
56	MG	2A	3330	1/1	0.90	0.11	71,71,71,71	0
56	MG	2A	3154	1/1	0.90	0.07	68,68,68,68	0
56	MG	2A	3334	1/1	0.90	0.11	50,50,50,50	0
56	MG	2a	3111	1/1	0.90	0.19	89,89,89,89	0
56	MG	1A	3133	1/1	0.90	0.11	46,46,46,46	0
56	MG	1A	3444	1/1	0.90	0.09	53,53,53,53	0
56	MG	1A	3549	1/1	0.90	0.40	46,46,46,46	0
56	MG	1a	1643	1/1	0.90	0.09	71,71,71,71	0
56	MG	1A	3551	1/1	0.90	0.07	59,59,59,59	0
56	MG	2A	3653	1/1	0.90	0.10	56,56,56,56	0
56	MG	2A	3658	1/1	0.90	0.13	54,54,54,54	0
56	MG	2A	3660	1/1	0.90	0.10	55,55,55,55	0
56	MG	1A	3560	1/1	0.90	0.14	47,47,47,47	0
56	MG	2A	3346	1/1	0.90	0.26	50,50,50,50	0
56	MG	1A	3009	1/1	0.90	0.18	51,51,51,51	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3118	1/1	0.90	0.20	48,48,48,48	0
56	MG	1a	1656	1/1	0.90	0.23	55,55,55,55	0
56	MG	1v	101	1/1	0.90	0.22	68,68,68,68	0
56	MG	1A	3344	1/1	0.90	0.08	40,40,40,40	0
56	MG	2a	3164	1/1	0.90	0.09	70,70,70,70	0
56	MG	2A	3692	1/1	0.90	0.15	62,62,62,62	0
56	MG	1a	1660	1/1	0.90	0.13	63,63,63,63	0
56	MG	2a	3170	1/1	0.90	0.23	60,60,60,60	0
56	MG	1A	3398	1/1	0.90	0.12	56,56,56,56	0
56	MG	1A	3156	1/1	0.90	0.19	61,61,61,61	0
56	MG	2A	3364	1/1	0.90	0.17	80,80,80,80	0
56	MG	2A	3707	1/1	0.90	0.06	63,63,63,63	0
56	MG	1A	3818	1/1	0.90	0.15	41,41,41,41	0
56	MG	1A	3461	1/1	0.90	0.14	54,54,54,54	0
56	MG	2a	3186	1/1	0.90	0.10	52,52,52,52	0
56	MG	2A	3716	1/1	0.90	0.10	68,68,68,68	0
56	MG	2a	3194	1/1	0.90	0.15	71,71,71,71	0
56	MG	2a	3197	1/1	0.90	0.10	58,58,58,58	0
56	MG	2A	3373	1/1	0.90	0.23	41,41,41,41	0
56	MG	2A	3719	1/1	0.90	0.12	74,74,74,74	0
56	MG	1A	3272	1/1	0.90	0.07	42,42,42,42	0
56	MG	2A	3200	1/1	0.90	0.12	47,47,47,47	0
56	MG	2A	3738	1/1	0.90	0.09	47,47,47,47	0
56	MG	1A	3217	1/1	0.90	0.07	68,68,68,68	0
56	MG	1A	3638	1/1	0.90	0.14	32,32,32,32	0
56	MG	2a	3212	1/1	0.90	0.09	67,67,67,67	0
56	MG	2A	3215	1/1	0.90	0.10	54,54,54,54	0
56	MG	1A	3644	1/1	0.90	0.23	55,55,55,55	0
56	MG	2A	3219	1/1	0.90	0.08	57,57,57,57	0
56	MG	2A	3397	1/1	0.90	0.13	39,39,39,39	0
56	MG	2A	3010	1/1	0.90	0.06	56,56,56,56	0
56	MG	1A	3360	1/1	0.90	0.14	53,53,53,53	0
56	MG	1a	1684	1/1	0.90	0.12	40,40,40,40	0
56	MG	1a	1687	1/1	0.90	0.06	49,49,49,49	0
56	MG	2A	3799	1/1	0.90	0.22	52,52,52,52	0
56	MG	2A	3408	1/1	0.90	0.26	44,44,44,44	0
56	MG	1A	3829	1/1	0.90	0.10	34,34,34,34	0
56	MG	2A	3021	1/1	0.90	0.14	54,54,54,54	0
56	MG	2A	3231	1/1	0.90	0.08	56,56,56,56	0
56	MG	1A	3840	1/1	0.90	0.09	69,69,69,69	0
56	MG	2B	206	1/1	0.90	0.28	57,57,57,57	0
56	MG	1A	3391	1/1	0.91	0.15	53,53,53,53	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3795	1/1	0.91	0.10	44,44,44,44	0
56	MG	2A	3383	1/1	0.91	0.10	53,53,53,53	0
56	MG	1A	3824	1/1	0.91	0.21	46,46,46,46	0
56	MG	2A	3802	1/1	0.91	0.21	60,60,60,60	0
56	MG	1A	3602	1/1	0.91	0.14	37,37,37,37	0
56	MG	1A	3607	1/1	0.91	0.10	42,42,42,42	0
56	MG	1A	3624	1/1	0.91	0.13	30,30,30,30	0
56	MG	1A	3632	1/1	0.91	0.13	51,51,51,51	0
56	MG	1A	3392	1/1	0.91	0.25	58,58,58,58	0
56	MG	1A	3835	1/1	0.91	0.13	28,28,28,28	0
56	MG	1a	1605	1/1	0.91	0.20	53,53,53,53	0
56	MG	2A	3405	1/1	0.91	0.18	43,43,43,43	0
56	MG	2B	215	1/1	0.91	0.15	71,71,71,71	0
56	MG	1A	3242	1/1	0.91	0.17	58,58,58,58	0
56	MG	2A	3188	1/1	0.91	0.13	50,50,50,50	0
56	MG	1a	1607	1/1	0.91	0.20	64,64,64,64	0
56	MG	1A	3046	1/1	0.91	0.08	50,50,50,50	0
56	MG	1a	1609	1/1	0.91	0.15	59,59,59,59	0
56	MG	2Q	201	1/1	0.91	0.25	56,56,56,56	0
56	MG	2A	3194	1/1	0.91	0.13	63,63,63,63	0
56	MG	1A	3475	1/1	0.91	0.21	54,54,54,54	0
56	MG	2T	204	1/1	0.91	0.09	47,47,47,47	0
56	MG	1a	1614	1/1	0.91	0.06	72,72,72,72	0
56	MG	2X	101	1/1	0.91	0.15	53,53,53,53	0
56	MG	2Y	201	1/1	0.91	0.21	49,49,49,49	0
56	MG	1A	3162	1/1	0.91	0.18	52,52,52,52	0
56	MG	1a	1792	1/1	0.91	0.06	53,53,53,53	0
56	MG	1A	3049	1/1	0.91	0.25	39,39,39,39	0
56	MG	25	104	1/1	0.91	0.21	61,61,61,61	0
56	MG	28	101	1/1	0.91	0.13	47,47,47,47	0
56	MG	2A	3444	1/1	0.91	0.31	54,54,54,54	0
56	MG	1A	3862	1/1	0.91	0.21	32,32,32,32	0
56	MG	1A	3171	1/1	0.91	0.10	67,67,67,67	0
56	MG	2A	3449	1/1	0.91	0.24	67,67,67,67	0
56	MG	1A	3880	1/1	0.91	0.14	56,56,56,56	0
56	MG	2A	3454	1/1	0.91	0.20	53,53,53,53	0
56	MG	1A	3666	1/1	0.91	0.09	53,53,53,53	0
56	MG	1A	3406	1/1	0.91	0.11	55,55,55,55	0
56	MG	1x	102	1/1	0.91	0.10	62,62,62,62	0
56	MG	2a	3012	1/1	0.91	0.19	47,47,47,47	0
56	MG	1A	3697	1/1	0.91	0.08	42,42,42,42	0
56	MG	1a	1628	1/1	0.91	0.21	66,66,66,66	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3703	1/1	0.91	0.09	54,54,54,54	0
56	MG	1A	3704	1/1	0.91	0.21	41,41,41,41	0
56	MG	2A	3236	1/1	0.91	0.26	52,52,52,52	0
56	MG	2A	3473	1/1	0.91	0.11	58,58,58,58	0
56	MG	1A	3923	1/1	0.91	0.10	72,72,72,72	0
56	MG	1A	3710	1/1	0.91	0.07	46,46,46,46	0
56	MG	2A	3479	1/1	0.91	0.16	40,40,40,40	0
56	MG	1a	1634	1/1	0.91	0.14	46,46,46,46	0
56	MG	1A	3932	1/1	0.91	0.10	50,50,50,50	0
56	MG	2A	3486	1/1	0.91	0.12	49,49,49,49	0
56	MG	2A	3493	1/1	0.91	0.24	57,57,57,57	0
56	MG	1A	3506	1/1	0.91	0.14	38,38,38,38	0
56	MG	2A	3004	1/1	0.91	0.27	51,51,51,51	0
56	MG	2A	3243	1/1	0.91	0.11	60,60,60,60	0
56	MG	1A	3939	1/1	0.91	0.15	64,64,64,64	0
56	MG	2A	3246	1/1	0.91	0.07	44,44,44,44	0
56	MG	2a	3047	1/1	0.91	0.07	55,55,55,55	0
56	MG	2A	3006	1/1	0.91	0.21	53,53,53,53	0
56	MG	2a	3053	1/1	0.91	0.10	54,54,54,54	0
56	MG	1A	3059	1/1	0.91	0.15	55,55,55,55	0
56	MG	1A	3063	1/1	0.91	0.11	60,60,60,60	0
56	MG	1A	3337	1/1	0.91	0.07	46,46,46,46	0
56	MG	2a	3061	1/1	0.91	0.15	63,63,63,63	0
56	MG	1A	3274	1/1	0.91	0.16	39,39,39,39	0
56	MG	1A	3425	1/1	0.91	0.31	73,73,73,73	0
56	MG	2a	3071	1/1	0.91	0.10	59,59,59,59	0
56	MG	2A	3537	1/1	0.91	0.09	52,52,52,52	0
56	MG	2A	3259	1/1	0.91	0.10	54,54,54,54	0
56	MG	1A	3189	1/1	0.91	0.10	31,31,31,31	0
56	MG	1A	3987	1/1	0.91	0.11	49,49,49,49	0
56	MG	1A	3190	1/1	0.91	0.08	32,32,32,32	0
56	MG	2A	3267	1/1	0.91	0.24	58,58,58,58	0
56	MG	2A	3029	1/1	0.91	0.16	54,54,54,54	0
56	MG	1A	3293	1/1	0.91	0.12	35,35,35,35	0
56	MG	2A	3272	1/1	0.91	0.07	46,46,46,46	0
56	MG	1A	3763	1/1	0.91	0.13	48,48,48,48	0
56	MG	1a	1664	1/1	0.91	0.17	72,72,72,72	0
56	MG	2A	3582	1/1	0.91	0.13	66,66,66,66	0
56	MG	2A	3044	1/1	0.91	0.08	55,55,55,55	0
56	MG	2A	3051	1/1	0.91	0.16	56,56,56,56	0
56	MG	2a	3098	1/1	0.91	0.09	70,70,70,70	0
56	MG	1A	3294	1/1	0.91	0.33	62,62,62,62	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2a	3101	1/1	0.91	0.15	62,62,62,62	0
56	MG	1A	3198	1/1	0.91	0.23	47,47,47,47	0
56	MG	1a	1672	1/1	0.91	0.16	56,56,56,56	0
56	MG	1A	3770	1/1	0.91	0.17	63,63,63,63	0
56	MG	2A	3599	1/1	0.91	0.10	38,38,38,38	0
56	MG	2A	3600	1/1	0.91	0.14	53,53,53,53	0
56	MG	2a	3113	1/1	0.91	0.10	43,43,43,43	0
56	MG	2A	3602	1/1	0.91	0.12	64,64,64,64	0
56	MG	2A	3062	1/1	0.91	0.36	71,71,71,71	0
56	MG	1A	3300	1/1	0.91	0.08	27,27,27,27	0
56	MG	2a	3117	1/1	0.91	0.11	53,53,53,53	0
56	MG	2a	3118	1/1	0.91	0.08	48,48,48,48	0
56	MG	2A	3064	1/1	0.91	0.16	49,49,49,49	0
56	MG	2A	3065	1/1	0.91	0.10	58,58,58,58	0
56	MG	2a	3121	1/1	0.91	0.19	63,63,63,63	0
56	MG	2a	3122	1/1	0.91	0.12	63,63,63,63	0
56	MG	2A	3066	1/1	0.91	0.20	67,67,67,67	0
56	MG	1A	3440	1/1	0.91	0.10	48,48,48,48	0
56	MG	1A	4030	1/1	0.91	0.13	62,62,62,62	0
56	MG	1A	3776	1/1	0.91	0.10	46,46,46,46	0
56	MG	2a	3131	1/1	0.91	0.06	73,73,73,73	0
56	MG	1a	1683	1/1	0.91	0.18	61,61,61,61	0
56	MG	2a	3137	1/1	0.91	0.09	66,66,66,66	0
56	MG	2A	3642	1/1	0.91	0.13	62,62,62,62	0
56	MG	2a	3142	1/1	0.91	0.09	63,63,63,63	0
56	MG	1A	4037	1/1	0.91	0.24	55,55,55,55	0
56	MG	1A	4039	1/1	0.91	0.20	76,76,76,76	0
56	MG	1A	3780	1/1	0.91	0.08	72,72,72,72	0
56	MG	1A	3371	1/1	0.91	0.52	59,59,59,59	0
56	MG	2a	3162	1/1	0.91	0.16	53,53,53,53	0
56	MG	2A	3088	1/1	0.91	0.18	49,49,49,49	0
56	MG	1A	3143	1/1	0.91	0.16	47,47,47,47	0
56	MG	1A	3210	1/1	0.91	0.17	52,52,52,52	0
56	MG	1B	221	1/1	0.91	0.08	66,66,66,66	0
56	MG	2A	3098	1/1	0.91	0.17	55,55,55,55	0
56	MG	2A	3326	1/1	0.91	0.13	66,66,66,66	0
56	MG	1B	225	1/1	0.91	0.09	62,62,62,62	0
56	MG	2A	3100	1/1	0.91	0.31	56,56,56,56	0
56	MG	2a	3179	1/1	0.91	0.25	70,70,70,70	0
56	MG	2a	3183	1/1	0.91	0.10	58,58,58,58	0
56	MG	2A	3683	1/1	0.91	0.11	44,44,44,44	0
56	MG	2A	3688	1/1	0.91	0.09	63,63,63,63	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3575	1/1	0.91	0.14	57,57,57,57	0
56	MG	2a	3190	1/1	0.91	0.32	61,61,61,61	0
56	MG	1A	3092	1/1	0.91	0.09	49,49,49,49	0
56	MG	1A	3800	1/1	0.91	0.13	57,57,57,57	0
56	MG	2a	3196	1/1	0.91	0.12	64,64,64,64	0
56	MG	1a	1707	1/1	0.91	0.29	61,61,61,61	0
56	MG	2A	3116	1/1	0.91	0.30	68,68,68,68	0
56	MG	1A	3093	1/1	0.91	0.19	50,50,50,50	0
56	MG	2A	3706	1/1	0.91	0.09	65,65,65,65	0
56	MG	2a	3201	1/1	0.91	0.24	49,49,49,49	0
56	MG	1a	1711	1/1	0.91	0.07	69,69,69,69	0
56	MG	2a	3204	1/1	0.91	0.16	58,58,58,58	0
56	MG	2a	3206	1/1	0.91	0.06	63,63,63,63	0
56	MG	1A	3586	1/1	0.91	0.13	65,65,65,65	0
56	MG	2A	3714	1/1	0.91	0.08	55,55,55,55	0
56	MG	1A	3587	1/1	0.91	0.07	49,49,49,49	0
56	MG	1G	202	1/1	0.91	0.12	49,49,49,49	0
56	MG	1G	203	1/1	0.91	0.06	51,51,51,51	0
56	MG	1A	3813	1/1	0.91	0.09	48,48,48,48	0
56	MG	1N	202	1/1	0.91	0.15	46,46,46,46	0
56	MG	2A	3141	1/1	0.91	0.20	64,64,64,64	0
56	MG	1T	201	1/1	0.91	0.14	59,59,59,59	0
56	MG	2A	3753	1/1	0.91	0.20	69,69,69,69	0
56	MG	2f	201	1/1	0.91	0.15	49,49,49,49	0
56	MG	2A	3754	1/1	0.91	0.14	63,63,63,63	0
56	MG	1a	1726	1/1	0.91	0.23	54,54,54,54	0
56	MG	1T	203	1/1	0.91	0.15	56,56,56,56	0
56	MG	2r	101	1/1	0.91	0.18	62,62,62,62	0
56	MG	2A	3147	1/1	0.91	0.17	65,65,65,65	0
56	MG	1A	3101	1/1	0.91	0.07	37,37,37,37	0
56	MG	1U	209	1/1	0.91	0.15	47,47,47,47	0
56	MG	1A	3236	1/1	0.91	0.07	57,57,57,57	0
56	MG	1A	3065	1/1	0.91	0.10	53,53,53,53	0
56	MG	10	105	1/1	0.91	0.24	52,52,52,52	0
56	MG	2A	3801	1/1	0.92	0.17	59,59,59,59	0
56	MG	1A	3875	1/1	0.92	0.10	57,57,57,57	0
56	MG	2A	3382	1/1	0.92	0.18	41,41,41,41	0
56	MG	1A	3499	1/1	0.92	0.27	51,51,51,51	0
56	MG	1A	3332	1/1	0.92	0.08	45,45,45,45	0
56	MG	1A	3896	1/1	0.92	0.06	89,89,89,89	0
56	MG	2A	3157	1/1	0.92	0.09	42,42,42,42	0
56	MG	1A	3898	1/1	0.92	0.07	46,46,46,46	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2B	207	1/1	0.92	0.08	55,55,55,55	0
56	MG	2B	210	1/1	0.92	0.25	42,42,42,42	0
56	MG	1A	3407	1/1	0.92	0.21	56,56,56,56	0
56	MG	1A	3408	1/1	0.92	0.19	54,54,54,54	0
56	MG	2A	3401	1/1	0.92	0.17	49,49,49,49	0
56	MG	1a	1765	1/1	0.92	0.14	53,53,53,53	0
56	MG	1A	3064	1/1	0.92	0.13	43,43,43,43	0
56	MG	1A	3909	1/1	0.92	0.14	55,55,55,55	0
56	MG	1A	3410	1/1	0.92	0.06	29,29,29,29	0
56	MG	2O	202	1/1	0.92	0.12	50,50,50,50	0
56	MG	2A	3178	1/1	0.92	0.16	52,52,52,52	0
56	MG	2A	3179	1/1	0.92	0.19	63,63,63,63	0
56	MG	2Q	202	1/1	0.92	0.21	34,34,34,34	0
56	MG	2R	201	1/1	0.92	0.14	48,48,48,48	0
56	MG	1a	1771	1/1	0.92	0.07	70,70,70,70	0
56	MG	2A	3413	1/1	0.92	0.24	45,45,45,45	0
56	MG	1A	3412	1/1	0.92	0.13	56,56,56,56	0
56	MG	2U	202	1/1	0.92	0.06	44,44,44,44	0
56	MG	2V	201	1/1	0.92	0.04	69,69,69,69	0
56	MG	1a	1775	1/1	0.92	0.10	56,56,56,56	0
56	MG	1A	3288	1/1	0.92	0.09	37,37,37,37	0
56	MG	2A	3423	1/1	0.92	0.05	70,70,70,70	0
56	MG	2A	3424	1/1	0.92	0.19	39,39,39,39	0
56	MG	1a	1778	1/1	0.92	0.07	69,69,69,69	0
56	MG	1a	1779	1/1	0.92	0.19	59,59,59,59	0
56	MG	2A	3431	1/1	0.92	0.16	51,51,51,51	0
56	MG	2A	3434	1/1	0.92	0.20	54,54,54,54	0
56	MG	1A	3532	1/1	0.92	0.18	42,42,42,42	0
56	MG	1a	1784	1/1	0.92	0.12	55,55,55,55	0
56	MG	1a	1620	1/1	0.92	0.17	65,65,65,65	0
56	MG	1a	1788	1/1	0.92	0.20	60,60,60,60	0
56	MG	1a	1790	1/1	0.92	0.08	51,51,51,51	0
56	MG	2A	3448	1/1	0.92	0.24	54,54,54,54	0
56	MG	2A	3199	1/1	0.92	0.14	52,52,52,52	0
56	MG	2a	3009	1/1	0.92	0.07	74,74,74,74	0
56	MG	1A	3751	1/1	0.92	0.06	34,34,34,34	0
56	MG	1a	1812	1/1	0.92	0.14	62,62,62,62	0
56	MG	1A	3938	1/1	0.92	0.14	52,52,52,52	0
56	MG	2A	3210	1/1	0.92	0.21	48,48,48,48	0
56	MG	2A	3211	1/1	0.92	0.10	44,44,44,44	0
56	MG	1A	3070	1/1	0.92	0.19	43,43,43,43	0
56	MG	1A	3090	1/1	0.92	0.13	50,50,50,50	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1f	202	1/1	0.92	0.15	60,60,60,60	0
56	MG	2a	3018	1/1	0.92	0.12	52,52,52,52	0
56	MG	2A	3465	1/1	0.92	0.28	58,58,58,58	0
56	MG	1A	3761	1/1	0.92	0.15	60,60,60,60	0
56	MG	1m	201	1/1	0.92	0.09	46,46,46,46	0
56	MG	1A	3349	1/1	0.92	0.23	56,56,56,56	0
56	MG	1A	3226	1/1	0.92	0.24	41,41,41,41	0
56	MG	1A	3427	1/1	0.92	0.24	56,56,56,56	0
56	MG	1A	3978	1/1	0.92	0.12	77,77,77,77	0
56	MG	2a	3029	1/1	0.92	0.07	73,73,73,73	0
56	MG	1x	106	1/1	0.92	0.09	72,72,72,72	0
56	MG	1A	3091	1/1	0.92	0.10	60,60,60,60	0
56	MG	1A	3356	1/1	0.92	0.09	51,51,51,51	0
56	MG	1A	3301	1/1	0.92	0.29	48,48,48,48	0
56	MG	2a	3039	1/1	0.92	0.22	47,47,47,47	0
56	MG	1A	3566	1/1	0.92	0.14	28,28,28,28	0
56	MG	1A	3126	1/1	0.92	0.09	44,44,44,44	0
56	MG	2A	3507	1/1	0.92	0.19	44,44,44,44	0
56	MG	2A	3509	1/1	0.92	0.10	46,46,46,46	0
56	MG	1a	1641	1/1	0.92	0.23	49,49,49,49	0
56	MG	1A	4016	1/1	0.92	0.09	40,40,40,40	0
56	MG	1A	4022	1/1	0.92	0.30	42,42,42,42	0
56	MG	2A	3517	1/1	0.92	0.12	73,73,73,73	0
56	MG	2a	3059	1/1	0.92	0.12	40,40,40,40	0
56	MG	1A	3781	1/1	0.92	0.32	61,61,61,61	0
56	MG	1a	1650	1/1	0.92	0.19	55,55,55,55	0
56	MG	1A	3172	1/1	0.92	0.09	48,48,48,48	0
56	MG	2a	3068	1/1	0.92	0.07	60,60,60,60	0
56	MG	2A	3248	1/1	0.92	0.14	53,53,53,53	0
56	MG	1A	3578	1/1	0.92	0.12	37,37,37,37	0
56	MG	1A	3306	1/1	0.92	0.24	55,55,55,55	0
56	MG	2A	3252	1/1	0.92	0.06	54,54,54,54	0
56	MG	1a	1658	1/1	0.92	0.15	52,52,52,52	0
56	MG	2A	3550	1/1	0.92	0.12	62,62,62,62	0
56	MG	1A	3175	1/1	0.92	0.31	55,55,55,55	0
56	MG	2A	3556	1/1	0.92	0.07	51,51,51,51	0
56	MG	2A	3017	1/1	0.92	0.15	46,46,46,46	0
56	MG	1A	3378	1/1	0.92	0.17	50,50,50,50	0
56	MG	1A	3309	1/1	0.92	0.13	59,59,59,59	0
56	MG	2A	3022	1/1	0.92	0.19	56,56,56,56	0
56	MG	1a	1662	1/1	0.92	0.11	67,67,67,67	0
56	MG	1A	3071	1/1	0.92	0.14	43,43,43,43	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3578	1/1	0.92	0.09	41,41,41,41	0
56	MG	1A	3802	1/1	0.92	0.09	33,33,33,33	0
56	MG	2A	3033	1/1	0.92	0.07	35,35,35,35	0
56	MG	2A	3581	1/1	0.92	0.20	54,54,54,54	0
56	MG	1A	3451	1/1	0.92	0.18	27,27,27,27	0
56	MG	1a	1668	1/1	0.92	0.18	70,70,70,70	0
56	MG	2a	3107	1/1	0.92	0.25	61,61,61,61	0
56	MG	1A	3181	1/1	0.92	0.28	48,48,48,48	0
56	MG	1B	214	1/1	0.92	0.06	52,52,52,52	0
56	MG	2A	3046	1/1	0.92	0.09	73,73,73,73	0
56	MG	1A	3074	1/1	0.92	0.23	42,42,42,42	0
56	MG	1A	3460	1/1	0.92	0.15	44,44,44,44	0
56	MG	2A	3053	1/1	0.92	0.07	57,57,57,57	0
56	MG	2A	3287	1/1	0.92	0.08	51,51,51,51	0
56	MG	1A	3188	1/1	0.92	0.06	48,48,48,48	0
56	MG	2A	3291	1/1	0.92	0.35	44,44,44,44	0
56	MG	2A	3610	1/1	0.92	0.19	48,48,48,48	0
56	MG	2A	3292	1/1	0.92	0.12	66,66,66,66	0
56	MG	1a	1678	1/1	0.92	0.25	60,60,60,60	0
56	MG	2A	3619	1/1	0.92	0.25	45,45,45,45	0
56	MG	2A	3622	1/1	0.92	0.14	56,56,56,56	0
56	MG	1A	3098	1/1	0.92	0.15	46,46,46,46	0
56	MG	1a	1681	1/1	0.92	0.23	62,62,62,62	0
56	MG	2A	3630	1/1	0.92	0.18	52,52,52,52	0
56	MG	1A	3269	1/1	0.92	0.41	54,54,54,54	0
56	MG	1A	3035	1/1	0.92	0.07	42,42,42,42	0
56	MG	2a	3134	1/1	0.92	0.09	77,77,77,77	0
56	MG	2a	3135	1/1	0.92	0.09	67,67,67,67	0
56	MG	1A	3191	1/1	0.92	0.05	46,46,46,46	0
56	MG	2A	3306	1/1	0.92	0.26	46,46,46,46	0
56	MG	1a	1686	1/1	0.92	0.21	50,50,50,50	0
56	MG	1D	305	1/1	0.92	0.14	44,44,44,44	0
56	MG	1A	3324	1/1	0.92	0.15	40,40,40,40	0
56	MG	1E	305	1/1	0.92	0.28	39,39,39,39	0
56	MG	2A	3312	1/1	0.92	0.10	50,50,50,50	0
56	MG	1A	3658	1/1	0.92	0.10	43,43,43,43	0
56	MG	1A	3473	1/1	0.92	0.12	47,47,47,47	0
56	MG	1A	3399	1/1	0.92	0.10	42,42,42,42	0
56	MG	2A	3318	1/1	0.92	0.08	53,53,53,53	0
56	MG	2A	3673	1/1	0.92	0.08	59,59,59,59	0
56	MG	1A	3197	1/1	0.92	0.14	47,47,47,47	0
56	MG	2A	3083	1/1	0.92	0.13	46,46,46,46	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3839	1/1	0.92	0.11	34,34,34,34	0
56	MG	1a	1698	1/1	0.92	0.11	43,43,43,43	0
56	MG	1N	201	1/1	0.92	0.34	52,52,52,52	0
56	MG	2a	3181	1/1	0.92	0.12	64,64,64,64	0
56	MG	2A	3325	1/1	0.92	0.07	48,48,48,48	0
56	MG	1A	3487	1/1	0.92	0.11	52,52,52,52	0
56	MG	1Q	201	1/1	0.92	0.17	44,44,44,44	0
56	MG	2A	3694	1/1	0.92	0.11	46,46,46,46	0
56	MG	1A	3402	1/1	0.92	0.09	47,47,47,47	0
56	MG	1a	1709	1/1	0.92	0.08	56,56,56,56	0
56	MG	1a	1710	1/1	0.92	0.21	58,58,58,58	0
56	MG	2A	3704	1/1	0.92	0.14	57,57,57,57	0
56	MG	2A	3333	1/1	0.92	0.05	37,37,37,37	0
56	MG	1A	3673	1/1	0.92	0.13	50,50,50,50	0
56	MG	2A	3110	1/1	0.92	0.14	40,40,40,40	0
56	MG	1A	3851	1/1	0.92	0.09	48,48,48,48	0
56	MG	1A	3853	1/1	0.92	0.17	47,47,47,47	0
56	MG	1V	206	1/1	0.92	0.07	47,47,47,47	0
56	MG	1A	3854	1/1	0.92	0.10	52,52,52,52	0
56	MG	2A	3343	1/1	0.92	0.09	54,54,54,54	0
56	MG	1A	3856	1/1	0.92	0.12	33,33,33,33	0
56	MG	1A	3674	1/1	0.92	0.07	64,64,64,64	0
56	MG	1a	1721	1/1	0.92	0.15	66,66,66,66	0
56	MG	13	102	1/1	0.92	0.09	41,41,41,41	0
56	MG	13	103	1/1	0.92	0.22	57,57,57,57	0
56	MG	1A	3491	1/1	0.92	0.09	44,44,44,44	0
56	MG	2A	3769	1/1	0.92	0.11	61,61,61,61	0
56	MG	15	102	1/1	0.92	0.27	47,47,47,47	0
56	MG	2A	3137	1/1	0.92	0.14	49,49,49,49	0
56	MG	15	105	1/1	0.92	0.13	48,48,48,48	0
56	MG	1A	3115	1/1	0.92	0.09	41,41,41,41	0
56	MG	2A	3779	1/1	0.92	0.18	50,50,50,50	0
56	MG	17	105	1/1	0.92	0.15	42,42,42,42	0
56	MG	1A	3863	1/1	0.92	0.21	57,57,57,57	0
56	MG	2A	3369	1/1	0.92	0.18	63,63,63,63	0
56	MG	2A	3789	1/1	0.92	0.14	52,52,52,52	0
56	MG	1A	3331	1/1	0.92	0.44	45,45,45,45	0
56	MG	1A	3873	1/1	0.92	0.11	31,31,31,31	0
56	MG	2A	3375	1/1	0.92	0.19	37,37,37,37	0
56	MG	2A	3149	1/1	0.92	0.17	52,52,52,52	0
56	MG	2A	3379	1/1	0.92	0.15	45,45,45,45	0
56	MG	1A	3743	1/1	0.93	0.09	27,27,27,27	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1X	101	1/1	0.93	0.31	43,43,43,43	0
56	MG	1X	102	1/1	0.93	0.17	49,49,49,49	0
56	MG	2A	3472	1/1	0.93	0.18	62,62,62,62	0
56	MG	2A	3054	1/1	0.93	0.21	55,55,55,55	0
56	MG	2A	3474	1/1	0.93	0.14	66,66,66,66	0
56	MG	1a	1705	1/1	0.93	0.14	45,45,45,45	0
56	MG	1A	3879	1/1	0.93	0.08	36,36,36,36	0
56	MG	2T	202	1/1	0.93	0.23	62,62,62,62	0
56	MG	2T	203	1/1	0.93	0.08	34,34,34,34	0
56	MG	1A	3336	1/1	0.93	0.16	56,56,56,56	0
56	MG	1A	3554	1/1	0.93	0.08	51,51,51,51	0
56	MG	10	106	1/1	0.93	0.20	63,63,63,63	0
56	MG	2A	3485	1/1	0.93	0.08	45,45,45,45	0
56	MG	13	101	1/1	0.93	0.16	43,43,43,43	0
56	MG	1A	3453	1/1	0.93	0.08	47,47,47,47	0
56	MG	1A	3152	1/1	0.93	0.09	42,42,42,42	0
56	MG	1A	3899	1/1	0.93	0.08	50,50,50,50	0
56	MG	2A	3070	1/1	0.93	0.25	38,38,38,38	0
56	MG	25	101	1/1	0.93	0.22	53,53,53,53	0
56	MG	1A	3755	1/1	0.93	0.10	58,58,58,58	0
56	MG	27	101	1/1	0.93	0.07	42,42,42,42	0
56	MG	1a	1716	1/1	0.93	0.14	56,56,56,56	0
56	MG	1A	3053	1/1	0.93	0.10	34,34,34,34	0
56	MG	2A	3280	1/1	0.93	0.27	43,43,43,43	0
56	MG	1A	3569	1/1	0.93	0.11	53,53,53,53	0
56	MG	1A	3241	1/1	0.93	0.07	39,39,39,39	0
56	MG	2A	3525	1/1	0.93	0.12	49,49,49,49	0
56	MG	1A	3571	1/1	0.93	0.12	33,33,33,33	0
56	MG	2A	3527	1/1	0.93	0.08	55,55,55,55	0
56	MG	1a	1722	1/1	0.93	0.25	51,51,51,51	0
56	MG	1A	3078	1/1	0.93	0.28	47,47,47,47	0
56	MG	2A	3087	1/1	0.93	0.10	54,54,54,54	0
56	MG	2A	3534	1/1	0.93	0.11	38,38,38,38	0
56	MG	1a	1724	1/1	0.93	0.27	47,47,47,47	0
56	MG	1A	3463	1/1	0.93	0.12	56,56,56,56	0
56	MG	1A	3927	1/1	0.93	0.18	65,65,65,65	0
56	MG	2A	3544	1/1	0.93	0.11	42,42,42,42	0
56	MG	2A	3093	1/1	0.93	0.19	63,63,63,63	0
56	MG	1A	3772	1/1	0.93	0.19	34,34,34,34	0
56	MG	1A	3404	1/1	0.93	0.17	32,32,32,32	0
56	MG	2A	3557	1/1	0.93	0.14	61,61,61,61	0
56	MG	2a	3021	1/1	0.93	0.10	75,75,75,75	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3179	1/1	0.93	0.10	35,35,35,35	0
56	MG	2A	3562	1/1	0.93	0.16	51,51,51,51	0
56	MG	1A	3351	1/1	0.93	0.12	64,64,64,64	0
56	MG	2A	3105	1/1	0.93	0.22	57,57,57,57	0
56	MG	1A	3353	1/1	0.93	0.21	52,52,52,52	0
56	MG	2a	3028	1/1	0.93	0.27	61,61,61,61	0
56	MG	1A	3250	1/1	0.93	0.07	36,36,36,36	0
56	MG	1a	1743	1/1	0.93	0.26	44,44,44,44	0
56	MG	1A	3946	1/1	0.93	0.10	35,35,35,35	0
56	MG	1A	3203	1/1	0.93	0.19	47,47,47,47	0
56	MG	1A	3784	1/1	0.93	0.12	59,59,59,59	0
56	MG	2a	3037	1/1	0.93	0.21	66,66,66,66	0
56	MG	2a	3038	1/1	0.93	0.16	41,41,41,41	0
56	MG	1a	1750	1/1	0.93	0.19	49,49,49,49	0
56	MG	2A	3119	1/1	0.93	0.05	46,46,46,46	0
56	MG	1A	3358	1/1	0.93	0.08	33,33,33,33	0
56	MG	2a	3044	1/1	0.93	0.07	54,54,54,54	0
56	MG	2a	3045	1/1	0.93	0.09	47,47,47,47	0
56	MG	1A	3974	1/1	0.93	0.09	75,75,75,75	0
56	MG	1A	3788	1/1	0.93	0.10	43,43,43,43	0
56	MG	1A	3596	1/1	0.93	0.12	38,38,38,38	0
56	MG	1A	3597	1/1	0.93	0.09	41,41,41,41	0
56	MG	1A	3204	1/1	0.93	0.09	53,53,53,53	0
56	MG	2a	3057	1/1	0.93	0.09	62,62,62,62	0
56	MG	1A	4006	1/1	0.93	0.10	54,54,54,54	0
56	MG	2A	3138	1/1	0.93	0.10	65,65,65,65	0
56	MG	1a	1625	1/1	0.93	0.10	44,44,44,44	0
56	MG	1A	3479	1/1	0.93	0.09	37,37,37,37	0
56	MG	2a	3063	1/1	0.93	0.17	54,54,54,54	0
56	MG	1A	3482	1/1	0.93	0.45	37,37,37,37	0
56	MG	1A	3485	1/1	0.93	0.09	33,33,33,33	0
56	MG	1A	3104	1/1	0.93	0.11	33,33,33,33	0
56	MG	1A	4024	1/1	0.93	0.20	61,61,61,61	0
56	MG	2a	3073	1/1	0.93	0.23	66,66,66,66	0
56	MG	1A	3807	1/1	0.93	0.13	37,37,37,37	0
56	MG	2A	3338	1/1	0.93	0.14	55,55,55,55	0
56	MG	1A	3810	1/1	0.93	0.06	43,43,43,43	0
56	MG	2a	3077	1/1	0.93	0.15	70,70,70,70	0
56	MG	2A	3627	1/1	0.93	0.11	55,55,55,55	0
56	MG	1A	3420	1/1	0.93	0.12	37,37,37,37	0
56	MG	2A	3632	1/1	0.93	0.12	60,60,60,60	0
56	MG	2A	3153	1/1	0.93	0.16	68,68,68,68	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2a	3086	1/1	0.93	0.24	63,63,63,63	0
56	MG	1A	3642	1/1	0.93	0.11	36,36,36,36	0
56	MG	1A	3363	1/1	0.93	0.08	43,43,43,43	0
56	MG	2A	3637	1/1	0.93	0.13	74,74,74,74	0
56	MG	1A	3815	1/1	0.93	0.27	58,58,58,58	0
56	MG	1A	3262	1/1	0.93	0.18	50,50,50,50	0
56	MG	2A	3161	1/1	0.93	0.09	59,59,59,59	0
56	MG	1A	3652	1/1	0.93	0.08	52,52,52,52	0
56	MG	1a	1804	1/1	0.93	0.11	46,46,46,46	0
56	MG	2A	3651	1/1	0.93	0.10	70,70,70,70	0
56	MG	2A	3169	1/1	0.93	0.32	54,54,54,54	0
56	MG	2a	3104	1/1	0.93	0.12	57,57,57,57	0
56	MG	1A	3657	1/1	0.93	0.12	48,48,48,48	0
56	MG	1a	1647	1/1	0.93	0.17	48,48,48,48	0
56	MG	1A	3822	1/1	0.93	0.14	38,38,38,38	0
56	MG	2A	3663	1/1	0.93	0.08	50,50,50,50	0
56	MG	2A	3665	1/1	0.93	0.07	57,57,57,57	0
56	MG	1A	3823	1/1	0.93	0.14	42,42,42,42	0
56	MG	2A	3670	1/1	0.93	0.06	62,62,62,62	0
56	MG	2A	3671	1/1	0.93	0.13	45,45,45,45	0
56	MG	1a	1652	1/1	0.93	0.15	54,54,54,54	0
56	MG	1B	206	1/1	0.93	0.15	55,55,55,55	0
56	MG	1B	208	1/1	0.93	0.18	50,50,50,50	0
56	MG	1a	1655	1/1	0.93	0.10	41,41,41,41	0
56	MG	2A	3680	1/1	0.93	0.12	58,58,58,58	0
56	MG	1B	211	1/1	0.93	0.06	45,45,45,45	0
56	MG	2A	3377	1/1	0.93	0.20	41,41,41,41	0
56	MG	2A	3687	1/1	0.93	0.21	55,55,55,55	0
56	MG	1A	3495	1/1	0.93	0.11	64,64,64,64	0
56	MG	2a	3125	1/1	0.93	0.27	38,38,38,38	0
56	MG	2A	3187	1/1	0.93	0.09	58,58,58,58	0
56	MG	1B	218	1/1	0.93	0.07	36,36,36,36	0
56	MG	2A	3693	1/1	0.93	0.07	48,48,48,48	0
56	MG	2A	3189	1/1	0.93	0.07	33,33,33,33	0
56	MG	1A	3212	1/1	0.93	0.11	50,50,50,50	0
56	MG	2A	3191	1/1	0.93	0.16	51,51,51,51	0
56	MG	2A	3386	1/1	0.93	0.28	61,61,61,61	0
56	MG	1A	3215	1/1	0.93	0.13	53,53,53,53	0
56	MG	1A	3661	1/1	0.93	0.06	69,69,69,69	0
56	MG	1A	3216	1/1	0.93	0.09	55,55,55,55	0
56	MG	1A	3012	1/1	0.93	0.14	38,38,38,38	0
56	MG	2A	3396	1/1	0.93	0.23	45,45,45,45	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2a	3158	1/1	0.93	0.13	71,71,71,71	0
56	MG	2A	3196	1/1	0.93	0.07	57,57,57,57	0
56	MG	1A	3509	1/1	0.93	0.21	65,65,65,65	0
56	MG	1a	1667	1/1	0.93	0.16	82,82,82,82	0
56	MG	1A	3138	1/1	0.93	0.35	37,37,37,37	0
56	MG	1A	3227	1/1	0.93	0.18	37,37,37,37	0
56	MG	2a	3169	1/1	0.93	0.16	65,65,65,65	0
56	MG	2A	3725	1/1	0.93	0.14	60,60,60,60	0
56	MG	1D	309	1/1	0.93	0.11	33,33,33,33	0
56	MG	1A	3384	1/1	0.93	0.17	48,48,48,48	0
56	MG	2A	3731	1/1	0.93	0.07	59,59,59,59	0
56	MG	1A	3228	1/1	0.93	0.12	57,57,57,57	0
56	MG	2A	3007	1/1	0.93	0.12	49,49,49,49	0
56	MG	2a	3180	1/1	0.93	0.22	62,62,62,62	0
56	MG	2A	3009	1/1	0.93	0.12	57,57,57,57	0
56	MG	2A	3765	1/1	0.93	0.07	67,67,67,67	0
56	MG	1A	3094	1/1	0.93	0.17	33,33,33,33	0
56	MG	2A	3416	1/1	0.93	0.10	68,68,68,68	0
56	MG	1A	3441	1/1	0.93	0.16	51,51,51,51	0
56	MG	2a	3189	1/1	0.93	0.10	72,72,72,72	0
56	MG	2A	3221	1/1	0.93	0.13	58,58,58,58	0
56	MG	1A	3706	1/1	0.93	0.09	27,27,27,27	0
56	MG	2a	3193	1/1	0.93	0.08	81,81,81,81	0
56	MG	2A	3778	1/1	0.93	0.20	45,45,45,45	0
56	MG	1a	1680	1/1	0.93	0.23	60,60,60,60	0
56	MG	1A	3097	1/1	0.93	0.11	59,59,59,59	0
56	MG	2A	3428	1/1	0.93	0.14	57,57,57,57	0
56	MG	1A	3297	1/1	0.93	0.06	44,44,44,44	0
56	MG	2A	3020	1/1	0.93	0.11	55,55,55,55	0
56	MG	2A	3433	1/1	0.93	0.19	29,29,29,29	0
56	MG	2A	3230	1/1	0.93	0.07	47,47,47,47	0
56	MG	2A	3794	1/1	0.93	0.20	58,58,58,58	0
56	MG	1A	3333	1/1	0.93	0.36	45,45,45,45	0
56	MG	2A	3440	1/1	0.93	0.41	49,49,49,49	0
56	MG	1A	3861	1/1	0.93	0.08	55,55,55,55	0
56	MG	2A	3800	1/1	0.93	0.16	38,38,38,38	0
56	MG	1A	3544	1/1	0.93	0.18	42,42,42,42	0
56	MG	1Q	205	1/1	0.93	0.09	36,36,36,36	0
56	MG	2A	3446	1/1	0.93	0.11	36,36,36,36	0
56	MG	1a	1689	1/1	0.93	0.17	55,55,55,55	0
56	MG	1A	3725	1/1	0.93	0.09	36,36,36,36	0
56	MG	1A	3864	1/1	0.93	0.08	56,56,56,56	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1U	207	1/1	0.93	0.21	38,38,38,38	0
56	MG	2A	3041	1/1	0.93	0.21	35,35,35,35	0
56	MG	1A	3233	1/1	0.93	0.12	57,57,57,57	0
56	MG	2A	3245	1/1	0.93	0.07	49,49,49,49	0
56	MG	2A	3457	1/1	0.93	0.20	48,48,48,48	0
56	MG	1A	3449	1/1	0.93	0.19	58,58,58,58	0
56	MG	2A	3460	1/1	0.93	0.30	51,51,51,51	0
56	MG	2D	304	1/1	0.93	0.11	54,54,54,54	0
56	MG	1V	205	1/1	0.93	0.12	49,49,49,49	0
56	MG	2E	304	1/1	0.93	0.15	50,50,50,50	0
56	MG	2A	3047	1/1	0.93	0.07	53,53,53,53	0
56	MG	2A	3050	1/1	0.93	0.20	50,50,50,50	0
56	MG	1S	202	1/1	0.94	0.11	35,35,35,35	0
56	MG	1A	3767	1/1	0.94	0.10	49,49,49,49	0
56	MG	1A	3085	1/1	0.94	0.11	40,40,40,40	0
56	MG	1T	205	1/1	0.94	0.07	55,55,55,55	0
56	MG	2B	209	1/1	0.94	0.14	70,70,70,70	0
56	MG	2A	3233	1/1	0.94	0.09	59,59,59,59	0
56	MG	2B	211	1/1	0.94	0.22	51,51,51,51	0
56	MG	2A	3234	1/1	0.94	0.05	50,50,50,50	0
56	MG	1U	204	1/1	0.94	0.10	40,40,40,40	0
56	MG	1A	3184	1/1	0.94	0.12	40,40,40,40	0
56	MG	2D	302	1/1	0.94	0.23	62,62,62,62	0
56	MG	2A	3030	1/1	0.94	0.28	54,54,54,54	0
56	MG	2A	3458	1/1	0.94	0.07	38,38,38,38	0
56	MG	2E	302	1/1	0.94	0.10	52,52,52,52	0
56	MG	2E	303	1/1	0.94	0.09	64,64,64,64	0
56	MG	2A	3031	1/1	0.94	0.08	59,59,59,59	0
56	MG	1A	3593	1/1	0.94	0.07	44,44,44,44	0
56	MG	2E	308	1/1	0.94	0.09	51,51,51,51	0
56	MG	1A	3161	1/1	0.94	0.12	47,47,47,47	0
56	MG	1V	204	1/1	0.94	0.13	43,43,43,43	0
56	MG	1A	3245	1/1	0.94	0.12	37,37,37,37	0
56	MG	1A	3921	1/1	0.94	0.07	63,63,63,63	0
56	MG	2A	3466	1/1	0.94	0.24	44,44,44,44	0
56	MG	2A	3043	1/1	0.94	0.10	58,58,58,58	0
56	MG	1A	3388	1/1	0.94	0.14	51,51,51,51	0
56	MG	2A	3469	1/1	0.94	0.27	53,53,53,53	0
56	MG	2R	204	1/1	0.94	0.07	42,42,42,42	0
56	MG	1A	3779	1/1	0.94	0.13	38,38,38,38	0
56	MG	1a	1699	1/1	0.94	0.21	41,41,41,41	0
56	MG	2A	3048	1/1	0.94	0.13	50,50,50,50	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3049	1/1	0.94	0.06	47,47,47,47	0
56	MG	2U	201	1/1	0.94	0.09	55,55,55,55	0
56	MG	1A	3497	1/1	0.94	0.15	43,43,43,43	0
56	MG	1a	1702	1/1	0.94	0.13	51,51,51,51	0
56	MG	1a	1703	1/1	0.94	0.18	58,58,58,58	0
56	MG	2A	3256	1/1	0.94	0.11	57,57,57,57	0
56	MG	2A	3484	1/1	0.94	0.19	63,63,63,63	0
56	MG	1Z	302	1/1	0.94	0.07	42,42,42,42	0
56	MG	1A	3248	1/1	0.94	0.14	53,53,53,53	0
56	MG	2A	3490	1/1	0.94	0.13	43,43,43,43	0
56	MG	2A	3491	1/1	0.94	0.07	42,42,42,42	0
56	MG	2A	3492	1/1	0.94	0.35	49,49,49,49	0
56	MG	26	101	1/1	0.94	0.07	53,53,53,53	0
56	MG	1A	3504	1/1	0.94	0.18	55,55,55,55	0
56	MG	2A	3496	1/1	0.94	0.17	45,45,45,45	0
56	MG	1A	3139	1/1	0.94	0.12	29,29,29,29	0
56	MG	10	108	1/1	0.94	0.14	62,62,62,62	0
56	MG	2A	3265	1/1	0.94	0.09	58,58,58,58	0
56	MG	2A	3266	1/1	0.94	0.06	38,38,38,38	0
56	MG	2A	3059	1/1	0.94	0.18	52,52,52,52	0
56	MG	1A	3630	1/1	0.94	0.09	65,65,65,65	0
56	MG	2A	3269	1/1	0.94	0.23	50,50,50,50	0
56	MG	2A	3270	1/1	0.94	0.19	56,56,56,56	0
56	MG	2A	3519	1/1	0.94	0.22	49,49,49,49	0
56	MG	2A	3523	1/1	0.94	0.16	65,65,65,65	0
56	MG	1A	3941	1/1	0.94	0.13	55,55,55,55	0
56	MG	1A	3786	1/1	0.94	0.13	51,51,51,51	0
56	MG	1A	3943	1/1	0.94	0.08	64,64,64,64	0
56	MG	15	101	1/1	0.94	0.18	36,36,36,36	0
56	MG	1A	3442	1/1	0.94	0.08	49,49,49,49	0
56	MG	2A	3529	1/1	0.94	0.14	51,51,51,51	0
56	MG	2A	3278	1/1	0.94	0.08	56,56,56,56	0
56	MG	1A	3251	1/1	0.94	0.06	39,39,39,39	0
56	MG	1A	3640	1/1	0.94	0.14	37,37,37,37	0
56	MG	1a	1719	1/1	0.94	0.10	45,45,45,45	0
56	MG	2A	3283	1/1	0.94	0.09	60,60,60,60	0
56	MG	16	102	1/1	0.94	0.10	50,50,50,50	0
56	MG	17	101	1/1	0.94	0.10	39,39,39,39	0
56	MG	1A	3512	1/1	0.94	0.26	42,42,42,42	0
56	MG	2A	3288	1/1	0.94	0.09	44,44,44,44	0
56	MG	2A	3081	1/1	0.94	0.10	62,62,62,62	0
56	MG	1A	3956	1/1	0.94	0.10	36,36,36,36	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3394	1/1	0.94	0.10	57,57,57,57	0
56	MG	2A	3560	1/1	0.94	0.12	55,55,55,55	0
56	MG	1a	1725	1/1	0.94	0.15	36,36,36,36	0
56	MG	19	101	1/1	0.94	0.13	52,52,52,52	0
56	MG	2A	3299	1/1	0.94	0.07	48,48,48,48	0
56	MG	1A	3342	1/1	0.94	0.10	45,45,45,45	0
56	MG	2A	3573	1/1	0.94	0.09	66,66,66,66	0
56	MG	1A	3975	1/1	0.94	0.08	63,63,63,63	0
56	MG	2A	3090	1/1	0.94	0.18	38,38,38,38	0
56	MG	2a	3043	1/1	0.94	0.09	68,68,68,68	0
56	MG	1A	3253	1/1	0.94	0.16	46,46,46,46	0
56	MG	1A	3982	1/1	0.94	0.20	59,59,59,59	0
56	MG	1a	1734	1/1	0.94	0.19	61,61,61,61	0
56	MG	1A	3803	1/1	0.94	0.08	55,55,55,55	0
56	MG	2a	3050	1/1	0.94	0.09	68,68,68,68	0
56	MG	1A	3986	1/1	0.94	0.07	45,45,45,45	0
56	MG	1A	3653	1/1	0.94	0.17	28,28,28,28	0
56	MG	2A	3101	1/1	0.94	0.17	56,56,56,56	0
56	MG	2A	3102	1/1	0.94	0.23	50,50,50,50	0
56	MG	2A	3588	1/1	0.94	0.16	43,43,43,43	0
56	MG	1A	3996	1/1	0.94	0.08	38,38,38,38	0
56	MG	1a	1745	1/1	0.94	0.16	49,49,49,49	0
56	MG	2A	3317	1/1	0.94	0.09	51,51,51,51	0
56	MG	1A	3516	1/1	0.94	0.08	44,44,44,44	0
56	MG	2a	3065	1/1	0.94	0.11	47,47,47,47	0
56	MG	1a	1610	1/1	0.94	0.16	66,66,66,66	0
56	MG	2A	3601	1/1	0.94	0.12	45,45,45,45	0
56	MG	1A	3518	1/1	0.94	0.22	52,52,52,52	0
56	MG	2A	3604	1/1	0.94	0.06	38,38,38,38	0
56	MG	1A	3048	1/1	0.94	0.19	28,28,28,28	0
56	MG	2A	3114	1/1	0.94	0.11	53,53,53,53	0
56	MG	2A	3613	1/1	0.94	0.20	55,55,55,55	0
56	MG	1A	3096	1/1	0.94	0.16	43,43,43,43	0
56	MG	1A	3527	1/1	0.94	0.05	53,53,53,53	0
56	MG	1a	1753	1/1	0.94	0.14	58,58,58,58	0
56	MG	2A	3120	1/1	0.94	0.04	66,66,66,66	0
56	MG	2A	3121	1/1	0.94	0.27	49,49,49,49	0
56	MG	2A	3624	1/1	0.94	0.19	49,49,49,49	0
56	MG	1A	4017	1/1	0.94	0.08	54,54,54,54	0
56	MG	2a	3087	1/1	0.94	0.12	76,76,76,76	0
56	MG	1A	3194	1/1	0.94	0.19	36,36,36,36	0
56	MG	2A	3628	1/1	0.94	0.15	57,57,57,57	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3332	1/1	0.94	0.10	51,51,51,51	0
56	MG	2A	3631	1/1	0.94	0.09	68,68,68,68	0
56	MG	2a	3094	1/1	0.94	0.06	49,49,49,49	0
56	MG	1a	1757	1/1	0.94	0.12	65,65,65,65	0
56	MG	1A	3014	1/1	0.94	0.11	28,28,28,28	0
56	MG	1A	3536	1/1	0.94	0.14	45,45,45,45	0
56	MG	2A	3336	1/1	0.94	0.08	47,47,47,47	0
56	MG	1A	3539	1/1	0.94	0.29	43,43,43,43	0
56	MG	2A	3638	1/1	0.94	0.15	56,56,56,56	0
56	MG	2A	3136	1/1	0.94	0.20	43,43,43,43	0
56	MG	1A	3015	1/1	0.94	0.10	47,47,47,47	0
56	MG	1A	3459	1/1	0.94	0.12	44,44,44,44	0
56	MG	1A	3683	1/1	0.94	0.17	54,54,54,54	0
56	MG	2A	3140	1/1	0.94	0.10	61,61,61,61	0
56	MG	1a	1773	1/1	0.94	0.05	63,63,63,63	0
56	MG	2a	3112	1/1	0.94	0.28	51,51,51,51	0
56	MG	2A	3345	1/1	0.94	0.15	44,44,44,44	0
56	MG	1A	3685	1/1	0.94	0.19	59,59,59,59	0
56	MG	1A	4032	1/1	0.94	0.14	21,21,21,21	0
56	MG	2A	3349	1/1	0.94	0.05	58,58,58,58	0
56	MG	1A	3688	1/1	0.94	0.09	50,50,50,50	0
56	MG	2A	3351	1/1	0.94	0.07	62,62,62,62	0
56	MG	1A	3694	1/1	0.94	0.11	70,70,70,70	0
56	MG	1A	3066	1/1	0.94	0.08	54,54,54,54	0
56	MG	2A	3150	1/1	0.94	0.25	54,54,54,54	0
56	MG	1A	4040	1/1	0.94	0.13	34,34,34,34	0
56	MG	1A	3545	1/1	0.94	0.14	58,58,58,58	0
56	MG	2A	3675	1/1	0.94	0.09	70,70,70,70	0
56	MG	1B	203	1/1	0.94	0.10	47,47,47,47	0
56	MG	2a	3126	1/1	0.94	0.10	84,84,84,84	0
56	MG	1A	3832	1/1	0.94	0.13	42,42,42,42	0
56	MG	1a	1639	1/1	0.94	0.20	47,47,47,47	0
56	MG	2A	3368	1/1	0.94	0.13	49,49,49,49	0
56	MG	2a	3132	1/1	0.94	0.10	80,80,80,80	0
56	MG	1a	1640	1/1	0.94	0.12	59,59,59,59	0
56	MG	2A	3370	1/1	0.94	0.11	62,62,62,62	0
56	MG	1A	3200	1/1	0.94	0.05	35,35,35,35	0
56	MG	1A	3234	1/1	0.94	0.12	56,56,56,56	0
56	MG	1a	1814	1/1	0.94	0.05	63,63,63,63	0
56	MG	1a	1816	1/1	0.94	0.06	76,76,76,76	0
56	MG	2a	3146	1/1	0.94	0.06	81,81,81,81	0
56	MG	2a	3147	1/1	0.94	0.12	70,70,70,70	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1B	209	1/1	0.94	0.11	48,48,48,48	0
56	MG	2A	3695	1/1	0.94	0.11	51,51,51,51	0
56	MG	1a	1820	1/1	0.94	0.07	44,44,44,44	0
56	MG	1B	210	1/1	0.94	0.23	49,49,49,49	0
56	MG	2A	3381	1/1	0.94	0.18	33,33,33,33	0
56	MG	2A	3175	1/1	0.94	0.12	40,40,40,40	0
56	MG	1A	3157	1/1	0.94	0.11	39,39,39,39	0
56	MG	2a	3165	1/1	0.94	0.10	78,78,78,78	0
56	MG	1A	3279	1/1	0.94	0.18	41,41,41,41	0
56	MG	1A	3556	1/1	0.94	0.19	50,50,50,50	0
56	MG	1l	202	1/1	0.94	0.10	52,52,52,52	0
56	MG	1A	3047	1/1	0.94	0.23	44,44,44,44	0
56	MG	1n	101	1/1	0.94	0.27	51,51,51,51	0
56	MG	1A	3724	1/1	0.94	0.09	33,33,33,33	0
56	MG	2a	3176	1/1	0.94	0.12	67,67,67,67	0
56	MG	1A	3369	1/1	0.94	0.12	41,41,41,41	0
56	MG	1A	3855	1/1	0.94	0.09	60,60,60,60	0
56	MG	2A	3722	1/1	0.94	0.09	64,64,64,64	0
56	MG	1x	103	1/1	0.94	0.14	65,65,65,65	0
56	MG	1A	3240	1/1	0.94	0.05	41,41,41,41	0
56	MG	1x	105	1/1	0.94	0.14	57,57,57,57	0
56	MG	2A	3730	1/1	0.94	0.06	71,71,71,71	0
56	MG	1A	3568	1/1	0.94	0.19	39,39,39,39	0
56	MG	2A	3734	1/1	0.94	0.07	45,45,45,45	0
56	MG	2A	3736	1/1	0.94	0.11	60,60,60,60	0
56	MG	1A	3740	1/1	0.94	0.14	44,44,44,44	0
56	MG	2A	3745	1/1	0.94	0.08	45,45,45,45	0
56	MG	1A	3419	1/1	0.94	0.18	43,43,43,43	0
56	MG	1A	3325	1/1	0.94	0.13	43,43,43,43	0
56	MG	2A	3761	1/1	0.94	0.07	55,55,55,55	0
56	MG	2A	3764	1/1	0.94	0.09	52,52,52,52	0
56	MG	1A	3476	1/1	0.94	0.07	41,41,41,41	0
56	MG	2A	3412	1/1	0.94	0.23	57,57,57,57	0
56	MG	1A	3376	1/1	0.94	0.17	26,26,26,26	0
56	MG	1A	3867	1/1	0.94	0.09	78,78,78,78	0
56	MG	1E	309	1/1	0.94	0.07	56,56,56,56	0
56	MG	1F	301	1/1	0.94	0.10	40,40,40,40	0
56	MG	2A	3202	1/1	0.94	0.22	51,51,51,51	0
56	MG	2A	3003	1/1	0.94	0.09	40,40,40,40	0
56	MG	1A	3289	1/1	0.94	0.11	36,36,36,36	0
56	MG	2A	3784	1/1	0.94	0.10	58,58,58,58	0
56	MG	1a	1671	1/1	0.94	0.06	47,47,47,47	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1G	201	1/1	0.94	0.08	50,50,50,50	0
56	MG	2A	3788	1/1	0.94	0.07	55,55,55,55	0
56	MG	2A	3213	1/1	0.94	0.09	41,41,41,41	0
56	MG	2A	3790	1/1	0.94	0.10	62,62,62,62	0
56	MG	1A	3379	1/1	0.94	0.18	52,52,52,52	0
56	MG	2A	3432	1/1	0.94	0.16	26,26,26,26	0
56	MG	1A	3327	1/1	0.94	0.21	49,49,49,49	0
56	MG	1A	3758	1/1	0.94	0.08	48,48,48,48	0
56	MG	2A	3796	1/1	0.94	0.13	53,53,53,53	0
56	MG	2A	3435	1/1	0.94	0.20	64,64,64,64	0
56	MG	2A	3436	1/1	0.94	0.29	51,51,51,51	0
56	MG	2A	3437	1/1	0.94	0.37	30,30,30,30	0
56	MG	1A	3759	1/1	0.94	0.06	48,48,48,48	0
56	MG	1A	3486	1/1	0.94	0.10	54,54,54,54	0
56	MG	1P	204	1/1	0.94	0.20	54,54,54,54	0
56	MG	2x	103	1/1	0.94	0.18	59,59,59,59	0
56	MG	1A	3292	1/1	0.94	0.19	49,49,49,49	0
56	MG	1A	3588	1/1	0.94	0.07	46,46,46,46	0
56	MG	1Q	204	1/1	0.95	0.06	20,20,20,20	0
56	MG	1A	3140	1/1	0.95	0.14	48,48,48,48	0
56	MG	2A	3135	1/1	0.95	0.16	36,36,36,36	0
56	MG	1R	202	1/1	0.95	0.14	51,51,51,51	0
56	MG	2A	3762	1/1	0.95	0.07	65,65,65,65	0
56	MG	2A	3763	1/1	0.95	0.07	65,65,65,65	0
56	MG	1A	3500	1/1	0.95	0.10	29,29,29,29	0
56	MG	1A	3502	1/1	0.95	0.13	37,37,37,37	0
56	MG	2A	3767	1/1	0.95	0.08	62,62,62,62	0
56	MG	1T	202	1/1	0.95	0.17	49,49,49,49	0
56	MG	1a	1727	1/1	0.95	0.23	52,52,52,52	0
56	MG	1A	3270	1/1	0.95	0.07	49,49,49,49	0
56	MG	2A	3142	1/1	0.95	0.14	39,39,39,39	0
56	MG	1T	204	1/1	0.95	0.04	35,35,35,35	0
56	MG	1A	3271	1/1	0.95	0.07	27,27,27,27	0
56	MG	1A	3866	1/1	0.95	0.20	73,73,73,73	0
56	MG	2A	3780	1/1	0.95	0.13	70,70,70,70	0
56	MG	2A	3398	1/1	0.95	0.15	33,33,33,33	0
56	MG	2A	3146	1/1	0.95	0.18	46,46,46,46	0
56	MG	2A	3402	1/1	0.95	0.18	51,51,51,51	0
56	MG	1U	205	1/1	0.95	0.06	37,37,37,37	0
56	MG	1A	3684	1/1	0.95	0.06	43,43,43,43	0
56	MG	1A	3507	1/1	0.95	0.16	40,40,40,40	0
56	MG	1A	3334	1/1	0.95	0.14	53,53,53,53	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1U	210	1/1	0.95	0.15	47,47,47,47	0
56	MG	1A	3690	1/1	0.95	0.12	44,44,44,44	0
56	MG	1A	3219	1/1	0.95	0.11	37,37,37,37	0
56	MG	2A	3410	1/1	0.95	0.25	64,64,64,64	0
56	MG	1A	3696	1/1	0.95	0.08	48,48,48,48	0
56	MG	2A	3797	1/1	0.95	0.15	42,42,42,42	0
56	MG	1W	201	1/1	0.95	0.14	33,33,33,33	0
56	MG	1A	3886	1/1	0.95	0.06	45,45,45,45	0
56	MG	1A	3887	1/1	0.95	0.08	65,65,65,65	0
56	MG	2A	3418	1/1	0.95	0.16	42,42,42,42	0
56	MG	2A	3419	1/1	0.95	0.14	60,60,60,60	0
56	MG	2A	3162	1/1	0.95	0.19	54,54,54,54	0
56	MG	1A	3510	1/1	0.95	0.14	53,53,53,53	0
56	MG	2A	3165	1/1	0.95	0.12	42,42,42,42	0
56	MG	1Z	301	1/1	0.95	0.07	32,32,32,32	0
56	MG	1A	3511	1/1	0.95	0.09	48,48,48,48	0
56	MG	2A	3427	1/1	0.95	0.29	41,41,41,41	0
56	MG	10	101	1/1	0.95	0.10	42,42,42,42	0
56	MG	2B	208	1/1	0.95	0.09	48,48,48,48	0
56	MG	2A	3171	1/1	0.95	0.16	50,50,50,50	0
56	MG	1A	3221	1/1	0.95	0.10	35,35,35,35	0
56	MG	1a	1760	1/1	0.95	0.06	55,55,55,55	0
56	MG	10	103	1/1	0.95	0.10	39,39,39,39	0
56	MG	1A	3414	1/1	0.95	0.19	44,44,44,44	0
56	MG	1A	3707	1/1	0.95	0.15	41,41,41,41	0
56	MG	1A	3415	1/1	0.95	0.07	58,58,58,58	0
56	MG	2D	303	1/1	0.95	0.09	48,48,48,48	0
56	MG	1A	3416	1/1	0.95	0.06	36,36,36,36	0
56	MG	2A	3438	1/1	0.95	0.22	54,54,54,54	0
56	MG	2A	3182	1/1	0.95	0.13	41,41,41,41	0
56	MG	1A	3418	1/1	0.95	0.14	46,46,46,46	0
56	MG	1A	3912	1/1	0.95	0.10	44,44,44,44	0
56	MG	2E	305	1/1	0.95	0.07	42,42,42,42	0
56	MG	1A	3915	1/1	0.95	0.12	51,51,51,51	0
56	MG	1A	3180	1/1	0.95	0.12	40,40,40,40	0
56	MG	2E	309	1/1	0.95	0.07	39,39,39,39	0
56	MG	1A	3099	1/1	0.95	0.09	33,33,33,33	0
56	MG	2F	302	1/1	0.95	0.13	54,54,54,54	0
56	MG	1A	3922	1/1	0.95	0.11	83,83,83,83	0
56	MG	15	106	1/1	0.95	0.28	40,40,40,40	0
56	MG	1A	3523	1/1	0.95	0.06	46,46,46,46	0
56	MG	2A	3451	1/1	0.95	0.14	51,51,51,51	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3524	1/1	0.95	0.20	36,36,36,36	0
56	MG	1A	3422	1/1	0.95	0.20	46,46,46,46	0
56	MG	1A	3277	1/1	0.95	0.08	37,37,37,37	0
56	MG	1A	3934	1/1	0.95	0.07	49,49,49,49	0
56	MG	18	101	1/1	0.95	0.22	53,53,53,53	0
56	MG	1a	1793	1/1	0.95	0.09	80,80,80,80	0
56	MG	1a	1794	1/1	0.95	0.07	60,60,60,60	0
56	MG	1a	1800	1/1	0.95	0.06	57,57,57,57	0
56	MG	2A	3201	1/1	0.95	0.10	44,44,44,44	0
56	MG	1A	3935	1/1	0.95	0.17	46,46,46,46	0
56	MG	1A	3741	1/1	0.95	0.09	35,35,35,35	0
56	MG	1A	3937	1/1	0.95	0.15	81,81,81,81	0
56	MG	1A	3278	1/1	0.95	0.20	31,31,31,31	0
56	MG	1a	1818	1/1	0.95	0.09	44,44,44,44	0
56	MG	2A	3212	1/1	0.95	0.07	47,47,47,47	0
56	MG	1A	3146	1/1	0.95	0.08	42,42,42,42	0
56	MG	20	103	1/1	0.95	0.14	52,52,52,52	0
56	MG	2A	3470	1/1	0.95	0.06	66,66,66,66	0
56	MG	2A	3471	1/1	0.95	0.34	53,53,53,53	0
56	MG	25	102	1/1	0.95	0.10	52,52,52,52	0
56	MG	2A	3214	1/1	0.95	0.23	48,48,48,48	0
56	MG	1A	3747	1/1	0.95	0.12	56,56,56,56	0
56	MG	1A	3748	1/1	0.95	0.11	59,59,59,59	0
56	MG	1A	3280	1/1	0.95	0.21	35,35,35,35	0
56	MG	1A	3944	1/1	0.95	0.08	45,45,45,45	0
56	MG	1A	3282	1/1	0.95	0.14	37,37,37,37	0
56	MG	2A	3480	1/1	0.95	0.21	43,43,43,43	0
56	MG	2a	3004	1/1	0.95	0.12	47,47,47,47	0
56	MG	1l	201	1/1	0.95	0.23	67,67,67,67	0
56	MG	2A	3482	1/1	0.95	0.12	49,49,49,49	0
56	MG	1A	3352	1/1	0.95	0.22	54,54,54,54	0
56	MG	1A	3283	1/1	0.95	0.20	41,41,41,41	0
56	MG	2A	3226	1/1	0.95	0.13	49,49,49,49	0
56	MG	1a	1611	1/1	0.95	0.07	28,28,28,28	0
56	MG	2A	3488	1/1	0.95	0.10	40,40,40,40	0
56	MG	1n	102	1/1	0.95	0.10	71,71,71,71	0
56	MG	1A	3284	1/1	0.95	0.24	38,38,38,38	0
56	MG	1t	201	1/1	0.95	0.31	55,55,55,55	0
56	MG	2A	3232	1/1	0.95	0.07	55,55,55,55	0
56	MG	1A	3955	1/1	0.95	0.07	43,43,43,43	0
56	MG	1x	101	1/1	0.95	0.16	42,42,42,42	0
56	MG	2A	3235	1/1	0.95	0.08	49,49,49,49	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3501	1/1	0.95	0.11	49,49,49,49	0
56	MG	2A	3503	1/1	0.95	0.07	54,54,54,54	0
56	MG	2A	3506	1/1	0.95	0.13	48,48,48,48	0
56	MG	1A	3028	1/1	0.95	0.16	34,34,34,34	0
56	MG	1A	3959	1/1	0.95	0.04	48,48,48,48	0
56	MG	1A	3150	1/1	0.95	0.13	38,38,38,38	0
56	MG	1a	1619	1/1	0.95	0.15	51,51,51,51	0
56	MG	2A	3514	1/1	0.95	0.12	61,61,61,61	0
56	MG	1A	3969	1/1	0.95	0.15	62,62,62,62	0
56	MG	1A	3232	1/1	0.95	0.12	45,45,45,45	0
56	MG	2a	3030	1/1	0.95	0.07	64,64,64,64	0
56	MG	1A	3290	1/1	0.95	0.09	42,42,42,42	0
56	MG	1A	3362	1/1	0.95	0.04	38,38,38,38	0
56	MG	1A	3043	1/1	0.95	0.15	36,36,36,36	0
56	MG	1A	3984	1/1	0.95	0.07	65,65,65,65	0
56	MG	1A	3557	1/1	0.95	0.09	34,34,34,34	0
56	MG	1A	3559	1/1	0.95	0.10	34,34,34,34	0
56	MG	1A	3154	1/1	0.95	0.06	37,37,37,37	0
56	MG	2A	3002	1/1	0.95	0.11	41,41,41,41	0
56	MG	2a	3041	1/1	0.95	0.14	55,55,55,55	0
56	MG	1A	3990	1/1	0.95	0.06	31,31,31,31	0
56	MG	1A	3992	1/1	0.95	0.10	40,40,40,40	0
56	MG	1A	3993	1/1	0.95	0.09	85,85,85,85	0
56	MG	1A	3368	1/1	0.95	0.09	32,32,32,32	0
56	MG	2a	3046	1/1	0.95	0.06	72,72,72,72	0
56	MG	1A	3774	1/1	0.95	0.11	54,54,54,54	0
56	MG	2A	3257	1/1	0.95	0.18	47,47,47,47	0
56	MG	1A	3999	1/1	0.95	0.08	45,45,45,45	0
56	MG	1A	4004	1/1	0.95	0.10	46,46,46,46	0
56	MG	2A	3554	1/1	0.95	0.09	58,58,58,58	0
56	MG	2a	3055	1/1	0.95	0.06	64,64,64,64	0
56	MG	2A	3011	1/1	0.95	0.08	52,52,52,52	0
56	MG	1A	3110	1/1	0.95	0.14	41,41,41,41	0
56	MG	2A	3262	1/1	0.95	0.07	46,46,46,46	0
56	MG	1A	3370	1/1	0.95	0.10	48,48,48,48	0
56	MG	1A	4008	1/1	0.95	0.07	40,40,40,40	0
56	MG	2A	3015	1/1	0.95	0.11	44,44,44,44	0
56	MG	1a	1642	1/1	0.95	0.06	42,42,42,42	0
56	MG	1A	3193	1/1	0.95	0.08	58,58,58,58	0
56	MG	2A	3568	1/1	0.95	0.07	40,40,40,40	0
56	MG	1A	3238	1/1	0.95	0.07	63,63,63,63	0
56	MG	2a	3070	1/1	0.95	0.07	44,44,44,44	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1a	1645	1/1	0.95	0.19	65,65,65,65	0
56	MG	1a	1646	1/1	0.95	0.10	48,48,48,48	0
56	MG	2A	3575	1/1	0.95	0.15	37,37,37,37	0
56	MG	2A	3024	1/1	0.95	0.14	54,54,54,54	0
56	MG	1A	3455	1/1	0.95	0.09	46,46,46,46	0
56	MG	1A	4018	1/1	0.95	0.08	27,27,27,27	0
56	MG	1a	1649	1/1	0.95	0.30	62,62,62,62	0
56	MG	2a	3078	1/1	0.95	0.23	58,58,58,58	0
56	MG	1A	4019	1/1	0.95	0.18	53,53,53,53	0
56	MG	1a	1651	1/1	0.95	0.11	39,39,39,39	0
56	MG	2A	3583	1/1	0.95	0.10	56,56,56,56	0
56	MG	2A	3584	1/1	0.95	0.07	48,48,48,48	0
56	MG	1A	4020	1/1	0.95	0.09	42,42,42,42	0
56	MG	1A	3032	1/1	0.95	0.11	47,47,47,47	0
56	MG	2a	3088	1/1	0.95	0.13	53,53,53,53	0
56	MG	2A	3282	1/1	0.95	0.15	45,45,45,45	0
56	MG	1A	4023	1/1	0.95	0.09	57,57,57,57	0
56	MG	2A	3589	1/1	0.95	0.15	39,39,39,39	0
56	MG	2a	3092	1/1	0.95	0.07	60,60,60,60	0
56	MG	2A	3591	1/1	0.95	0.11	45,45,45,45	0
56	MG	2A	3039	1/1	0.95	0.19	53,53,53,53	0
56	MG	1A	3377	1/1	0.95	0.09	33,33,33,33	0
56	MG	2A	3286	1/1	0.95	0.08	57,57,57,57	0
56	MG	1A	3034	1/1	0.95	0.25	45,45,45,45	0
56	MG	1a	1657	1/1	0.95	0.15	58,58,58,58	0
56	MG	1A	3001	1/1	0.95	0.09	39,39,39,39	0
56	MG	1A	3061	1/1	0.95	0.20	47,47,47,47	0
56	MG	2a	3103	1/1	0.95	0.13	60,60,60,60	0
56	MG	1A	3462	1/1	0.95	0.12	43,43,43,43	0
56	MG	2a	3105	1/1	0.95	0.12	49,49,49,49	0
56	MG	2A	3607	1/1	0.95	0.14	35,35,35,35	0
56	MG	1A	3790	1/1	0.95	0.06	50,50,50,50	0
56	MG	1A	3794	1/1	0.95	0.06	51,51,51,51	0
56	MG	1A	3381	1/1	0.95	0.11	60,60,60,60	0
56	MG	1A	3075	1/1	0.95	0.14	36,36,36,36	0
56	MG	2A	3615	1/1	0.95	0.12	52,52,52,52	0
56	MG	1a	1665	1/1	0.95	0.17	60,60,60,60	0
56	MG	2A	3303	1/1	0.95	0.06	67,67,67,67	0
56	MG	1A	3246	1/1	0.95	0.14	31,31,31,31	0
56	MG	1A	3467	1/1	0.95	0.14	46,46,46,46	0
56	MG	1A	3076	1/1	0.95	0.06	38,38,38,38	0
56	MG	1A	3311	1/1	0.95	0.18	46,46,46,46	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3057	1/1	0.95	0.12	45,45,45,45	0
56	MG	1a	1670	1/1	0.95	0.19	60,60,60,60	0
56	MG	1B	201	1/1	0.95	0.15	56,56,56,56	0
56	MG	2A	3311	1/1	0.95	0.07	43,43,43,43	0
56	MG	2A	3060	1/1	0.95	0.06	44,44,44,44	0
56	MG	2A	3633	1/1	0.95	0.19	51,51,51,51	0
56	MG	1A	3127	1/1	0.95	0.27	50,50,50,50	0
56	MG	1A	3598	1/1	0.95	0.15	57,57,57,57	0
56	MG	1A	3472	1/1	0.95	0.05	49,49,49,49	0
56	MG	2A	3316	1/1	0.95	0.05	53,53,53,53	0
56	MG	1a	1676	1/1	0.95	0.11	35,35,35,35	0
56	MG	1A	3208	1/1	0.95	0.16	59,59,59,59	0
56	MG	2A	3641	1/1	0.95	0.12	58,58,58,58	0
56	MG	1A	3474	1/1	0.95	0.07	40,40,40,40	0
56	MG	1A	3608	1/1	0.95	0.07	42,42,42,42	0
56	MG	1A	3609	1/1	0.95	0.09	42,42,42,42	0
56	MG	1A	3612	1/1	0.95	0.05	36,36,36,36	0
56	MG	2a	3140	1/1	0.95	0.07	61,61,61,61	0
56	MG	2A	3647	1/1	0.95	0.07	72,72,72,72	0
56	MG	2a	3144	1/1	0.95	0.07	58,58,58,58	0
56	MG	2A	3650	1/1	0.95	0.13	62,62,62,62	0
56	MG	1A	3621	1/1	0.95	0.11	40,40,40,40	0
56	MG	2a	3151	1/1	0.95	0.05	82,82,82,82	0
56	MG	1A	3314	1/1	0.95	0.13	43,43,43,43	0
56	MG	2a	3153	1/1	0.95	0.05	76,76,76,76	0
56	MG	2A	3654	1/1	0.95	0.06	62,62,62,62	0
56	MG	2A	3079	1/1	0.95	0.14	52,52,52,52	0
56	MG	1A	3626	1/1	0.95	0.09	39,39,39,39	0
56	MG	2a	3159	1/1	0.95	0.12	59,59,59,59	0
56	MG	2a	3160	1/1	0.95	0.13	67,67,67,67	0
56	MG	1A	3315	1/1	0.95	0.06	34,34,34,34	0
56	MG	1B	223	1/1	0.95	0.09	58,58,58,58	0
56	MG	1a	1688	1/1	0.95	0.16	52,52,52,52	0
56	MG	1A	3252	1/1	0.95	0.12	59,59,59,59	0
56	MG	2A	3669	1/1	0.95	0.06	43,43,43,43	0
56	MG	1A	3634	1/1	0.95	0.06	65,65,65,65	0
56	MG	1A	3636	1/1	0.95	0.09	34,34,34,34	0
56	MG	1A	3037	1/1	0.95	0.12	37,37,37,37	0
56	MG	1B	230	1/1	0.95	0.07	61,61,61,61	0
56	MG	2a	3173	1/1	0.95	0.10	42,42,42,42	0
56	MG	1D	303	1/1	0.95	0.14	39,39,39,39	0
56	MG	1A	3480	1/1	0.95	0.13	57,57,57,57	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3254	1/1	0.95	0.10	55,55,55,55	0
56	MG	2A	3679	1/1	0.95	0.11	51,51,51,51	0
56	MG	2A	3096	1/1	0.95	0.11	59,59,59,59	0
56	MG	2A	3341	1/1	0.95	0.04	47,47,47,47	0
56	MG	2A	3682	1/1	0.95	0.07	58,58,58,58	0
56	MG	2A	3097	1/1	0.95	0.14	51,51,51,51	0
56	MG	1A	3484	1/1	0.95	0.25	39,39,39,39	0
56	MG	1E	303	1/1	0.95	0.19	44,44,44,44	0
56	MG	2A	3689	1/1	0.95	0.09	46,46,46,46	0
56	MG	2a	3187	1/1	0.95	0.07	47,47,47,47	0
56	MG	1E	304	1/1	0.95	0.11	38,38,38,38	0
56	MG	1A	3136	1/1	0.95	0.06	35,35,35,35	0
56	MG	1A	3214	1/1	0.95	0.18	50,50,50,50	0
56	MG	1A	3400	1/1	0.95	0.06	54,54,54,54	0
56	MG	2A	3108	1/1	0.95	0.07	50,50,50,50	0
56	MG	1A	3002	1/1	0.95	0.13	52,52,52,52	0
56	MG	1F	303	1/1	0.95	0.12	43,43,43,43	0
56	MG	2A	3353	1/1	0.95	0.12	44,44,44,44	0
56	MG	2A	3700	1/1	0.95	0.09	61,61,61,61	0
56	MG	1A	3258	1/1	0.95	0.09	53,53,53,53	0
56	MG	1F	308	1/1	0.95	0.06	32,32,32,32	0
56	MG	2a	3202	1/1	0.95	0.20	53,53,53,53	0
56	MG	1F	309	1/1	0.95	0.11	52,52,52,52	0
56	MG	1A	3848	1/1	0.95	0.06	43,43,43,43	0
56	MG	2a	3205	1/1	0.95	0.08	36,36,36,36	0
56	MG	2A	3115	1/1	0.95	0.17	57,57,57,57	0
56	MG	2a	3207	1/1	0.95	0.05	68,68,68,68	0
56	MG	2A	3362	1/1	0.95	0.08	54,54,54,54	0
56	MG	1A	3850	1/1	0.95	0.09	52,52,52,52	0
56	MG	2A	3365	1/1	0.95	0.07	46,46,46,46	0
56	MG	1a	1713	1/1	0.95	0.14	41,41,41,41	0
56	MG	2A	3367	1/1	0.95	0.07	41,41,41,41	0
56	MG	2A	3720	1/1	0.95	0.10	48,48,48,48	0
56	MG	1A	3084	1/1	0.95	0.12	50,50,50,50	0
56	MG	1A	3263	1/1	0.95	0.15	36,36,36,36	0
56	MG	2A	3727	1/1	0.95	0.12	63,63,63,63	0
56	MG	1A	3267	1/1	0.95	0.07	52,52,52,52	0
56	MG	2e	201	1/1	0.95	0.07	81,81,81,81	0
56	MG	1A	3268	1/1	0.95	0.23	57,57,57,57	0
56	MG	1O	201	1/1	0.95	0.10	43,43,43,43	0
56	MG	2A	3374	1/1	0.95	0.17	37,37,37,37	0
56	MG	2A	3732	1/1	0.95	0.11	74,74,74,74	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3663	1/1	0.95	0.10	32,32,32,32	0
56	MG	2A	3735	1/1	0.95	0.09	67,67,67,67	0
56	MG	1A	3498	1/1	0.95	0.06	38,38,38,38	0
56	MG	2A	3737	1/1	0.95	0.10	54,54,54,54	0
56	MG	2A	3129	1/1	0.95	0.08	59,59,59,59	0
56	MG	2A	3740	1/1	0.95	0.06	71,71,71,71	0
56	MG	2x	104	1/1	0.95	0.17	50,50,50,50	0
56	MG	2A	3741	1/1	0.95	0.10	68,68,68,68	0
56	MG	2A	3744	1/1	0.95	0.06	59,59,59,59	0
56	MG	1A	3576	1/1	0.96	0.08	34,34,34,34	0
56	MG	2A	3502	1/1	0.96	0.12	58,58,58,58	0
56	MG	1U	206	1/1	0.96	0.23	34,34,34,34	0
56	MG	1A	3201	1/1	0.96	0.10	41,41,41,41	0
56	MG	2A	3068	1/1	0.96	0.12	54,54,54,54	0
56	MG	2A	3508	1/1	0.96	0.05	75,75,75,75	0
56	MG	1A	3762	1/1	0.96	0.10	51,51,51,51	0
56	MG	2A	3511	1/1	0.96	0.10	70,70,70,70	0
56	MG	1A	3477	1/1	0.96	0.24	50,50,50,50	0
56	MG	1A	3109	1/1	0.96	0.09	52,52,52,52	0
56	MG	1V	203	1/1	0.96	0.19	44,44,44,44	0
56	MG	1A	3060	1/1	0.96	0.24	49,49,49,49	0
56	MG	1A	3940	1/1	0.96	0.07	79,79,79,79	0
56	MG	2A	3076	1/1	0.96	0.07	56,56,56,56	0
56	MG	2G	201	1/1	0.96	0.17	52,52,52,52	0
56	MG	2A	3078	1/1	0.96	0.10	40,40,40,40	0
56	MG	1A	3302	1/1	0.96	0.08	52,52,52,52	0
56	MG	1A	3206	1/1	0.96	0.27	44,44,44,44	0
56	MG	2A	3289	1/1	0.96	0.05	49,49,49,49	0
56	MG	1W	204	1/1	0.96	0.14	36,36,36,36	0
56	MG	1W	205	1/1	0.96	0.06	39,39,39,39	0
56	MG	1A	3589	1/1	0.96	0.11	37,37,37,37	0
56	MG	2A	3084	1/1	0.96	0.10	35,35,35,35	0
56	MG	2A	3532	1/1	0.96	0.15	39,39,39,39	0
56	MG	1A	3357	1/1	0.96	0.06	39,39,39,39	0
56	MG	2A	3086	1/1	0.96	0.06	49,49,49,49	0
56	MG	1X	104	1/1	0.96	0.26	44,44,44,44	0
56	MG	1X	105	1/1	0.96	0.10	45,45,45,45	0
56	MG	2A	3538	1/1	0.96	0.05	57,57,57,57	0
56	MG	2A	3540	1/1	0.96	0.05	53,53,53,53	0
56	MG	2V	202	1/1	0.96	0.05	38,38,38,38	0
56	MG	2A	3541	1/1	0.96	0.12	46,46,46,46	0
56	MG	2A	3302	1/1	0.96	0.17	46,46,46,46	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3113	1/1	0.96	0.07	51,51,51,51	0
56	MG	2A	3547	1/1	0.96	0.10	44,44,44,44	0
56	MG	1A	3305	1/1	0.96	0.28	49,49,49,49	0
56	MG	1A	3417	1/1	0.96	0.18	46,46,46,46	0
56	MG	2A	3092	1/1	0.96	0.05	53,53,53,53	0
56	MG	1A	3953	1/1	0.96	0.09	39,39,39,39	0
56	MG	1A	3777	1/1	0.96	0.09	52,52,52,52	0
56	MG	1a	1728	1/1	0.96	0.11	62,62,62,62	0
56	MG	1A	3083	1/1	0.96	0.19	39,39,39,39	0
56	MG	10	104	1/1	0.96	0.12	46,46,46,46	0
56	MG	1A	3307	1/1	0.96	0.11	55,55,55,55	0
56	MG	1A	3957	1/1	0.96	0.07	31,31,31,31	0
56	MG	1A	3045	1/1	0.96	0.11	41,41,41,41	0
56	MG	1a	1736	1/1	0.96	0.23	60,60,60,60	0
56	MG	2A	3571	1/1	0.96	0.10	52,52,52,52	0
56	MG	2A	3104	1/1	0.96	0.16	39,39,39,39	0
56	MG	11	101	1/1	0.96	0.07	39,39,39,39	0
56	MG	1A	3117	1/1	0.96	0.11	47,47,47,47	0
56	MG	1A	3366	1/1	0.96	0.18	59,59,59,59	0
56	MG	1A	3261	1/1	0.96	0.11	62,62,62,62	0
56	MG	1A	3062	1/1	0.96	0.10	49,49,49,49	0
56	MG	1A	3976	1/1	0.96	0.13	67,67,67,67	0
56	MG	1A	3031	1/1	0.96	0.20	25,25,25,25	0
56	MG	1a	1748	1/1	0.96	0.16	55,55,55,55	0
56	MG	15	104	1/1	0.96	0.16	38,38,38,38	0
56	MG	1A	3120	1/1	0.96	0.25	40,40,40,40	0
56	MG	1A	3619	1/1	0.96	0.06	43,43,43,43	0
56	MG	1A	3374	1/1	0.96	0.07	38,38,38,38	0
56	MG	1A	3122	1/1	0.96	0.14	53,53,53,53	0
56	MG	1a	1754	1/1	0.96	0.06	53,53,53,53	0
56	MG	2A	3122	1/1	0.96	0.08	55,55,55,55	0
56	MG	1A	3505	1/1	0.96	0.25	38,38,38,38	0
56	MG	1A	3989	1/1	0.96	0.08	52,52,52,52	0
56	MG	2A	3125	1/1	0.96	0.13	46,46,46,46	0
56	MG	2a	3024	1/1	0.96	0.06	53,53,53,53	0
56	MG	2A	3594	1/1	0.96	0.05	40,40,40,40	0
56	MG	1A	3799	1/1	0.96	0.06	36,36,36,36	0
56	MG	2A	3598	1/1	0.96	0.14	60,60,60,60	0
56	MG	17	107	1/1	0.96	0.11	29,29,29,29	0
56	MG	1A	3173	1/1	0.96	0.06	41,41,41,41	0
56	MG	2A	3130	1/1	0.96	0.18	32,32,32,32	0
56	MG	1A	3432	1/1	0.96	0.21	33,33,33,33	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2a	3032	1/1	0.96	0.14	37,37,37,37	0
56	MG	18	103	1/1	0.96	0.07	33,33,33,33	0
56	MG	1A	3434	1/1	0.96	0.11	39,39,39,39	0
56	MG	1A	3224	1/1	0.96	0.32	37,37,37,37	0
56	MG	1A	3804	1/1	0.96	0.16	40,40,40,40	0
56	MG	1A	3805	1/1	0.96	0.05	45,45,45,45	0
56	MG	2A	3347	1/1	0.96	0.12	45,45,45,45	0
56	MG	1A	3437	1/1	0.96	0.14	41,41,41,41	0
56	MG	1A	3319	1/1	0.96	0.06	30,30,30,30	0
56	MG	2A	3617	1/1	0.96	0.08	59,59,59,59	0
56	MG	1A	3439	1/1	0.96	0.27	44,44,44,44	0
56	MG	1A	4012	1/1	0.96	0.14	56,56,56,56	0
56	MG	1A	3123	1/1	0.96	0.25	40,40,40,40	0
56	MG	1A	3006	1/1	0.96	0.04	35,35,35,35	0
56	MG	2A	3625	1/1	0.96	0.07	58,58,58,58	0
56	MG	1A	3651	1/1	0.96	0.08	30,30,30,30	0
56	MG	1A	3025	1/1	0.96	0.15	55,55,55,55	0
56	MG	2a	3051	1/1	0.96	0.07	81,81,81,81	0
56	MG	1a	1612	1/1	0.96	0.06	35,35,35,35	0
56	MG	1A	3016	1/1	0.96	0.05	39,39,39,39	0
56	MG	1a	1791	1/1	0.96	0.06	59,59,59,59	0
56	MG	1A	3654	1/1	0.96	0.09	31,31,31,31	0
56	MG	2A	3363	1/1	0.96	0.09	63,63,63,63	0
56	MG	1A	4021	1/1	0.96	0.06	64,64,64,64	0
56	MG	1A	3128	1/1	0.96	0.12	25,25,25,25	0
56	MG	2a	3060	1/1	0.96	0.07	78,78,78,78	0
56	MG	1a	1795	1/1	0.96	0.13	86,86,86,86	0
56	MG	1A	3821	1/1	0.96	0.24	34,34,34,34	0
56	MG	1A	3446	1/1	0.96	0.05	37,37,37,37	0
56	MG	2A	3639	1/1	0.96	0.07	59,59,59,59	0
56	MG	1a	1807	1/1	0.96	0.05	66,66,66,66	0
56	MG	1a	1808	1/1	0.96	0.06	82,82,82,82	0
56	MG	1a	1810	1/1	0.96	0.07	75,75,75,75	0
56	MG	1A	3520	1/1	0.96	0.07	36,36,36,36	0
56	MG	2A	3644	1/1	0.96	0.07	58,58,58,58	0
56	MG	1A	3522	1/1	0.96	0.14	37,37,37,37	0
56	MG	2A	3166	1/1	0.96	0.18	48,48,48,48	0
56	MG	1A	3067	1/1	0.96	0.07	34,34,34,34	0
56	MG	1A	3385	1/1	0.96	0.15	48,48,48,48	0
56	MG	1A	3005	1/1	0.96	0.04	42,42,42,42	0
56	MG	1A	3526	1/1	0.96	0.25	24,24,24,24	0
56	MG	1a	1821	1/1	0.96	0.11	49,49,49,49	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3173	1/1	0.96	0.21	58,58,58,58	0
56	MG	2A	3659	1/1	0.96	0.08	36,36,36,36	0
56	MG	2A	3174	1/1	0.96	0.32	55,55,55,55	0
56	MG	2a	3084	1/1	0.96	0.24	52,52,52,52	0
56	MG	1A	3450	1/1	0.96	0.08	53,53,53,53	0
56	MG	1A	3529	1/1	0.96	0.07	36,36,36,36	0
56	MG	1A	3530	1/1	0.96	0.13	37,37,37,37	0
56	MG	2A	3388	1/1	0.96	0.15	52,52,52,52	0
56	MG	2A	3389	1/1	0.96	0.20	42,42,42,42	0
56	MG	2A	3390	1/1	0.96	0.20	48,48,48,48	0
56	MG	2A	3391	1/1	0.96	0.20	54,54,54,54	0
56	MG	1A	4038	1/1	0.96	0.06	41,41,41,41	0
56	MG	1A	3837	1/1	0.96	0.10	41,41,41,41	0
56	MG	2A	3394	1/1	0.96	0.11	61,61,61,61	0
56	MG	1A	3676	1/1	0.96	0.06	42,42,42,42	0
56	MG	1A	3531	1/1	0.96	0.13	53,53,53,53	0
56	MG	1a	1635	1/1	0.96	0.04	43,43,43,43	0
56	MG	1A	3187	1/1	0.96	0.20	49,49,49,49	0
56	MG	2A	3399	1/1	0.96	0.21	41,41,41,41	0
56	MG	2A	3400	1/1	0.96	0.11	60,60,60,60	0
56	MG	1B	202	1/1	0.96	0.10	46,46,46,46	0
56	MG	2A	3684	1/1	0.96	0.06	65,65,65,65	0
56	MG	1A	3452	1/1	0.96	0.37	41,41,41,41	0
56	MG	1A	3846	1/1	0.96	0.05	53,53,53,53	0
56	MG	1A	3534	1/1	0.96	0.13	26,26,26,26	0
56	MG	2A	3690	1/1	0.96	0.08	43,43,43,43	0
56	MG	2a	3110	1/1	0.96	0.13	53,53,53,53	0
56	MG	1A	3686	1/1	0.96	0.06	47,47,47,47	0
56	MG	1A	3535	1/1	0.96	0.17	28,28,28,28	0
56	MG	1A	3235	1/1	0.96	0.11	50,50,50,50	0
56	MG	1A	3693	1/1	0.96	0.06	31,31,31,31	0
56	MG	1A	3538	1/1	0.96	0.04	28,28,28,28	0
56	MG	1x	107	1/1	0.96	0.29	67,67,67,67	0
56	MG	1A	3019	1/1	0.96	0.13	48,48,48,48	0
56	MG	1A	3052	1/1	0.96	0.08	41,41,41,41	0
56	MG	1A	3699	1/1	0.96	0.09	58,58,58,58	0
56	MG	2A	3701	1/1	0.96	0.09	51,51,51,51	0
56	MG	2A	3702	1/1	0.96	0.06	50,50,50,50	0
56	MG	2A	3415	1/1	0.96	0.11	43,43,43,43	0
56	MG	1A	3072	1/1	0.96	0.05	45,45,45,45	0
56	MG	2A	3417	1/1	0.96	0.23	42,42,42,42	0
56	MG	1A	3543	1/1	0.96	0.05	33,33,33,33	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3705	1/1	0.96	0.07	63,63,63,63	0
56	MG	2A	3713	1/1	0.96	0.12	58,58,58,58	0
56	MG	1A	3393	1/1	0.96	0.07	41,41,41,41	0
56	MG	2A	3204	1/1	0.96	0.07	40,40,40,40	0
56	MG	2A	3205	1/1	0.96	0.24	52,52,52,52	0
56	MG	1A	3286	1/1	0.96	0.11	41,41,41,41	0
56	MG	1A	3395	1/1	0.96	0.07	59,59,59,59	0
56	MG	1B	229	1/1	0.96	0.06	64,64,64,64	0
56	MG	1A	3871	1/1	0.96	0.07	57,57,57,57	0
56	MG	2A	3429	1/1	0.96	0.09	67,67,67,67	0
56	MG	2a	3139	1/1	0.96	0.06	75,75,75,75	0
56	MG	2A	3726	1/1	0.96	0.06	56,56,56,56	0
56	MG	1A	3547	1/1	0.96	0.05	42,42,42,42	0
56	MG	1A	3396	1/1	0.96	0.18	53,53,53,53	0
56	MG	1D	307	1/1	0.96	0.08	38,38,38,38	0
56	MG	2A	3216	1/1	0.96	0.12	37,37,37,37	0
56	MG	2a	3150	1/1	0.96	0.06	53,53,53,53	0
56	MG	2A	3217	1/1	0.96	0.18	46,46,46,46	0
56	MG	1D	308	1/1	0.96	0.06	47,47,47,47	0
56	MG	1A	3716	1/1	0.96	0.13	28,28,28,28	0
56	MG	1A	3550	1/1	0.96	0.14	27,27,27,27	0
56	MG	1E	301	1/1	0.96	0.07	45,45,45,45	0
56	MG	1A	3719	1/1	0.96	0.08	60,60,60,60	0
56	MG	2A	3223	1/1	0.96	0.07	52,52,52,52	0
56	MG	2A	3441	1/1	0.96	0.19	47,47,47,47	0
56	MG	1A	3884	1/1	0.96	0.07	57,57,57,57	0
56	MG	1A	3885	1/1	0.96	0.05	58,58,58,58	0
56	MG	2a	3163	1/1	0.96	0.12	50,50,50,50	0
56	MG	2A	3016	1/1	0.96	0.09	57,57,57,57	0
56	MG	1A	3142	1/1	0.96	0.17	43,43,43,43	0
56	MG	1A	3192	1/1	0.96	0.10	44,44,44,44	0
56	MG	2A	3755	1/1	0.96	0.08	62,62,62,62	0
56	MG	2A	3758	1/1	0.96	0.07	52,52,52,52	0
56	MG	2A	3019	1/1	0.96	0.06	46,46,46,46	0
56	MG	1A	3029	1/1	0.96	0.12	51,51,51,51	0
56	MG	1A	3892	1/1	0.96	0.06	63,63,63,63	0
56	MG	1A	3893	1/1	0.96	0.09	51,51,51,51	0
56	MG	2A	3453	1/1	0.96	0.29	47,47,47,47	0
56	MG	2A	3766	1/1	0.96	0.07	65,65,65,65	0
56	MG	1F	305	1/1	0.96	0.10	51,51,51,51	0
56	MG	2A	3768	1/1	0.96	0.13	43,43,43,43	0
56	MG	2A	3025	1/1	0.96	0.04	44,44,44,44	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3772	1/1	0.96	0.06	46,46,46,46	0
56	MG	2a	3182	1/1	0.96	0.09	60,60,60,60	0
56	MG	1F	306	1/1	0.96	0.11	31,31,31,31	0
56	MG	1F	307	1/1	0.96	0.12	34,34,34,34	0
56	MG	1A	3733	1/1	0.96	0.06	66,66,66,66	0
56	MG	1A	3466	1/1	0.96	0.17	51,51,51,51	0
56	MG	2A	3777	1/1	0.96	0.14	65,65,65,65	0
56	MG	1A	3041	1/1	0.96	0.11	45,45,45,45	0
56	MG	1A	3340	1/1	0.96	0.09	61,61,61,61	0
56	MG	1A	3469	1/1	0.96	0.05	33,33,33,33	0
56	MG	2a	3192	1/1	0.96	0.07	70,70,70,70	0
56	MG	2A	3781	1/1	0.96	0.14	52,52,52,52	0
56	MG	1A	3562	1/1	0.96	0.11	43,43,43,43	0
56	MG	2A	3037	1/1	0.96	0.28	50,50,50,50	0
56	MG	1A	3908	1/1	0.96	0.13	72,72,72,72	0
56	MG	2A	3040	1/1	0.96	0.07	51,51,51,51	0
56	MG	1A	3564	1/1	0.96	0.08	36,36,36,36	0
56	MG	1A	3030	1/1	0.96	0.10	49,49,49,49	0
56	MG	1a	1685	1/1	0.96	0.19	42,42,42,42	0
56	MG	1O	202	1/1	0.96	0.08	56,56,56,56	0
56	MG	2A	3045	1/1	0.96	0.07	52,52,52,52	0
56	MG	1A	3749	1/1	0.96	0.07	41,41,41,41	0
56	MG	1A	3044	1/1	0.96	0.11	40,40,40,40	0
56	MG	1Q	203	1/1	0.96	0.07	43,43,43,43	0
56	MG	1a	1690	1/1	0.96	0.10	65,65,65,65	0
56	MG	2A	3477	1/1	0.96	0.17	47,47,47,47	0
56	MG	1A	3918	1/1	0.96	0.13	47,47,47,47	0
56	MG	1A	3345	1/1	0.96	0.07	46,46,46,46	0
56	MG	2a	3211	1/1	0.96	0.09	66,66,66,66	0
56	MG	1A	3346	1/1	0.96	0.09	40,40,40,40	0
56	MG	1R	203	1/1	0.96	0.09	48,48,48,48	0
56	MG	2A	3803	1/1	0.96	0.04	39,39,39,39	0
56	MG	2A	3804	1/1	0.96	0.14	52,52,52,52	0
56	MG	2A	3806	1/1	0.96	0.10	51,51,51,51	0
56	MG	1S	201	1/1	0.96	0.10	61,61,61,61	0
56	MG	1A	3106	1/1	0.96	0.12	49,49,49,49	0
56	MG	2B	201	1/1	0.96	0.13	49,49,49,49	0
56	MG	2B	202	1/1	0.96	0.12	56,56,56,56	0
56	MG	2A	3264	1/1	0.96	0.09	38,38,38,38	0
56	MG	1A	3924	1/1	0.96	0.08	67,67,67,67	0
56	MG	1A	3573	1/1	0.96	0.21	35,35,35,35	0
56	MG	1A	3926	1/1	0.96	0.13	61,61,61,61	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3757	1/1	0.96	0.05	41,41,41,41	0
56	MG	1A	3930	1/1	0.96	0.06	39,39,39,39	0
56	MG	2A	3061	1/1	0.96	0.07	37,37,37,37	0
56	MG	1U	201	1/1	0.96	0.21	42,42,42,42	0
56	MG	2A	3497	1/1	0.96	0.08	58,58,58,58	0
56	MG	1A	3108	1/1	0.96	0.05	43,43,43,43	0
56	MG	2B	213	1/1	0.96	0.28	46,46,46,46	0
56	MG	2A	3274	1/1	0.96	0.22	48,48,48,48	0
56	MG	1A	4014	1/1	0.97	0.06	49,49,49,49	0
56	MG	1A	3421	1/1	0.97	0.14	44,44,44,44	0
56	MG	2A	3561	1/1	0.97	0.07	59,59,59,59	0
56	MG	2A	3328	1/1	0.97	0.06	65,65,65,65	0
56	MG	2A	3564	1/1	0.97	0.08	49,49,49,49	0
56	MG	2P	201	1/1	0.97	0.12	53,53,53,53	0
56	MG	1A	3565	1/1	0.97	0.06	41,41,41,41	0
56	MG	1A	3213	1/1	0.97	0.06	56,56,56,56	0
56	MG	2A	3567	1/1	0.97	0.05	52,52,52,52	0
56	MG	1A	3488	1/1	0.97	0.07	49,49,49,49	0
56	MG	2A	3569	1/1	0.97	0.12	41,41,41,41	0
56	MG	1A	3702	1/1	0.97	0.06	55,55,55,55	0
56	MG	1A	3364	1/1	0.97	0.12	44,44,44,44	0
56	MG	1A	3833	1/1	0.97	0.06	38,38,38,38	0
56	MG	2A	3132	1/1	0.97	0.07	40,40,40,40	0
56	MG	1a	1782	1/1	0.97	0.06	49,49,49,49	0
56	MG	1a	1783	1/1	0.97	0.08	59,59,59,59	0
56	MG	1A	3089	1/1	0.97	0.10	39,39,39,39	0
56	MG	1a	1785	1/1	0.97	0.06	68,68,68,68	0
56	MG	1A	3100	1/1	0.97	0.13	37,37,37,37	0
56	MG	2W	201	1/1	0.97	0.09	44,44,44,44	0
56	MG	1a	1787	1/1	0.97	0.06	53,53,53,53	0
56	MG	1A	3494	1/1	0.97	0.10	36,36,36,36	0
56	MG	2X	102	1/1	0.97	0.10	57,57,57,57	0
56	MG	1A	3310	1/1	0.97	0.20	48,48,48,48	0
56	MG	1A	3709	1/1	0.97	0.09	28,28,28,28	0
56	MG	1A	3178	1/1	0.97	0.16	43,43,43,43	0
56	MG	1A	3843	1/1	0.97	0.07	52,52,52,52	0
56	MG	1A	3844	1/1	0.97	0.14	53,53,53,53	0
56	MG	1A	3845	1/1	0.97	0.06	62,62,62,62	0
56	MG	1A	4031	1/1	0.97	0.12	47,47,47,47	0
56	MG	1a	1803	1/1	0.97	0.15	67,67,67,67	0
56	MG	1A	3079	1/1	0.97	0.07	40,40,40,40	0
56	MG	1a	1805	1/1	0.97	0.05	44,44,44,44	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	4035	1/1	0.97	0.06	46,46,46,46	0
56	MG	1A	3847	1/1	0.97	0.08	30,30,30,30	0
56	MG	2A	3596	1/1	0.97	0.06	32,32,32,32	0
56	MG	1A	3579	1/1	0.97	0.06	45,45,45,45	0
56	MG	2A	3356	1/1	0.97	0.05	55,55,55,55	0
56	MG	1A	3429	1/1	0.97	0.07	54,54,54,54	0
56	MG	2A	3358	1/1	0.97	0.07	38,38,38,38	0
56	MG	2A	3155	1/1	0.97	0.12	41,41,41,41	0
56	MG	2A	3603	1/1	0.97	0.08	33,33,33,33	0
56	MG	1a	1622	1/1	0.97	0.05	55,55,55,55	0
56	MG	2A	3606	1/1	0.97	0.08	48,48,48,48	0
56	MG	1A	3218	1/1	0.97	0.20	47,47,47,47	0
56	MG	1A	3373	1/1	0.97	0.04	33,33,33,33	0
56	MG	2A	3609	1/1	0.97	0.12	45,45,45,45	0
56	MG	2A	3159	1/1	0.97	0.16	45,45,45,45	0
56	MG	2A	3160	1/1	0.97	0.04	50,50,50,50	0
56	MG	1A	3721	1/1	0.97	0.05	31,31,31,31	0
56	MG	1A	3722	1/1	0.97	0.06	58,58,58,58	0
56	MG	1A	3723	1/1	0.97	0.04	37,37,37,37	0
56	MG	2A	3164	1/1	0.97	0.04	57,57,57,57	0
56	MG	1A	3102	1/1	0.97	0.23	38,38,38,38	0
56	MG	1a	1629	1/1	0.97	0.12	46,46,46,46	0
56	MG	1A	3503	1/1	0.97	0.17	25,25,25,25	0
56	MG	1B	205	1/1	0.97	0.22	50,50,50,50	0
56	MG	1A	3727	1/1	0.97	0.06	45,45,45,45	0
56	MG	1B	207	1/1	0.97	0.07	55,55,55,55	0
56	MG	1l	203	1/1	0.97	0.03	61,61,61,61	0
56	MG	1A	3729	1/1	0.97	0.14	37,37,37,37	0
56	MG	1A	3730	1/1	0.97	0.05	60,60,60,60	0
56	MG	1A	3433	1/1	0.97	0.07	37,37,37,37	0
56	MG	1A	3264	1/1	0.97	0.27	45,45,45,45	0
56	MG	1B	213	1/1	0.97	0.05	37,37,37,37	0
56	MG	2A	3384	1/1	0.97	0.37	37,37,37,37	0
56	MG	1A	3735	1/1	0.97	0.07	35,35,35,35	0
56	MG	1B	216	1/1	0.97	0.08	41,41,41,41	0
56	MG	1B	217	1/1	0.97	0.04	37,37,37,37	0
56	MG	2A	3181	1/1	0.97	0.22	49,49,49,49	0
56	MG	1A	3868	1/1	0.97	0.07	46,46,46,46	0
56	MG	1A	3737	1/1	0.97	0.05	48,48,48,48	0
56	MG	1A	3738	1/1	0.97	0.07	55,55,55,55	0
56	MG	1A	3266	1/1	0.97	0.06	40,40,40,40	0
56	MG	1A	3220	1/1	0.97	0.10	42,42,42,42	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3080	1/1	0.97	0.08	31,31,31,31	0
56	MG	1A	3595	1/1	0.97	0.06	41,41,41,41	0
56	MG	1A	3222	1/1	0.97	0.15	41,41,41,41	0
56	MG	1x	111	1/1	0.97	0.10	70,70,70,70	0
56	MG	2A	3648	1/1	0.97	0.07	41,41,41,41	0
56	MG	1A	3745	1/1	0.97	0.06	46,46,46,46	0
56	MG	1A	3746	1/1	0.97	0.09	51,51,51,51	0
56	MG	1A	3223	1/1	0.97	0.10	42,42,42,42	0
56	MG	1D	302	1/1	0.97	0.06	51,51,51,51	0
56	MG	2A	3655	1/1	0.97	0.09	59,59,59,59	0
56	MG	1A	3105	1/1	0.97	0.05	42,42,42,42	0
56	MG	2A	3197	1/1	0.97	0.18	45,45,45,45	0
56	MG	1A	3891	1/1	0.97	0.09	67,67,67,67	0
56	MG	1D	306	1/1	0.97	0.24	34,34,34,34	0
56	MG	1A	3055	1/1	0.97	0.07	41,41,41,41	0
56	MG	1A	3185	1/1	0.97	0.14	32,32,32,32	0
56	MG	1A	3895	1/1	0.97	0.06	72,72,72,72	0
56	MG	1A	3605	1/1	0.97	0.10	27,27,27,27	0
56	MG	2A	3008	1/1	0.97	0.07	58,58,58,58	0
56	MG	2A	3411	1/1	0.97	0.38	52,52,52,52	0
56	MG	2a	3066	1/1	0.97	0.07	43,43,43,43	0
56	MG	1A	3151	1/1	0.97	0.14	44,44,44,44	0
56	MG	2A	3207	1/1	0.97	0.06	46,46,46,46	0
56	MG	2a	3069	1/1	0.97	0.14	53,53,53,53	0
56	MG	2A	3208	1/1	0.97	0.11	48,48,48,48	0
56	MG	1A	3107	1/1	0.97	0.12	48,48,48,48	0
56	MG	1A	3230	1/1	0.97	0.12	55,55,55,55	0
56	MG	1A	3901	1/1	0.97	0.06	63,63,63,63	0
56	MG	1A	3902	1/1	0.97	0.04	49,49,49,49	0
56	MG	1A	3517	1/1	0.97	0.08	45,45,45,45	0
56	MG	1A	3905	1/1	0.97	0.10	44,44,44,44	0
56	MG	1F	302	1/1	0.97	0.10	53,53,53,53	0
56	MG	1A	3613	1/1	0.97	0.06	43,43,43,43	0
56	MG	2A	3686	1/1	0.97	0.07	68,68,68,68	0
56	MG	1A	3615	1/1	0.97	0.07	30,30,30,30	0
56	MG	2A	3425	1/1	0.97	0.26	31,31,31,31	0
56	MG	1A	3760	1/1	0.97	0.15	59,59,59,59	0
56	MG	1A	3329	1/1	0.97	0.12	44,44,44,44	0
56	MG	2a	3085	1/1	0.97	0.08	67,67,67,67	0
56	MG	1A	3913	1/1	0.97	0.07	47,47,47,47	0
56	MG	1A	3125	1/1	0.97	0.10	42,42,42,42	0
56	MG	2A	3023	1/1	0.97	0.18	55,55,55,55	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3389	1/1	0.97	0.07	52,52,52,52	0
56	MG	1A	3917	1/1	0.97	0.10	72,72,72,72	0
56	MG	2A	3026	1/1	0.97	0.14	39,39,39,39	0
56	MG	1A	3764	1/1	0.97	0.20	41,41,41,41	0
56	MG	2A	3227	1/1	0.97	0.06	59,59,59,59	0
56	MG	1A	3919	1/1	0.97	0.15	56,56,56,56	0
56	MG	1A	3765	1/1	0.97	0.08	53,53,53,53	0
56	MG	1A	3073	1/1	0.97	0.10	41,41,41,41	0
56	MG	2a	3097	1/1	0.97	0.14	35,35,35,35	0
56	MG	1A	3628	1/1	0.97	0.06	40,40,40,40	0
56	MG	2a	3099	1/1	0.97	0.10	55,55,55,55	0
56	MG	2A	3032	1/1	0.97	0.15	47,47,47,47	0
56	MG	1A	3768	1/1	0.97	0.07	38,38,38,38	0
56	MG	1A	3011	1/1	0.97	0.19	32,32,32,32	0
56	MG	2A	3708	1/1	0.97	0.06	45,45,45,45	0
56	MG	2A	3443	1/1	0.97	0.12	38,38,38,38	0
56	MG	2A	3712	1/1	0.97	0.10	67,67,67,67	0
56	MG	1P	202	1/1	0.97	0.08	33,33,33,33	0
56	MG	2A	3036	1/1	0.97	0.23	42,42,42,42	0
56	MG	1P	203	1/1	0.97	0.23	43,43,43,43	0
56	MG	2A	3038	1/1	0.97	0.07	44,44,44,44	0
56	MG	1A	3020	1/1	0.97	0.20	24,24,24,24	0
56	MG	1A	3454	1/1	0.97	0.14	48,48,48,48	0
56	MG	2A	3450	1/1	0.97	0.15	51,51,51,51	0
56	MG	2A	3721	1/1	0.97	0.05	56,56,56,56	0
56	MG	1A	3129	1/1	0.97	0.05	47,47,47,47	0
56	MG	2A	3723	1/1	0.97	0.06	59,59,59,59	0
56	MG	1A	3931	1/1	0.97	0.04	34,34,34,34	0
56	MG	1A	3130	1/1	0.97	0.10	41,41,41,41	0
56	MG	1A	3933	1/1	0.97	0.07	38,38,38,38	0
56	MG	1A	3639	1/1	0.97	0.08	24,24,24,24	0
56	MG	1A	3285	1/1	0.97	0.14	42,42,42,42	0
56	MG	1A	3641	1/1	0.97	0.06	56,56,56,56	0
56	MG	1A	3195	1/1	0.97	0.11	45,45,45,45	0
56	MG	1A	3196	1/1	0.97	0.14	37,37,37,37	0
56	MG	2A	3733	1/1	0.97	0.05	76,76,76,76	0
56	MG	1A	3646	1/1	0.97	0.12	46,46,46,46	0
56	MG	1A	3339	1/1	0.97	0.10	32,32,32,32	0
56	MG	2A	3462	1/1	0.97	0.08	54,54,54,54	0
56	MG	2a	3129	1/1	0.97	0.05	62,62,62,62	0
56	MG	1a	1700	1/1	0.97	0.19	48,48,48,48	0
56	MG	1A	3648	1/1	0.97	0.10	64,64,64,64	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3739	1/1	0.97	0.08	62,62,62,62	0
56	MG	1A	3239	1/1	0.97	0.08	42,42,42,42	0
56	MG	1U	203	1/1	0.97	0.13	36,36,36,36	0
56	MG	2A	3743	1/1	0.97	0.05	47,47,47,47	0
56	MG	2a	3136	1/1	0.97	0.07	75,75,75,75	0
56	MG	1A	3341	1/1	0.97	0.20	50,50,50,50	0
56	MG	1A	3132	1/1	0.97	0.13	25,25,25,25	0
56	MG	2A	3747	1/1	0.97	0.05	58,58,58,58	0
56	MG	2A	3751	1/1	0.97	0.06	54,54,54,54	0
56	MG	1A	3343	1/1	0.97	0.16	45,45,45,45	0
56	MG	2a	3143	1/1	0.97	0.09	57,57,57,57	0
56	MG	1A	3017	1/1	0.97	0.07	44,44,44,44	0
56	MG	1A	3792	1/1	0.97	0.12	51,51,51,51	0
56	MG	1A	3950	1/1	0.97	0.08	82,82,82,82	0
56	MG	2a	3148	1/1	0.97	0.04	60,60,60,60	0
56	MG	1A	3793	1/1	0.97	0.05	45,45,45,45	0
56	MG	1V	201	1/1	0.97	0.13	39,39,39,39	0
56	MG	1A	3291	1/1	0.97	0.16	46,46,46,46	0
56	MG	1A	3166	1/1	0.97	0.04	33,33,33,33	0
56	MG	1A	3347	1/1	0.97	0.06	45,45,45,45	0
56	MG	2A	3478	1/1	0.97	0.18	56,56,56,56	0
56	MG	1A	3348	1/1	0.97	0.06	38,38,38,38	0
56	MG	1A	3134	1/1	0.97	0.22	36,36,36,36	0
56	MG	1W	203	1/1	0.97	0.06	36,36,36,36	0
56	MG	2A	3771	1/1	0.97	0.11	42,42,42,42	0
56	MG	1A	3961	1/1	0.97	0.09	40,40,40,40	0
56	MG	2A	3273	1/1	0.97	0.04	71,71,71,71	0
56	MG	1A	3244	1/1	0.97	0.07	49,49,49,49	0
56	MG	1A	3964	1/1	0.97	0.07	50,50,50,50	0
56	MG	1A	3965	1/1	0.97	0.05	76,76,76,76	0
56	MG	2A	3075	1/1	0.97	0.08	52,52,52,52	0
56	MG	1X	103	1/1	0.97	0.06	34,34,34,34	0
56	MG	1A	3967	1/1	0.97	0.05	50,50,50,50	0
56	MG	1A	3968	1/1	0.97	0.06	80,80,80,80	0
56	MG	1A	3296	1/1	0.97	0.24	44,44,44,44	0
56	MG	2A	3494	1/1	0.97	0.05	69,69,69,69	0
56	MG	2A	3783	1/1	0.97	0.29	29,29,29,29	0
56	MG	1A	3970	1/1	0.97	0.09	79,79,79,79	0
56	MG	2A	3785	1/1	0.97	0.14	41,41,41,41	0
56	MG	1A	3973	1/1	0.97	0.05	78,78,78,78	0
56	MG	2A	3498	1/1	0.97	0.06	51,51,51,51	0
56	MG	1a	1729	1/1	0.97	0.16	44,44,44,44	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3411	1/1	0.97	0.09	61,61,61,61	0
56	MG	1A	3667	1/1	0.97	0.04	36,36,36,36	0
56	MG	1A	3669	1/1	0.97	0.09	37,37,37,37	0
56	MG	2A	3792	1/1	0.97	0.04	63,63,63,63	0
56	MG	1A	3168	1/1	0.97	0.05	37,37,37,37	0
56	MG	2A	3504	1/1	0.97	0.04	47,47,47,47	0
56	MG	2a	3188	1/1	0.97	0.07	58,58,58,58	0
56	MG	1A	3169	1/1	0.97	0.12	22,22,22,22	0
56	MG	1a	1735	1/1	0.97	0.11	46,46,46,46	0
56	MG	1A	3808	1/1	0.97	0.05	55,55,55,55	0
56	MG	10	107	1/1	0.97	0.11	30,30,30,30	0
56	MG	1a	1738	1/1	0.97	0.07	38,38,38,38	0
56	MG	1A	3809	1/1	0.97	0.07	48,48,48,48	0
56	MG	2A	3295	1/1	0.97	0.15	52,52,52,52	0
56	MG	2A	3298	1/1	0.97	0.06	66,66,66,66	0
56	MG	1A	3247	1/1	0.97	0.23	41,41,41,41	0
56	MG	1A	3681	1/1	0.97	0.05	59,59,59,59	0
56	MG	2A	3805	1/1	0.97	0.08	43,43,43,43	0
56	MG	2A	3518	1/1	0.97	0.07	45,45,45,45	0
56	MG	1A	3988	1/1	0.97	0.06	50,50,50,50	0
56	MG	2A	3809	1/1	0.97	0.20	38,38,38,38	0
56	MG	1A	3552	1/1	0.97	0.15	40,40,40,40	0
56	MG	2A	3811	1/1	0.97	0.10	77,77,77,77	0
56	MG	1A	3170	1/1	0.97	0.14	44,44,44,44	0
56	MG	1A	3991	1/1	0.97	0.13	31,31,31,31	0
56	MG	1A	3135	1/1	0.97	0.10	34,34,34,34	0
56	MG	15	103	1/1	0.97	0.12	37,37,37,37	0
56	MG	2A	3103	1/1	0.97	0.12	32,32,32,32	0
56	MG	1A	3816	1/1	0.97	0.07	61,61,61,61	0
56	MG	1A	3817	1/1	0.97	0.20	30,30,30,30	0
56	MG	2A	3531	1/1	0.97	0.05	35,35,35,35	0
56	MG	2A	3106	1/1	0.97	0.09	48,48,48,48	0
56	MG	2A	3107	1/1	0.97	0.25	39,39,39,39	0
56	MG	1A	3207	1/1	0.97	0.07	47,47,47,47	0
56	MG	15	107	1/1	0.97	0.05	29,29,29,29	0
56	MG	2A	3536	1/1	0.97	0.07	56,56,56,56	0
56	MG	1A	3481	1/1	0.97	0.38	36,36,36,36	0
56	MG	1A	3687	1/1	0.97	0.04	45,45,45,45	0
56	MG	1A	3114	1/1	0.97	0.11	43,43,43,43	0
56	MG	1a	1758	1/1	0.97	0.05	54,54,54,54	0
56	MG	2l	201	1/1	0.97	0.06	51,51,51,51	0
56	MG	17	102	1/1	0.97	0.04	34,34,34,34	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2q	201	1/1	0.97	0.27	60,60,60,60	0
56	MG	1a	1763	1/1	0.97	0.05	46,46,46,46	0
56	MG	17	103	1/1	0.97	0.16	48,48,48,48	0
56	MG	2A	3548	1/1	0.97	0.11	43,43,43,43	0
56	MG	1A	3004	1/1	0.97	0.11	38,38,38,38	0
56	MG	1A	3692	1/1	0.97	0.20	36,36,36,36	0
56	MG	2E	306	1/1	0.97	0.05	53,53,53,53	0
56	MG	2A	3323	1/1	0.97	0.11	42,42,42,42	0
56	MG	1A	3174	1/1	0.97	0.06	39,39,39,39	0
56	MG	1A	4013	1/1	0.97	0.06	43,43,43,43	0
56	MG	1A	3714	1/1	0.98	0.10	26,26,26,26	0
56	MG	1A	3611	1/1	0.98	0.05	29,29,29,29	0
56	MG	1A	3960	1/1	0.98	0.07	27,27,27,27	0
56	MG	2A	3685	1/1	0.98	0.06	37,37,37,37	0
56	MG	1Q	202	1/1	0.98	0.07	45,45,45,45	0
56	MG	1A	3367	1/1	0.98	0.11	44,44,44,44	0
56	MG	1A	3717	1/1	0.98	0.06	32,32,32,32	0
56	MG	1A	3147	1/1	0.98	0.04	41,41,41,41	0
56	MG	1a	1674	1/1	0.98	0.07	37,37,37,37	0
56	MG	1R	201	1/1	0.98	0.10	45,45,45,45	0
56	MG	1A	3202	1/1	0.98	0.17	37,37,37,37	0
56	MG	2A	3487	1/1	0.98	0.11	30,30,30,30	0
56	MG	1A	3720	1/1	0.98	0.05	21,21,21,21	0
56	MG	2A	3489	1/1	0.98	0.08	55,55,55,55	0
56	MG	1A	3616	1/1	0.98	0.07	26,26,26,26	0
56	MG	1A	3618	1/1	0.98	0.10	27,27,27,27	0
56	MG	2a	3033	1/1	0.98	0.27	57,57,57,57	0
56	MG	1A	3830	1/1	0.98	0.07	27,27,27,27	0
56	MG	1A	3971	1/1	0.98	0.04	59,59,59,59	0
56	MG	1A	3295	1/1	0.98	0.10	62,62,62,62	0
56	MG	1A	3620	1/1	0.98	0.04	36,36,36,36	0
56	MG	2A	3703	1/1	0.98	0.11	38,38,38,38	0
56	MG	1A	3077	1/1	0.98	0.07	38,38,38,38	0
56	MG	1A	3836	1/1	0.98	0.04	29,29,29,29	0
56	MG	1A	3977	1/1	0.98	0.04	43,43,43,43	0
56	MG	2A	3167	1/1	0.98	0.10	29,29,29,29	0
56	MG	1A	3726	1/1	0.98	0.04	38,38,38,38	0
56	MG	1A	3838	1/1	0.98	0.06	41,41,41,41	0
56	MG	2A	3710	1/1	0.98	0.05	48,48,48,48	0
56	MG	2A	3711	1/1	0.98	0.04	67,67,67,67	0
56	MG	1A	3622	1/1	0.98	0.08	37,37,37,37	0
56	MG	1A	3728	1/1	0.98	0.08	57,57,57,57	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2a	3049	1/1	0.98	0.04	44,44,44,44	0
56	MG	2A	3505	1/1	0.98	0.08	34,34,34,34	0
56	MG	1A	3548	1/1	0.98	0.05	51,51,51,51	0
56	MG	2a	3052	1/1	0.98	0.04	54,54,54,54	0
56	MG	1A	3372	1/1	0.98	0.17	42,42,42,42	0
56	MG	1A	3731	1/1	0.98	0.05	56,56,56,56	0
56	MG	1A	3627	1/1	0.98	0.03	31,31,31,31	0
56	MG	2A	3510	1/1	0.98	0.11	44,44,44,44	0
56	MG	1A	3501	1/1	0.98	0.10	22,22,22,22	0
56	MG	1A	3734	1/1	0.98	0.04	40,40,40,40	0
56	MG	1A	3629	1/1	0.98	0.05	30,30,30,30	0
56	MG	2A	3724	1/1	0.98	0.05	46,46,46,46	0
56	MG	1A	3736	1/1	0.98	0.12	25,25,25,25	0
56	MG	2A	3515	1/1	0.98	0.07	43,43,43,43	0
56	MG	1A	3995	1/1	0.98	0.05	47,47,47,47	0
56	MG	2a	3064	1/1	0.98	0.04	58,58,58,58	0
56	MG	1W	202	1/1	0.98	0.14	40,40,40,40	0
56	MG	1A	3849	1/1	0.98	0.06	45,45,45,45	0
56	MG	1A	3042	1/1	0.98	0.03	33,33,33,33	0
56	MG	1A	3998	1/1	0.98	0.04	37,37,37,37	0
56	MG	1a	1704	1/1	0.98	0.18	38,38,38,38	0
56	MG	2A	3186	1/1	0.98	0.07	40,40,40,40	0
56	MG	1A	3631	1/1	0.98	0.09	35,35,35,35	0
56	MG	1A	4001	1/1	0.98	0.08	26,26,26,26	0
56	MG	1A	3265	1/1	0.98	0.12	36,36,36,36	0
56	MG	1A	4005	1/1	0.98	0.11	55,55,55,55	0
56	MG	1A	3633	1/1	0.98	0.05	23,23,23,23	0
56	MG	1A	3553	1/1	0.98	0.08	25,25,25,25	0
56	MG	1A	3635	1/1	0.98	0.05	43,43,43,43	0
56	MG	1A	4011	1/1	0.98	0.05	52,52,52,52	0
56	MG	2a	3079	1/1	0.98	0.23	45,45,45,45	0
56	MG	2A	3742	1/1	0.98	0.07	43,43,43,43	0
56	MG	1A	3299	1/1	0.98	0.05	49,49,49,49	0
56	MG	1A	3555	1/1	0.98	0.06	42,42,42,42	0
56	MG	2A	3361	1/1	0.98	0.11	53,53,53,53	0
56	MG	1A	3033	1/1	0.98	0.15	26,26,26,26	0
56	MG	1A	3095	1/1	0.98	0.14	35,35,35,35	0
56	MG	2A	3752	1/1	0.98	0.04	44,44,44,44	0
56	MG	2A	3539	1/1	0.98	0.07	38,38,38,38	0
56	MG	1A	3153	1/1	0.98	0.05	36,36,36,36	0
56	MG	1A	3209	1/1	0.98	0.08	51,51,51,51	0
56	MG	2A	3756	1/1	0.98	0.08	34,34,34,34	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3865	1/1	0.98	0.03	77,77,77,77	0
56	MG	2A	3760	1/1	0.98	0.04	65,65,65,65	0
56	MG	1A	3054	1/1	0.98	0.16	30,30,30,30	0
56	MG	2A	3545	1/1	0.98	0.06	44,44,44,44	0
56	MG	2A	3546	1/1	0.98	0.09	37,37,37,37	0
56	MG	1A	3645	1/1	0.98	0.05	23,23,23,23	0
56	MG	1A	3021	1/1	0.98	0.13	27,27,27,27	0
56	MG	1A	3183	1/1	0.98	0.16	50,50,50,50	0
56	MG	2A	3553	1/1	0.98	0.06	43,43,43,43	0
56	MG	2A	3371	1/1	0.98	0.14	31,31,31,31	0
56	MG	1A	3007	1/1	0.98	0.15	45,45,45,45	0
56	MG	2A	3770	1/1	0.98	0.04	60,60,60,60	0
56	MG	1A	3650	1/1	0.98	0.08	26,26,26,26	0
56	MG	1A	3874	1/1	0.98	0.04	38,38,38,38	0
56	MG	2A	3558	1/1	0.98	0.04	36,36,36,36	0
56	MG	1A	3036	1/1	0.98	0.09	27,27,27,27	0
56	MG	2A	3376	1/1	0.98	0.13	45,45,45,45	0
56	MG	1A	3877	1/1	0.98	0.05	52,52,52,52	0
56	MG	1A	3275	1/1	0.98	0.07	39,39,39,39	0
56	MG	2A	3563	1/1	0.98	0.16	36,36,36,36	0
56	MG	1A	3058	1/1	0.98	0.04	53,53,53,53	0
56	MG	1A	3881	1/1	0.98	0.04	63,63,63,63	0
56	MG	1A	3023	1/1	0.98	0.09	47,47,47,47	0
56	MG	1A	3655	1/1	0.98	0.05	42,42,42,42	0
56	MG	1A	4034	1/1	0.98	0.07	39,39,39,39	0
56	MG	1A	3656	1/1	0.98	0.17	39,39,39,39	0
56	MG	1A	3137	1/1	0.98	0.07	39,39,39,39	0
56	MG	1A	3889	1/1	0.98	0.06	33,33,33,33	0
56	MG	1A	3087	1/1	0.98	0.18	27,27,27,27	0
56	MG	1a	1739	1/1	0.98	0.20	38,38,38,38	0
56	MG	1a	1740	1/1	0.98	0.21	37,37,37,37	0
56	MG	2A	3576	1/1	0.98	0.06	47,47,47,47	0
56	MG	1A	3574	1/1	0.98	0.11	50,50,50,50	0
56	MG	1A	3163	1/1	0.98	0.04	48,48,48,48	0
56	MG	1A	3281	1/1	0.98	0.27	44,44,44,44	0
56	MG	1A	3577	1/1	0.98	0.09	52,52,52,52	0
56	MG	1A	3521	1/1	0.98	0.09	38,38,38,38	0
56	MG	2a	3128	1/1	0.98	0.04	67,67,67,67	0
56	MG	1A	3897	1/1	0.98	0.07	60,60,60,60	0
56	MG	1A	3249	1/1	0.98	0.09	26,26,26,26	0
56	MG	1A	3665	1/1	0.98	0.06	34,34,34,34	0
56	MG	1A	3580	1/1	0.98	0.07	30,30,30,30	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3581	1/1	0.98	0.11	31,31,31,31	0
56	MG	1A	3668	1/1	0.98	0.05	45,45,45,45	0
56	MG	1A	3582	1/1	0.98	0.09	39,39,39,39	0
56	MG	1A	3904	1/1	0.98	0.05	47,47,47,47	0
56	MG	2A	3590	1/1	0.98	0.17	37,37,37,37	0
56	MG	1A	3671	1/1	0.98	0.05	51,51,51,51	0
56	MG	1B	212	1/1	0.98	0.05	41,41,41,41	0
56	MG	1A	3906	1/1	0.98	0.04	67,67,67,67	0
56	MG	2a	3141	1/1	0.98	0.05	61,61,61,61	0
56	MG	2A	3808	1/1	0.98	0.11	46,46,46,46	0
56	MG	2A	3077	1/1	0.98	0.06	42,42,42,42	0
56	MG	1A	3672	1/1	0.98	0.09	37,37,37,37	0
56	MG	2a	3145	1/1	0.98	0.05	67,67,67,67	0
56	MG	1a	1759	1/1	0.98	0.05	45,45,45,45	0
56	MG	1B	215	1/1	0.98	0.04	44,44,44,44	0
56	MG	1a	1762	1/1	0.98	0.08	44,44,44,44	0
56	MG	2a	3149	1/1	0.98	0.13	67,67,67,67	0
56	MG	1A	3317	1/1	0.98	0.27	43,43,43,43	0
56	MG	1A	3782	1/1	0.98	0.04	38,38,38,38	0
56	MG	1A	3911	1/1	0.98	0.08	26,26,26,26	0
56	MG	1a	1616	1/1	0.98	0.06	64,64,64,64	0
56	MG	2A	3249	1/1	0.98	0.08	55,55,55,55	0
56	MG	2A	3605	1/1	0.98	0.09	55,55,55,55	0
56	MG	2a	3157	1/1	0.98	0.04	58,58,58,58	0
56	MG	1A	3584	1/1	0.98	0.11	40,40,40,40	0
56	MG	1A	3675	1/1	0.98	0.05	57,57,57,57	0
56	MG	1A	3914	1/1	0.98	0.06	54,54,54,54	0
56	MG	1B	222	1/1	0.98	0.09	67,67,67,67	0
56	MG	1A	3354	1/1	0.98	0.06	43,43,43,43	0
56	MG	2A	3611	1/1	0.98	0.09	31,31,31,31	0
56	MG	2A	3612	1/1	0.98	0.09	49,49,49,49	0
56	MG	2D	301	1/1	0.98	0.07	39,39,39,39	0
56	MG	2a	3166	1/1	0.98	0.09	41,41,41,41	0
56	MG	1A	3677	1/1	0.98	0.04	31,31,31,31	0
56	MG	1A	3787	1/1	0.98	0.06	41,41,41,41	0
56	MG	1A	3678	1/1	0.98	0.06	39,39,39,39	0
56	MG	1A	3164	1/1	0.98	0.14	40,40,40,40	0
56	MG	2A	3095	1/1	0.98	0.15	47,47,47,47	0
56	MG	2a	3172	1/1	0.98	0.07	39,39,39,39	0
56	MG	2A	3618	1/1	0.98	0.05	59,59,59,59	0
56	MG	2a	3174	1/1	0.98	0.04	78,78,78,78	0
56	MG	1A	3920	1/1	0.98	0.11	31,31,31,31	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3621	1/1	0.98	0.06	42,42,42,42	0
56	MG	1A	3436	1/1	0.98	0.14	34,34,34,34	0
56	MG	1B	231	1/1	0.98	0.06	36,36,36,36	0
56	MG	1D	301	1/1	0.98	0.05	44,44,44,44	0
56	MG	1A	3121	1/1	0.98	0.04	61,61,61,61	0
56	MG	1A	3528	1/1	0.98	0.12	23,23,23,23	0
56	MG	1D	304	1/1	0.98	0.05	42,42,42,42	0
56	MG	1A	3590	1/1	0.98	0.07	31,31,31,31	0
56	MG	1A	3024	1/1	0.98	0.19	44,44,44,44	0
56	MG	1A	3796	1/1	0.98	0.05	51,51,51,51	0
56	MG	1A	3141	1/1	0.98	0.13	43,43,43,43	0
56	MG	1A	3928	1/1	0.98	0.04	58,58,58,58	0
56	MG	1A	3929	1/1	0.98	0.08	26,26,26,26	0
56	MG	1A	3798	1/1	0.98	0.09	20,20,20,20	0
56	MG	1a	1796	1/1	0.98	0.05	67,67,67,67	0
56	MG	1a	1798	1/1	0.98	0.05	72,72,72,72	0
56	MG	2R	203	1/1	0.98	0.10	39,39,39,39	0
56	MG	1E	302	1/1	0.98	0.07	47,47,47,47	0
56	MG	1a	1802	1/1	0.98	0.05	64,64,64,64	0
56	MG	2a	3195	1/1	0.98	0.07	52,52,52,52	0
56	MG	1A	3039	1/1	0.98	0.17	37,37,37,37	0
56	MG	1A	3003	1/1	0.98	0.05	33,33,33,33	0
56	MG	1A	3691	1/1	0.98	0.08	28,28,28,28	0
56	MG	1E	306	1/1	0.98	0.24	33,33,33,33	0
56	MG	1A	3361	1/1	0.98	0.04	24,24,24,24	0
56	MG	1a	1809	1/1	0.98	0.05	48,48,48,48	0
56	MG	1E	308	1/1	0.98	0.08	26,26,26,26	0
56	MG	1A	3443	1/1	0.98	0.20	44,44,44,44	0
56	MG	1a	1813	1/1	0.98	0.06	72,72,72,72	0
56	MG	2A	3649	1/1	0.98	0.07	49,49,49,49	0
56	MG	1A	3144	1/1	0.98	0.07	42,42,42,42	0
56	MG	1A	3145	1/1	0.98	0.03	56,56,56,56	0
56	MG	2A	3652	1/1	0.98	0.08	31,31,31,31	0
56	MG	1a	1817	1/1	0.98	0.04	70,70,70,70	0
56	MG	1A	3537	1/1	0.98	0.07	31,31,31,31	0
56	MG	2A	3128	1/1	0.98	0.16	34,34,34,34	0
56	MG	2A	3656	1/1	0.98	0.05	66,66,66,66	0
56	MG	1A	3600	1/1	0.98	0.04	29,29,29,29	0
56	MG	25	103	1/1	0.98	0.15	46,46,46,46	0
56	MG	1A	3601	1/1	0.98	0.11	33,33,33,33	0
56	MG	1A	3010	1/1	0.98	0.04	44,44,44,44	0
56	MG	2A	3296	1/1	0.98	0.06	54,54,54,54	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3297	1/1	0.98	0.07	54,54,54,54	0
56	MG	1A	3603	1/1	0.98	0.04	54,54,54,54	0
56	MG	2A	3666	1/1	0.98	0.02	44,44,44,44	0
56	MG	2A	3667	1/1	0.98	0.05	37,37,37,37	0
56	MG	1A	3811	1/1	0.98	0.11	56,56,56,56	0
56	MG	1A	3604	1/1	0.98	0.08	25,25,25,25	0
56	MG	1A	3492	1/1	0.98	0.05	45,45,45,45	0
56	MG	1A	3606	1/1	0.98	0.06	40,40,40,40	0
56	MG	1A	3708	1/1	0.98	0.04	46,46,46,46	0
56	MG	1A	3259	1/1	0.98	0.05	37,37,37,37	0
56	MG	1A	3951	1/1	0.98	0.07	50,50,50,50	0
56	MG	2A	3676	1/1	0.98	0.06	45,45,45,45	0
56	MG	1A	3541	1/1	0.98	0.04	51,51,51,51	0
56	MG	1A	3711	1/1	0.98	0.06	25,25,25,25	0
56	MG	1A	3712	1/1	0.98	0.05	42,42,42,42	0
56	MG	1P	201	1/1	0.98	0.11	39,39,39,39	0
57	ZN	24	501	1/1	0.98	0.07	114,114,114,114	0
57	ZN	2n	102	1/1	0.98	0.04	98,98,98,98	0
56	MG	1A	3328	1/1	0.98	0.06	39,39,39,39	0
56	MG	2A	3664	1/1	0.99	0.04	43,43,43,43	0
56	MG	1A	3558	1/1	0.99	0.05	47,47,47,47	0
56	MG	1a	1801	1/1	0.99	0.03	60,60,60,60	0
56	MG	2A	3117	1/1	0.99	0.03	49,49,49,49	0
56	MG	1A	3870	1/1	0.99	0.04	62,62,62,62	0
56	MG	1A	3211	1/1	0.99	0.04	40,40,40,40	0
56	MG	2A	3206	1/1	0.99	0.03	55,55,55,55	0
56	MG	1A	3979	1/1	0.99	0.04	50,50,50,50	0
56	MG	2A	3672	1/1	0.99	0.04	46,46,46,46	0
56	MG	1A	3980	1/1	0.99	0.03	40,40,40,40	0
56	MG	1a	1806	1/1	0.99	0.03	65,65,65,65	0
56	MG	1A	3483	1/1	0.99	0.09	37,37,37,37	0
56	MG	2A	3572	1/1	0.99	0.04	57,57,57,57	0
56	MG	17	104	1/1	0.99	0.03	36,36,36,36	0
56	MG	1A	3983	1/1	0.99	0.08	47,47,47,47	0
56	MG	1A	3186	1/1	0.99	0.06	39,39,39,39	0
56	MG	1a	1811	1/1	0.99	0.04	45,45,45,45	0
56	MG	1A	3165	1/1	0.99	0.03	30,30,30,30	0
56	MG	1A	3637	1/1	0.99	0.08	29,29,29,29	0
56	MG	1A	3876	1/1	0.99	0.07	65,65,65,65	0
56	MG	2A	3131	1/1	0.99	0.11	36,36,36,36	0
56	MG	1a	1815	1/1	0.99	0.03	60,60,60,60	0
56	MG	1A	3563	1/1	0.99	0.13	45,45,45,45	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3610	1/1	0.99	0.05	32,32,32,32	0
56	MG	1A	3131	1/1	0.99	0.04	33,33,33,33	0
56	MG	1A	3260	1/1	0.99	0.10	36,36,36,36	0
56	MG	1A	3883	1/1	0.99	0.04	34,34,34,34	0
56	MG	1A	3791	1/1	0.99	0.03	56,56,56,56	0
56	MG	1a	1604	1/1	0.99	0.04	48,48,48,48	0
56	MG	1e	201	1/1	0.99	0.27	42,42,42,42	0
56	MG	2a	3154	1/1	0.99	0.03	69,69,69,69	0
56	MG	1A	3994	1/1	0.99	0.04	39,39,39,39	0
56	MG	1A	3834	1/1	0.99	0.03	45,45,45,45	0
56	MG	2A	3696	1/1	0.99	0.05	47,47,47,47	0
56	MG	2A	3495	1/1	0.99	0.04	61,61,61,61	0
56	MG	1A	3177	1/1	0.99	0.07	36,36,36,36	0
56	MG	1a	1744	1/1	0.99	0.19	40,40,40,40	0
56	MG	1U	202	1/1	0.99	0.08	43,43,43,43	0
56	MG	1A	3643	1/1	0.99	0.04	32,32,32,32	0
56	MG	2A	3597	1/1	0.99	0.06	37,37,37,37	0
56	MG	1A	3888	1/1	0.99	0.04	59,59,59,59	0
56	MG	2A	3148	1/1	0.99	0.11	50,50,50,50	0
56	MG	1A	3752	1/1	0.99	0.04	42,42,42,42	0
56	MG	1A	4000	1/1	0.99	0.05	41,41,41,41	0
56	MG	1A	3614	1/1	0.99	0.08	36,36,36,36	0
56	MG	1A	4003	1/1	0.99	0.10	61,61,61,61	0
56	MG	2A	3067	1/1	0.99	0.04	46,46,46,46	0
56	MG	1A	3567	1/1	0.99	0.05	36,36,36,36	0
56	MG	1A	3489	1/1	0.99	0.06	58,58,58,58	0
56	MG	1A	3680	1/1	0.99	0.05	22,22,22,22	0
56	MG	1A	3894	1/1	0.99	0.03	56,56,56,56	0
56	MG	1A	3617	1/1	0.99	0.08	27,27,27,27	0
56	MG	1A	4009	1/1	0.99	0.04	26,26,26,26	0
56	MG	1A	4010	1/1	0.99	0.03	49,49,49,49	0
56	MG	1A	3008	1/1	0.99	0.02	34,34,34,34	0
56	MG	2A	3718	1/1	0.99	0.04	79,79,79,79	0
56	MG	1A	3649	1/1	0.99	0.08	31,31,31,31	0
56	MG	1a	1761	1/1	0.99	0.04	47,47,47,47	0
56	MG	1A	3158	1/1	0.99	0.12	39,39,39,39	0
56	MG	1A	3948	1/1	0.99	0.10	25,25,25,25	0
56	MG	1A	3949	1/1	0.99	0.04	55,55,55,55	0
56	MG	2A	3520	1/1	0.99	0.08	44,44,44,44	0
56	MG	2A	3521	1/1	0.99	0.05	52,52,52,52	0
56	MG	2A	3620	1/1	0.99	0.06	48,48,48,48	0
56	MG	2A	3522	1/1	0.99	0.09	27,27,27,27	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3254	1/1	0.99	0.11	42,42,42,42	0
56	MG	1A	3456	1/1	0.99	0.08	40,40,40,40	0
56	MG	1A	3572	1/1	0.99	0.08	34,34,34,34	0
56	MG	1A	3952	1/1	0.99	0.03	40,40,40,40	0
56	MG	1a	1768	1/1	0.99	0.03	39,39,39,39	0
56	MG	1A	3111	1/1	0.99	0.09	35,35,35,35	0
56	MG	1A	3623	1/1	0.99	0.06	21,21,21,21	0
56	MG	2A	3629	1/1	0.99	0.05	56,56,56,56	0
56	MG	1a	1772	1/1	0.99	0.06	52,52,52,52	0
56	MG	1A	3689	1/1	0.99	0.03	45,45,45,45	0
56	MG	1A	3205	1/1	0.99	0.10	32,32,32,32	0
56	MG	1A	3852	1/1	0.99	0.05	36,36,36,36	0
56	MG	1a	1776	1/1	0.99	0.05	56,56,56,56	0
56	MG	1A	3958	1/1	0.99	0.03	38,38,38,38	0
56	MG	1A	3625	1/1	0.99	0.05	34,34,34,34	0
56	MG	1A	3112	1/1	0.99	0.06	51,51,51,51	0
56	MG	1A	3069	1/1	0.99	0.02	28,28,28,28	0
56	MG	1a	1781	1/1	0.99	0.05	49,49,49,49	0
56	MG	2A	3746	1/1	0.99	0.07	33,33,33,33	0
56	MG	1A	3771	1/1	0.99	0.11	40,40,40,40	0
56	MG	2A	3748	1/1	0.99	0.05	47,47,47,47	0
56	MG	2A	3749	1/1	0.99	0.06	42,42,42,42	0
56	MG	2A	3750	1/1	0.99	0.03	54,54,54,54	0
56	MG	1A	3963	1/1	0.99	0.03	41,41,41,41	0
56	MG	1A	3910	1/1	0.99	0.07	19,19,19,19	0
56	MG	2A	3543	1/1	0.99	0.06	35,35,35,35	0
56	MG	1A	3082	1/1	0.99	0.04	39,39,39,39	0
56	MG	1A	3966	1/1	0.99	0.04	46,46,46,46	0
56	MG	1A	4033	1/1	0.99	0.06	34,34,34,34	0
56	MG	2A	3757	1/1	0.99	0.04	59,59,59,59	0
56	MG	1A	3695	1/1	0.99	0.04	44,44,44,44	0
56	MG	2A	3759	1/1	0.99	0.05	33,33,33,33	0
56	MG	1a	1789	1/1	0.99	0.04	61,61,61,61	0
56	MG	2A	3549	1/1	0.99	0.03	35,35,35,35	0
56	MG	1A	3103	1/1	0.99	0.15	42,42,42,42	0
56	MG	2A	3551	1/1	0.99	0.04	41,41,41,41	0
56	MG	2A	3552	1/1	0.99	0.02	50,50,50,50	0
56	MG	1A	3013	1/1	0.99	0.07	41,41,41,41	0
56	MG	1A	3698	1/1	0.99	0.05	35,35,35,35	0
56	MG	1A	3225	1/1	0.99	0.04	49,49,49,49	0
56	MG	1A	3972	1/1	0.99	0.05	64,64,64,64	0
56	MG	2A	3657	1/1	0.99	0.04	36,36,36,36	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3778	1/1	0.99	0.07	38,38,38,38	0
56	MG	1A	3700	1/1	0.99	0.03	55,55,55,55	0
56	MG	1a	1797	1/1	0.99	0.03	58,58,58,58	0
57	ZN	14	501	1/1	0.99	0.05	90,90,90,90	0
57	ZN	16	103	1/1	0.99	0.02	41,41,41,41	0
56	MG	1A	3701	1/1	0.99	0.03	39,39,39,39	0
57	ZN	26	102	1/1	0.99	0.06	62,62,62,62	0
57	ZN	29	501	1/1	0.99	0.03	72,72,72,72	0
56	MG	2A	3662	1/1	0.99	0.10	51,51,51,51	0
58	SF4	1d	501	8/8	0.99	0.03	64,70,81,85	0
58	SF4	2d	302	8/8	0.99	0.03	63,75,80,93	0
56	MG	1a	1799	1/1	0.99	0.04	66,66,66,66	0
56	MG	1A	3858	1/1	1.00	0.04	27,27,27,27	0
56	MG	1a	1769	1/1	1.00	0.05	30,30,30,30	0
56	MG	1A	3859	1/1	1.00	0.02	36,36,36,36	0
56	MG	1B	224	1/1	1.00	0.02	48,48,48,48	0
56	MG	1A	3753	1/1	1.00	0.03	31,31,31,31	0
56	MG	1A	3878	1/1	1.00	0.05	43,43,43,43	0
56	MG	1A	4002	1/1	1.00	0.03	47,47,47,47	0
57	ZN	1Y	202	1/1	1.00	0.02	65,65,65,65	0
56	MG	1V	202	1/1	1.00	0.02	41,41,41,41	0
57	ZN	15	108	1/1	1.00	0.01	40,40,40,40	0
56	MG	1A	3869	1/1	1.00	0.02	43,43,43,43	0
57	ZN	19	103	1/1	1.00	0.01	44,44,44,44	0
57	ZN	1n	103	1/1	1.00	0.02	70,70,70,70	0
57	ZN	2Y	202	1/1	1.00	0.02	79,79,79,79	0
56	MG	1A	3670	1/1	1.00	0.05	25,25,25,25	0
57	ZN	25	105	1/1	1.00	0.04	58,58,58,58	0
56	MG	1A	3742	1/1	1.00	0.09	32,32,32,32	0
56	MG	1A	3981	1/1	1.00	0.03	40,40,40,40	0
56	MG	1A	3882	1/1	1.00	0.06	20,20,20,20	0
56	MG	1A	3831	1/1	1.00	0.05	33,33,33,33	0
56	MG	1A	3679	1/1	1.00	0.05	31,31,31,31	0
56	MG	1A	3148	1/1	1.00	0.04	45,45,45,45	0

6.5 Other polymers (i)

There are no such residues in this entry.