wwPDB X-ray Structure Validation Summary Report (i)

Sep 16, 2026 – 07:36 AM EDT

PDB ID	:	7RQA / pdb_00007rqa
Title	:	Crystal structure of the Thermus thermophilus 70S ribosome in complex with protein Y, A-site aminoacyl-tRNA analog ACC-PMN, and P-site MTI-tripeptidyl-tRNA analog ACCA-ITM at 2.40A resolution
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Deposited on	:	2021-08-06
Resolution	:	2.40 Å(reported)

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

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

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

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

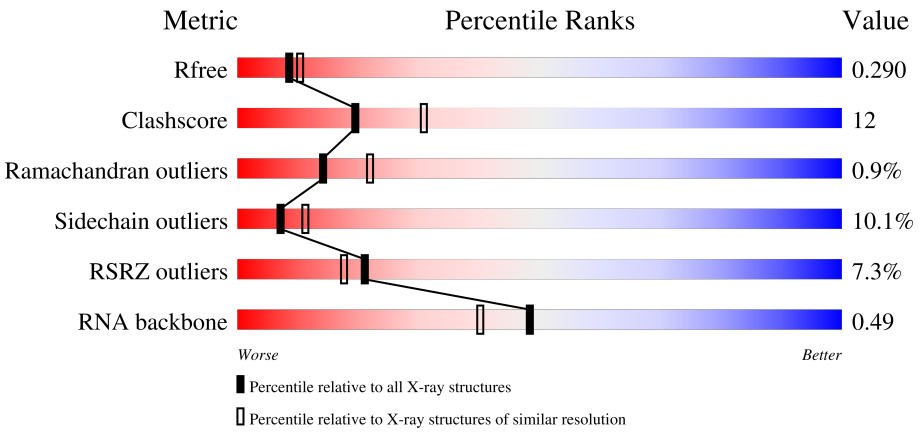
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)
RNA backbone	3983	1155 (2.70-2.10)

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	4% 57% 34% 7% •
1	2A	2915	5% 53% 37% 8% •
2	1B	121	53% 40% 6% •

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Mol	Chain	Length	Quality of chain
2	2B	121	2%, 60%, 36%
3	1D	276	%, 70%, 25%
3	2D	276	%, 74%, 21%
4	1E	206	%, 77%, 20%
4	2E	206	3%, 62%, 33%
5	1F	210	2%, 68%, 25%
5	2F	210	4%, 51%, 40%, 6%
6	1G	182	7%, 60%, 34%, 5%
6	2G	182	26%, 56%, 34%, 9%
7	1H	180	%, 68%, 27%
7	2H	180	14%, 49%, 43%
8	1I	148	9%, 64%, 30%, 5%
8	2I	148	21%, 64%, 30%, 5%
9	1N	140	68%, 30%
9	2N	140	4%, 76%, 21%
10	1O	122	64%, 35%
10	2O	122	%, 66%, 33%
11	1P	150	%, 74%, 23%
11	2P	150	6%, 70%, 27%
12	1Q	141	78%, 18%
12	2Q	141	4%, 63%, 33%
13	1R	118	71%, 24%, 5%
13	2R	118	%, 69%, 27%
14	1S	112	%, 69%, 25%
14	2S	112	12%, 63%, 32%

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Mol	Chain	Length	Quality of chain
15	1T	146	6% 64% 24% 10%
15	2T	146	2% 59% 27% 10%
16	1U	118	% 77% 19%
16	2U	118	3% 63% 34%
17	1V	101	% 78% 20%
17	2V	101	3% 68% 28%
18	1W	113	% 71% 25%
18	2W	113	2% 73% 22%
19	1X	96	3% 63% 35%
19	2X	96	4% 60% 35%
20	1Y	110	70% 24%
20	2Y	110	16% 64% 29% 5%
21	1Z	206	% 65% 29% 5%
21	2Z	206	7% 56% 34% 7%
22	10	85	% 75% 22%
22	20	85	11% 79% 18%
23	11	98	% 67% 23% 8%
23	21	98	3% 62% 31% 6%
24	12	72	% 71% 25%
24	22	72	% 61% 35%
25	13	60	70% 28%
25	23	60	5% 58% 37%
26	14	71	24% 52% 30% 15%
26	24	71	34% 38% 48% 8%
27	15	60	3% 72% 23%

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Mol	Chain	Length	Quality of chain
27	25	60	72% 25%
28	16	54	69% 26%
28	26	54	4% 59% 30% 9%
29	17	49	4% 76% 22%
29	27	49	6% 65% 29%
30	18	65	66% 31%
30	28	65	68% 31%
31	19	37	3% 89% 8%
31	29	37	5% 51% 49%
32	1a	1521	2% 48% 41% 10%
32	2a	1521	3% 46% 43% 10%
33	1b	256	20% 42% 42% 5% 10%
33	2b	256	31% 43% 41% 7% 10%
34	1c	239	13% 53% 31% 14%
34	2c	239	21% 47% 34% 5% 14%
35	1d	209	18% 54% 39% 7%
35	2d	209	8% 53% 40% 7%
36	1e	162	4% 57% 31% 9%
36	2e	162	6% 60% 27% 5% 9%
37	1f	101	3% 52% 44%
37	2f	101	3% 66% 29%
38	1g	156	10% 62% 35%
38	2g	156	17% 65% 28% 6%
39	1h	138	7% 57% 37% 6%
39	2h	138	7% 62% 33%

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Mol	Chain	Length	Quality of chain
40	1i	128	32% 52% 43% 5%
40	2i	128	45% 46% 47% 5%
41	1j	105	26% 60% 30% 8%
41	2j	105	45% 57% 30% 9%
42	1k	129	5% 63% 21% 5% 12%
42	2k	129	5% 60% 26% 12%
43	1l	132	3% 68% 23% 8%
43	2l	132	5% 67% 24% 8%
44	1m	126	9% 49% 41% 8%
44	2m	126	27% 40% 44% 6% 10%
45	1n	61	20% 67% 28%
45	2n	61	41% 49% 43% 7%
46	1o	89	4% 66% 31%
46	2o	89	6% 64% 34%
47	1p	88	28% 48% 44% 7%
47	2p	88	10% 53% 33% 7% 7%
48	1q	105	6% 55% 34% 5% 6%
48	2q	105	5% 59% 30% 5% 6%
49	1r	88	5% 43% 32% 23%
49	2r	88	6% 45% 32% 23%
50	1s	93	14% 52% 38% 11%
50	2s	93	27% 46% 40% 11%
51	1t	106	23% 49% 38% 9%
51	2t	106	10% 61% 29% 8%
52	1u	27	19% 56% 30% 15%

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Mol	Chain	Length	Quality of chain
52	2u	27	41% 59% 26% 15%
53	1y	113	12% 63% 20% • 14%
53	2y	113	38% 50% 30% • 15%
54	1w	4	75% 25%
54	2w	4	75% 25%
55	1x	4	25% 75% 25%
55	2x	4	75% 25%
56	1v	3	100%
56	2v	3	67% 33%

2 Entry composition (i)

There are 63 unique types of molecules in this entry. The entry contains 297986 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	2872	61869	27540	11574	19884	2871	0	0	0
1	2A	2867	61758	27491	11552	19850	2865	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	2572	1145	476	832	119	0	0	0
2	2B	120	2573	1146	476	832	119	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	2131	1346	422	360	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	1426	916	253	253	4	0	0	0
6	2G	181	1424	912	259	249	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	173	1324	842	247	234	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	147	1094	699	191	203	1	0	0	0
8	2I	146	1076	687	186	202	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	1121	722	208	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

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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	877	553	175	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	775	498	141	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	810	520	153	131	6	0	0	0
20	2Y	107	810	519	153	132	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	203	1587	1011	282	292	2	0	0	0
21	2Z	201	1557	995	274	286	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	83	653	404	139	109	1	0	0	0
22	20	83	650	401	139	109	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	754	475	148	130	1	0	0	0
23	21	97	759	478	149	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	592	368	119	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	546	346	96	99	5	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
26	24	69	536	342	98	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	459	288	90	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	1504	32331	14396	5990	10441	1504	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	1842	1175	330	332	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	1558	979	305	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	1665	1043	329	286	7	0	0	0
35	2d	208	1668	1047	330	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	1133	716	214	199	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	814	516	144	151	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	1235	769	244	216	6	0	0	0
38	2g	155	1229	766	241	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	1098	694	210	192	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	986	625	193	168	0	0	0
40	2i	126	966	613	186	167	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	719	446	142	131	0	0	0
41	2j	96	710	442	137	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	834	520	156	155	3	0	0	0

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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	116	914	564	189	159	2	0	0	0
44	2m	114	895	550	186	157	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	648	415	120	111	2	0	0	0
50	2s	83	645	410	118	115	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	732	449	157	124	2	0	0	0
51	2t	98	733	451	154	126	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 protein called Ribosome-associated inhibitor A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
53	1y	97	764	478	144	139	3	0	0	0
53	2y	96	749	468	141	137	3	0	0	0

- Molecule 54 is a RNA chain called A-site Aminoacyl-tRNA Analog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
54	1w	4	78	40	13	22	3	0	0	1
54	2w	4	78	40	13	22	3	0	0	1

- Molecule 55 is a RNA chain called P-site Peptidyl-tRNA Analog RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
55	1x	4	63	28	12	20	3	0	0	1
55	2x	4	63	28	12	20	3	0	0	1

- Molecule 56 is a protein called P-site Peptidyl-tRNA Analog Peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
56	1v	3	23	15	3	4	1	0	0	0
56	2v	3	23	15	3	4	1	0	0	0

- Molecule 57 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
57	1A	1028	1028	1028	0	0
57	1B	30	30	30	0	0
57	1D	18	18	18	0	0
57	1E	10	10	10	0	0
57	1F	16	16	16	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
57	1G	4	4	4	0	0
57	1H	2	2	2	0	0
57	1N	4	4	4	0	0
57	1O	1	1	1	0	0
57	1P	4	4	4	0	0
57	1Q	5	5	5	0	0
57	1R	4	4	4	0	0
57	1T	4	4	4	0	0
57	1U	8	8	8	0	0
57	1V	7	7	7	0	0
57	1W	2	2	2	0	0
57	1X	1	1	1	0	0
57	1Z	1	1	1	0	0
57	10	8	8	8	0	0
57	11	5	5	5	0	0
57	13	3	3	3	0	0
57	15	8	8	8	0	0
57	17	5	5	5	0	0
57	18	3	3	3	0	0
57	19	3	3	3	0	0
57	1a	280	280	280	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
57	1b	1	1	1	0	0
57	1d	6	6	6	0	0
57	1e	3	3	3	0	0
57	1f	2	2	2	0	0
57	1g	2	2	2	0	0
57	1h	2	2	2	0	0
57	1i	1	1	1	0	0
57	1l	2	2	2	0	0
57	1m	1	1	1	0	0
57	1n	1	1	1	0	0
57	1o	2	2	2	0	0
57	1t	2	2	2	0	0
57	1y	3	3	3	0	0
57	1w	1	1	1	0	0
57	1x	2	2	2	0	0
57	2A	737	737	737	0	0
57	2B	20	20	20	0	0
57	2D	11	11	11	0	0
57	2E	6	6	6	0	0
57	2F	4	4	4	0	0
57	2G	2	2	2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
57	2I	1	1	1	0	0
57	2N	1	1	1	0	0
57	2O	1	1	1	0	0
57	2P	3	3	3	0	0
57	2Q	4	4	4	0	0
57	2R	3	3	3	0	0
57	2T	4	4	4	0	0
57	2U	1	1	1	0	0
57	2V	3	3	3	0	0
57	2W	2	2	2	0	0
57	2Y	1	1	1	0	0
57	20	2	2	2	0	0
57	21	1	1	1	0	0
57	23	1	1	1	0	0
57	25	3	3	3	0	0
57	26	1	1	1	0	0
57	27	1	1	1	0	0
57	28	1	1	1	0	0
57	2a	191	191	191	0	0
57	2e	2	2	2	0	0
57	2f	1	1	1	0	0

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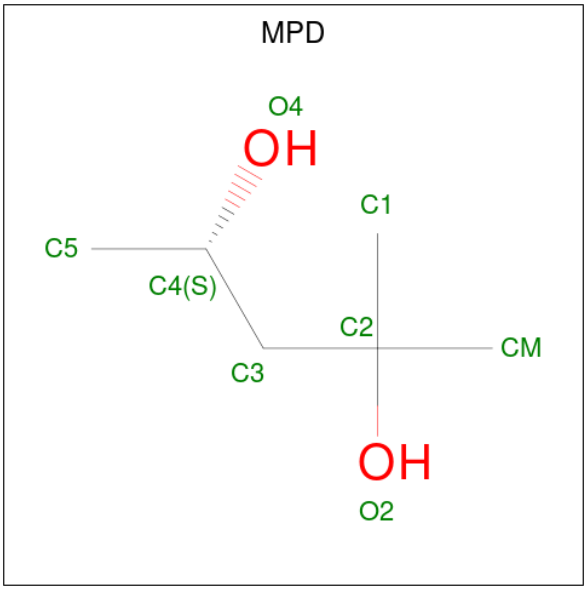
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	2h	1	Total Mg 1 1	0	0
57	2j	1	Total Mg 1 1	0	0
57	2k	2	Total Mg 2 2	0	0
57	2p	1	Total Mg 1 1	0	0
57	2r	1	Total Mg 1 1	0	0
57	2t	1	Total Mg 1 1	0	0
57	2x	1	Total Mg 1 1	0	0

- Molecule 58 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	1A	1	Total C O 8 6 2	0	0
58	1T	1	Total C O 8 6 2	0	0
58	18	1	Total C O 8 6 2	0	0
58	1a	1	Total C O 8 6 2	0	0

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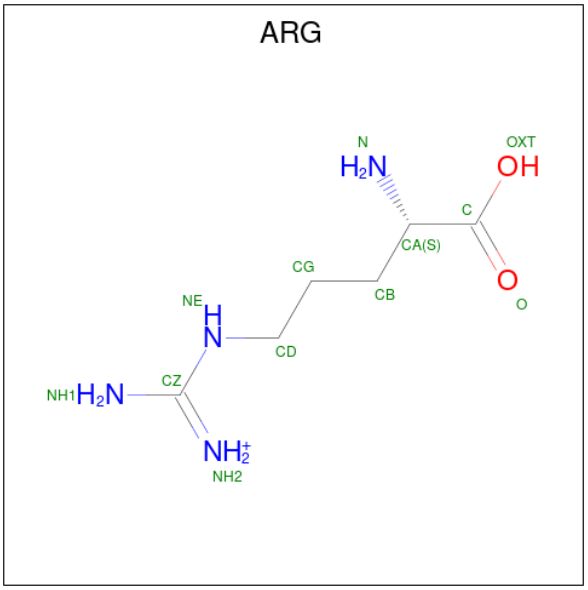
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	2A	1	Total C O 8 6 2	0	0
58	2B	1	Total C O 8 6 2	0	0

- Molecule 59 is ARGININE (CCD ID: ARG) (formula: $C_6H_{15}N_4O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	1B	1	Total C N O 12 6 4 2	0	0
59	1F	1	Total C N O 12 6 4 2	0	0

- Molecule 60 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	1Y	1	Total Zn 1 1	0	0
60	14	1	Total Zn 1 1	0	0
60	15	1	Total Zn 1 1	0	0
60	16	1	Total Zn 1 1	0	0
60	19	1	Total Zn 1 1	0	0

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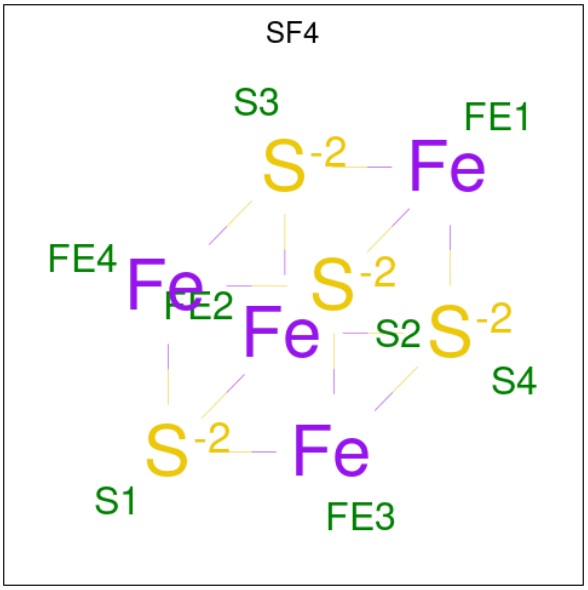
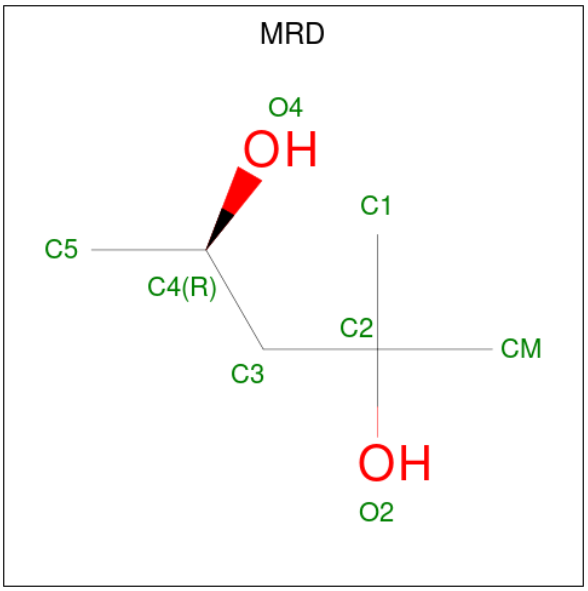
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	1n	1	Total Zn 1 1	0	0
60	2Y	1	Total Zn 1 1	0	0
60	24	1	Total Zn 1 1	0	0
60	25	1	Total Zn 1 1	0	0
60	26	1	Total Zn 1 1	0	0
60	29	1	Total Zn 1 1	0	0
60	2n	1	Total Zn 1 1	0	0

- Molecule 61 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1d	1	Total Fe S 8 4 4	0	0
61	2d	1	Total Fe S 8 4 4	0	0

- Molecule 62 is (4R)-2-METHYLPENTANE-2,4-DIOL (CCD ID: MRD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
62	2A	1	Total C O 8 6 2	0	0

- Molecule 63 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
63	1A	3988	Total O 3988 3988	0	0
63	1B	97	Total O 97 97	0	0
63	1D	113	Total O 113 113	0	0
63	1E	76	Total O 76 76	0	0
63	1F	67	Total O 67 67	0	0
63	1G	19	Total O 19 19	0	0
63	1H	11	Total O 11 11	0	0
63	1I	8	Total O 8 8	0	0
63	1N	52	Total O 52 52	0	0
63	1O	22	Total O 22 22	0	0
63	1P	66	Total O 66 66	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
63	1Q	36	Total O 36 36	0	0
63	1R	32	Total O 32 32	0	0
63	1S	12	Total O 12 12	0	0
63	1T	34	Total O 34 34	0	0
63	1U	47	Total O 47 47	0	0
63	1V	40	Total O 40 40	0	0
63	1W	33	Total O 33 33	0	0
63	1X	26	Total O 26 26	0	0
63	1Y	16	Total O 16 16	0	0
63	1Z	14	Total O 14 14	0	0
63	10	24	Total O 24 24	0	0
63	11	27	Total O 27 27	0	0
63	12	18	Total O 18 18	0	0
63	13	24	Total O 24 24	0	0
63	14	3	Total O 3 3	0	0
63	15	24	Total O 24 24	0	0
63	16	18	Total O 18 18	0	0
63	17	12	Total O 12 12	0	0
63	18	27	Total O 27 27	0	0
63	19	6	Total O 6 6	0	0
63	1a	511	Total O 511 511	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
63	1b	1	Total O 1 1	0	0
63	1d	8	Total O 8 8	0	0
63	1e	3	Total O 3 3	0	0
63	1f	2	Total O 2 2	0	0
63	1j	1	Total O 1 1	0	0
63	1k	1	Total O 1 1	0	0
63	1l	3	Total O 3 3	0	0
63	1m	1	Total O 1 1	0	0
63	1o	3	Total O 3 3	0	0
63	1p	2	Total O 2 2	0	0
63	1t	1	Total O 1 1	0	0
63	1y	7	Total O 7 7	0	0
63	1w	6	Total O 6 6	0	0
63	1x	5	Total O 5 5	0	0
63	2A	2224	Total O 2224 2224	0	0
63	2B	45	Total O 45 45	0	0
63	2D	50	Total O 50 50	0	0
63	2E	29	Total O 29 29	0	0
63	2F	22	Total O 22 22	0	0
63	2G	7	Total O 7 7	0	0
63	2H	2	Total O 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
63	2I	3	Total O 3 3	0	0
63	2N	2	Total O 2 2	0	0
63	2O	16	Total O 16 16	0	0
63	2P	25	Total O 25 25	0	0
63	2Q	16	Total O 16 16	0	0
63	2R	20	Total O 20 20	0	0
63	2S	5	Total O 5 5	0	0
63	2T	10	Total O 10 10	0	0
63	2U	12	Total O 12 12	0	0
63	2V	9	Total O 9 9	0	0
63	2W	23	Total O 23 23	0	0
63	2X	7	Total O 7 7	0	0
63	2Y	6	Total O 6 6	0	0
63	2Z	11	Total O 11 11	0	0
63	20	14	Total O 14 14	0	0
63	21	20	Total O 20 20	0	0
63	22	3	Total O 3 3	0	0
63	23	4	Total O 4 4	0	0
63	24	2	Total O 2 2	0	0
63	25	9	Total O 9 9	0	0
63	26	5	Total O 5 5	0	0

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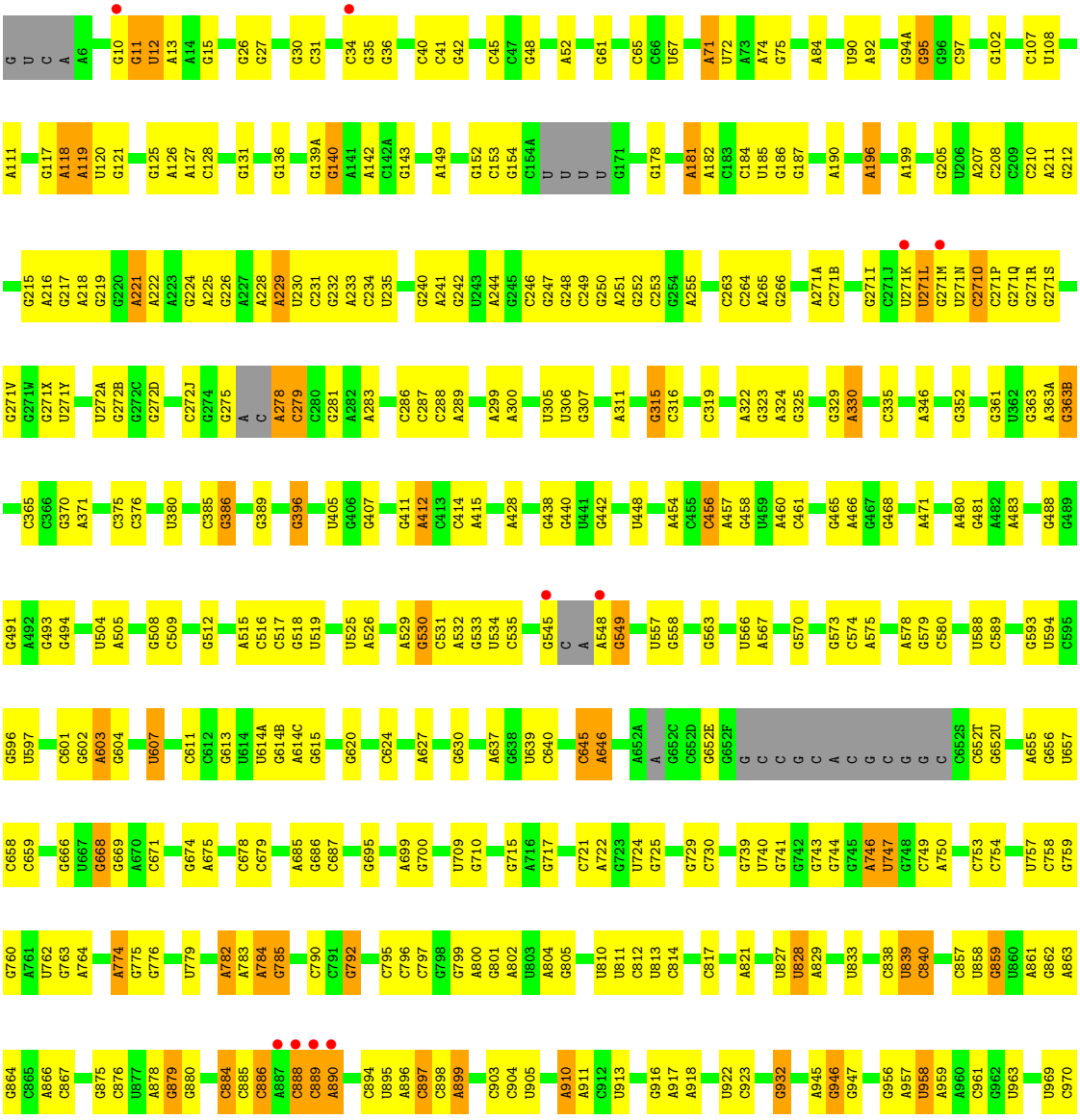
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
63	27	9	Total O 9 9	0	0
63	28	12	Total O 12 12	0	0
63	29	1	Total O 1 1	0	0
63	2a	384	Total O 384 384	0	0
63	2d	4	Total O 4 4	0	0
63	2e	2	Total O 2 2	0	0
63	2f	3	Total O 3 3	0	0
63	2j	2	Total O 2 2	0	0
63	2l	4	Total O 4 4	0	0
63	2m	1	Total O 1 1	0	0
63	2o	4	Total O 4 4	0	0
63	2p	1	Total O 1 1	0	0
63	2q	1	Total O 1 1	0	0
63	2r	3	Total O 3 3	0	0
63	2t	2	Total O 2 2	0	0
63	2u	1	Total O 1 1	0	0
63	2y	3	Total O 3 3	0	0
63	2w	3	Total O 3 3	0	0
63	2x	3	Total O 3 3	0	0

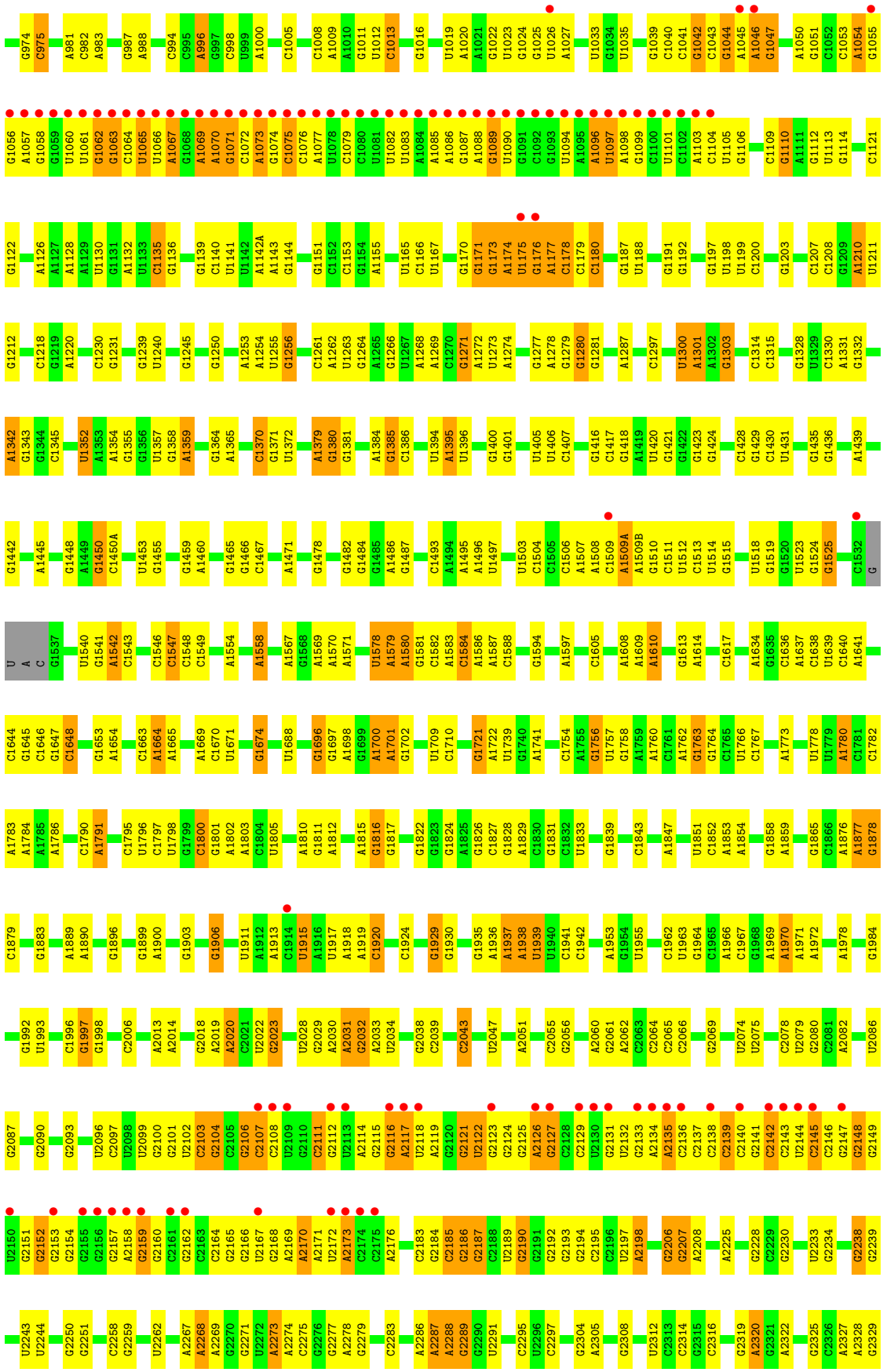
3 Residue-property plots (i)

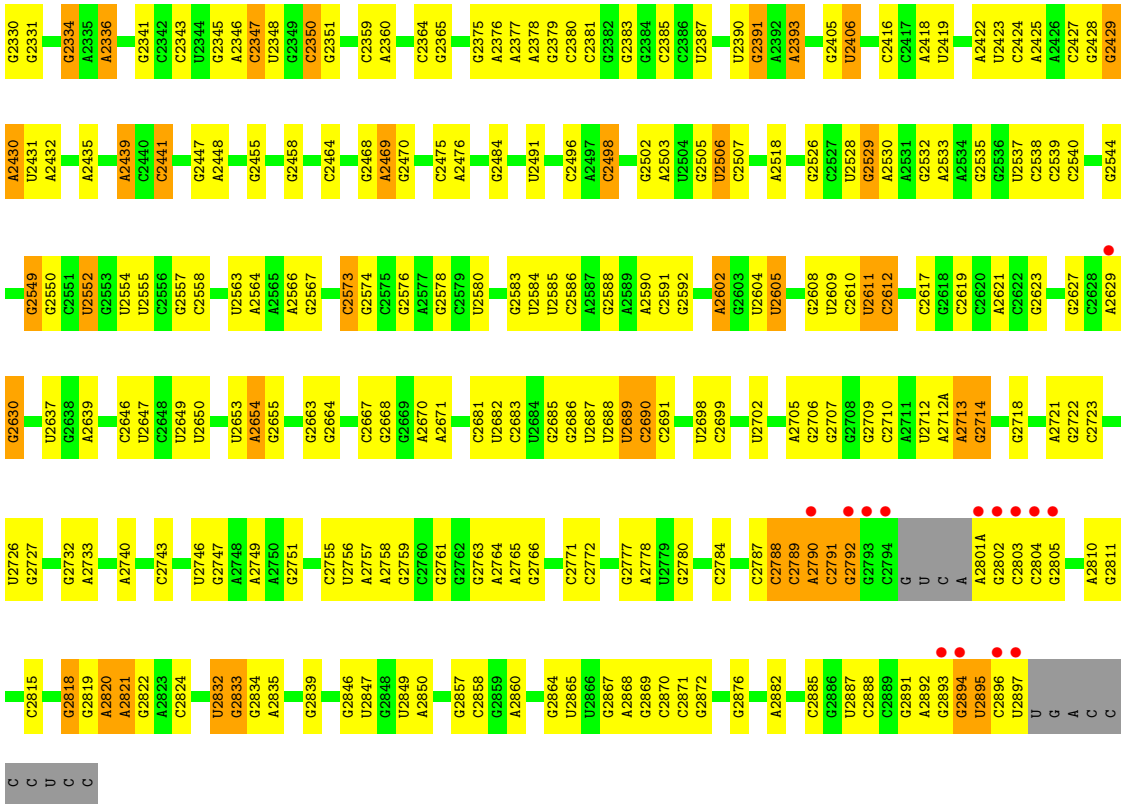
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: 23S Ribosomal RNA

Chain 1A: 4% 57% 34% 7%

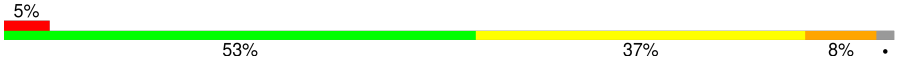


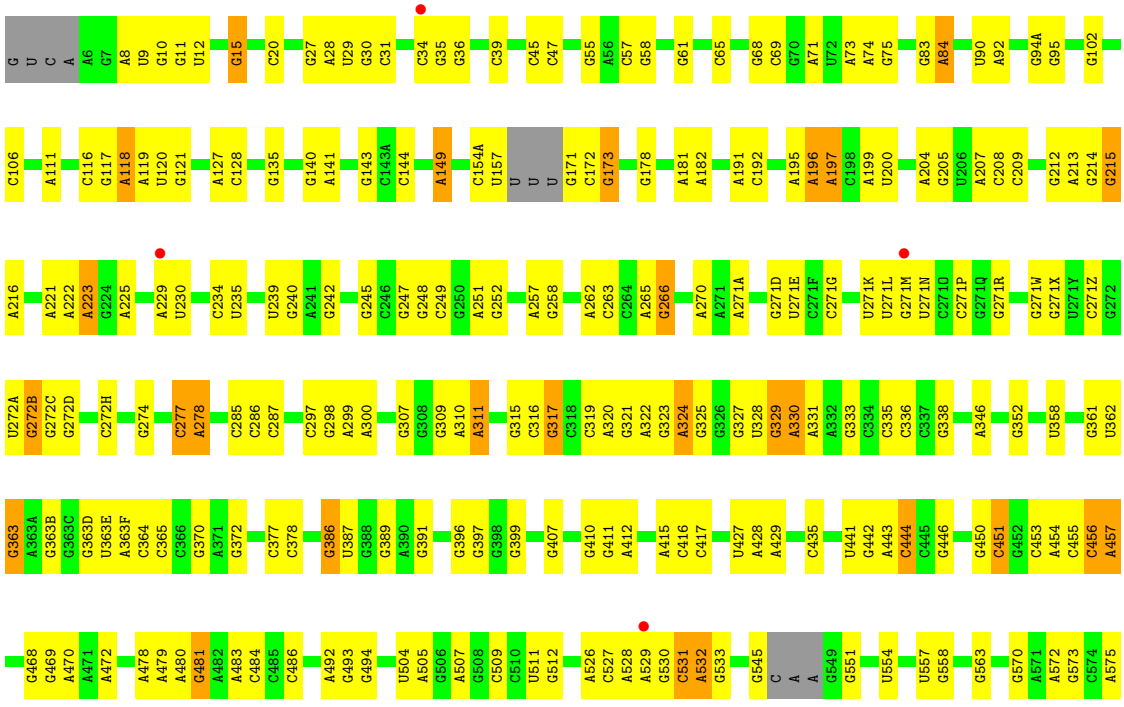

G974 C975 A981 C982 A983 G987 A988 C994 C995 A996 C997 C998 U999 A1000 C1005 C1008 A1009 A1010 G1011 U1012 C1013 G1016 U1019 A1020 A1021 G1022 U1023 G1024 G1025 U1026 A1027 U1033 G1034 U1035 G1039 C1040 C1041 G1042 C1043 G1044 A1045 A1046 G1047 A1050 G1051 C1052 C1053 A1054 G1055
G1056 A1057 G1058 G1059 U1060 U1061 G1062 G1063 C1064 U1065 U1066 A1067 G1068 A1069 A1070 G1071 C1072 A1073 G1074 C1075 C1076 A1077 U1078 C1079 C1080 U1081 U1082 U1083 A1084 A1085 A1086 G1087 A1088 G1089 U1090 G1091 C1092 G1093 U1094 A1095 A1096 U1097 A1098 G1099 C1100 U1101 C1102 A1103 C1104 U1105 G1106 C1109 G1110 A1111 G1112 U1113 G1114 C1121
G1122 A1126 A1127 A1128 A1129 U1130 G1131 A1132 U1133 C1135 G1136 G1139 C1140 U1141 U1142 A1142A A1143 G1144 G1151 C1152 C1153 G1154 A1155 U1165 C1166 U1167 G1170 G1171 G1173 A1174 U1175 G1176 A1177 C1178 C1179 C1180 G1187 U1188 G1191 G1192 G1197 U1198 U1199 C1200 G1203 C1207 C1208 G1209 A1210 U1211
G1212 C1218 G1219 A1220 C1230 G1231 G1239 U1240 G1245 G1250 A1253 A1254 U1255 G1256 C1261 A1262 U1263 G1264 A1265 G1266 U1267 A1268 A1269 C1270 G1271 A1272 U1273 A1274 G1277 A1278 G1279 G1280 G1281 A1287 C1297 U1300 A1301 A1302 G1303 C1314 C1315 G1328 U1329 C1330 A1331 G1332
A1342 G1343 G1344 C1345 U1352 A1353 A1354 G1355 G1356 U1357 U1358 A1359 G1364 A1365 C1370 G1371 U1372 A1379 G1380 G1381 A1384 G1385 C1386 U1394 A1395 U1396 G1400 G1401 U1405 U1406 C1407 G1416 C1417 G1418 A1419 U1420 G1421 G1422 G1423 G1424 C1428 G1429 C1430 U1431 G1435 G1436 A1439
G1442 A1445 G1448 A1449 G1450 C1450A U1453 G1455 G1459 A1460 G1465 G1466 C1467 A1471 G1478 G1482 G1484 G1485 A1486 G1487 C1493 A1494 A1495 A1496 U1497 U1503 C1504 C1505 C1506 A1507 A1508 C1509 A1509A A1509B G1510 C1511 U1512 C1513 U1514 G1515 U1518 G1519 G1520 U1523 G1524 G1525 C1532 G
U A C G1537 U1540 G1541 A1542 C1543 C1546 C1547 C1548 C1549 A1554 A1558 A1567 G1568 A1569 A1570 A1571 U1578 A1579 A1580 G1581 C1582 A1583 C1584 A1586 A1587 C1588 G1594 A1597 C1605 A1608 A1609 A1610 G1613 A1614 C1617 A1634 G1635 C1636 A1637 C1638 U1639 C1640 A1641
C1644 G1645 A1646 G1647 C1648 G1653 A1654 C1663 A1664 A1665 A1669 C1670 U1671 G1674 U1688 G1696 G1697 A1698 G1699 A1700 A1701 G1702 U1709 C1710 G1721 A1722 U1739 G1740 A1741 C1754 A1755 G1756 U1757 G1758 A1759 A1760 C1761 A1762 G1763 G1764 C1765 U1766 C1767 A1773 U1778 U1779 A1780 C1781 C1782
A1783 A1784 A1785 A1786 C1790 A1791 C1795 U1796 C1797 U1798 G1799 C1800 G1801 A1802 A1803 C1804 U1805 A1810 G1811 A1812 A1815 G1816 G1817 G1822 G1823 G1824 A1825 G1826 C1827 G1828 A1829 C1830 G1831 C1832 U1833 G1839 C1843 A1847 U1851 C1852 A1853 A1854 G1858 A1859 G1865 C1866 A1876 A1877 G1878
C1879 G1883 A1889 A1890 G1896 G1899 A1900 G1903 G1906 U1911 A1912 A1913 C1914 U1915 A1916 U1917 A1918 A1919 C1920 C1924 G1929 G1930 G1935 A1936 A1937 A1938 U1939 U1940 C1941 C1942 A1953 G1954 U1955 C1962 U1963 G1964 C1965 A1966 C1967 G1968 A1969 A1970 A1971 A1972 A1978 G1984
G1992 U1993 C1996 G1997 G1998 C2006 A2013 A2014 G2018 A2019 A2020 C2021 U2022 G2023 U2028 G2029 A2030 A2031 G2032 A2033 U2034 G2038 C2039 C2043 U2047 A2051 C2055 G2056 A2060 G2061 A2062 C2063 C2064 C2065 C2066 G2069 U2074 U2075 C2078 U2079 G2080 C2081 A2082 U2086
G2087 G2090 G2093 U2096 C2097 U2098 U2099 G2100 G2101 U2102 C2103 G2104 C2105 G2106 C2107 C2108 U2109 C2110 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 C2174 C2175 A2176 C2183 G2184 C2185 G2186 G2187 C2188 U2189 G2190 G2191 G2192 G2193 G2194 C2195 C2196 U2197 A2198 G2206 G2207 A2208 A2225 G2228 C2229 G2230 U2233 G2234 G2238 G2239
U2243 U2244 G2250 G2251 C2258 G2259 U2262 A2267 A2268 A2269 G2270 G2271 U2272 A2273 A2274 C2275 G2276 G2277 A2278 G2279 C2283 A2286 A2287 A2288 G2289 G2290 U2291 C2295 U2296 C2297 G2304 A2305 G2308 U2312 C2313 C2314 G2315 C2316 G2319 A2320 G2321 A2322 G2325 C2326 A2327 A2328 G2329

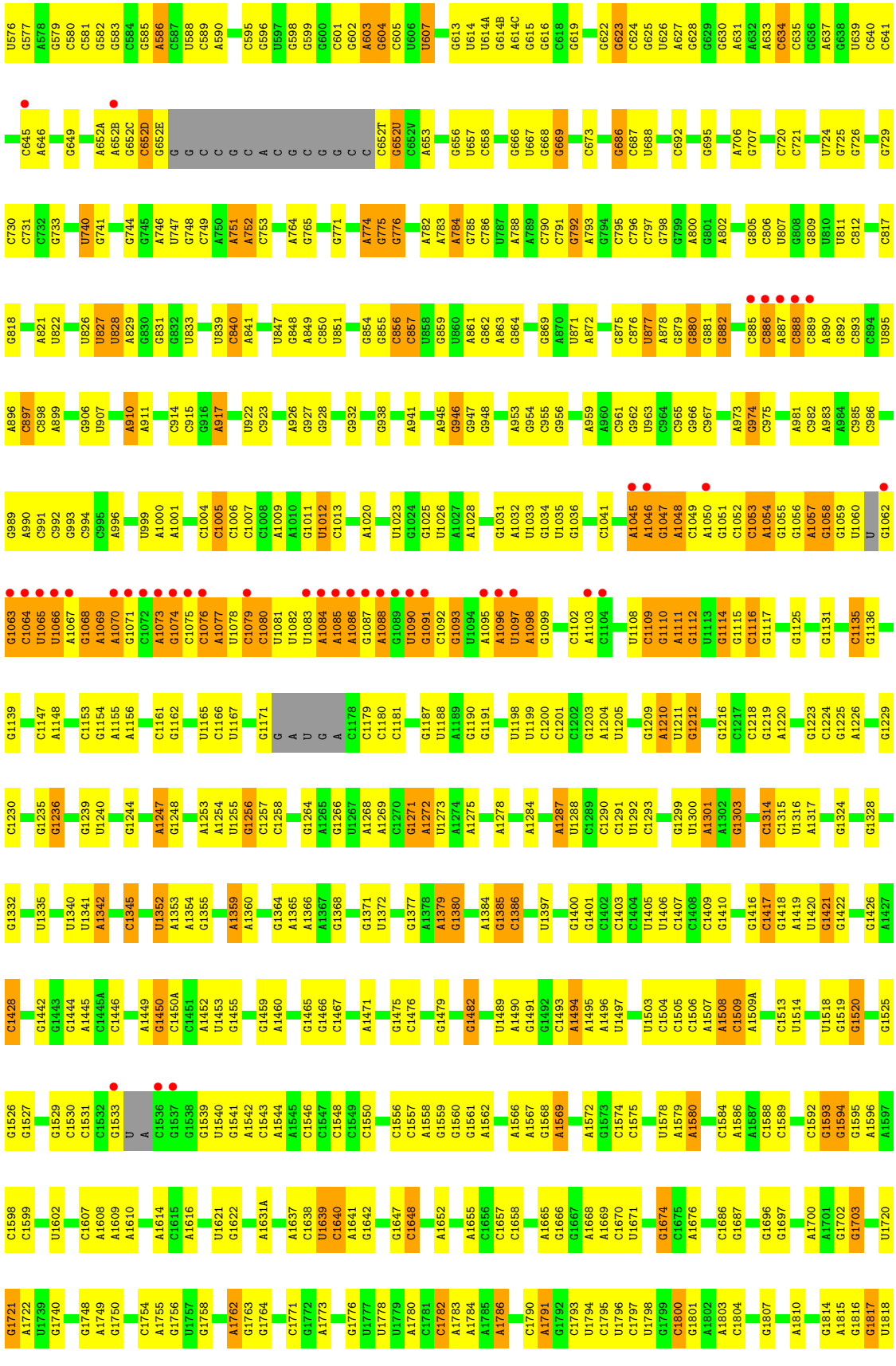


• Molecule 1: 23S Ribosomal RNA

Chain 2A:



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C645 A646 G649 A652A A652B G652C C652D G652E G G C C G C A C G G C C C652T G652U C652V A653 G656 U657 C658 G666 U667 G668 G669 C673 G686 C687 U688 C692 G695 A706 G707 C720 C721 U724 G725 G726 G729
C730 C731 C732 G733 U740 G741 G744 G745 A746 U747 G748 C749 A750 A751 A752 C753 A764 A765 G771 A774 G775 G776 A782 A783 A784 G785 C786 U787 A788 A789 C790 C791 G792 A793 G794 C795 C796 C797 G798 G799 A800 G801 A802 G805 C806 U807 G808 G809 U810 U811 C812 C817
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G1332 U1335 U1340 U1341 A1342 C1345 U1352 A1353 A1354 G1355 A1359 A1360 G1364 A1365 A1366 A1367 G1368 G1371 U1372 G1377 A1378 A1379 G1380 A1384 G1385 C1386 U1397 G1400 G1401 C1402 C1403 C1404 U1405 U1406 C1407 C1408 C1409 G1410 G1416 C1417 G1418 A1419 U1420 G1421 G1422 G1426 A1427
C1428 G1442 G1443 G1444 A1445 C1445A C1446 A1449 G1450 C1450A C1451 A1452 U1453 G1455 G1459 A1460 G1465 G1466 C1467 A1471 G1475 C1476 G1479 G1482 U1489 A1490 G1491 G1492 C1493 A1494 A1495 A1496 U1497 U1503 C1504 C1505 C1506 A1507 A1508 C1509 A1509A C1513 U1514 U1518 G1519 G1520 G1525
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C1598 C1599 U1602 C1607 A1608 A1609 A1610 A1614 C1615 A1616 U1621 G1622 A1631A A1637 C1638 U1639 C1640 A1641 G1642 G1647 C1648 A1652 A1655 C1656 C1657 C1658 A1665 G1666 G1667 A1668 A1669 C1670 U1671 G1674 C1675 A1676 C1686 G1687 G1696 G1697 A1700 A1701 G1702 G1703 U1720
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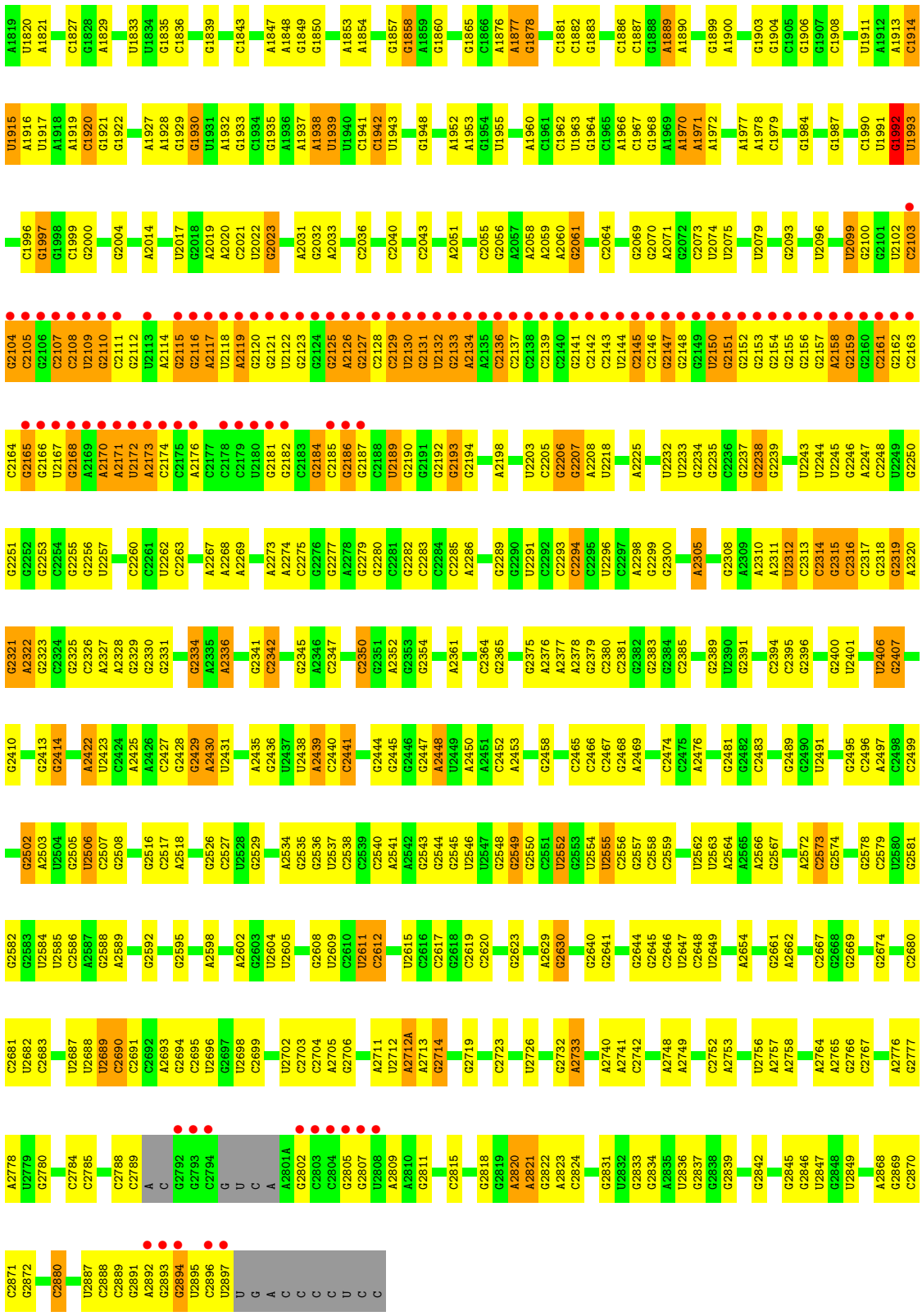
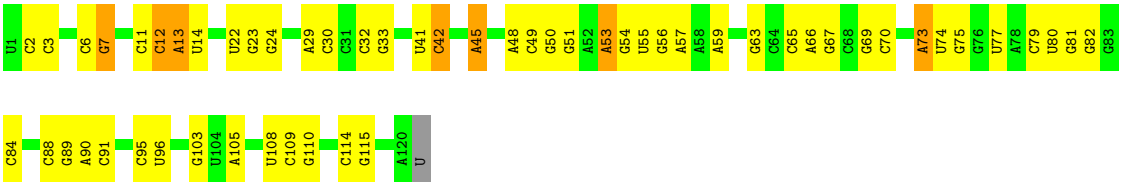


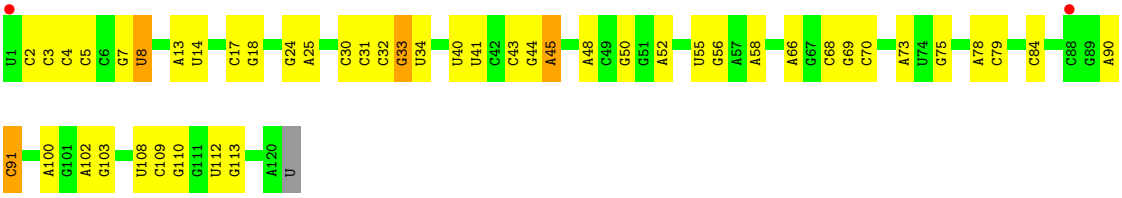
- Molecule 2: 5S Ribosomal RNA

Chain 1B:



• Molecule 2: 5S Ribosomal RNA

Chain 2B:

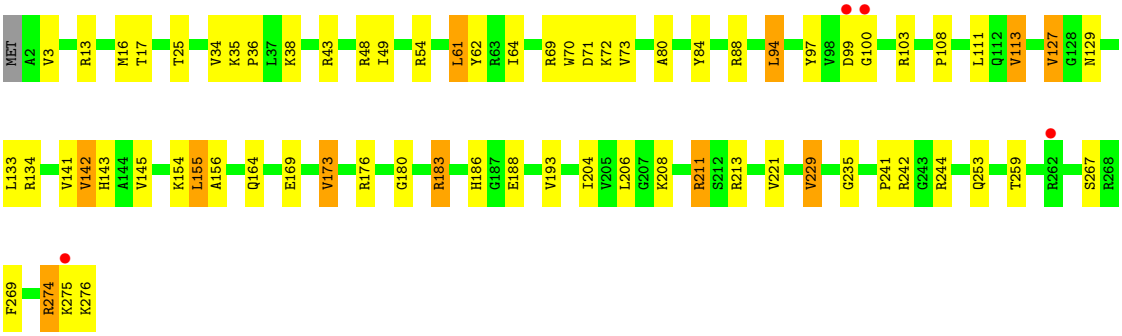


• Molecule 3: 50S ribosomal protein L2

Chain 1D:

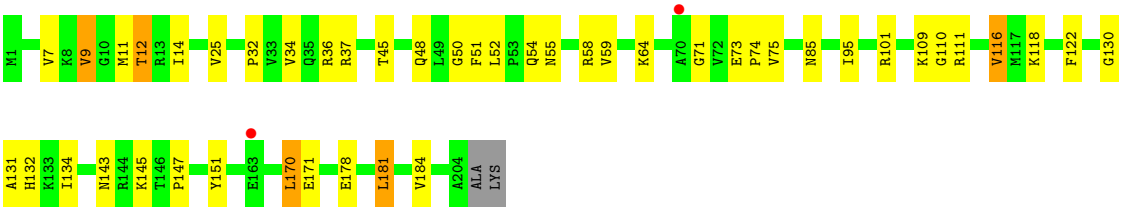
• Molecule 3: 50S ribosomal protein L2

Chain 2D:



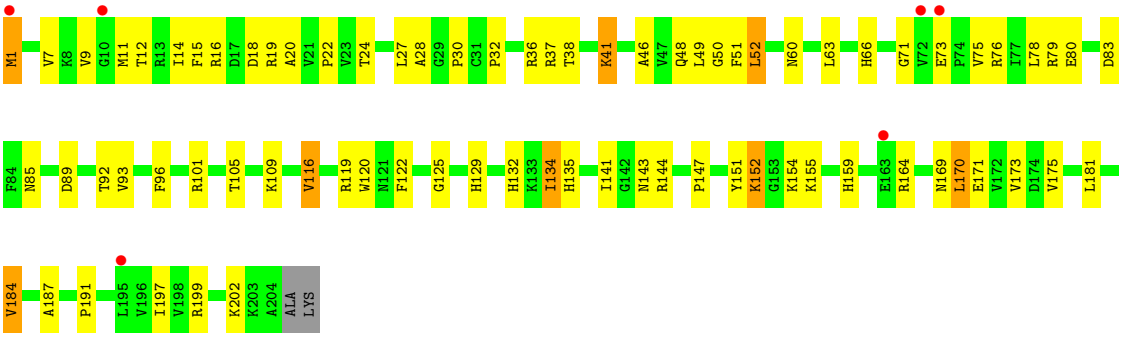
• Molecule 4: 50S ribosomal protein L3

Chain 1E:



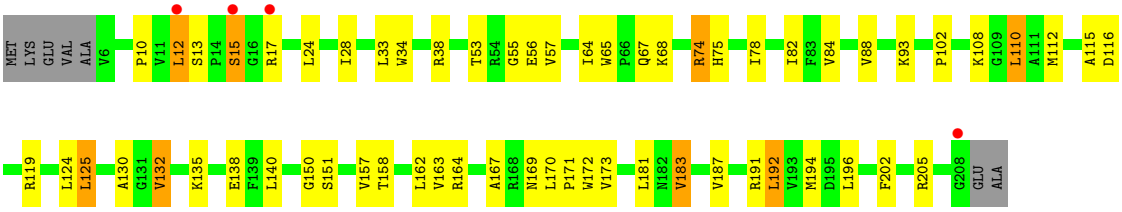
• Molecule 4: 50S ribosomal protein L3

Chain 2E:



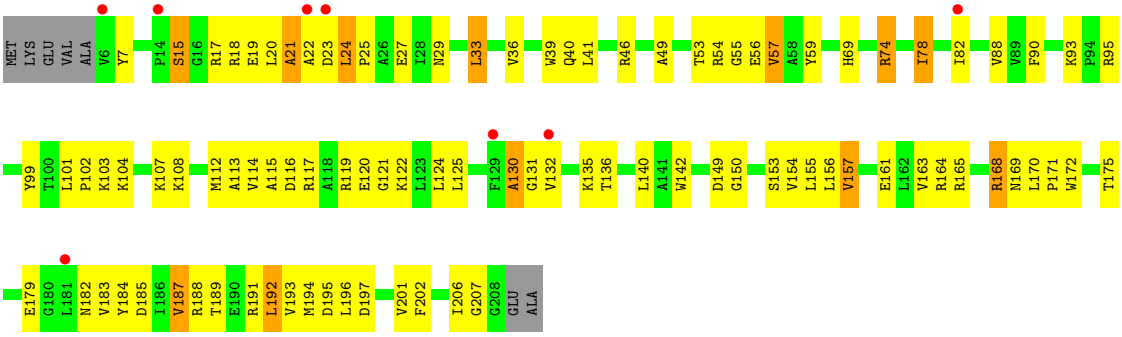
• Molecule 5: 50S ribosomal protein L4

Chain 1F:



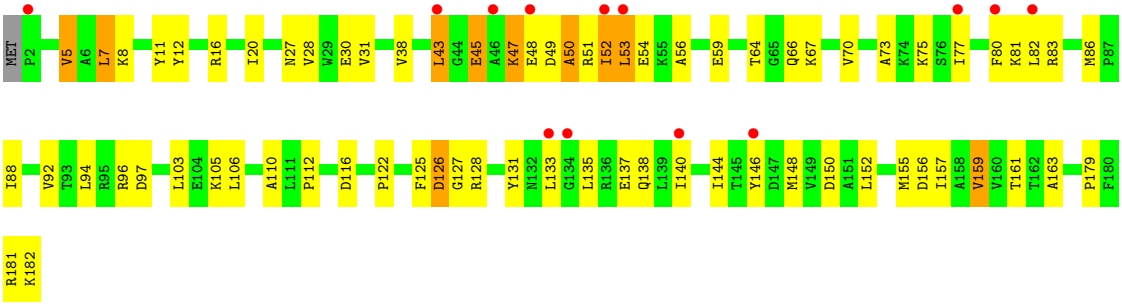
• Molecule 5: 50S ribosomal protein L4

Chain 2F:



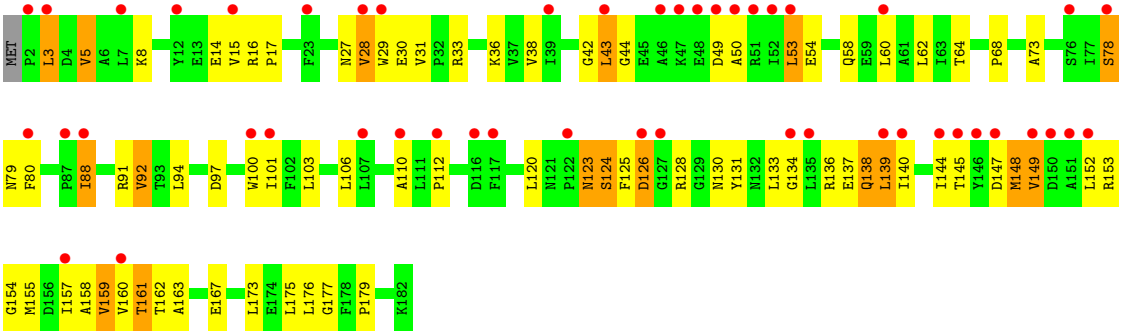
• Molecule 6: 50S ribosomal protein L5

Chain 1G:



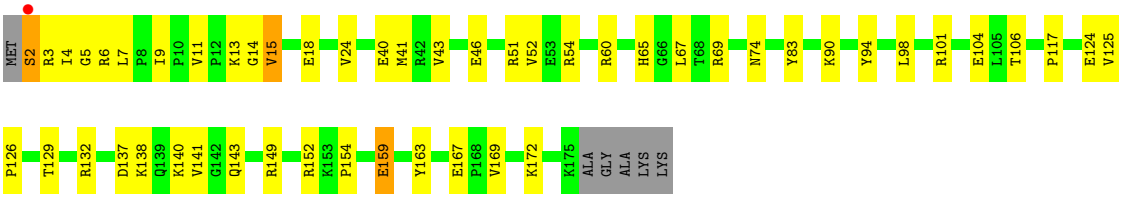
• Molecule 6: 50S ribosomal protein L5

Chain 2G:



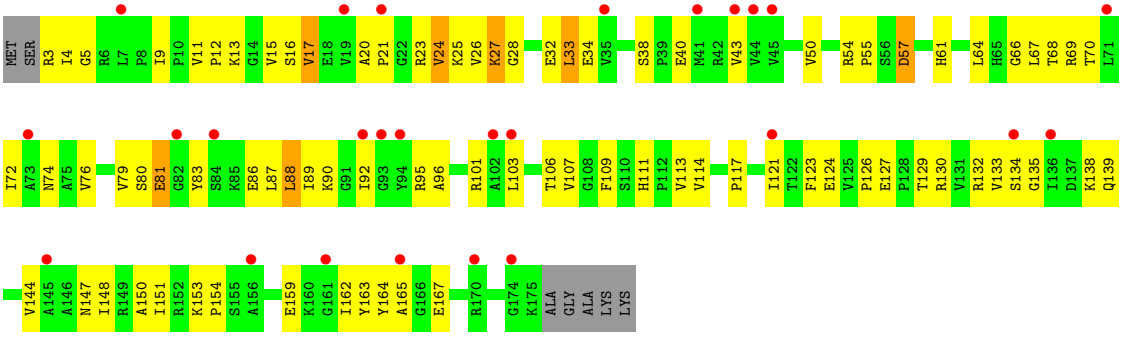
• Molecule 7: 50S ribosomal protein L6

Chain 1H:



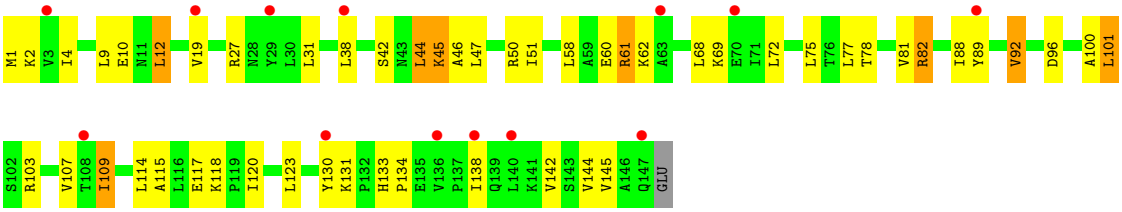
• Molecule 7: 50S ribosomal protein L6

Chain 2H:



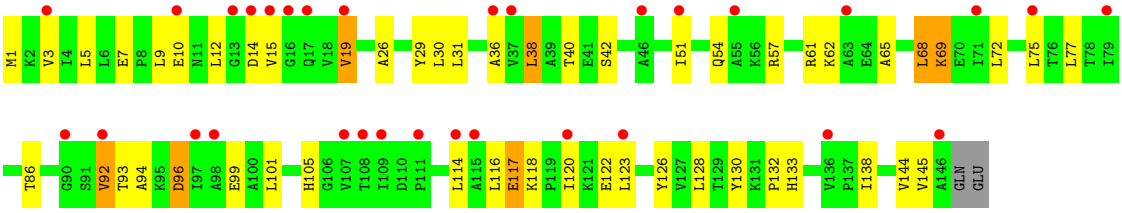
• Molecule 8: 50S ribosomal protein L9

Chain 1I:



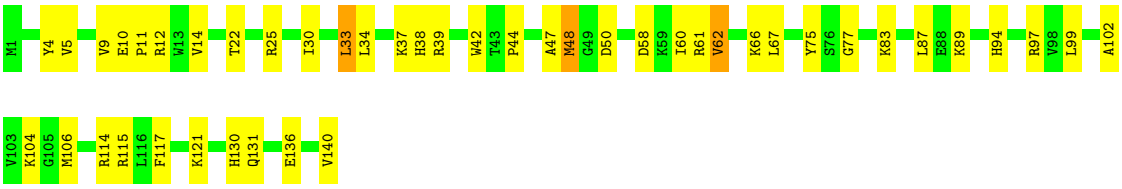
- Molecule 8: 50S ribosomal protein L9

Chain 2I:



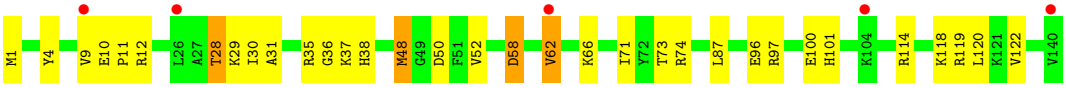
- Molecule 9: 50S ribosomal protein L13

Chain 1N:



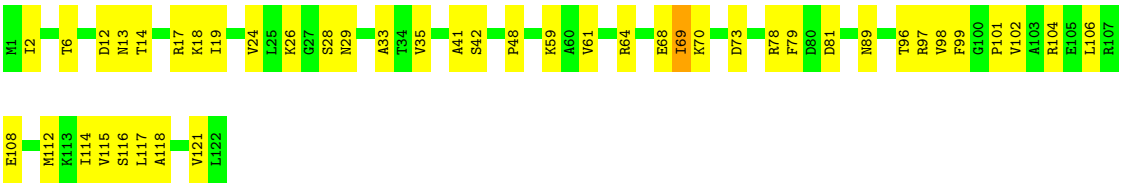
- Molecule 9: 50S ribosomal protein L13

Chain 2N:



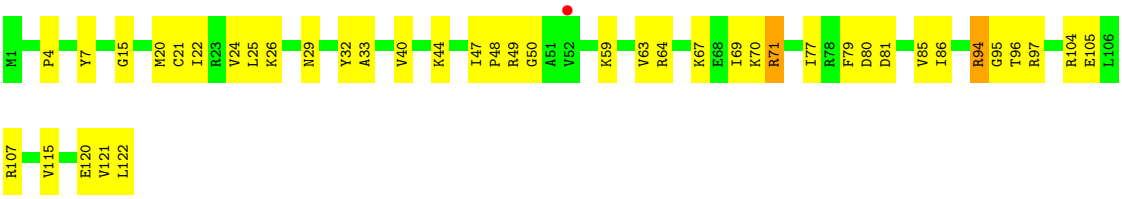
- Molecule 10: 50S ribosomal protein L14

Chain 1O:



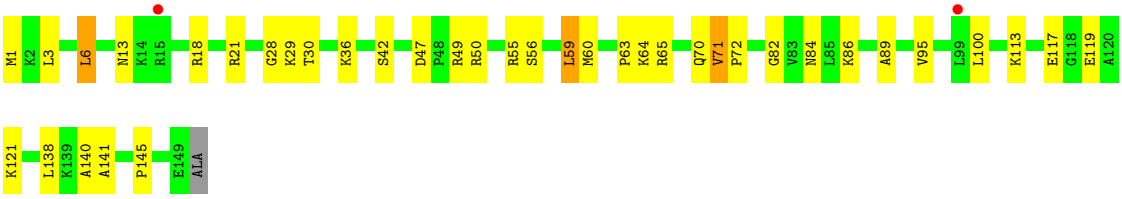
- Molecule 10: 50S ribosomal protein L14

Chain 2O:



- Molecule 11: 50S ribosomal protein L15

Chain 1P:

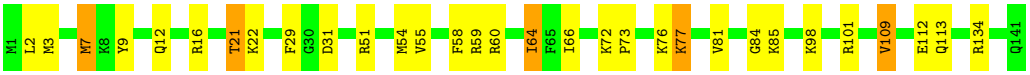


- Molecule 11: 50S ribosomal protein L15

Chain 2P:

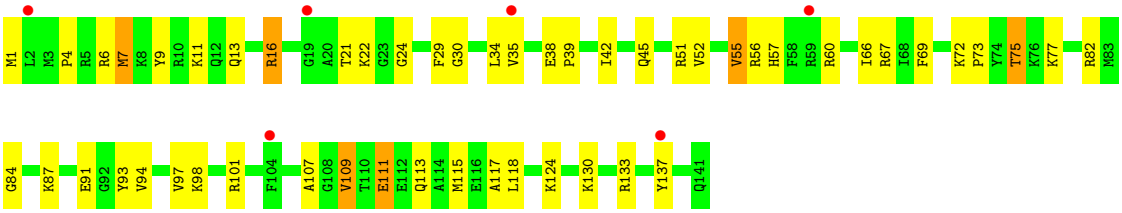
- Molecule 12: 50S ribosomal protein L16

Chain 1Q:



- Molecule 12: 50S ribosomal protein L16

Chain 2Q:



- Molecule 13: 50S ribosomal protein L17

Chain 1R: 71% 24% 5%

M1 R2 H3 L4 K5 N11 R17 L28 L29 T30 H31 T36 T37 V38 P39 G46 F47 V48 H53 V66 L67 L70 Q71 D72 L75 V76 R77 K78 L79 I83 R86 Y94 T95 R96 V97 L100 R104 D107 L113 V114 E118

• Molecule 13: 50S ribosomal protein L17

Chain 2R: % 69% 27% •

M1 R2 R8 K9 R12 R17 L18 A19 L20 Y21 R22 N23 Q24 L29 G32 R33 T36 T37 V38 P39 E43 G46 A55 K56 R63 D69 L70 L75 F80 D81 E82 P85 R86 Y87 R90 R96 V97 L100 R103 R104 V114

E115 L116 V117 E118

• Molecule 14: 50S ribosomal protein L18

Chain 1S: % 69% 25% • •

MET ALA R3 R9 R10 V14 R15 N16 R17 I18 T21 G22 R23 S27 A37 Q38 E43 V46 T47 S50 K59 K62 A66 R67 Q68 V69 G70 R71 A74 G81 I82 K83 Q84 F87 D88 R97 E103 R106 E107 L110 E111 F112

• Molecule 14: 50S ribosomal protein L18

Chain 2S: 12% 63% 32% • •

MET ALA R3 R9 R10 K11 V14 R15 N16 R17 I18 K19 R23 L24 R25 L26 S27 V28 F29 L32 K33 Y36 A37 Q38 D41 D42 F43 K44 G45 V46 V49 S50 L54 L58 K59 G60 N61 K62 T63 E64 V65 A66 V69 L73 A86 F87 D88 R89

G90 P91 Y92 K93 Y94 H95 V98 A102 A105 R106 L110 E111 F112

• Molecule 15: 50S ribosomal protein L19

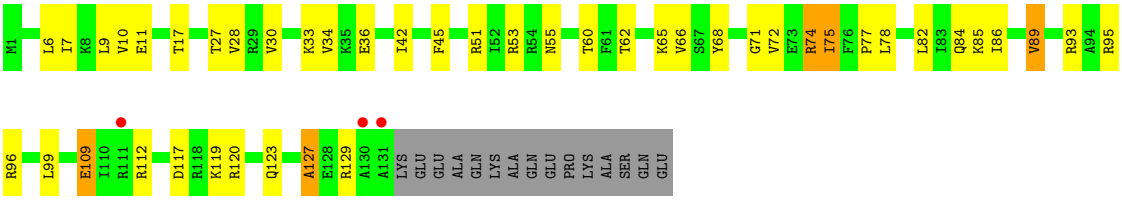
Chain 1T: 6% 64% 24% • 10%

M1 N2 R3 L19 P20 R23 V28 K33 V34 G37 N38 V49 I50 R51 I52 R53 R54 N55 G56 F57 N58 T59 S67 L82 I83 Q84 K85 I86 G92 R93 A94 R95 R96 N104 L105 S106 D107 R108 E109 I110 R111 R112 K113 D117 R118 K119 R120 Q123

D124 R125 A130 A131 LYS GLU GLU ALA GLN LYS ALA GLN GLU PRO LYS ALA SER GLN GLU

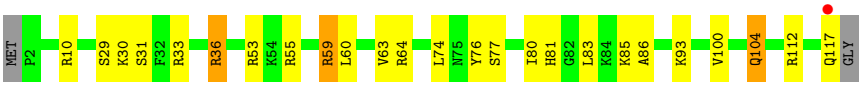
• Molecule 15: 50S ribosomal protein L19

Chain 2T: 2% 59% 27% • 10%



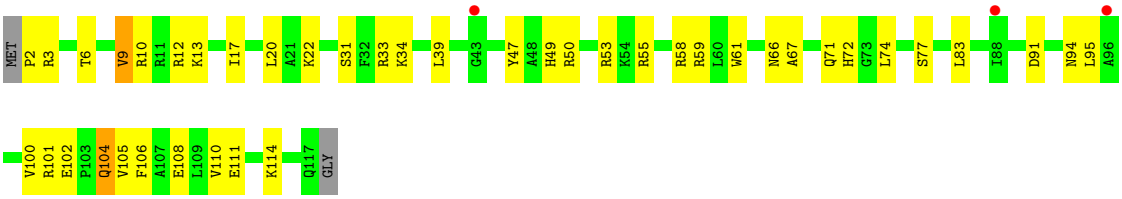
- Molecule 16: 50S ribosomal protein L20

Chain 1U:



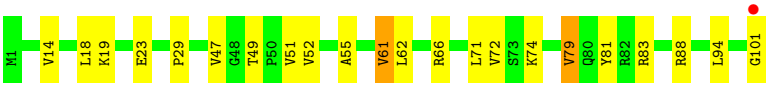
- Molecule 16: 50S ribosomal protein L20

Chain 2U:



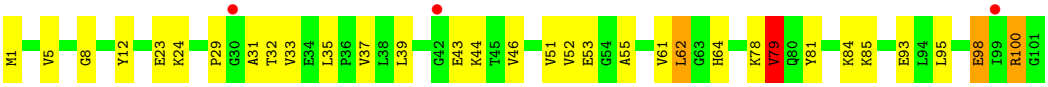
- Molecule 17: 50S ribosomal protein L21

Chain 1V:



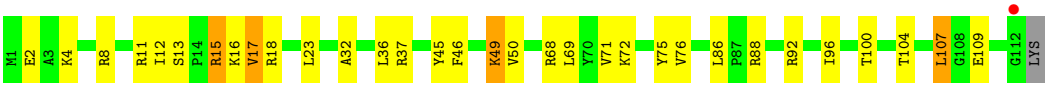
- Molecule 17: 50S ribosomal protein L21

Chain 2V:



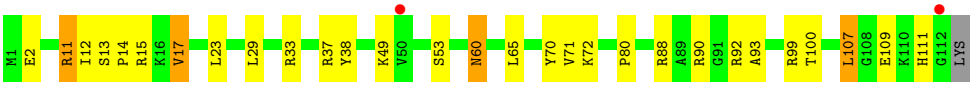
- Molecule 18: 50S ribosomal protein L22

Chain 1W:



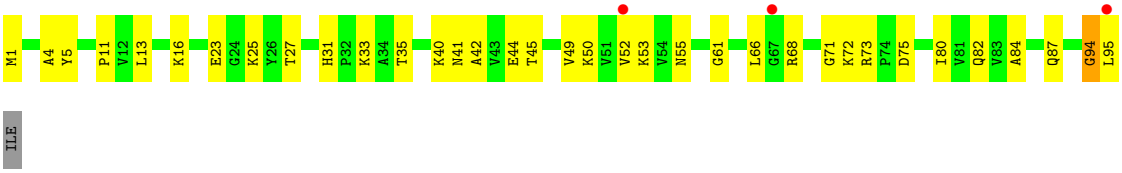
- Molecule 18: 50S ribosomal protein L22

Chain 2W:



• Molecule 19: 50S ribosomal protein L23

Chain 1X:

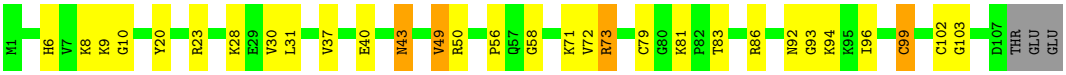


• Molecule 19: 50S ribosomal protein L23

Chain 2X:

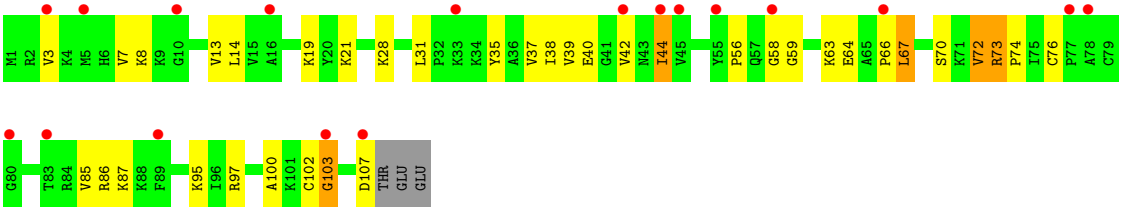
• Molecule 20: 50S ribosomal protein L24

Chain 1Y:



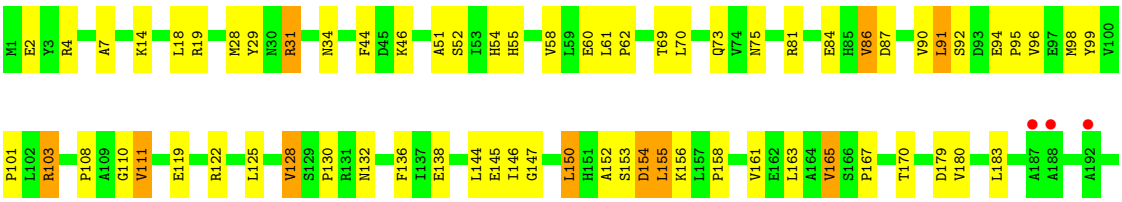
• Molecule 20: 50S ribosomal protein L24

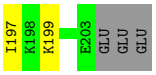
Chain 2Y:



• Molecule 21: 50S ribosomal protein L25

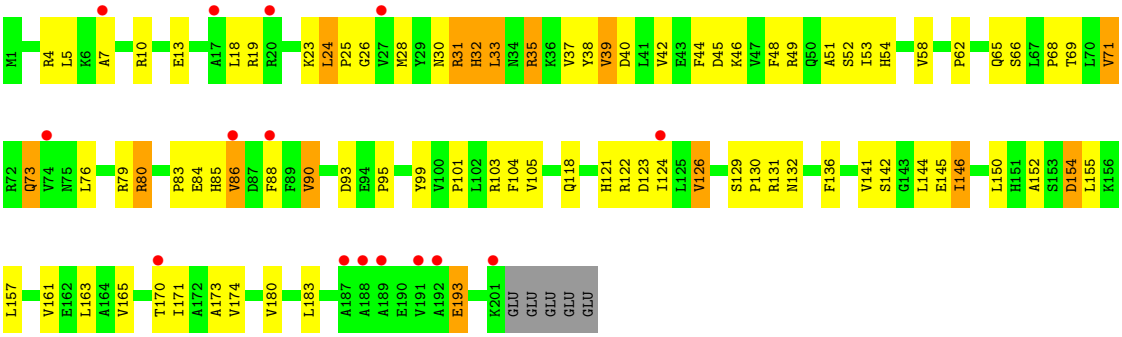
Chain 1Z:





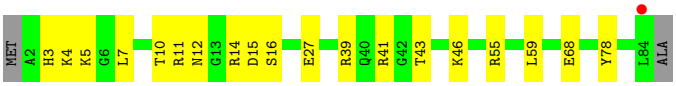
• Molecule 21: 50S ribosomal protein L25

Chain 2Z:



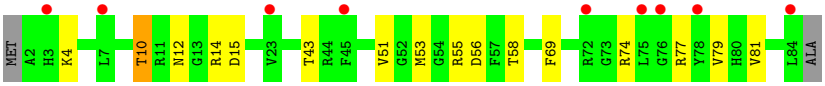
• Molecule 22: 50S ribosomal protein L27

Chain 10:



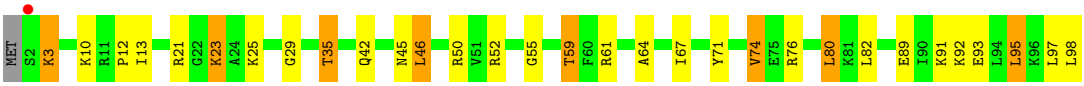
• Molecule 22: 50S ribosomal protein L27

Chain 20:



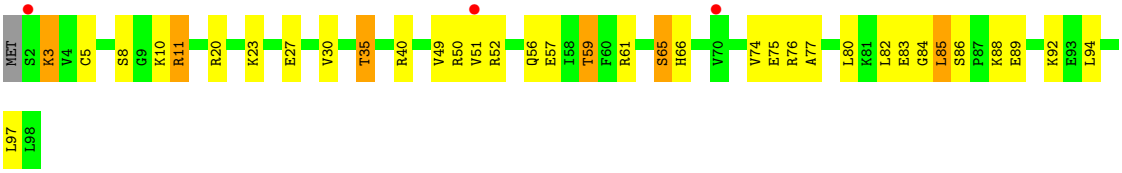
• Molecule 23: 50S ribosomal protein L28

Chain 11:



• Molecule 23: 50S ribosomal protein L28

Chain 21:

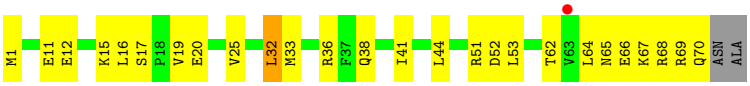


• Molecule 24: 50S ribosomal protein L29

Chain 12:

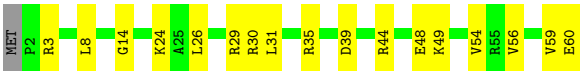
• Molecule 24: 50S ribosomal protein L29

Chain 22:



• Molecule 25: 50S ribosomal protein L30

Chain 13:

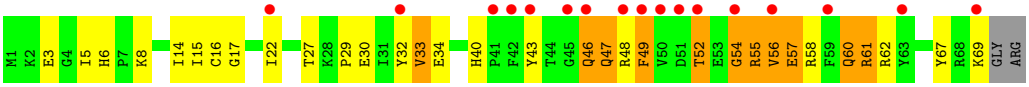


• Molecule 25: 50S ribosomal protein L30

Chain 23:

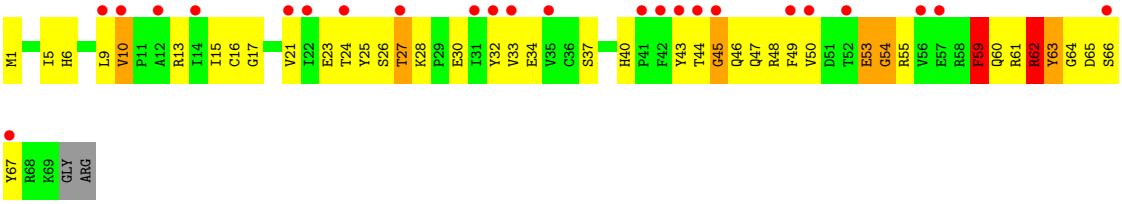
• Molecule 26: 50S ribosomal protein L31

Chain 14:



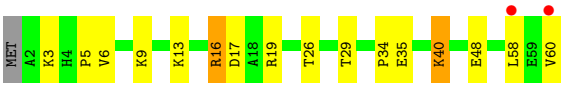
• Molecule 26: 50S ribosomal protein L31

Chain 24:



• Molecule 27: 50S ribosomal protein L32

Chain 15:

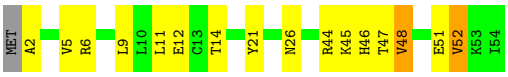


• Molecule 27: 50S ribosomal protein L32

Chain 25:

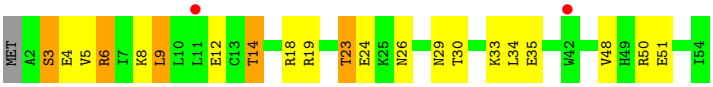
• Molecule 28: 50S ribosomal protein L33

Chain 16:



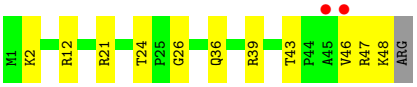
• Molecule 28: 50S ribosomal protein L33

Chain 26:



• Molecule 29: 50S ribosomal protein L34

Chain 17:

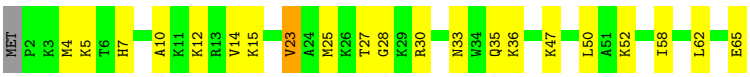


• Molecule 29: 50S ribosomal protein L34

Chain 27:

• Molecule 30: 50S ribosomal protein L35

Chain 18:



• Molecule 30: 50S ribosomal protein L35

Chain 28: 68% 31%

MET P2 K5 T6 H7 K8 G9 A10 R13 V14 K15 V23 K26 N33 W34 Q35 K36 Q43 R46 K47 F48 V49 E54 R57 E65

• Molecule 31: 50S ribosomal protein L36

Chain 19: 3% 89% 8%

M1 I17 Y24 K33 Q34 R35 Q36 G37

• Molecule 31: 50S ribosomal protein L36

Chain 29: 5% 51% 49%

M1 K2 A5 S6 V7 C14 K15 V16 I17 R18 R19 H20 G21 R22 V25 I26 C27 E28 N29 P30 K31 H32 K33 Q34 G37

• Molecule 32: 16S Ribosomal RNA

Chain 1a: 2% 48% 41% 10%

U U G U4 U5 G6 G7 A8 G9 A16 U17 C18 C19 G22 C23 G28 G29 A32 A33 C34 G38 G39 G42 C43 G44 U45 G46 C47 C48 U49 A50 A51 G52 A53 U56 G57 C58 A59 A60 G61 U62 C67 G68 G69 G70 G78 G79 G U U U

U A C U90 C91 C92 G93 U96 G97 C100 A101 G102 C103 G107 G108 A109 G113 U114 G115 A116 A119 A120 C121 G122 C123 A130 C131 C132 U133 A134 C137 G138 A141 G142 A143 G144 G145 A151 A160 A161 A162 C163 U164 C165 G166 G167 G168 C169 U170 A171 A172

U173 C174 C175 C176 C177 C178 A179 U180 G181 U182 G183 G184 A185 C186 C189B C189C C189D U189E U189F U189K G189L C194 A195 A196 A197 C201 U202 U203 U204 G216 G220 C221 U222 U223 C224 C225 G226 G227 A228 U229 G230 G231 C235 G236 G247 G251 G254 G255 U256 G257 G258

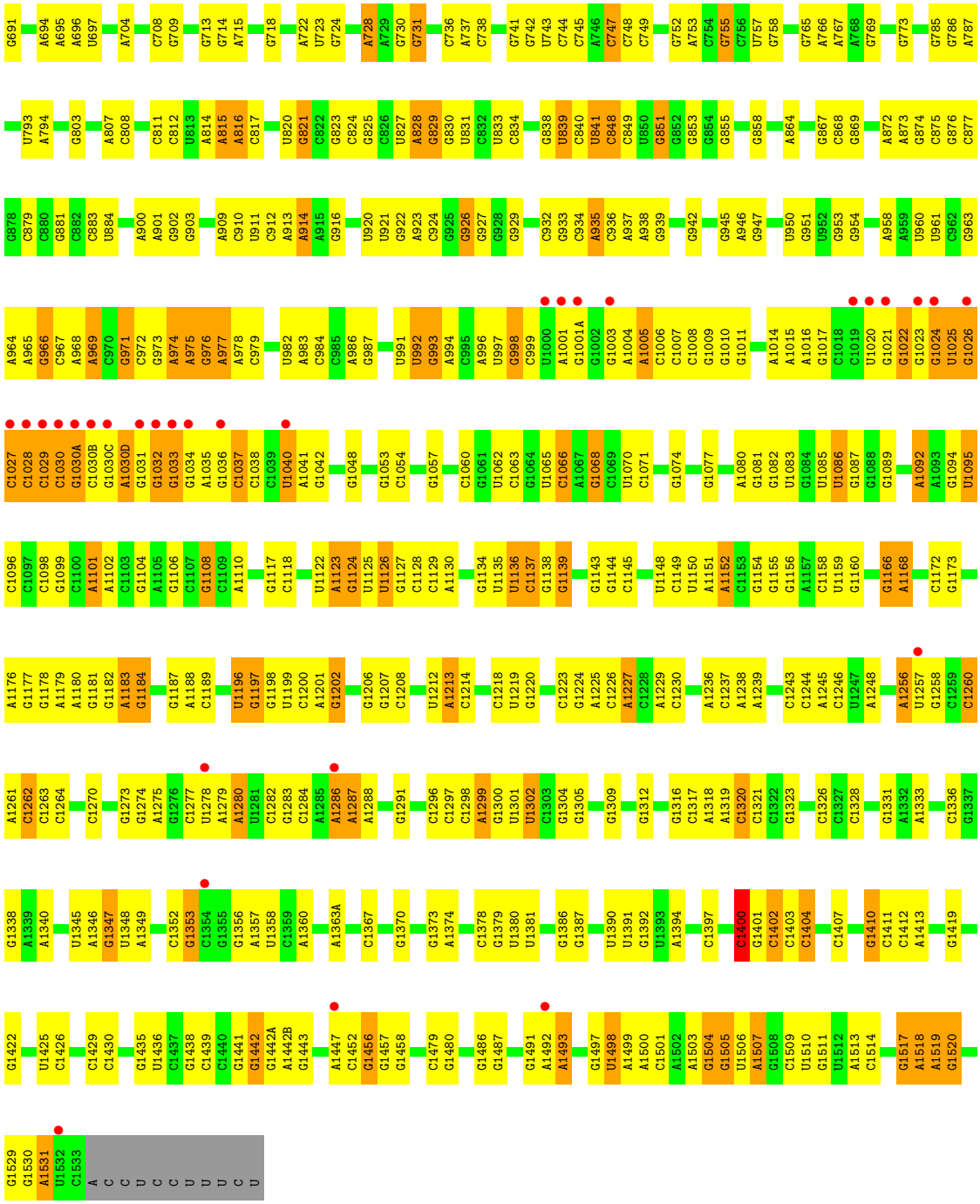
G259 A262 A263 G266 C267 C268 C271 C272 G275 G278 C283 G284 G289 G292 A298 G299 A300 G301 G302 A303 U304 G305 G309 G310 G316 C320 A321 G324 A325 C328 A329 C330 G331 G332 C341 C342 U343 A344 C345 G346 G347 G348 G351 C352

A353 G354 C355 A356 U359 A360 U367 U368 C372 A373 A374 U375 G376 C379 G380 C381 A382 A383 A389 C390 G396 A397 C398 G399 C400 C401 G402 C403 U404 U405 G406 G407 A408 G409 G410 A411 A412 G413 A414 G423 G424 G428 U429 A430 A431 A432 C433 U434 C435 C436 U437 G438

A439 A441 C442 C443 G446 G447 A448 C449 A452 A453 C454 C457 C458 G460 A461 C470 G471 A472 G473 G474 G475 G476 A477 G485 U486 A487 G490 G491 G492 A495 A496 U498 C501 G502 C503 C504 G505 G506 C507 C508 A509 A510 C511 C514 G515 U516 G517 C518 C519 A520 G527

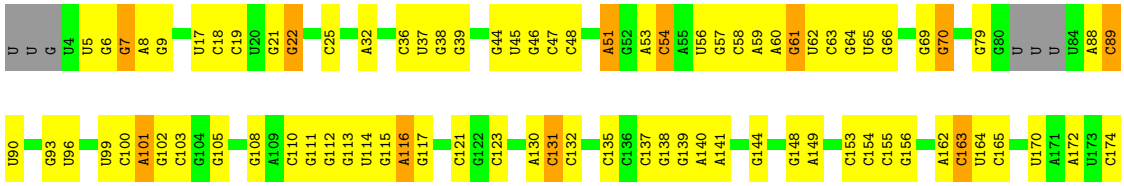
C528 G529 G530 U531 A532 A533 U534 A535 C536 G537 G538 A539 G540 G544 A547 G548 C549 G550 U551 U552 C555 G558 A559 U560 U561 C562 A563 C564 G567 G568 A572 A573 A574 G575 G576 G577 U582 A583 G584 G585 G588 G593 G594 G595 C596 C600 C601 A602 A607

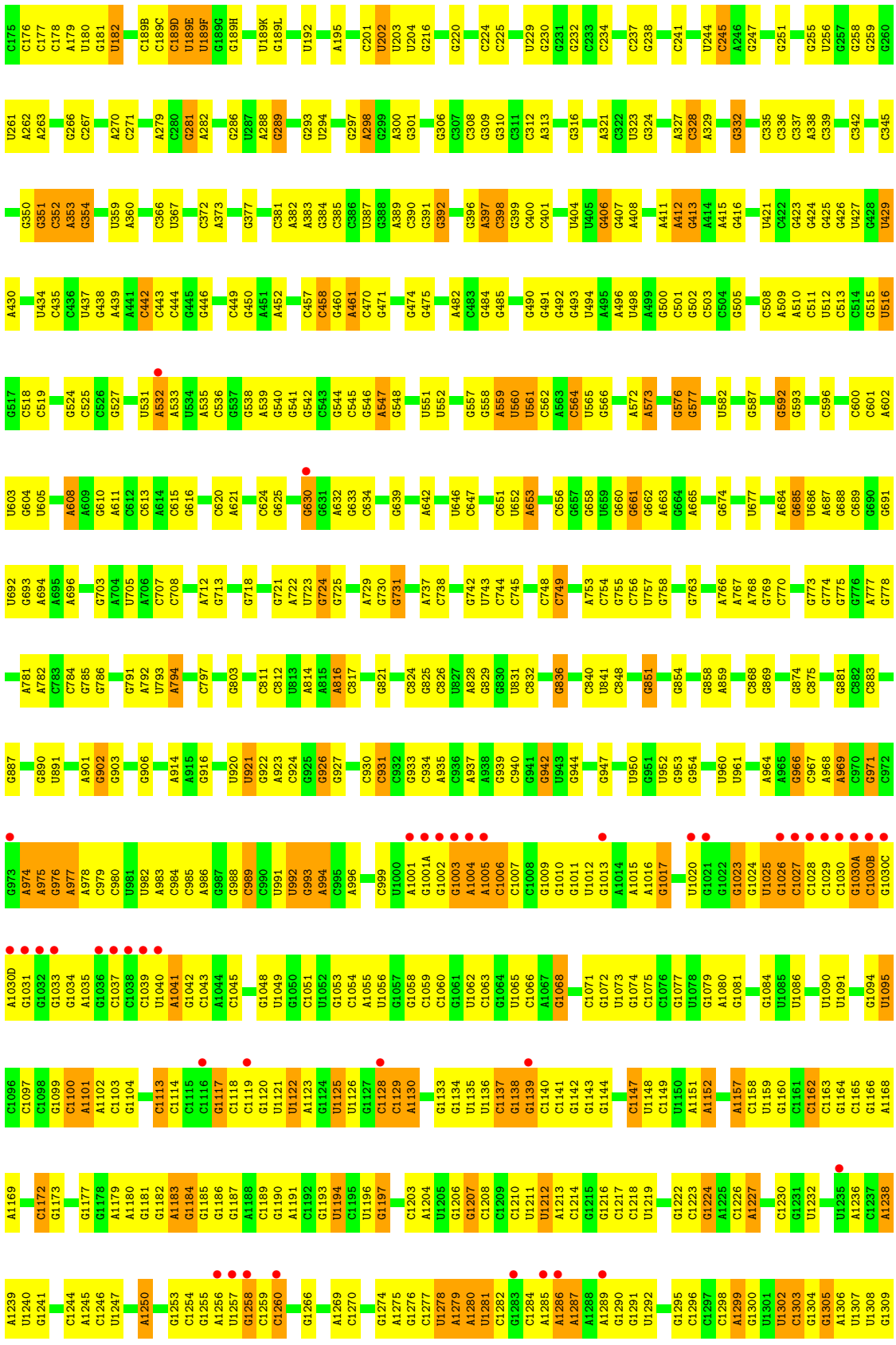
A608 A609 C612 C613 A614 C615 G616 U619 C620 A621 C624 G625 U626 G627 G628 G629 G630 G631 A632 G633 C634 C643 U646 C647 C651 U652 A653 C656 G657 G658 G661 G664 A665 U669 G670 G673 G674 A675 A676 U677 G682 G685 U686 A687 G688 C689 G690

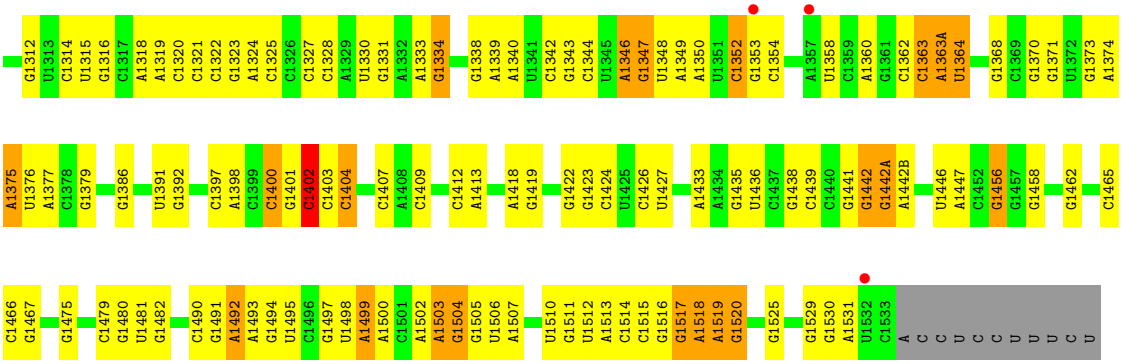


- Molecule 32: 16S Ribosomal RNA

Chain 2a:

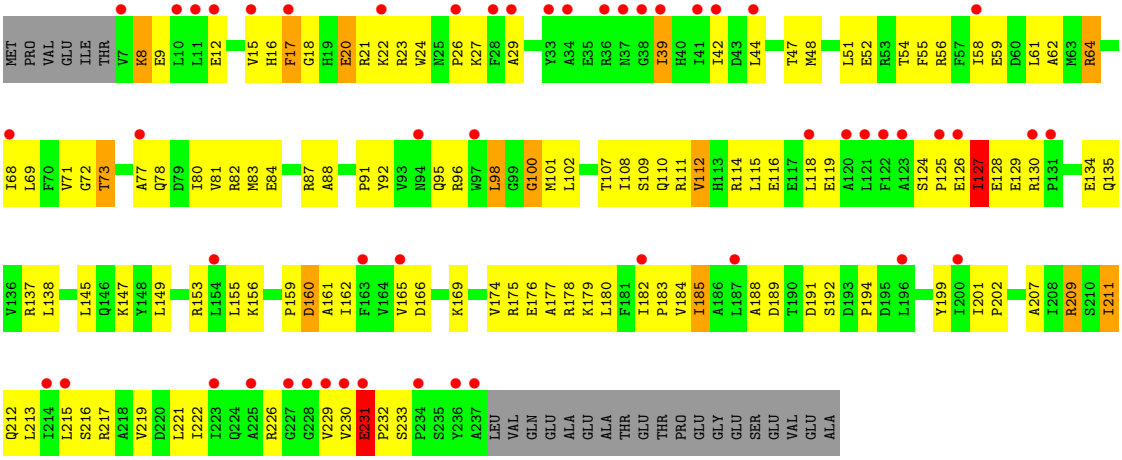



C175 C176 C177 C178 A179 U180 G181 U182 C189B C189C C189D U189E U189F G189G G189H U189K G189L U192 A195 C201 U202 U203 U204 G216 G220 C224 C225 U229 G230 G231 G232 C233 C234 C237 G238 C241 U244 C245 A246 G247 G251 G255 U256 G257 G258 G259 G260
U261 A262 A263 G266 C267 A270 C271 A279 C280 G281 A282 G286 U287 A288 G289 G293 U294 G297 A298 G299 A300 G301 G306 C307 C308 G309 G310 C311 C312 A313 G316 A321 C322 U323 G324 A327 C328 A329 G332 C335 C336 C337 A338 C339 C342 C345
G350 G351 C352 A353 G354 U359 A360 C366 U367 C372 A373 G377 C381 A382 A383 G384 C385 C386 U387 G388 A389 C390 G391 G392 G396 A397 C398 G399 C400 C401 U404 U405 G406 C407 A408 A411 A412 G413 A414 A415 G416 U421 C422 G423 G424 G425 G426 U427 G428 U429
A430 U434 C435 C436 U437 G438 A439 A441 C442 C443 C444 G445 G446 C449 G450 A451 A452 C457 C458 G460 A461 C470 G471 G474 G475 A482 C483 G484 G485 G490 G491 G492 G493 U494 A495 A496 U498 A499 G500 C501 G502 C503 C504 G505 C508 A509 A510 C511 U512 C513 C514 G515 U516
G517 C518 C519 G524 C525 C526 G527 U531 A532 A533 U534 A535 C536 G537 G538 A539 G540 G541 G542 C543 C544 C545 G546 A547 G548 U551 U552 G557 G558 A559 U560 U561 C562 A563 C564 U565 G566 A572 A573 G576 G577 U582 G587 G592 G593 C596 C600 C601 A602
U603 G604 U605 A608 A609 G610 A611 C612 C613 A614 C615 G616 C620 A621 C624 G625 G630 G631 A632 G633 C634 G639 A642 U646 C647 C651 U652 A653 C656 G657 G658 U659 G660 G661 G662 A663 G664 A665 G674 U677 A684 G685 U686 A687 G688 C689 G690 G691
U692 G693 A694 A695 A696 G703 A704 U705 A706 C707 C708 A712 G713 G718 G721 A722 U723 G724 G725 A729 G730 G731 A737 C738 G742 U743 C744 C745 C748 C749 A753 C754 G755 C756 U757 G758 G763 A766 A767 A768 G769 C770 G773 G774 G775 G776 A777 G778
A781 A782 C783 C784 G785 G786 G791 A792 U793 A794 C797 G803 C811 C812 U813 A814 A815 A816 C817 G821 C824 G825 G826 U827 A828 G829 G830 U831 C832 G836 C840 U841 C848 G851 G854 G858 A859 C868 G869 G874 C875 G881 C882 C883
G887 G890 U891 A901 G902 G903 G906 A914 A915 G916 U920 U921 G922 A923 C924 G925 G926 G927 C930 C931 C932 G933 C934 A935 C936 A937 A938 G939 C940 G941 G942 U943 G944 G947 U950 G951 U952 G953 G954 U960 U961 A964 A965 G966 C967 A968 A969 C970 G971 C972
G973 A974 A975 G976 A977 A978 C979 C980 U981 U982 A983 C984 C985 A986 G987 G988 G989 C990 U991 U992 G993 A994 C995 A996 C999 U1000 A1001 G1001A G1002 G1003 A1004 A1005 C1006 C1007 C1008 G1009 G1010 G1011 U1012 G1013 A1014 A1015 A1016 G1017 U1020 G1021 G1022 G1023 G1024 U1025 G1026 C1027 C1028 C1029 C1030 G1030A C1030B C1030C
A1030D G1031 G1032 G1033 G1034 A1035 G1036 C1037 C1038 C1039 U1040 A1041 G1042 C1043 A1044 C1045 G1048 U1049 G1050 C1051 U1052 G1053 C1054 A1055 U1056 G1057 G1058 C1059 C1060 G1061 U1062 C1063 G1064 U1065 C1066 A1067 G1068 C1071 G1072 U1073 G1074 C1075 C1076 G1077 U1078 G1079 A1080 G1081 G1084 U1085 U1086 U1090 U1091 G1094 U1095
C1096 C1097 C1098 G1099 C1100 A1101 A1102 C1103 G1104 C1113 C1114 C1115 C1116 G1117 C1118 C1119 C1120 U1121 U1122 A1123 G1124 G1125 U1126 G1127 C1128 C1129 A1130 G1133 G1134 U1135 U1136 C1137 G1138 G1139 C1140 C1141 G1142 G1143 G1144 C1147 U1148 C1149 U1150 A1151 A1152 A1157 C1158 U1159 G1160 C1161 C1162 C1163 G1164 C1165 G1166 A1168
A1169 C1172 G1173 G1177 G1178 A1179 A1180 G1181 G1182 A1183 G1184 G1185 G1186 G1187 A1188 C1189 G1190 A1191 C1192 G1193 U1194 C1195 U1196 G1197 C1203 A1204 U1205 G1206 G1207 C1208 C1209 C1210 U1211 U1212 A1213 C1214 G1215 G1216 C1217 C1218 U1219 G1222 C1223 G1224 A1225 C1226 A1227 C1230 G1231 U1232 U1235 A1236 C1237 A1238
A1239 U1240 G1241 C1244 A1245 C1246 U1247 A1250 G1253 C1254 G1255 A1256 U1257 G1258 C1259 C1260 G1266 A1269 C1270 G1274 A1275 G1276 C1277 U1278 A1279 A1280 U1281 C1282 G1283 C1284 A1285 A1286 A1287 A1288 A1289 G1290 G1291 U1292 G1295 C1296 C1297 C1298 A1299 G1300 U1301 U1302 C1303 G1304 G1305 A1306 U1307 U1308 G1309



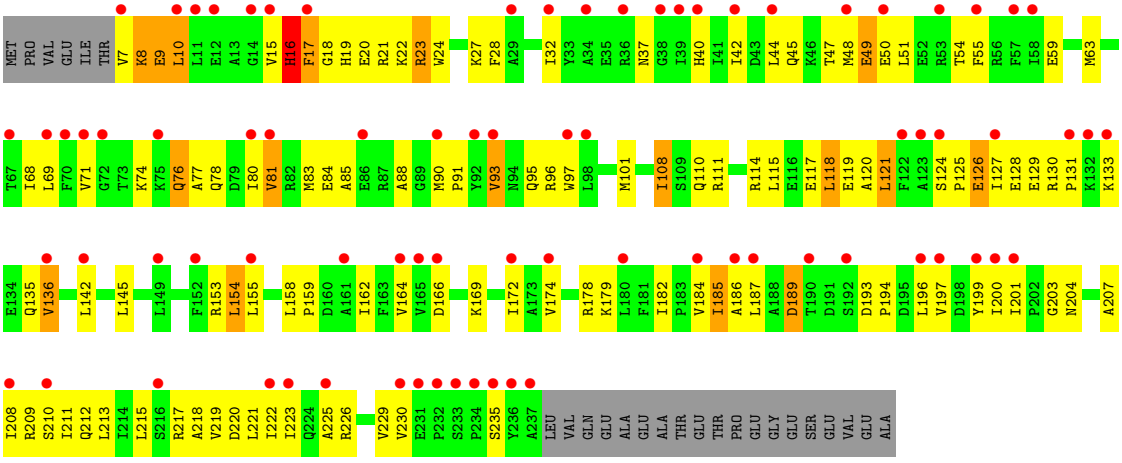
- Molecule 33: 30S ribosomal protein S2

Chain 1b:



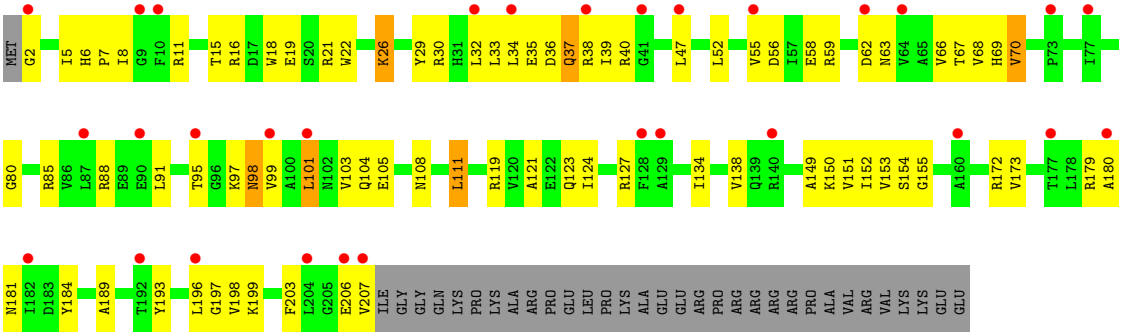
- Molecule 33: 30S ribosomal protein S2

Chain 2b:



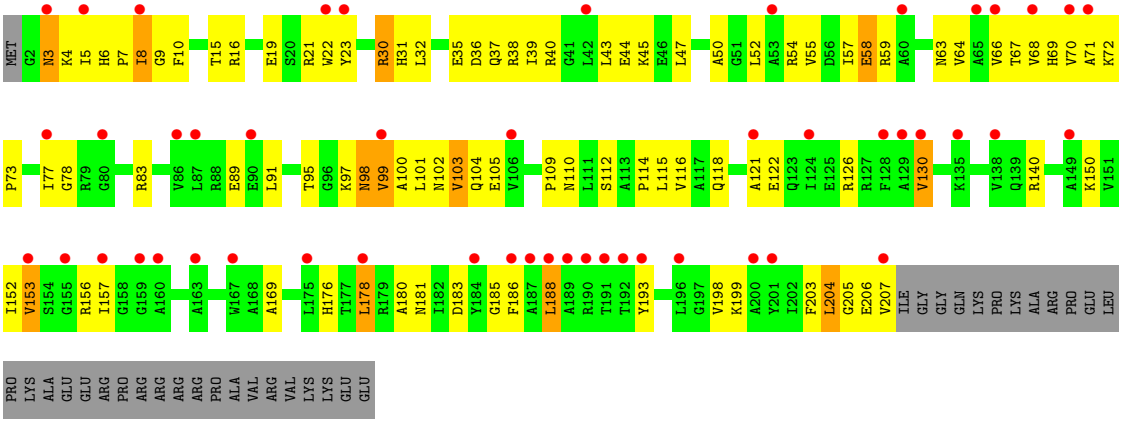
- Molecule 34: 30S ribosomal protein S3

Chain 1c:



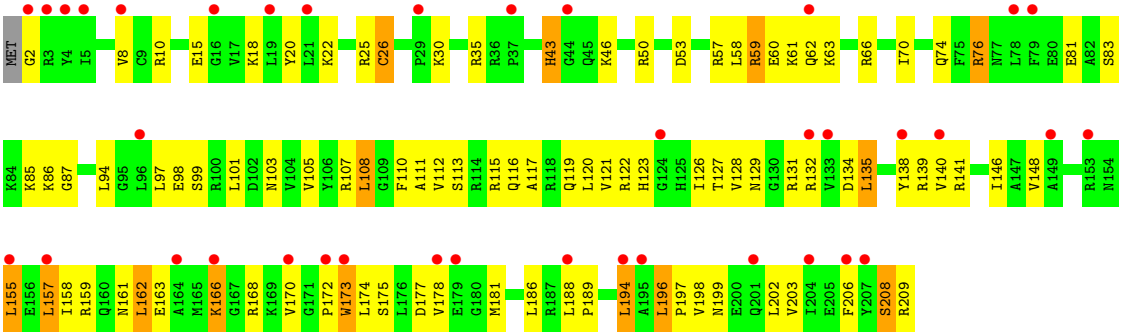
- Molecule 34: 30S ribosomal protein S3

Chain 2c:



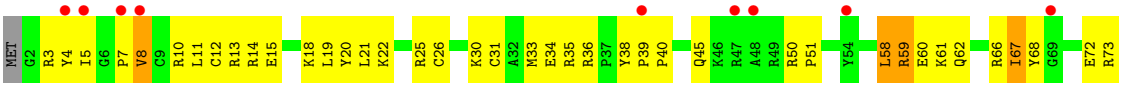
- Molecule 35: 30S ribosomal protein S4

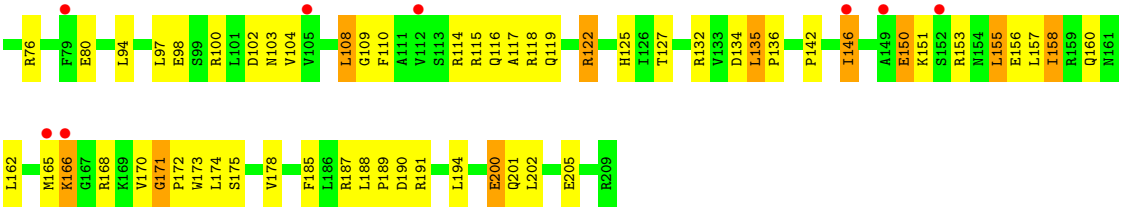
Chain 1d:



- Molecule 35: 30S ribosomal protein S4

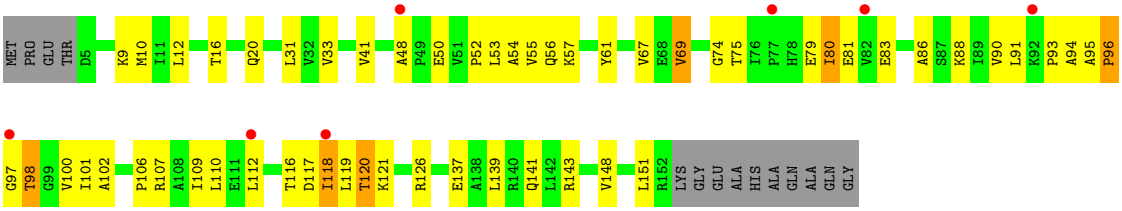
Chain 2d:





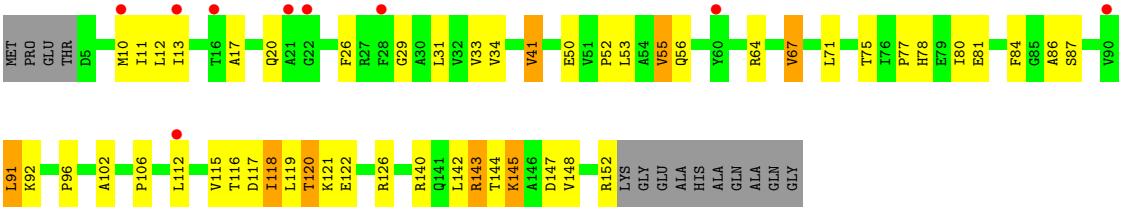
- Molecule 36: 30S ribosomal protein S5

Chain 1e:



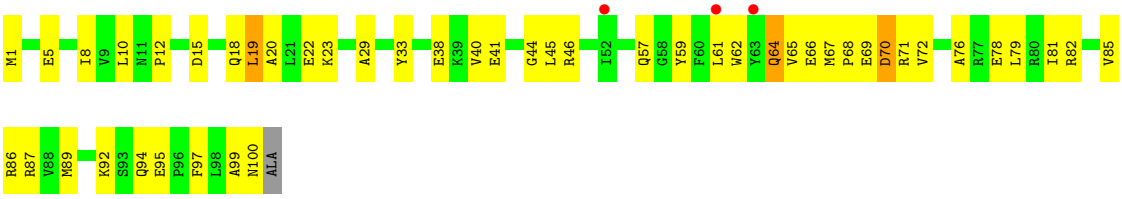
- Molecule 36: 30S ribosomal protein S5

Chain 2e:



- Molecule 37: 30S ribosomal protein S6

Chain 1f:

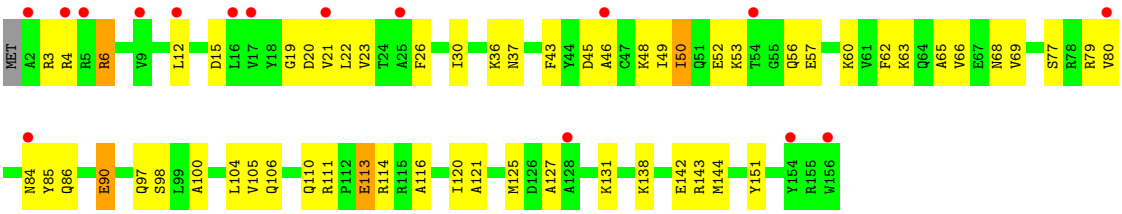


- Molecule 37: 30S ribosomal protein S6

Chain 2f:

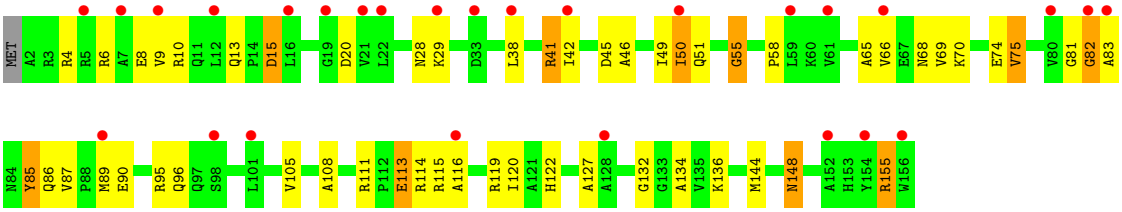
- Molecule 38: 30S ribosomal protein S7

Chain 1g:



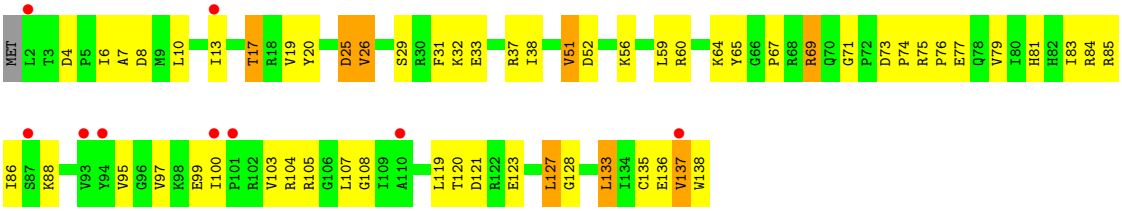
- Molecule 38: 30S ribosomal protein S7

Chain 2g:



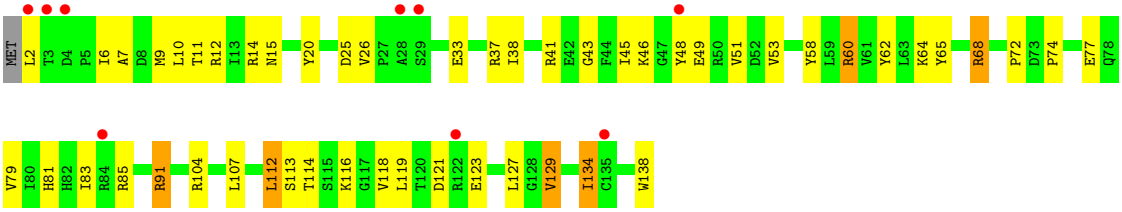
- Molecule 39: 30S ribosomal protein S8

Chain 1h:



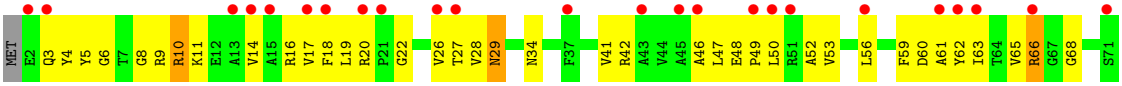
- Molecule 39: 30S ribosomal protein S8

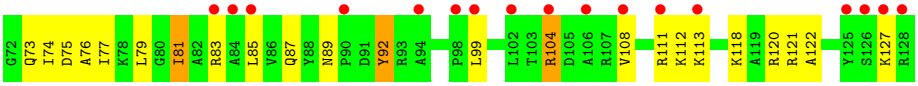
Chain 2h:



- Molecule 40: 30S ribosomal protein S9

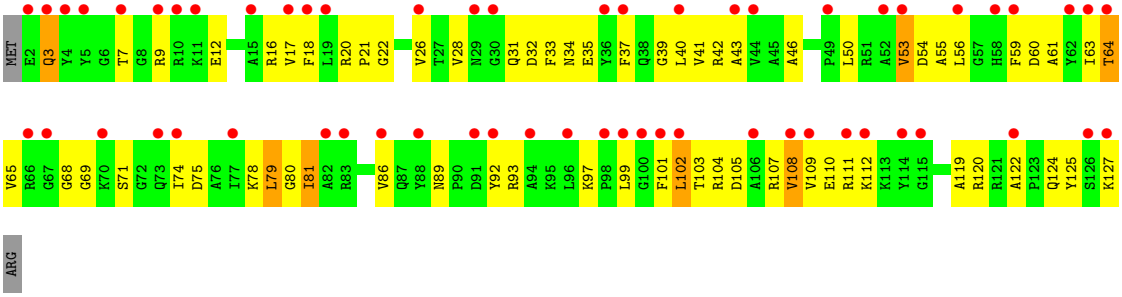
Chain 1i:





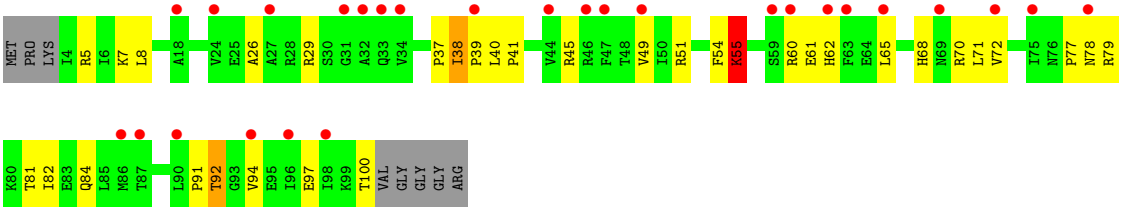
• Molecule 40: 30S ribosomal protein S9

Chain 2i:



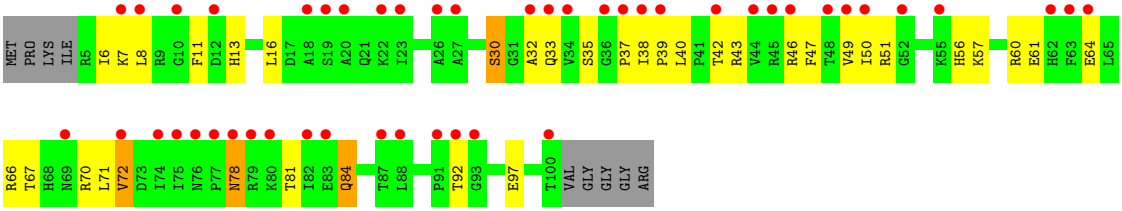
• Molecule 41: 30S ribosomal protein S10

Chain 1j:



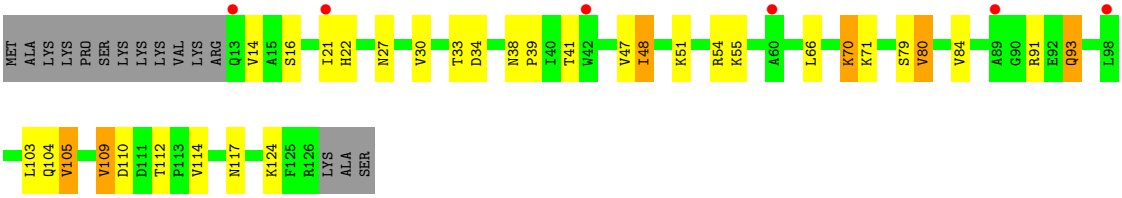
• Molecule 41: 30S ribosomal protein S10

Chain 2j:



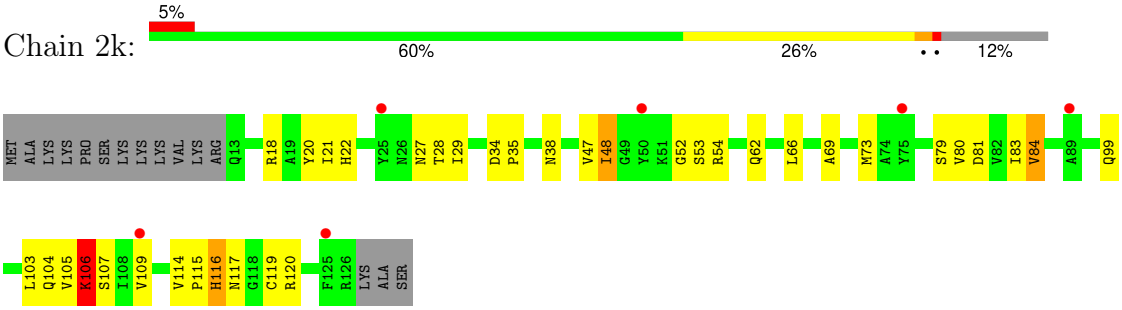
• Molecule 42: 30S ribosomal protein S11

Chain 1k:



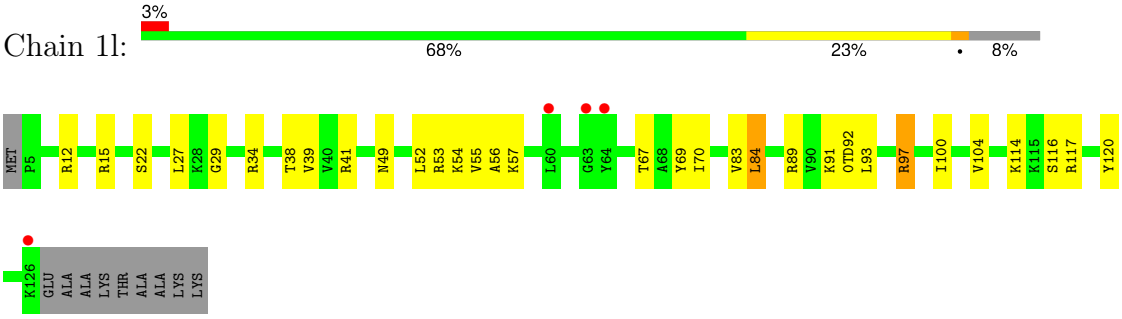
- Molecule 42: 30S ribosomal protein S11

Chain 2k:



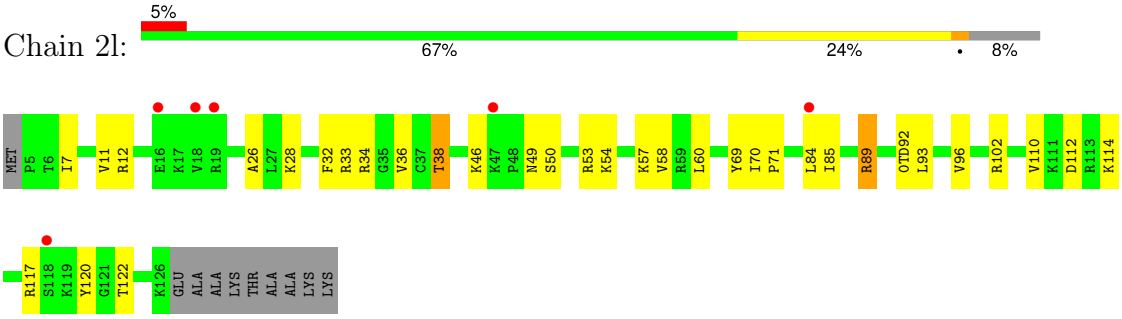
- Molecule 43: 30S ribosomal protein S12

Chain 1l:



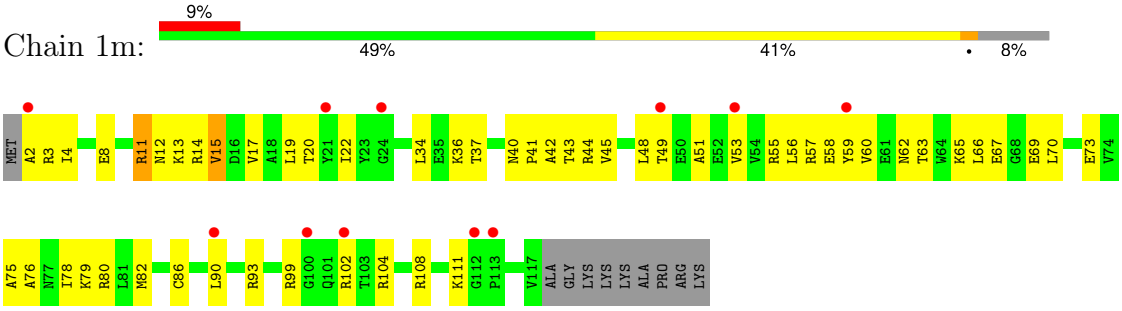
- Molecule 43: 30S ribosomal protein S12

Chain 2l:



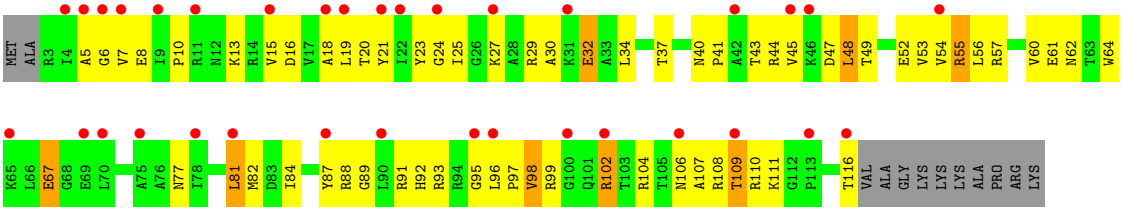
- Molecule 44: 30S ribosomal protein S13

Chain 1m:



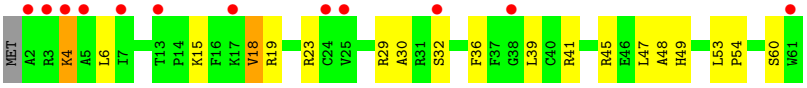
- Molecule 44: 30S ribosomal protein S13

Chain 2m:



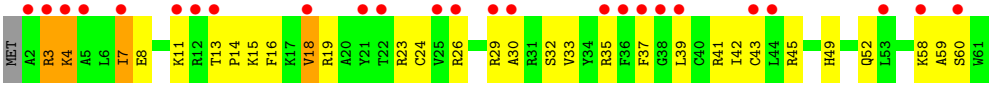
• Molecule 45: 30S ribosomal protein S14 type Z

Chain 1n:



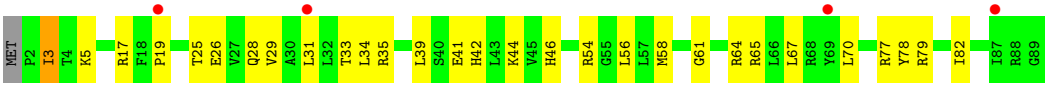
• Molecule 45: 30S ribosomal protein S14 type Z

Chain 2n:



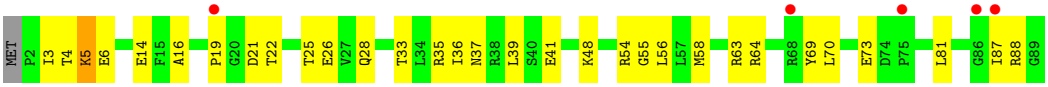
• Molecule 46: 30S ribosomal protein S15

Chain 1o:



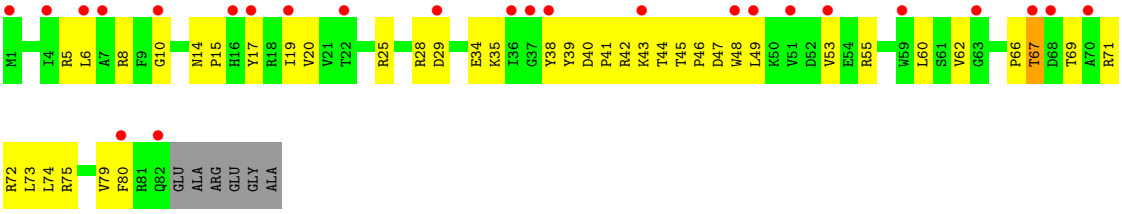
• Molecule 46: 30S ribosomal protein S15

Chain 2o:



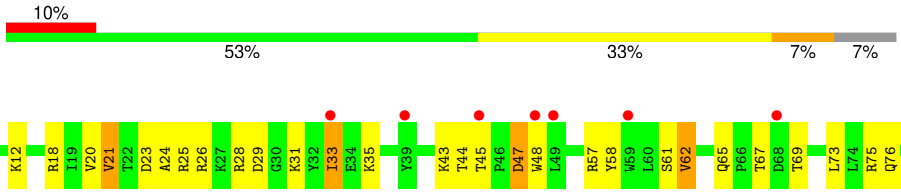
• Molecule 47: 30S ribosomal protein S16

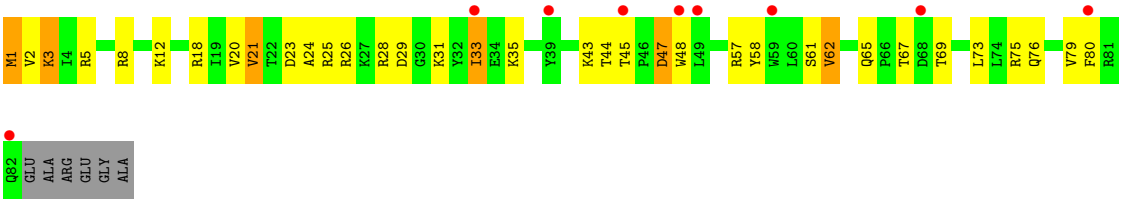
Chain 1p:



• Molecule 47: 30S ribosomal protein S16

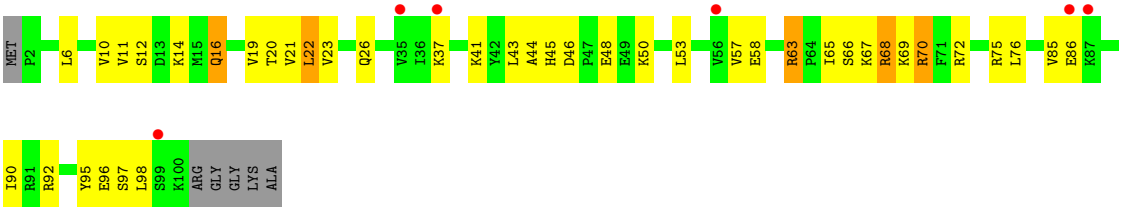
Chain 2p:





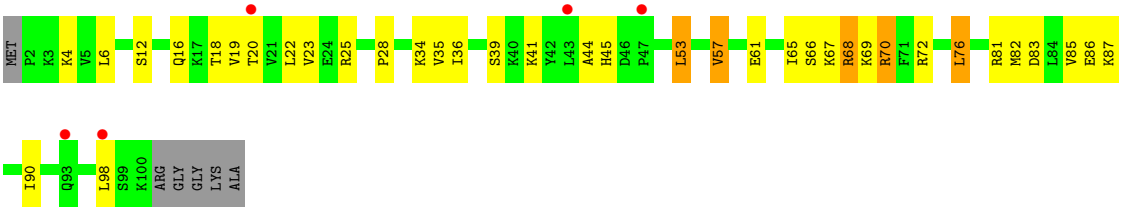
- Molecule 48: 30S ribosomal protein S17

Chain 1q:



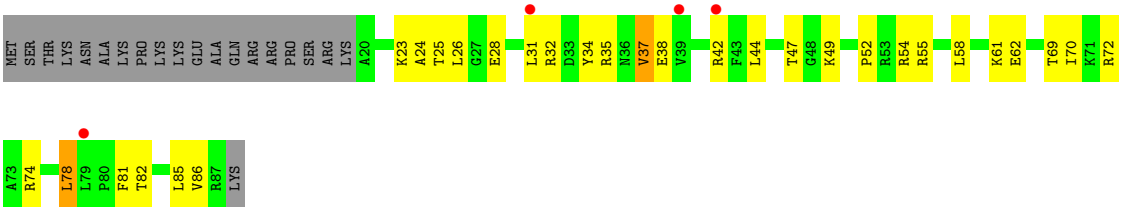
- Molecule 48: 30S ribosomal protein S17

Chain 2q:



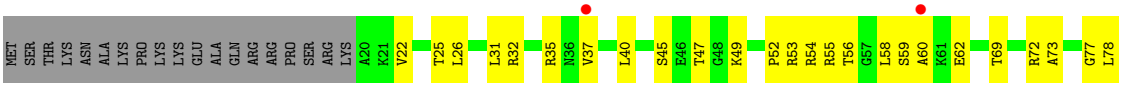
- Molecule 49: 30S ribosomal protein S18

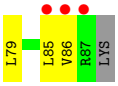
Chain 1r:



- Molecule 49: 30S ribosomal protein S18

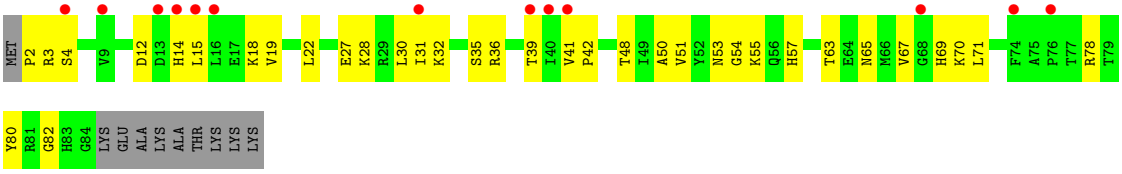
Chain 2r:





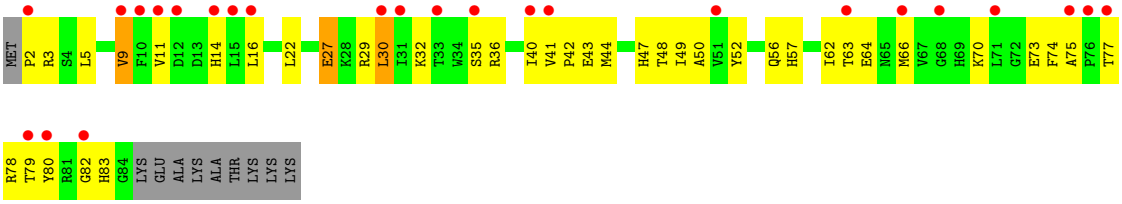
- Molecule 50: 30S ribosomal protein S19

Chain 1s:



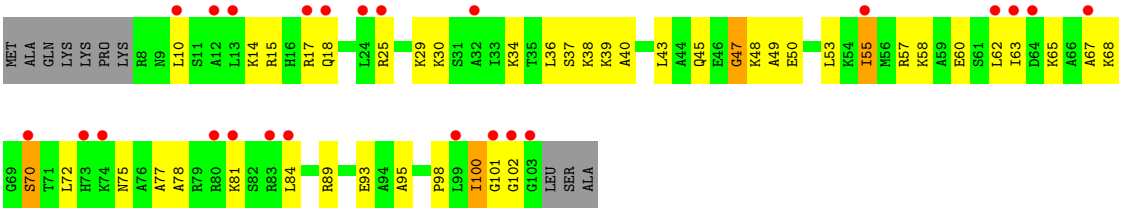
- Molecule 50: 30S ribosomal protein S19

Chain 2s:



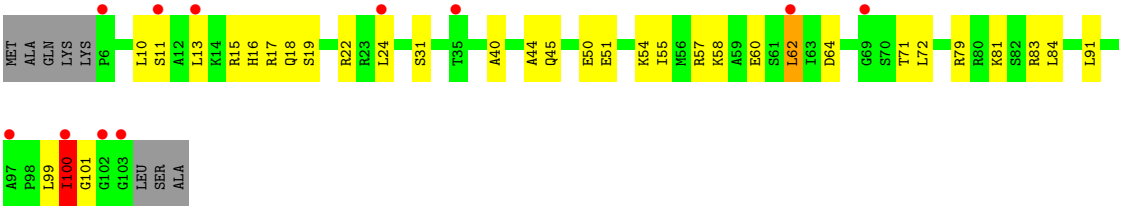
- Molecule 51: 30S ribosomal protein S20

Chain 1t:



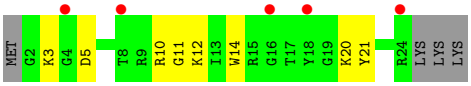
- Molecule 51: 30S ribosomal protein S20

Chain 2t:



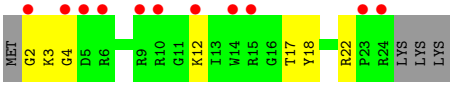
- Molecule 52: 30S ribosomal protein Thx

Chain 1u:



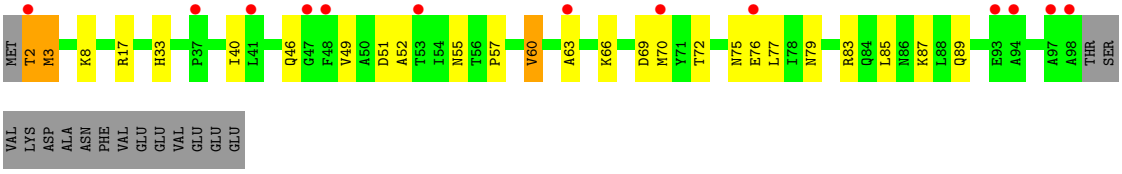
• Molecule 52: 30S ribosomal protein Thx

Chain 2u:



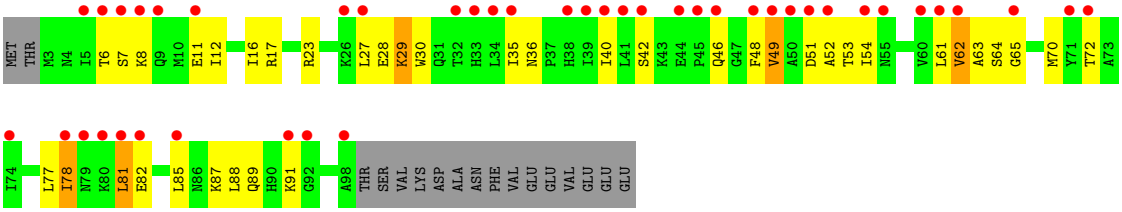
• Molecule 53: Ribosome-associated inhibitor A

Chain 1y:



• Molecule 53: Ribosome-associated inhibitor A

Chain 2y:



• Molecule 54: A-site Aminoacyl-tRNA Analog

Chain 1w:

• Molecule 54: A-site Aminoacyl-tRNA Analog

Chain 2w:

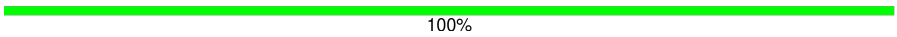
• Molecule 55: P-site Peptidyl-tRNA Analog RNA

Chain 1x:

• Molecule 55: P-site Peptidyl-tRNA Analog RNA

Chain 2x:

• Molecule 56: P-site Peptidyl-tRNA Analog Peptide

Chain 1v: 

There are no outlier residues recorded for this chain.

• Molecule 56: P-site Peptidyl-tRNA Analog Peptide

Chain 2v:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	209.64Å 448.67Å 619.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	181.72 – 2.40 181.72 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.7 (181.72-2.40) 99.7 (181.72-2.40)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.16 (at 2.40Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.239 , 0.289 0.241 , 0.290	Depositor DCC
R_{free} test set	112220 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	44.8	Xtriage
Anisotropy	0.085	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 58.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.33$, $< L^2 > = 0.16$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	297986	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.64% 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: 2MA, OMU, MA6, M2G, 0TD, PPU, UR3, PSU, SF4, 2MG, MG, G7M, 5MU, 4OC, 5MC, OMC, OMG, ZN, 8AN, MPD, MRD

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	0.30	0/69031	0.50	2/107754 (0.0%)
1	2A	0.23	0/68903	0.42	1/107552 (0.0%)
2	1B	0.25	0/2876	0.45	0/4486
2	2B	0.19	0/2878	0.37	0/4490
3	1D	0.28	0/2181	0.53	0/2940
3	2D	0.23	0/2186	0.49	0/2944
4	1E	0.27	0/1592	0.53	0/2149
4	2E	0.23	0/1592	0.46	0/2149
5	1F	0.28	0/1619	0.50	0/2193
5	2F	0.22	0/1615	0.49	3/2188 (0.1%)
6	1G	0.22	0/1451	0.45	0/1961
6	2G	0.20	0/1449	0.44	0/1957
7	1H	0.23	0/1356	0.45	0/1834
7	2H	0.21	0/1350	0.43	0/1826
8	1I	0.20	0/1109	0.43	0/1512
8	2I	0.19	0/1091	0.41	0/1490
9	1N	0.27	0/1148	0.49	0/1547
9	2N	0.20	0/1144	0.42	0/1543
10	1O	0.25	0/943	0.47	0/1269
10	2O	0.23	0/943	0.44	0/1269
11	1P	0.28	0/1152	0.52	0/1533
11	2P	0.20	0/1152	0.49	0/1533
12	1Q	0.26	0/1143	0.49	0/1527
12	2Q	0.21	0/1143	0.42	0/1527
13	1R	0.30	0/982	0.52	0/1312
13	2R	0.22	0/982	0.44	0/1312
14	1S	0.24	0/887	0.49	0/1180
14	2S	0.21	0/880	0.49	0/1172
15	1T	0.28	0/1105	0.54	0/1477
15	2T	0.22	0/1097	0.47	0/1468
16	1U	0.31	0/977	0.54	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
16	2U	0.21	0/977	0.43	0/1301
17	1V	0.30	0/786	0.53	0/1053
17	2V	0.23	0/782	0.48	0/1049
18	1W	0.30	0/897	0.49	0/1205
18	2W	0.23	0/897	0.44	0/1205
19	1X	0.26	0/764	0.51	0/1025
19	2X	0.21	0/764	0.44	0/1025
20	1Y	0.25	0/823	0.53	0/1099
20	2Y	0.21	0/823	0.40	0/1100
21	1Z	0.25	0/1620	0.52	0/2200
21	2Z	0.22	0/1590	0.47	0/2162
22	10	0.29	0/662	0.53	0/881
22	20	0.23	0/659	0.53	0/877
23	11	0.25	0/761	0.48	0/1013
23	21	0.24	0/766	0.44	0/1018
24	12	0.24	0/590	0.46	0/781
24	22	0.21	0/594	0.43	0/785
25	13	0.31	0/474	0.52	0/635
25	23	0.21	0/469	0.44	0/630
26	14	0.26	0/559	0.66	2/754 (0.3%)
26	24	0.30	0/549	0.71	3/741 (0.4%)
27	15	0.33	0/473	0.55	0/639
27	25	0.23	0/469	0.52	0/635
28	16	0.27	0/460	0.50	0/613
28	26	0.22	0/456	0.43	0/608
29	17	0.34	0/426	0.60	0/561
29	27	0.24	0/426	0.47	0/561
30	18	0.30	0/525	0.50	0/691
30	28	0.21	0/525	0.40	0/691
31	19	0.29	0/310	0.50	0/407
31	29	0.20	0/310	0.44	0/407
32	1a	0.21	0/35795	0.40	0/55864
32	2a	0.20	1/35890 (0.0%)	0.39	0/56012
33	1b	0.24	0/1876	0.53	1/2533 (0.0%)
33	2b	0.23	0/1860	0.54	2/2518 (0.1%)
34	1c	0.21	0/1582	0.43	0/2137
34	2c	0.23	0/1566	0.45	0/2119
35	1d	0.20	0/1695	0.46	0/2274
35	2d	0.19	0/1698	0.44	0/2277
36	1e	0.20	0/1149	0.44	0/1548
36	2e	0.20	0/1149	0.45	0/1548
37	1f	0.20	0/827	0.41	0/1120
37	2f	0.20	0/829	0.44	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
38	1g	0.20	0/1254	0.40	0/1683
38	2g	0.18	0/1248	0.40	0/1676
39	1h	0.20	0/1118	0.41	0/1506
39	2h	0.19	0/1108	0.43	0/1494
40	1i	0.19	0/1005	0.46	0/1351
40	2i	0.21	0/985	0.47	0/1329
41	1j	0.20	0/732	0.48	1/993 (0.1%)
41	2j	0.22	0/723	0.49	0/984
42	1k	0.21	0/849	0.46	0/1150
42	2k	0.20	0/848	0.49	0/1149
43	1l	0.21	0/937	0.43	0/1260
43	2l	0.21	0/937	0.44	0/1260
44	1m	0.21	0/924	0.49	0/1242
44	2m	0.25	0/905	0.55	0/1217
45	1n	0.22	0/501	0.46	0/664
45	2n	0.21	0/501	0.45	0/664
46	1o	0.19	0/739	0.38	0/985
46	2o	0.19	0/739	0.40	0/985
47	1p	0.20	0/697	0.44	0/939
47	2p	0.22	0/693	0.51	0/935
48	1q	0.20	0/836	0.44	0/1117
48	2q	0.19	0/836	0.48	0/1117
49	1r	0.20	0/560	0.41	0/746
49	2r	0.20	0/560	0.44	0/746
50	1s	0.20	0/663	0.47	0/895
50	2s	0.21	0/660	0.46	0/893
51	1t	0.20	0/734	0.46	0/969
51	2t	0.20	0/736	0.41	0/976
52	1u	0.23	0/203	0.44	0/266
52	2u	0.20	0/203	0.42	0/266
53	1y	0.22	0/776	0.39	0/1048
53	2y	0.20	0/761	0.42	0/1030
54	1w	0.24	0/44	0.58	0/67
54	2w	0.21	0/44	0.45	0/67
55	1x	0.36	0/44	0.62	0/67
55	2x	0.22	0/44	0.53	0/67
56	1v	0.32	0/22	0.42	0/28
56	2v	0.30	0/22	0.37	0/28
All	All	0.24	1/310250 (0.0%)	0.45	15/463679 (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
21	2Z	0	1
26	14	0	1
33	1b	0	2
33	2b	0	1
All	All	0	5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	2a	1498	UR3	O3'-P	5.26	1.61	1.56

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1A	1042	G	OP1-P-O3'	-9.05	80.86	108.00
26	24	65	ASP	N-CA-C	-7.46	102.38	113.72
1	1A	1042	G	OP2-P-O3'	-6.62	88.14	108.00
33	2b	23	ARG	N-CA-C	-6.51	105.21	112.57
5	2F	121	GLY	N-CA-C	-6.32	107.05	115.40

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
26	14	52	THR	Peptide
33	1b	127	ILE	Peptide
33	1b	231	GLU	Peptide
21	2Z	136	PHE	Peptide
33	2b	126	GLU	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	61869	0	31206	853	0
1	2A	61758	0	31149	979	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	1B	2572	0	1305	39	0
2	2B	2573	0	1306	33	0
3	1D	2131	0	2207	71	0
3	2D	2136	0	2218	51	0
4	1E	1559	0	1618	32	0
4	2E	1559	0	1618	51	0
5	1F	1584	0	1625	42	0
5	2F	1580	0	1619	65	0
6	1G	1426	0	1445	54	0
6	2G	1424	0	1441	57	0
7	1H	1330	0	1407	34	0
7	2H	1324	0	1402	49	0
8	1I	1094	0	1127	30	0
8	2I	1076	0	1094	30	0
9	1N	1121	0	1193	27	0
9	2N	1117	0	1184	24	0
10	1O	933	0	996	27	0
10	2O	933	0	996	30	0
11	1P	1135	0	1212	37	0
11	2P	1135	0	1212	34	0
12	1Q	1122	0	1179	25	0
12	2Q	1122	0	1179	38	0
13	1R	968	0	1033	29	0
13	2R	968	0	1033	27	0
14	1S	877	0	938	27	0
14	2S	870	0	923	30	0
15	1T	1091	0	1151	29	0
15	2T	1083	0	1136	23	0
16	1U	959	0	1019	20	0
16	2U	959	0	1019	28	0
17	1V	775	0	841	18	0
17	2V	771	0	830	18	0
18	1W	886	0	940	19	0
18	2W	886	0	940	17	0
19	1X	750	0	814	27	0
19	2X	750	0	814	23	0
20	1Y	810	0	892	19	0
20	2Y	810	0	887	26	0
21	1Z	1587	0	1598	45	0
21	2Z	1557	0	1564	52	0
22	10	653	0	674	13	0
22	20	650	0	665	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	11	754	0	823	23	0
23	21	759	0	837	29	0
24	12	588	0	643	16	0
24	22	592	0	654	13	0
25	13	469	0	518	9	0
25	23	464	0	514	20	0
26	14	546	0	522	22	0
26	24	536	0	514	35	0
27	15	459	0	476	15	0
27	25	455	0	465	12	0
28	16	453	0	473	9	0
28	26	449	0	469	15	0
29	17	418	0	467	9	0
29	27	418	0	466	12	0
30	18	517	0	582	23	0
30	28	517	0	582	17	0
31	19	307	0	335	5	0
31	29	307	0	335	16	0
32	1a	32246	0	16293	582	0
32	2a	32331	0	16338	597	0
33	1b	1842	0	1862	92	0
33	2b	1825	0	1828	81	0
34	1c	1558	0	1557	57	0
34	2c	1542	0	1517	62	0
35	1d	1665	0	1687	76	0
35	2d	1668	0	1703	87	0
36	1e	1133	0	1191	37	0
36	2e	1133	0	1191	33	0
37	1f	814	0	808	30	0
37	2f	816	0	808	23	0
38	1g	1235	0	1249	43	0
38	2g	1229	0	1238	44	0
39	1h	1098	0	1143	43	0
39	2h	1088	0	1126	36	0
40	1i	986	0	990	51	0
40	2i	966	0	953	53	0
41	1j	719	0	672	21	0
41	2j	710	0	661	31	0
42	1k	834	0	838	19	0
42	2k	833	0	836	29	0
43	1l	932	0	980	19	0
43	2l	932	0	981	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	1m	914	0	954	41	0
44	2m	895	0	920	50	0
45	1n	492	0	529	20	0
45	2n	492	0	529	27	0
46	1o	728	0	760	18	0
46	2o	728	0	760	20	0
47	1p	681	0	697	31	0
47	2p	677	0	686	24	0
48	1q	823	0	891	25	0
48	2q	823	0	891	30	0
49	1r	555	0	618	24	0
49	2r	555	0	618	21	0
50	1s	648	0	658	24	0
50	2s	645	0	635	29	0
51	1t	732	0	809	26	0
51	2t	733	0	795	20	0
52	1u	199	0	208	7	0
52	2u	199	0	208	6	0
53	1y	764	0	786	25	0
53	2y	749	0	757	29	0
54	1w	78	0	50	3	0
54	2w	78	0	50	4	0
55	1x	63	0	33	2	0
55	2x	63	0	33	2	0
56	1v	23	0	29	0	0
56	2v	23	0	29	1	0
57	10	8	0	0	0	0
57	11	5	0	0	0	0
57	13	3	0	0	0	0
57	15	8	0	0	0	0
57	17	5	0	0	0	0
57	18	3	0	0	0	0
57	19	3	0	0	0	0
57	1A	1028	0	0	0	0
57	1B	30	0	0	0	0
57	1D	18	0	0	0	0
57	1E	10	0	0	0	0
57	1F	16	0	0	0	0
57	1G	4	0	0	0	0
57	1H	2	0	0	0	0
57	1N	4	0	0	0	0
57	1O	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	1P	4	0	0	0	0
57	1Q	5	0	0	0	0
57	1R	4	0	0	0	0
57	1T	4	0	0	0	0
57	1U	8	0	0	0	0
57	1V	7	0	0	0	0
57	1W	2	0	0	0	0
57	1X	1	0	0	0	0
57	1Z	1	0	0	0	0
57	1a	280	0	0	0	0
57	1b	1	0	0	0	0
57	1d	6	0	0	0	0
57	1e	3	0	0	0	0
57	1f	2	0	0	0	0
57	1g	2	0	0	0	0
57	1h	2	0	0	0	0
57	1i	1	0	0	0	0
57	1l	2	0	0	0	0
57	1m	1	0	0	0	0
57	1n	1	0	0	0	0
57	1o	2	0	0	0	0
57	1t	2	0	0	0	0
57	1w	1	0	0	0	0
57	1x	2	0	0	0	0
57	1y	3	0	0	0	0
57	20	2	0	0	0	0
57	21	1	0	0	0	0
57	23	1	0	0	0	0
57	25	3	0	0	0	0
57	26	1	0	0	0	0
57	27	1	0	0	0	0
57	28	1	0	0	0	0
57	2A	737	0	0	0	0
57	2B	20	0	0	0	0
57	2D	11	0	0	0	0
57	2E	6	0	0	0	0
57	2F	4	0	0	0	0
57	2G	2	0	0	0	0
57	2I	1	0	0	0	0
57	2N	1	0	0	0	0
57	2O	1	0	0	0	0
57	2P	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	2Q	4	0	0	0	0
57	2R	3	0	0	0	0
57	2T	4	0	0	0	0
57	2U	1	0	0	0	0
57	2V	3	0	0	0	0
57	2W	2	0	0	0	0
57	2Y	1	0	0	0	0
57	2a	191	0	0	0	0
57	2e	2	0	0	0	0
57	2f	1	0	0	0	0
57	2h	1	0	0	0	0
57	2j	1	0	0	0	0
57	2k	2	0	0	0	0
57	2p	1	0	0	0	0
57	2r	1	0	0	0	0
57	2t	1	0	0	0	0
57	2x	1	0	0	0	0
58	18	8	0	14	2	0
58	1A	8	0	14	1	0
58	1T	8	0	14	1	0
58	1a	8	0	14	2	0
58	2A	8	0	14	0	0
58	2B	8	0	14	0	0
59	1B	12	0	12	4	0
59	1F	12	0	12	2	0
60	14	1	0	0	0	0
60	15	1	0	0	0	0
60	16	1	0	0	0	0
60	19	1	0	0	0	0
60	1Y	1	0	0	0	0
60	1n	1	0	0	0	0
60	24	1	0	0	0	0
60	25	1	0	0	0	0
60	26	1	0	0	0	0
60	29	1	0	0	0	0
60	2Y	1	0	0	0	0
60	2n	1	0	0	0	0
61	1d	8	0	0	0	0
61	2d	8	0	0	1	0
62	2A	8	0	14	0	0
63	10	24	0	0	1	0
63	11	27	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
63	12	18	0	0	4	0
63	13	24	0	0	1	0
63	14	3	0	0	0	0
63	15	24	0	0	3	0
63	16	18	0	0	2	0
63	17	12	0	0	1	0
63	18	27	0	0	1	0
63	19	6	0	0	1	0
63	1A	3988	0	0	192	0
63	1B	97	0	0	8	0
63	1D	113	0	0	9	0
63	1E	76	0	0	4	0
63	1F	67	0	0	5	0
63	1G	19	0	0	0	0
63	1H	11	0	0	0	0
63	1I	8	0	0	0	0
63	1N	52	0	0	4	0
63	1O	22	0	0	0	0
63	1P	66	0	0	3	0
63	1Q	36	0	0	3	0
63	1R	32	0	0	2	0
63	1S	12	0	0	2	0
63	1T	34	0	0	3	0
63	1U	47	0	0	5	0
63	1V	40	0	0	6	0
63	1W	33	0	0	2	0
63	1X	26	0	0	4	0
63	1Y	16	0	0	1	0
63	1Z	14	0	0	3	0
63	1a	511	0	0	45	0
63	1b	1	0	0	0	0
63	1d	8	0	0	2	0
63	1e	3	0	0	0	0
63	1f	2	0	0	0	0
63	1j	1	0	0	0	0
63	1k	1	0	0	1	0
63	1l	3	0	0	2	0
63	1m	1	0	0	0	0
63	1o	3	0	0	0	0
63	1p	2	0	0	0	0
63	1t	1	0	0	0	0
63	1w	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
63	1x	5	0	0	0	0
63	1y	7	0	0	0	0
63	20	14	0	0	0	0
63	21	20	0	0	1	0
63	22	3	0	0	0	0
63	23	4	0	0	2	0
63	24	2	0	0	2	0
63	25	9	0	0	1	0
63	26	5	0	0	1	0
63	27	9	0	0	0	0
63	28	12	0	0	2	0
63	29	1	0	0	0	0
63	2A	2224	0	0	191	0
63	2B	45	0	0	4	0
63	2D	50	0	0	3	0
63	2E	29	0	0	2	0
63	2F	22	0	0	1	0
63	2G	7	0	0	0	0
63	2H	2	0	0	0	0
63	2I	3	0	0	0	0
63	2N	2	0	0	1	0
63	2O	16	0	0	1	0
63	2P	25	0	0	3	0
63	2Q	16	0	0	3	0
63	2R	20	0	0	2	0
63	2S	5	0	0	1	0
63	2T	10	0	0	0	0
63	2U	12	0	0	2	0
63	2V	9	0	0	2	0
63	2W	23	0	0	1	0
63	2X	7	0	0	0	0
63	2Y	6	0	0	2	0
63	2Z	11	0	0	1	0
63	2a	384	0	0	29	0
63	2d	4	0	0	1	0
63	2e	2	0	0	0	0
63	2f	3	0	0	0	0
63	2j	2	0	0	0	0
63	2l	4	0	0	1	0
63	2m	1	0	0	0	0
63	2o	4	0	0	0	0
63	2p	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
63	2q	1	0	0	0	0
63	2r	3	0	0	0	0
63	2t	2	0	0	0	0
63	2u	1	0	0	0	0
63	2w	3	0	0	0	0
63	2x	3	0	0	1	0
63	2y	3	0	0	0	0
All	All	297986	0	194829	5395	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

The worst 5 of 5395 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)
32:2a:1003:G:H2'	32:2a:1004:A:H4'	1.38	1.05
1:1A:1063:G:H1	1:1A:1075:C:N4	1.60	1.00
32:2a:1129:C:N4	32:2a:1143:G:H1	1.59	0.99
1:1A:2096:U:H3	1:1A:2193:G:H1	1.09	0.99
1:1A:2319:G:H22	14:1S:3:ARG:HD3	1.27	0.98

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	1D	273/276 (99%)	254 (93%)	19 (7%)	0	100	100
3	2D	273/276 (99%)	259 (95%)	14 (5%)	0	100	100
4	1E	202/206 (98%)	189 (94%)	11 (5%)	2 (1%)	12	20
4	2E	202/206 (98%)	192 (95%)	8 (4%)	2 (1%)	12	20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	1F	201/210 (96%)	192 (96%)	8 (4%)	1 (0%)	24	37
5	2F	201/210 (96%)	189 (94%)	10 (5%)	2 (1%)	12	20
6	1G	179/182 (98%)	162 (90%)	12 (7%)	5 (3%)	4	3
6	2G	179/182 (98%)	153 (86%)	23 (13%)	3 (2%)	7	10
7	1H	172/180 (96%)	159 (92%)	11 (6%)	2 (1%)	10	16
7	2H	171/180 (95%)	150 (88%)	20 (12%)	1 (1%)	21	32
8	1I	145/148 (98%)	128 (88%)	17 (12%)	0	100	100
8	2I	144/148 (97%)	125 (87%)	18 (12%)	1 (1%)	18	28
9	1N	138/140 (99%)	131 (95%)	7 (5%)	0	100	100
9	2N	138/140 (99%)	127 (92%)	11 (8%)	0	100	100
10	1O	120/122 (98%)	112 (93%)	7 (6%)	1 (1%)	16	25
10	2O	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
11	1P	147/150 (98%)	138 (94%)	8 (5%)	1 (1%)	18	28
11	2P	147/150 (98%)	138 (94%)	8 (5%)	1 (1%)	18	28
12	1Q	139/141 (99%)	131 (94%)	7 (5%)	1 (1%)	18	28
12	2Q	139/141 (99%)	130 (94%)	9 (6%)	0	100	100
13	1R	116/118 (98%)	109 (94%)	7 (6%)	0	100	100
13	2R	116/118 (98%)	114 (98%)	2 (2%)	0	100	100
14	1S	108/112 (96%)	99 (92%)	8 (7%)	1 (1%)	14	22
14	2S	108/112 (96%)	98 (91%)	10 (9%)	0	100	100
15	1T	129/146 (88%)	121 (94%)	8 (6%)	0	100	100
15	2T	129/146 (88%)	121 (94%)	7 (5%)	1 (1%)	16	25
16	1U	114/118 (97%)	114 (100%)	0	0	100	100
16	2U	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
17	1V	99/101 (98%)	93 (94%)	6 (6%)	0	100	100
17	2V	99/101 (98%)	93 (94%)	5 (5%)	1 (1%)	12	20
18	1W	110/113 (97%)	107 (97%)	3 (3%)	0	100	100
18	2W	110/113 (97%)	108 (98%)	1 (1%)	1 (1%)	14	22
19	1X	93/96 (97%)	91 (98%)	1 (1%)	1 (1%)	11	18
19	2X	93/96 (97%)	87 (94%)	5 (5%)	1 (1%)	11	18
20	1Y	105/110 (96%)	97 (92%)	8 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	2Y	105/110 (96%)	97 (92%)	7 (7%)	1 (1%)	12	20
21	1Z	201/206 (98%)	186 (92%)	14 (7%)	1 (0%)	24	37
21	2Z	199/206 (97%)	169 (85%)	26 (13%)	4 (2%)	6	7
22	10	81/85 (95%)	78 (96%)	3 (4%)	0	100	100
22	20	81/85 (95%)	78 (96%)	2 (2%)	1 (1%)	10	16
23	11	95/98 (97%)	90 (95%)	4 (4%)	1 (1%)	11	18
23	21	95/98 (97%)	91 (96%)	3 (3%)	1 (1%)	11	18
24	12	68/72 (94%)	68 (100%)	0	0	100	100
24	22	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
25	13	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
25	23	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
26	14	67/71 (94%)	50 (75%)	12 (18%)	5 (8%)	1	0
26	24	67/71 (94%)	43 (64%)	18 (27%)	6 (9%)	0	0
27	15	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
27	25	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
28	16	51/54 (94%)	47 (92%)	4 (8%)	0	100	100
28	26	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
29	17	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
29	27	46/49 (94%)	46 (100%)	0	0	100	100
30	18	62/65 (95%)	61 (98%)	1 (2%)	0	100	100
30	28	62/65 (95%)	62 (100%)	0	0	100	100
31	19	35/37 (95%)	35 (100%)	0	0	100	100
31	29	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
33	1b	229/256 (90%)	193 (84%)	26 (11%)	10 (4%)	2	1
33	2b	229/256 (90%)	194 (85%)	31 (14%)	4 (2%)	7	10
34	1c	204/239 (85%)	179 (88%)	25 (12%)	0	100	100
34	2c	204/239 (85%)	171 (84%)	29 (14%)	4 (2%)	6	7
35	1d	206/209 (99%)	182 (88%)	23 (11%)	1 (0%)	24	37
35	2d	206/209 (99%)	188 (91%)	17 (8%)	1 (0%)	24	37
36	1e	146/162 (90%)	133 (91%)	11 (8%)	2 (1%)	9	13
36	2e	146/162 (90%)	138 (94%)	8 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	1f	98/101 (97%)	94 (96%)	4 (4%)	0	100	100
37	2f	98/101 (97%)	89 (91%)	9 (9%)	0	100	100
38	1g	153/156 (98%)	139 (91%)	14 (9%)	0	100	100
38	2g	153/156 (98%)	143 (94%)	7 (5%)	3 (2%)	6	7
39	1h	135/138 (98%)	130 (96%)	5 (4%)	0	100	100
39	2h	135/138 (98%)	122 (90%)	12 (9%)	1 (1%)	18	28
40	1i	125/128 (98%)	108 (86%)	13 (10%)	4 (3%)	3	3
40	2i	124/128 (97%)	102 (82%)	21 (17%)	1 (1%)	16	25
41	1j	95/105 (90%)	80 (84%)	9 (10%)	6 (6%)	1	0
41	2j	94/105 (90%)	81 (86%)	12 (13%)	1 (1%)	11	18
42	1k	112/129 (87%)	99 (88%)	12 (11%)	1 (1%)	14	22
42	2k	112/129 (87%)	102 (91%)	9 (8%)	1 (1%)	14	22
43	1l	119/132 (90%)	113 (95%)	6 (5%)	0	100	100
43	2l	119/132 (90%)	111 (93%)	8 (7%)	0	100	100
44	1m	114/126 (90%)	100 (88%)	11 (10%)	3 (3%)	4	4
44	2m	112/126 (89%)	93 (83%)	16 (14%)	3 (3%)	4	4
45	1n	58/61 (95%)	54 (93%)	4 (7%)	0	100	100
45	2n	58/61 (95%)	53 (91%)	4 (7%)	1 (2%)	7	10
46	1o	86/89 (97%)	81 (94%)	4 (5%)	1 (1%)	10	16
46	2o	86/89 (97%)	81 (94%)	4 (5%)	1 (1%)	10	16
47	1p	80/88 (91%)	72 (90%)	7 (9%)	1 (1%)	9	14
47	2p	80/88 (91%)	68 (85%)	12 (15%)	0	100	100
48	1q	97/105 (92%)	87 (90%)	9 (9%)	1 (1%)	12	20
48	2q	97/105 (92%)	89 (92%)	7 (7%)	1 (1%)	12	20
49	1r	66/88 (75%)	64 (97%)	1 (2%)	1 (2%)	8	12
49	2r	66/88 (75%)	63 (96%)	3 (4%)	0	100	100
50	1s	81/93 (87%)	66 (82%)	15 (18%)	0	100	100
50	2s	81/93 (87%)	67 (83%)	12 (15%)	2 (2%)	4	5
51	1t	94/106 (89%)	87 (93%)	5 (5%)	2 (2%)	5	7
51	2t	96/106 (91%)	87 (91%)	7 (7%)	2 (2%)	5	7
52	1u	21/27 (78%)	19 (90%)	2 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
52	2u	21/27 (78%)	18 (86%)	3 (14%)	0	100	100
53	1y	95/113 (84%)	92 (97%)	3 (3%)	0	100	100
53	2y	94/113 (83%)	85 (90%)	7 (7%)	2 (2%)	5	7
56	1v	1/3 (33%)	1 (100%)	0	0	100	100
56	2v	1/3 (33%)	1 (100%)	0	0	100	100
All	All	11643/12360 (94%)	10671 (92%)	862 (7%)	110 (1%)	14	22

5 of 110 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
21	1Z	52	SER
26	14	55	ARG
33	1b	8	LYS
33	1b	17	PHE
33	1b	22	LYS

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	1D	214/218 (98%)	195 (91%)	19 (9%)	9	15
3	2D	215/218 (99%)	195 (91%)	20 (9%)	8	14
4	1E	164/166 (99%)	156 (95%)	8 (5%)	22	39
4	2E	164/166 (99%)	148 (90%)	16 (10%)	7	12
5	1F	160/166 (96%)	142 (89%)	18 (11%)	5	8
5	2F	159/166 (96%)	136 (86%)	23 (14%)	3	4
6	1G	144/156 (92%)	133 (92%)	11 (8%)	12	21
6	2G	142/156 (91%)	120 (84%)	22 (16%)	2	3
7	1H	144/148 (97%)	135 (94%)	9 (6%)	16	29
7	2H	143/148 (97%)	123 (86%)	20 (14%)	3	4
8	1I	111/124 (90%)	92 (83%)	19 (17%)	2	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	2I	108/124 (87%)	93 (86%)	15 (14%)	3	4
9	1N	119/119 (100%)	105 (88%)	14 (12%)	5	7
9	2N	118/119 (99%)	111 (94%)	7 (6%)	18	31
10	1O	100/100 (100%)	93 (93%)	7 (7%)	14	24
10	2O	100/100 (100%)	94 (94%)	6 (6%)	17	31
11	1P	115/116 (99%)	110 (96%)	5 (4%)	26	44
11	2P	115/116 (99%)	106 (92%)	9 (8%)	11	20
12	1Q	111/111 (100%)	104 (94%)	7 (6%)	16	29
12	2Q	111/111 (100%)	100 (90%)	11 (10%)	7	11
13	1R	101/101 (100%)	94 (93%)	7 (7%)	14	24
13	2R	101/101 (100%)	93 (92%)	8 (8%)	11	19
14	1S	87/88 (99%)	81 (93%)	6 (7%)	14	24
14	2S	85/88 (97%)	76 (89%)	9 (11%)	6	10
15	1T	115/127 (91%)	109 (95%)	6 (5%)	21	36
15	2T	113/127 (89%)	98 (87%)	15 (13%)	4	5
16	1U	93/94 (99%)	85 (91%)	8 (9%)	10	16
16	2U	93/94 (99%)	84 (90%)	9 (10%)	8	12
17	1V	81/82 (99%)	75 (93%)	6 (7%)	13	22
17	2V	80/82 (98%)	69 (86%)	11 (14%)	3	4
18	1W	90/92 (98%)	83 (92%)	7 (8%)	11	20
18	2W	90/92 (98%)	83 (92%)	7 (8%)	11	20
19	1X	77/78 (99%)	73 (95%)	4 (5%)	21	36
19	2X	77/78 (99%)	69 (90%)	8 (10%)	7	10
20	1Y	86/91 (94%)	78 (91%)	8 (9%)	8	14
20	2Y	86/91 (94%)	76 (88%)	10 (12%)	5	8
21	1Z	169/179 (94%)	150 (89%)	19 (11%)	6	9
21	2Z	165/179 (92%)	144 (87%)	21 (13%)	4	6
22	10	65/67 (97%)	60 (92%)	5 (8%)	12	20
22	20	64/67 (96%)	61 (95%)	3 (5%)	23	41
23	11	79/83 (95%)	69 (87%)	10 (13%)	4	6
23	21	81/83 (98%)	73 (90%)	8 (10%)	7	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	12	65/67 (97%)	61 (94%)	4 (6%)	16	29
24	22	66/67 (98%)	57 (86%)	9 (14%)	3	5
25	13	51/52 (98%)	48 (94%)	3 (6%)	18	31
25	23	50/52 (96%)	46 (92%)	4 (8%)	11	19
26	14	58/63 (92%)	47 (81%)	11 (19%)	1	2
26	24	54/63 (86%)	45 (83%)	9 (17%)	2	3
27	15	51/52 (98%)	45 (88%)	6 (12%)	5	7
27	25	50/52 (96%)	46 (92%)	4 (8%)	11	19
28	16	51/52 (98%)	47 (92%)	4 (8%)	11	20
28	26	50/52 (96%)	42 (84%)	8 (16%)	2	3
29	17	41/42 (98%)	39 (95%)	2 (5%)	22	39
29	27	41/42 (98%)	36 (88%)	5 (12%)	5	7
30	18	54/55 (98%)	51 (94%)	3 (6%)	19	33
30	28	54/55 (98%)	51 (94%)	3 (6%)	19	33
31	19	34/34 (100%)	33 (97%)	1 (3%)	37	60
31	29	34/34 (100%)	33 (97%)	1 (3%)	37	60
33	1b	191/220 (87%)	168 (88%)	23 (12%)	5	7
33	2b	187/220 (85%)	155 (83%)	32 (17%)	2	2
34	1c	144/188 (77%)	133 (92%)	11 (8%)	12	21
34	2c	140/188 (74%)	121 (86%)	19 (14%)	3	5
35	1d	171/181 (94%)	146 (85%)	25 (15%)	3	4
35	2d	172/181 (95%)	150 (87%)	22 (13%)	4	6
36	1e	114/123 (93%)	104 (91%)	10 (9%)	9	15
36	2e	114/123 (93%)	99 (87%)	15 (13%)	4	5
37	1f	85/90 (94%)	73 (86%)	12 (14%)	3	4
37	2f	85/90 (94%)	76 (89%)	9 (11%)	6	10
38	1g	120/127 (94%)	107 (89%)	13 (11%)	6	9
38	2g	119/127 (94%)	108 (91%)	11 (9%)	8	14
39	1h	116/119 (98%)	103 (89%)	13 (11%)	6	9
39	2h	114/119 (96%)	102 (90%)	12 (10%)	6	10
40	1i	91/99 (92%)	82 (90%)	9 (10%)	7	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	2i	88/99 (89%)	76 (86%)	12 (14%)	3	5
41	1j	68/92 (74%)	61 (90%)	7 (10%)	7	11
41	2j	68/92 (74%)	62 (91%)	6 (9%)	9	15
42	1k	83/99 (84%)	71 (86%)	12 (14%)	3	4
42	2k	83/99 (84%)	74 (89%)	9 (11%)	6	9
43	1l	96/108 (89%)	89 (93%)	7 (7%)	13	22
43	2l	96/108 (89%)	89 (93%)	7 (7%)	13	22
44	1m	90/101 (89%)	86 (96%)	4 (4%)	25	43
44	2m	87/101 (86%)	74 (85%)	13 (15%)	3	3
45	1n	49/50 (98%)	45 (92%)	4 (8%)	10	18
45	2n	49/50 (98%)	42 (86%)	7 (14%)	3	4
46	1o	78/80 (98%)	73 (94%)	5 (6%)	16	28
46	2o	78/80 (98%)	72 (92%)	6 (8%)	12	20
47	1p	69/74 (93%)	64 (93%)	5 (7%)	13	23
47	2p	68/74 (92%)	55 (81%)	13 (19%)	1	2
48	1q	94/97 (97%)	83 (88%)	11 (12%)	5	7
48	2q	94/97 (97%)	88 (94%)	6 (6%)	16	28
49	1r	59/77 (77%)	54 (92%)	5 (8%)	10	16
49	2r	59/77 (77%)	57 (97%)	2 (3%)	32	54
50	1s	68/80 (85%)	63 (93%)	5 (7%)	13	22
50	2s	67/80 (84%)	58 (87%)	9 (13%)	4	5
51	1t	71/82 (87%)	61 (86%)	10 (14%)	3	4
51	2t	70/82 (85%)	63 (90%)	7 (10%)	7	11
52	1u	18/22 (82%)	18 (100%)	0	100	100
52	2u	18/22 (82%)	18 (100%)	0	100	100
53	1y	82/98 (84%)	78 (95%)	4 (5%)	22	39
53	2y	79/98 (81%)	70 (89%)	9 (11%)	5	8
56	1v	3/3 (100%)	3 (100%)	0	100	100
56	2v	3/3 (100%)	3 (100%)	0	100	100
All	All	9537/10266 (93%)	8578 (90%)	959 (10%)	7	11

5 of 959 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	2E	152	LYS
43	2l	112	ASP
12	2Q	21	THR
42	2k	106	LYS
51	2t	71	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 147 such sidechains are listed below:

Mol	Chain	Res	Type
35	2d	119	GLN
50	2s	14	HIS
36	2e	78	HIS
40	2i	73	GLN
37	1f	57	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2865/2915 (98%)	449 (15%)	32 (1%)
1	2A	2858/2915 (98%)	500 (17%)	32 (1%)
2	1B	119/121 (98%)	17 (14%)	0
2	2B	119/121 (98%)	13 (10%)	0
32	1a	1497/1521 (98%)	253 (16%)	0
32	2a	1501/1521 (98%)	281 (18%)	0
54	1w	1/4 (25%)	0	0
54	2w	1/4 (25%)	0	0
55	1x	1/4 (25%)	0	0
55	2x	1/4 (25%)	0	0
All	All	8963/9130 (98%)	1513 (16%)	64 (0%)

5 of 1513 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	10	G
1	1A	11	G
1	1A	12	U
1	1A	15	G
1	1A	34	C

5 of 64 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2A	2126	A
1	2A	2172	U
1	1A	2126	A
1	1A	1663	C
1	2A	2321	G

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

52 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	1518	32	23,26,27	0.39	0	33,38,41	2.06	10 (30%)
32	5MC	2a	1407	32	19,22,23	1.67	3 (15%)	26,32,35	1.23	3 (11%)
32	G7M	2a	527	32	23,26,27	1.48	3 (13%)	34,39,42	1.74	5 (14%)
1	2MA	1A	2503	1,57	22,25,26	1.50	5 (22%)	32,37,40	2.27	9 (28%)
43	0TD	2l	92	43	8,9,10	4.62	1 (12%)	6,11,13	5.01	3 (50%)
32	5MC	1a	967	32	19,22,23	1.70	3 (15%)	26,32,35	1.16	3 (11%)
32	PSU	1a	516	57,32	18,21,22	1.39	2 (11%)	21,30,33	2.02	5 (23%)
32	M2G	2a	966	32	24,27,28	1.32	4 (16%)	33,40,43	1.85	5 (15%)
32	5MC	2a	1404	32	19,22,23	1.73	3 (15%)	26,32,35	1.22	3 (11%)
54	PPU	2w	76	1,54	37,40,41	1.24	4 (10%)	47,57,60	2.01	14 (29%)
1	PSU	2A	1911	1	18,21,22	1.39	2 (11%)	21,30,33	1.95	3 (14%)
1	OMG	1A	2251	1,57,55	23,26,27	1.23	3 (13%)	32,38,41	2.06	6 (18%)
1	OMU	2A	2552	1,57	19,22,23	1.17	2 (10%)	25,31,34	1.94	6 (24%)
1	5MU	1A	1939	1,57	19,22,23	1.43	5 (26%)	27,32,35	2.21	7 (25%)
1	5MU	2A	1915	1	19,22,23	1.41	4 (21%)	27,32,35	2.18	7 (25%)
32	5MC	2a	967	32	19,22,23	1.81	3 (15%)	26,32,35	1.02	2 (7%)
1	PSU	2A	2605	1	18,21,22	1.34	3 (16%)	21,30,33	2.02	4 (19%)
1	PSU	1A	1911	1	18,21,22	1.35	2 (11%)	21,30,33	2.00	4 (19%)
1	5MC	1A	1942	1	19,22,23	1.72	3 (15%)	26,32,35	1.15	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
32	4OC	2a	1402	32	20,23,24	0.75	0	25,32,35	0.93	1 (4%)
54	PPU	1w	76	1,54	37,40,41	1.26	3 (8%)	47,57,60	2.02	13 (27%)
43	0TD	1l	92	43	8,9,10	4.60	1 (12%)	6,11,13	6.80	3 (50%)
1	PSU	1A	1917	1	18,21,22	1.35	2 (11%)	21,30,33	2.05	3 (14%)
32	MA6	1a	1519	32	23,26,27	0.43	0	33,38,41	2.01	10 (30%)
1	OMC	2A	1920	1	19,22,23	0.84	0	25,31,34	1.05	2 (8%)
1	2MA	2A	2503	1,57	22,25,26	1.45	4 (18%)	32,37,40	2.42	9 (28%)
1	5MC	1A	1962	1,57	19,22,23	1.68	3 (15%)	26,32,35	1.16	2 (7%)
1	PSU	1A	2605	1	18,21,22	1.42	3 (16%)	21,30,33	1.91	4 (19%)
1	5MC	2A	1962	1,57	19,22,23	1.66	3 (15%)	26,32,35	1.13	3 (11%)
32	UR3	2a	1498	57,32	19,22,23	1.02	1 (5%)	26,32,35	1.60	3 (11%)
1	OMC	1A	1920	1	19,22,23	0.82	0	25,31,34	1.01	1 (4%)
1	PSU	2A	1917	1	18,21,22	1.33	2 (11%)	21,30,33	1.96	3 (14%)
32	M2G	1a	966	32	24,27,28	1.28	4 (16%)	33,40,43	1.84	6 (18%)
1	5MC	2A	1942	1	19,22,23	1.54	3 (15%)	26,32,35	1.15	2 (7%)
1	5MU	2A	1939	1,57	19,22,23	1.44	4 (21%)	27,32,35	2.17	6 (22%)
32	UR3	1a	1498	32	19,22,23	1.00	2 (10%)	26,32,35	1.79	4 (15%)
32	5MC	1a	1404	32	19,22,23	1.73	3 (15%)	26,32,35	1.18	2 (7%)
32	MA6	1a	1518	32	23,26,27	0.40	0	33,38,41	1.96	10 (30%)
1	OMG	2A	2251	1,57,55	23,26,27	1.23	3 (13%)	32,38,41	1.88	6 (18%)
32	G7M	1a	527	57,32	23,26,27	1.56	4 (17%)	34,39,42	1.66	4 (11%)
32	5MC	1a	1400	32	19,22,23	1.82	3 (15%)	26,32,35	1.21	2 (7%)
32	5MC	2a	1400	32	19,22,23	1.63	3 (15%)	26,32,35	1.22	3 (11%)
32	4OC	1a	1402	32	20,23,24	0.77	0	25,32,35	0.84	1 (4%)
32	PSU	2a	516	57,32	18,21,22	1.36	3 (16%)	21,30,33	2.06	5 (23%)
32	MA6	2a	1519	32	23,26,27	0.44	0	33,38,41	2.16	10 (30%)
32	2MG	2a	1207	32	23,26,27	1.25	4 (17%)	33,38,41	2.11	7 (21%)
55	8AN	2x	76	57,56,55	21,24,25	1.40	3 (14%)	26,35,38	2.25	10 (38%)
32	2MG	1a	1207	32	23,26,27	1.25	3 (13%)	33,38,41	2.30	8 (24%)
55	8AN	1x	76	57,56,55	21,24,25	1.41	3 (14%)	26,35,38	2.40	11 (42%)
1	OMU	1A	2552	1,57	19,22,23	1.26	3 (15%)	25,31,34	1.88	6 (24%)
32	5MC	1a	1407	32	19,22,23	1.76	2 (10%)	26,32,35	1.10	2 (7%)
1	5MU	1A	1915	1	19,22,23	1.39	4 (21%)	27,32,35	2.33	8 (29%)

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	1518	32	-	0/11/29/30	0/3/3/3
32	5MC	2a	1407	32	-	0/7/25/26	0/2/2/2
32	G7M	2a	527	32	-	1/7/25/26	0/3/3/3
1	2MA	1A	2503	1,57	-	0/7/25/26	0/3/3/3
43	0TD	2l	92	43	-	1/7/12/14	-
32	5MC	1a	967	32	-	0/7/25/26	0/2/2/2
32	PSU	1a	516	57,32	-	0/7/25/26	0/2/2/2
32	M2G	2a	966	32	-	0/11/29/30	0/3/3/3
32	5MC	2a	1404	32	-	0/7/25/26	0/2/2/2
54	PPU	2w	76	1,54	-	0/25/43/44	0/4/4/4
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
1	OMG	1A	2251	1,57,55	-	1/9/27/28	0/3/3/3
1	OMU	2A	2552	1,57	-	1/9/27/28	0/2/2/2
1	5MU	1A	1939	1,57	-	0/7/25/26	0/2/2/2
1	5MU	2A	1915	1	-	4/7/25/26	0/2/2/2
32	5MC	2a	967	32	-	0/7/25/26	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
1	5MC	1A	1942	1	-	0/7/25/26	0/2/2/2
32	4OC	2a	1402	32	-	2/9/29/30	0/2/2/2
54	PPU	1w	76	1,54	-	1/25/43/44	0/4/4/4
43	0TD	1l	92	43	-	2/7/12/14	-
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
32	MA6	1a	1519	32	-	3/11/29/30	0/3/3/3
1	OMC	2A	1920	1	-	1/9/27/28	0/2/2/2
1	2MA	2A	2503	1,57	-	0/7/25/26	0/3/3/3
1	5MC	1A	1962	1,57	-	2/7/25/26	0/2/2/2
1	PSU	1A	2605	1	-	0/7/25/26	0/2/2/2
1	5MC	2A	1962	1,57	-	0/7/25/26	0/2/2/2
32	UR3	2a	1498	57,32	-	0/7/25/26	0/2/2/2
1	OMC	1A	1920	1	-	1/9/27/28	0/2/2/2
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
32	M2G	1a	966	32	-	0/11/29/30	0/3/3/3
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
1	5MU	2A	1939	1,57	-	0/7/25/26	0/2/2/2
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
32	MA6	1a	1518	32	-	0/11/29/30	0/3/3/3
1	OMG	2A	2251	1,57,55	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	G7M	1a	527	57,32	-	2/7/25/26	0/3/3/3
32	5MC	1a	1400	32	-	2/7/25/26	0/2/2/2
32	5MC	2a	1400	32	-	0/7/25/26	0/2/2/2
32	4OC	1a	1402	32	-	2/9/29/30	0/2/2/2
32	PSU	2a	516	57,32	-	2/7/25/26	0/2/2/2
32	MA6	2a	1519	32	-	2/11/29/30	0/3/3/3
32	2MG	2a	1207	32	-	2/9/27/28	0/3/3/3
55	8AN	2x	76	57,56,55	-	3/7/25/26	0/3/3/3
32	2MG	1a	1207	32	-	2/9/27/28	0/3/3/3
55	8AN	1x	76	57,56,55	-	3/7/25/26	0/3/3/3
1	OMU	1A	2552	1,57	-	0/9/27/28	0/2/2/2
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
1	5MU	1A	1915	1	-	2/7/25/26	0/2/2/2

The worst 5 of 131 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	2l	92	0TD	CB-SB	-12.71	1.69	1.82
43	1l	92	0TD	CB-SB	-12.64	1.69	1.82
32	2a	967	5MC	C5-C4	6.79	1.49	1.44
32	1a	1400	5MC	C5-C4	6.72	1.49	1.44
32	1a	1407	5MC	C5-C4	6.55	1.49	1.44

The worst 5 of 271 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	1l	92	0TD	CSB-SB-CB	-16.13	73.36	102.36
43	2l	92	0TD	CSB-SB-CB	-11.71	81.31	102.36
1	2A	2503	2MA	C5-C4-N3	-8.11	118.64	127.18
1	1A	2503	2MA	C5-C4-N3	-7.71	119.06	127.18
32	1a	1207	2MG	C2-N3-C4	7.21	121.02	112.00

There are no chirality outliers.

5 of 42 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1A	1915	5MU	O4'-C1'-N1-C2
1	1A	1915	5MU	O4'-C1'-N1-C6
1	1A	2251	OMG	C1'-C2'-O2'-CM2

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Mol	Chain	Res	Type	Atoms
32	1a	1207	2MG	N1-C2-N2-CM2
32	1a	1207	2MG	N3-C2-N2-CM2

There are no ring outliers.

27 monomers are involved in 44 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	2a	1518	MA6	2	0
32	2a	1404	5MC	1	0
54	2w	76	PPU	4	0
1	2A	2552	OMU	1	0
1	1A	1939	5MU	1	0
1	2A	1915	5MU	1	0
32	2a	1402	4OC	3	0
54	1w	76	PPU	3	0
32	1a	1519	MA6	3	0
1	2A	1920	OMC	1	0
1	1A	2605	PSU	1	0
1	1A	1920	OMC	1	0
32	1a	966	M2G	1	0
1	2A	1942	5MC	1	0
1	2A	1939	5MU	2	0
32	1a	1498	UR3	1	0
32	1a	1404	5MC	1	0
32	1a	1518	MA6	2	0
32	1a	1400	5MC	1	0
32	2a	1400	5MC	1	0
32	1a	1402	4OC	2	0
32	2a	516	PSU	1	0
32	2a	1519	MA6	6	0
32	2a	1207	2MG	4	0
55	2x	76	8AN	2	0
55	1x	76	8AN	2	0
1	1A	2552	OMU	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2534 ligands modelled in this entry, 2523 are monoatomic - leaving 11 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
59	ARG	1F	317	-	10,11,11	0.76	1 (10%)	9,13,13	0.97	1 (11%)
62	MRD	2A	3738	-	7,7,7	0.31	0	9,10,10	0.42	0
58	MPD	2A	3739	-	7,7,7	0.29	0	9,10,10	0.22	0
58	MPD	1a	1881	-	7,7,7	0.37	0	9,10,10	0.29	0
61	SF4	2d	501	35	0,12,12	-	-	-		
58	MPD	1T	205	-	7,7,7	0.26	0	9,10,10	0.29	0
58	MPD	2B	221	-	7,7,7	0.31	0	9,10,10	0.15	0
58	MPD	18	104	-	7,7,7	0.40	0	9,10,10	0.35	0
58	MPD	1A	4029	-	7,7,7	0.41	0	9,10,10	0.38	0
59	ARG	1B	231	57	10,11,11	0.81	1 (10%)	9,13,13	1.04	1 (11%)
61	SF4	1d	307	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
59	ARG	1F	317	-	-	1/11/11/11	-
62	MRD	2A	3738	-	-	1/5/5/5	-
58	MPD	2A	3739	-	-	5/5/5/5	-
58	MPD	1a	1881	-	-	3/5/5/5	-
61	SF4	2d	501	35	-	-	0/6/5/5
58	MPD	1T	205	-	-	3/5/5/5	-
58	MPD	2B	221	-	-	4/5/5/5	-
58	MPD	18	104	-	-	1/5/5/5	-
58	MPD	1A	4029	-	-	2/5/5/5	-
59	ARG	1B	231	57	-	0/11/11/11	-
61	SF4	1d	307	35	-	-	0/6/5/5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	1B	231	ARG	OXT-C	-2.37	1.23	1.30
59	1F	317	ARG	OXT-C	-2.20	1.23	1.30

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
59	1B	231	ARG	OXT-C-O	-2.89	117.52	124.08
59	1F	317	ARG	OXT-C-O	-2.83	117.66	124.08

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	1T	205	MPD	C1-C2-C3-C4
58	2A	3739	MPD	C2-C3-C4-O4
58	2A	3739	MPD	C2-C3-C4-C5
58	1A	4029	MPD	O2-C2-C3-C4
58	1T	205	MPD	CM-C2-C3-C4

There are no ring outliers.

7 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
59	1F	317	ARG	2	0
58	1a	1881	MPD	2	0
61	2d	501	SF4	1	0
58	1T	205	MPD	1	0
58	18	104	MPD	2	0
58	1A	4029	MPD	1	0
59	1B	231	ARG	4	0

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	2861/2915 (98%)	-0.34	121 (4%)	40	36	19, 36, 80, 92	0
1	2A	2856/2915 (97%)	0.16	138 (4%)	35	32	33, 53, 81, 91	0
2	1B	120/121 (99%)	-0.10	0	100	100	28, 49, 63, 76	0
2	2B	120/121 (99%)	0.56	2 (1%)	69	65	52, 68, 73, 78	0
3	1D	275/276 (99%)	0.04	2 (0%)	84	81	22, 38, 48, 62	0
3	2D	275/276 (99%)	0.42	4 (1%)	72	68	34, 48, 58, 68	0
4	1E	204/206 (99%)	0.14	2 (0%)	79	76	20, 40, 57, 68	0
4	2E	204/206 (99%)	0.70	6 (2%)	53	50	32, 54, 64, 79	0
5	1F	203/210 (96%)	0.16	4 (1%)	65	60	18, 39, 63, 74	0
5	2F	203/210 (96%)	0.87	8 (3%)	43	39	37, 58, 68, 75	0
6	1G	181/182 (99%)	0.84	13 (7%)	21	18	42, 59, 67, 73	0
6	2G	181/182 (99%)	1.55	48 (26%)	1	1	60, 70, 75, 82	0
7	1H	174/180 (96%)	0.49	1 (0%)	85	83	34, 50, 59, 64	0
7	2H	173/180 (96%)	1.35	26 (15%)	5	4	59, 69, 74, 77	0
8	1I	147/148 (99%)	1.09	13 (8%)	15	12	41, 64, 71, 75	0
8	2I	146/148 (98%)	1.37	31 (21%)	2	2	50, 66, 73, 77	0
9	1N	140/140 (100%)	0.14	0	100	100	24, 36, 53, 64	0
9	2N	140/140 (100%)	0.77	5 (3%)	46	42	42, 57, 67, 71	0
10	1O	122/122 (100%)	0.16	0	100	100	29, 42, 56, 63	0
10	2O	122/122 (100%)	0.64	1 (0%)	82	80	44, 52, 62, 66	0
11	1P	149/150 (99%)	0.20	2 (1%)	75	71	20, 44, 59, 65	0
11	2P	149/150 (99%)	0.81	9 (6%)	27	24	36, 59, 70, 80	0
12	1Q	141/141 (100%)	0.14	0	100	100	26, 40, 50, 61	0
12	2Q	141/141 (100%)	0.75	6 (4%)	40	36	41, 56, 65, 75	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
13	1R	118/118 (100%)	0.06	0	100	100	26, 35, 47, 57	0
13	2R	118/118 (100%)	0.54	1 (0%)	82	80	39, 50, 58, 60	0
14	1S	110/112 (98%)	0.55	1 (0%)	81	78	36, 49, 58, 61	0
14	2S	110/112 (98%)	1.30	14 (12%)	8	6	56, 62, 70, 72	0
15	1T	131/146 (89%)	0.46	9 (6%)	23	19	34, 44, 60, 70	0
15	2T	131/146 (89%)	0.71	3 (2%)	61	57	45, 55, 65, 73	0
16	1U	116/118 (98%)	-0.19	1 (0%)	81	78	20, 29, 42, 53	0
16	2U	116/118 (98%)	0.71	3 (2%)	57	53	38, 53, 64, 69	0
17	1V	101/101 (100%)	-0.04	1 (0%)	79	76	21, 38, 52, 59	0
17	2V	101/101 (100%)	0.83	3 (2%)	52	48	37, 60, 67, 71	0
18	1W	112/113 (99%)	-0.05	1 (0%)	81	78	22, 30, 50, 66	0
18	2W	112/113 (99%)	0.46	2 (1%)	67	63	41, 49, 58, 71	0
19	1X	95/96 (98%)	0.30	3 (3%)	50	46	28, 38, 56, 65	0
19	2X	95/96 (98%)	0.87	4 (4%)	40	36	47, 55, 63, 67	0
20	1Y	107/110 (97%)	0.41	0	100	100	34, 46, 59, 67	0
20	2Y	107/110 (97%)	1.36	18 (16%)	4	3	52, 62, 69, 75	0
21	1Z	203/206 (98%)	0.71	3 (1%)	72	68	34, 52, 64, 70	0
21	2Z	201/206 (97%)	1.13	15 (7%)	20	17	54, 65, 71, 77	0
22	10	83/85 (97%)	0.08	1 (1%)	76	73	26, 37, 45, 54	0
22	20	83/85 (97%)	1.07	9 (10%)	11	8	41, 55, 62, 66	0
23	11	97/98 (98%)	0.32	1 (1%)	79	76	28, 43, 64, 66	0
23	21	97/98 (98%)	0.64	3 (3%)	51	47	41, 52, 63, 68	0
24	12	70/72 (97%)	0.50	1 (1%)	73	69	36, 47, 57, 71	0
24	22	70/72 (97%)	0.83	1 (1%)	73	69	51, 61, 67, 70	0
25	13	59/60 (98%)	-0.05	0	100	100	24, 34, 57, 63	0
25	23	59/60 (98%)	0.65	3 (5%)	33	30	46, 54, 68, 75	0
26	14	69/71 (97%)	1.37	17 (24%)	2	1	56, 70, 76, 80	0
26	24	69/71 (97%)	1.75	24 (34%)	1	1	65, 75, 82, 83	0
27	15	59/60 (98%)	0.07	2 (3%)	48	44	21, 34, 48, 54	0
27	25	59/60 (98%)	0.41	0	100	100	37, 47, 62, 72	0
28	16	53/54 (98%)	0.06	0	100	100	35, 41, 52, 57	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
28	26	53/54 (98%)	0.65	2 (3%) 44 40	49, 56, 62, 65	0
29	17	48/49 (97%)	0.06	2 (4%) 40 36	21, 28, 53, 60	0
29	27	48/49 (97%)	0.42	3 (6%) 26 22	34, 43, 58, 65	0
30	18	64/65 (98%)	0.01	0 100 100	27, 33, 42, 49	0
30	28	64/65 (98%)	0.81	0 100 100	42, 52, 57, 61	0
31	19	37/37 (100%)	0.24	1 (2%) 56 52	28, 39, 50, 59	0
31	29	37/37 (100%)	1.03	2 (5%) 31 28	53, 59, 64, 66	0
32	1a	1488/1521 (97%)	0.54	34 (2%) 61 57	37, 65, 80, 90	0
32	2a	1492/1521 (98%)	0.64	45 (3%) 52 48	47, 67, 80, 88	0
33	1b	231/256 (90%)	1.49	52 (22%) 2 2	58, 69, 76, 79	0
33	2b	231/256 (90%)	1.67	79 (34%) 1 1	61, 71, 76, 81	0
34	1c	206/239 (86%)	1.28	30 (14%) 6 4	56, 68, 75, 80	0
34	2c	206/239 (86%)	1.51	50 (24%) 2 1	60, 71, 76, 79	0
35	1d	208/209 (99%)	1.33	38 (18%) 3 3	54, 66, 72, 76	0
35	2d	208/209 (99%)	1.15	17 (8%) 17 14	55, 64, 70, 73	0
36	1e	148/162 (91%)	0.89	7 (4%) 36 32	45, 61, 67, 72	0
36	2e	148/162 (91%)	1.02	9 (6%) 27 23	52, 63, 71, 78	0
37	1f	100/101 (99%)	0.97	3 (3%) 52 48	52, 62, 67, 71	0
37	2f	100/101 (99%)	0.88	3 (3%) 52 48	52, 62, 68, 70	0
38	1g	155/156 (99%)	1.09	16 (10%) 12 9	58, 65, 72, 77	0
38	2g	155/156 (99%)	1.36	27 (17%) 4 3	60, 69, 73, 77	0
39	1h	137/138 (99%)	1.05	9 (6%) 24 20	53, 62, 68, 71	0
39	2h	137/138 (99%)	1.13	9 (6%) 24 20	57, 63, 68, 72	0
40	1i	127/128 (99%)	1.71	41 (32%) 1 1	58, 69, 74, 78	0
40	2i	126/128 (98%)	1.93	58 (46%) 0 0	64, 71, 76, 79	0
41	1j	97/105 (92%)	1.60	27 (27%) 1 1	57, 69, 76, 78	0
41	2j	96/105 (91%)	1.98	47 (48%) 0 0	63, 72, 75, 78	0
42	1k	114/129 (88%)	0.88	6 (5%) 32 28	45, 59, 66, 70	0
42	2k	114/129 (88%)	0.99	6 (5%) 32 28	54, 63, 70, 72	0
43	1l	121/132 (91%)	0.88	4 (3%) 49 45	50, 58, 64, 67	0
43	2l	121/132 (91%)	1.03	6 (4%) 34 30	52, 62, 68, 72	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
44	1m	116/126 (92%)	1.22	11 (9%)	14	11	56, 67, 71, 76	0
44	2m	114/126 (90%)	1.62	34 (29%)	1	1	64, 70, 75, 77	0
45	1n	60/61 (98%)	1.57	12 (20%)	3	2	60, 67, 71, 72	0
45	2n	60/61 (98%)	1.92	25 (41%)	0	0	63, 70, 76, 79	0
46	1o	88/89 (98%)	0.92	4 (4%)	38	34	47, 59, 68, 75	0
46	2o	88/89 (98%)	1.10	5 (5%)	29	25	54, 63, 69, 72	0
47	1p	82/88 (93%)	1.72	25 (30%)	1	1	57, 66, 72, 73	0
47	2p	82/88 (93%)	1.23	9 (10%)	10	8	56, 62, 68, 71	0
48	1q	99/105 (94%)	1.15	6 (6%)	27	23	53, 63, 69, 72	0
48	2q	99/105 (94%)	1.09	5 (5%)	33	30	54, 62, 68, 73	0
49	1r	68/88 (77%)	0.98	4 (5%)	28	24	54, 61, 69, 75	0
49	2r	68/88 (77%)	0.94	5 (7%)	20	17	56, 62, 69, 71	0
50	1s	83/93 (89%)	1.45	13 (15%)	5	4	53, 68, 73, 78	0
50	2s	83/93 (89%)	1.54	25 (30%)	1	1	66, 72, 76, 79	0
51	1t	96/106 (90%)	1.48	24 (25%)	2	1	56, 66, 72, 75	0
51	2t	98/106 (92%)	1.23	11 (11%)	10	7	53, 63, 70, 74	0
52	1u	23/27 (85%)	1.66	5 (21%)	2	2	63, 67, 70, 71	0
52	2u	23/27 (85%)	2.13	11 (47%)	0	0	65, 69, 72, 74	0
53	1y	97/113 (85%)	1.13	13 (13%)	7	5	50, 60, 67, 71	0
53	2y	96/113 (84%)	2.00	43 (44%)	0	0	62, 68, 74, 75	0
54	1w	3/4 (75%)	-0.20	0	100	100	28, 28, 36, 40	0
54	2w	3/4 (75%)	0.28	0	100	100	44, 44, 47, 53	0
55	1x	3/4 (75%)	0.19	1 (33%)	1	1	27, 27, 29, 44	0
55	2x	3/4 (75%)	0.36	0	100	100	43, 43, 46, 52	0
56	1v	3/3 (100%)	-0.50	0	100	100	22, 22, 23, 26	0
56	2v	3/3 (100%)	0.84	0	100	100	46, 46, 49, 52	0
All	All	20796/21490 (96%)	0.57	1510 (7%)	21	17	18, 58, 76, 92	0

The worst 5 of 1510 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1A	1091	G	6.7
1	1A	1090	U	6.5

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Mol	Chain	Res	Type	RSRZ
1	1A	1087	G	6.4
45	2n	2	ALA	6.4
45	1n	2	ALA	6.3

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
1	5MU	2A	1915	21/22	0.80	0.14	69,74,81,90	0
1	5MU	1A	1915	21/22	0.87	0.13	66,72,75,80	0
32	M2G	2a	966	25/26	0.87	0.17	55,68,78,84	0
32	2MG	2a	1207	24/25	0.87	0.13	70,78,81,86	0
43	0TD	2l	92	10/11	0.88	0.14	59,63,66,74	0
1	PSU	2A	1911	20/21	0.89	0.11	61,67,79,80	0
32	PSU	2a	516	20/21	0.90	0.11	66,71,77,78	0
1	PSU	1A	1917	20/21	0.90	0.12	58,67,76,76	0
32	2MG	1a	1207	24/25	0.90	0.12	61,67,72,75	0
1	PSU	2A	1917	20/21	0.90	0.11	59,73,81,83	0
1	PSU	1A	1911	20/21	0.92	0.10	52,63,68,72	0
1	OMC	2A	1920	21/22	0.92	0.11	57,62,65,66	0
43	0TD	1l	92	10/11	0.92	0.12	51,58,60,75	0
32	5MC	2a	967	21/22	0.93	0.13	60,67,70,78	0
32	G7M	1a	527	24/25	0.94	0.11	43,55,59,61	0
32	4OC	2a	1402	22/23	0.94	0.12	57,63,65,66	0
32	5MC	2a	1407	21/22	0.94	0.12	52,57,62,63	0
32	MA6	2a	1518	24/25	0.94	0.12	56,60,64,67	0
32	G7M	2a	527	24/25	0.94	0.10	52,63,66,68	0
32	5MC	1a	967	21/22	0.95	0.12	59,66,70,74	0
32	PSU	1a	516	20/21	0.95	0.09	55,60,66,67	0
32	5MC	1a	1400	21/22	0.95	0.11	51,57,63,66	0
32	5MC	2a	1400	21/22	0.95	0.12	56,63,67,67	0
32	UR3	1a	1498	21/22	0.95	0.10	40,53,56,66	0
32	5MC	2a	1404	21/22	0.95	0.09	54,58,61,62	0
1	5MC	2A	1942	21/22	0.95	0.10	47,54,57,58	0
32	UR3	2a	1498	21/22	0.95	0.12	52,62,65,67	0
32	MA6	1a	1519	24/25	0.95	0.11	44,48,53,53	0
32	MA6	2a	1519	24/25	0.95	0.12	46,58,62,63	0
1	OMC	1A	1920	21/22	0.95	0.11	44,56,61,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
32	4OC	1a	1402	22/23	0.96	0.10	46,54,57,66	0
32	5MC	1a	1404	21/22	0.96	0.11	47,54,59,66	0
32	5MC	1a	1407	21/22	0.96	0.10	43,52,57,61	0
32	M2G	1a	966	25/26	0.96	0.10	57,63,68,71	0
32	MA6	1a	1518	24/25	0.96	0.10	45,48,51,57	0
55	8AN	2x	76	22/23	0.96	0.10	34,41,51,60	0
1	OMG	2A	2251	24/25	0.97	0.10	33,38,44,44	0
1	2MA	2A	2503	23/24	0.97	0.09	22,36,41,43	0
1	OMU	2A	2552	21/22	0.97	0.08	33,40,43,53	0
1	PSU	2A	2605	20/21	0.97	0.09	33,38,45,48	0
1	5MC	1A	1942	21/22	0.97	0.08	28,40,44,46	0
1	5MC	1A	1962	21/22	0.97	0.08	30,41,45,47	0
1	5MU	2A	1939	21/22	0.97	0.08	34,43,48,49	0
1	PSU	1A	2605	20/21	0.97	0.07	18,28,32,34	0
54	PPU	2w	76	37/38	0.97	0.09	29,38,43,44	0
55	8AN	1x	76	22/23	0.97	0.08	18,24,29,40	0
1	5MC	2A	1962	21/22	0.97	0.09	35,46,49,52	0
1	OMG	1A	2251	24/25	0.98	0.06	18,25,29,35	0
54	PPU	1w	76	37/38	0.98	0.08	15,24,31,33	0
1	2MA	1A	2503	23/24	0.98	0.07	17,22,25,26	0
1	OMU	1A	2552	21/22	0.98	0.06	25,28,30,31	0
1	5MU	1A	1939	21/22	0.98	0.07	25,30,38,43	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
57	MG	2A	3726	1/1	0.58	0.21	65,65,65,65	0
57	MG	1a	1792	1/1	0.59	0.21	78,78,78,78	0
57	MG	1A	3703	1/1	0.65	0.17	64,64,64,64	0
57	MG	2A	3383	1/1	0.66	0.20	78,78,78,78	0
57	MG	2A	3437	1/1	0.66	0.19	72,72,72,72	0
57	MG	1A	3997	1/1	0.66	0.17	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3435	1/1	0.67	0.19	80,80,80,80	0
57	MG	1A	3533	1/1	0.70	0.20	64,64,64,64	0
57	MG	1a	1738	1/1	0.70	0.20	86,86,86,86	0
57	MG	2B	201	1/1	0.71	0.20	68,68,68,68	0
57	MG	1A	3440	1/1	0.72	0.17	43,43,43,43	0
57	MG	1a	1675	1/1	0.73	0.28	68,68,68,68	0
57	MG	1a	1722	1/1	0.73	0.21	77,77,77,77	0
57	MG	1A	3960	1/1	0.73	0.15	81,81,81,81	0
57	MG	1A	3902	1/1	0.73	0.19	41,41,41,41	0
57	MG	2A	3364	1/1	0.74	0.15	57,57,57,57	0
57	MG	1A	3448	1/1	0.74	0.13	29,29,29,29	0
57	MG	1E	304	1/1	0.74	0.10	34,34,34,34	0
57	MG	1A	3714	1/1	0.74	0.20	49,49,49,49	0
57	MG	2A	3223	1/1	0.74	0.26	69,69,69,69	0
57	MG	2A	3536	1/1	0.76	0.27	71,71,71,71	0
57	MG	1A	3812	1/1	0.77	0.15	55,55,55,55	0
57	MG	2A	3484	1/1	0.77	0.21	55,55,55,55	0
57	MG	2A	3323	1/1	0.77	0.16	70,70,70,70	0
57	MG	1a	1751	1/1	0.77	0.15	72,72,72,72	0
57	MG	2A	3731	1/1	0.77	0.21	59,59,59,59	0
57	MG	1A	3900	1/1	0.77	0.14	58,58,58,58	0
58	MPD	2B	221	8/8	0.77	0.27	52,63,69,73	0
57	MG	2A	3246	1/1	0.78	0.28	68,68,68,68	0
57	MG	2A	3582	1/1	0.78	0.15	64,64,64,64	0
57	MG	2a	3062	1/1	0.78	0.22	66,66,66,66	0
57	MG	1A	3803	1/1	0.78	0.23	53,53,53,53	0
62	MRD	2A	3738	8/8	0.78	0.29	46,55,58,59	0
57	MG	1R	202	1/1	0.79	0.21	48,48,48,48	0
57	MG	1a	1664	1/1	0.79	0.24	72,72,72,72	0
57	MG	2A	3489	1/1	0.79	0.14	48,48,48,48	0
57	MG	2A	3173	1/1	0.79	0.20	60,60,60,60	0
57	MG	2A	3199	1/1	0.79	0.20	64,64,64,64	0
57	MG	1A	3617	1/1	0.79	0.11	42,42,42,42	0
57	MG	1a	1682	1/1	0.79	0.22	66,66,66,66	0
57	MG	1a	1706	1/1	0.79	0.15	64,64,64,64	0
57	MG	1A	3463	1/1	0.79	0.16	70,70,70,70	0
57	MG	1P	204	1/1	0.79	0.13	73,73,73,73	0
57	MG	2A	3431	1/1	0.79	0.16	77,77,77,77	0
57	MG	1a	1808	1/1	0.80	0.16	70,70,70,70	0
57	MG	1a	1671	1/1	0.80	0.20	68,68,68,68	0
57	MG	2A	3423	1/1	0.80	0.19	67,67,67,67	0
57	MG	1a	1729	1/1	0.80	0.18	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3735	1/1	0.80	0.23	69,69,69,69	0
57	MG	1A	3779	1/1	0.80	0.13	41,41,41,41	0
57	MG	1a	1636	1/1	0.80	0.34	71,71,71,71	0
57	MG	2a	3091	1/1	0.80	0.27	70,70,70,70	0
57	MG	1A	4024	1/1	0.80	0.13	60,60,60,60	0
57	MG	2A	3529	1/1	0.80	0.20	67,67,67,67	0
57	MG	2A	3623	1/1	0.81	0.14	45,45,45,45	0
57	MG	1A	3627	1/1	0.81	0.22	30,30,30,30	0
57	MG	1A	3535	1/1	0.81	0.12	53,53,53,53	0
57	MG	2A	3733	1/1	0.81	0.15	65,65,65,65	0
57	MG	2A	3165	1/1	0.81	0.12	48,48,48,48	0
57	MG	2A	3526	1/1	0.81	0.28	55,55,55,55	0
57	MG	1B	230	1/1	0.81	0.11	56,56,56,56	0
57	MG	1a	1748	1/1	0.81	0.15	63,63,63,63	0
57	MG	2a	3156	1/1	0.81	0.17	77,77,77,77	0
57	MG	2a	3185	1/1	0.81	0.15	70,70,70,70	0
57	MG	1A	3852	1/1	0.81	0.12	54,54,54,54	0
57	MG	2A	3590	1/1	0.81	0.14	45,45,45,45	0
57	MG	1A	3995	1/1	0.82	0.12	66,66,66,66	0
57	MG	2A	3402	1/1	0.82	0.15	48,48,48,48	0
57	MG	1A	3097	1/1	0.82	0.19	61,61,61,61	0
57	MG	1a	1762	1/1	0.82	0.18	75,75,75,75	0
57	MG	1a	1779	1/1	0.82	0.13	65,65,65,65	0
57	MG	2A	3460	1/1	0.82	0.19	44,44,44,44	0
57	MG	2A	3464	1/1	0.82	0.11	65,65,65,65	0
57	MG	2A	3472	1/1	0.82	0.18	61,61,61,61	0
57	MG	2a	3010	1/1	0.82	0.14	70,70,70,70	0
57	MG	1A	3729	1/1	0.82	0.12	39,39,39,39	0
57	MG	2A	3247	1/1	0.82	0.27	77,77,77,77	0
57	MG	2A	3496	1/1	0.82	0.14	66,66,66,66	0
57	MG	2A	3320	1/1	0.82	0.21	68,68,68,68	0
57	MG	1A	3705	1/1	0.82	0.18	61,61,61,61	0
59	ARG	1F	317	12/12	0.82	0.19	42,62,67,68	0
57	MG	1a	1837	1/1	0.82	0.16	63,63,63,63	0
57	MG	2A	3146	1/1	0.83	0.20	60,60,60,60	0
57	MG	1A	4014	1/1	0.83	0.12	57,57,57,57	0
57	MG	1A	3630	1/1	0.83	0.20	58,58,58,58	0
57	MG	2A	3513	1/1	0.83	0.12	60,60,60,60	0
57	MG	1A	3768	1/1	0.83	0.23	57,57,57,57	0
57	MG	1A	3496	1/1	0.83	0.10	27,27,27,27	0
57	MG	1A	3969	1/1	0.83	0.12	63,63,63,63	0
57	MG	1A	3987	1/1	0.83	0.13	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1R	204	1/1	0.83	0.23	52,52,52,52	0
57	MG	1a	1609	1/1	0.83	0.17	68,68,68,68	0
57	MG	2A	3681	1/1	0.83	0.12	64,64,64,64	0
57	MG	2A	3694	1/1	0.83	0.21	59,59,59,59	0
57	MG	1A	3870	1/1	0.83	0.08	19,19,19,19	0
57	MG	1a	1776	1/1	0.83	0.12	66,66,66,66	0
57	MG	2A	3394	1/1	0.83	0.15	60,60,60,60	0
57	MG	1a	1777	1/1	0.83	0.14	69,69,69,69	0
57	MG	1a	1638	1/1	0.83	0.24	71,71,71,71	0
57	MG	1a	1663	1/1	0.83	0.17	70,70,70,70	0
57	MG	2A	3433	1/1	0.83	0.20	57,57,57,57	0
57	MG	1A	3885	1/1	0.83	0.11	72,72,72,72	0
57	MG	2a	3125	1/1	0.83	0.16	68,68,68,68	0
57	MG	2a	3135	1/1	0.83	0.19	61,61,61,61	0
57	MG	2a	3148	1/1	0.83	0.14	51,51,51,51	0
57	MG	2A	3447	1/1	0.83	0.14	55,55,55,55	0
57	MG	2a	3170	1/1	0.83	0.12	76,76,76,76	0
57	MG	2a	3175	1/1	0.83	0.14	68,68,68,68	0
57	MG	2A	3454	1/1	0.83	0.13	60,60,60,60	0
57	MG	1A	4000	1/1	0.83	0.27	51,51,51,51	0
57	MG	1a	1860	1/1	0.83	0.11	55,55,55,55	0
57	MG	1h	202	1/1	0.83	0.17	67,67,67,67	0
57	MG	1a	1667	1/1	0.84	0.28	74,74,74,74	0
57	MG	2A	3044	1/1	0.84	0.28	66,66,66,66	0
57	MG	2A	3132	1/1	0.84	0.20	70,70,70,70	0
57	MG	1a	1758	1/1	0.84	0.14	66,66,66,66	0
57	MG	1A	3849	1/1	0.84	0.12	50,50,50,50	0
57	MG	1A	3890	1/1	0.84	0.20	54,54,54,54	0
57	MG	2A	3178	1/1	0.84	0.15	53,53,53,53	0
57	MG	1A	3246	1/1	0.84	0.21	64,64,64,64	0
57	MG	2B	207	1/1	0.84	0.17	68,68,68,68	0
57	MG	1B	202	1/1	0.84	0.16	63,63,63,63	0
57	MG	2a	3060	1/1	0.84	0.24	64,64,64,64	0
57	MG	1B	225	1/1	0.84	0.18	60,60,60,60	0
57	MG	2a	3068	1/1	0.84	0.21	65,65,65,65	0
57	MG	1A	3292	1/1	0.84	0.17	74,74,74,74	0
57	MG	1D	313	1/1	0.84	0.14	48,48,48,48	0
57	MG	1a	1845	1/1	0.84	0.21	73,73,73,73	0
57	MG	2A	3522	1/1	0.84	0.22	56,56,56,56	0
57	MG	2A	3357	1/1	0.84	0.17	64,64,64,64	0
57	MG	2a	3166	1/1	0.84	0.15	60,60,60,60	0
57	MG	1a	1851	1/1	0.84	0.13	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3532	1/1	0.84	0.11	66,66,66,66	0
57	MG	2a	3177	1/1	0.84	0.22	72,72,72,72	0
57	MG	1a	1856	1/1	0.84	0.15	64,64,64,64	0
57	MG	1A	3951	1/1	0.84	0.09	51,51,51,51	0
57	MG	1f	202	1/1	0.84	0.12	52,52,52,52	0
57	MG	2A	3592	1/1	0.84	0.15	50,50,50,50	0
57	MG	1Z	301	1/1	0.85	0.12	52,52,52,52	0
57	MG	2A	3665	1/1	0.85	0.11	66,66,66,66	0
57	MG	2A	3422	1/1	0.85	0.13	50,50,50,50	0
57	MG	1A	3896	1/1	0.85	0.09	28,28,28,28	0
57	MG	2A	3703	1/1	0.85	0.15	56,56,56,56	0
57	MG	2A	3705	1/1	0.85	0.13	53,53,53,53	0
57	MG	1A	4003	1/1	0.85	0.14	54,54,54,54	0
57	MG	1A	3394	1/1	0.85	0.12	43,43,43,43	0
57	MG	1a	1774	1/1	0.85	0.14	67,67,67,67	0
57	MG	1A	3824	1/1	0.85	0.12	71,71,71,71	0
57	MG	1A	3198	1/1	0.85	0.18	63,63,63,63	0
57	MG	1A	3753	1/1	0.85	0.15	44,44,44,44	0
57	MG	2B	218	1/1	0.85	0.13	61,61,61,61	0
57	MG	2G	3302	1/1	0.85	0.16	70,70,70,70	0
57	MG	2A	3193	1/1	0.85	0.15	60,60,60,60	0
57	MG	2a	3021	1/1	0.85	0.15	70,70,70,70	0
57	MG	2a	3025	1/1	0.85	0.16	64,64,64,64	0
57	MG	1A	3967	1/1	0.85	0.12	59,59,59,59	0
57	MG	2A	3480	1/1	0.85	0.17	69,69,69,69	0
57	MG	1a	1803	1/1	0.85	0.16	67,67,67,67	0
57	MG	1A	3863	1/1	0.85	0.12	56,56,56,56	0
57	MG	1a	1809	1/1	0.85	0.14	70,70,70,70	0
57	MG	2A	3511	1/1	0.85	0.10	67,67,67,67	0
57	MG	2A	3282	1/1	0.85	0.16	66,66,66,66	0
57	MG	1A	3687	1/1	0.85	0.17	61,61,61,61	0
57	MG	1P	203	1/1	0.85	0.17	36,36,36,36	0
57	MG	1A	3993	1/1	0.85	0.09	29,29,29,29	0
57	MG	2A	3363	1/1	0.85	0.19	69,69,69,69	0
57	MG	1A	3612	1/1	0.85	0.11	40,40,40,40	0
57	MG	2a	3179	1/1	0.85	0.13	65,65,65,65	0
57	MG	2A	3372	1/1	0.85	0.17	61,61,61,61	0
57	MG	2e	201	1/1	0.85	0.30	70,70,70,70	0
57	MG	2A	3583	1/1	0.85	0.12	50,50,50,50	0
57	MG	1A	3355	1/1	0.85	0.14	57,57,57,57	0
57	MG	1a	1874	1/1	0.85	0.19	74,74,74,74	0
57	MG	2A	3441	1/1	0.86	0.13	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3171	1/1	0.86	0.12	65,65,65,65	0
57	MG	1A	3637	1/1	0.86	0.10	38,38,38,38	0
57	MG	1A	3311	1/1	0.86	0.27	67,67,67,67	0
57	MG	1a	1789	1/1	0.86	0.16	75,75,75,75	0
57	MG	1G	202	1/1	0.86	0.12	55,55,55,55	0
57	MG	1A	3593	1/1	0.86	0.18	40,40,40,40	0
57	MG	1a	1805	1/1	0.86	0.17	73,73,73,73	0
57	MG	1a	1696	1/1	0.86	0.19	70,70,70,70	0
57	MG	1a	1703	1/1	0.86	0.11	64,64,64,64	0
57	MG	2A	3318	1/1	0.86	0.26	68,68,68,68	0
57	MG	1a	1704	1/1	0.86	0.16	57,57,57,57	0
57	MG	1A	3454	1/1	0.86	0.18	62,62,62,62	0
57	MG	1a	1707	1/1	0.86	0.24	61,61,61,61	0
57	MG	2a	3066	1/1	0.86	0.13	74,74,74,74	0
57	MG	1A	3710	1/1	0.86	0.11	72,72,72,72	0
57	MG	1A	4007	1/1	0.86	0.12	73,73,73,73	0
57	MG	2A	3533	1/1	0.86	0.26	66,66,66,66	0
57	MG	1A	4011	1/1	0.86	0.23	53,53,53,53	0
57	MG	2a	3141	1/1	0.86	0.10	61,61,61,61	0
57	MG	2A	3558	1/1	0.86	0.12	62,62,62,62	0
57	MG	2A	3569	1/1	0.86	0.15	44,44,44,44	0
57	MG	1A	3841	1/1	0.86	0.18	34,34,34,34	0
57	MG	1a	1626	1/1	0.86	0.13	74,74,74,74	0
57	MG	2A	3399	1/1	0.86	0.13	58,58,58,58	0
57	MG	1A	3422	1/1	0.86	0.10	53,53,53,53	0
57	MG	2A	3093	1/1	0.86	0.25	67,67,67,67	0
57	MG	2A	3643	1/1	0.86	0.09	74,74,74,74	0
57	MG	2A	3107	1/1	0.86	0.20	56,56,56,56	0
57	MG	1A	3034	1/1	0.86	0.27	56,56,56,56	0
57	MG	1A	3361	1/1	0.86	0.20	50,50,50,50	0
57	MG	1A	3767	1/1	0.86	0.09	29,29,29,29	0
57	MG	2A	3331	1/1	0.87	0.18	57,57,57,57	0
57	MG	1A	3493	1/1	0.87	0.12	23,23,23,23	0
57	MG	1A	3078	1/1	0.87	0.13	56,56,56,56	0
57	MG	1A	4002	1/1	0.87	0.12	38,38,38,38	0
57	MG	2A	3626	1/1	0.87	0.13	59,59,59,59	0
57	MG	2A	3632	1/1	0.87	0.17	63,63,63,63	0
57	MG	1A	3521	1/1	0.87	0.12	49,49,49,49	0
57	MG	2A	3659	1/1	0.87	0.16	74,74,74,74	0
57	MG	1a	1725	1/1	0.87	0.13	74,74,74,74	0
57	MG	1A	3944	1/1	0.87	0.15	59,59,59,59	0
57	MG	1a	1880	1/1	0.87	0.15	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3749	1/1	0.87	0.13	47,47,47,47	0
57	MG	2A	3404	1/1	0.87	0.20	69,69,69,69	0
57	MG	2A	3715	1/1	0.87	0.17	72,72,72,72	0
57	MG	1h	201	1/1	0.87	0.13	57,57,57,57	0
57	MG	1A	3109	1/1	0.87	0.13	64,64,64,64	0
57	MG	1A	3666	1/1	0.87	0.12	42,42,42,42	0
57	MG	2A	3056	1/1	0.87	0.18	65,65,65,65	0
57	MG	1a	1658	1/1	0.87	0.17	71,71,71,71	0
57	MG	2A	3096	1/1	0.87	0.16	68,68,68,68	0
57	MG	2B	213	1/1	0.87	0.13	56,56,56,56	0
57	MG	2A	3106	1/1	0.87	0.26	69,69,69,69	0
57	MG	2A	3451	1/1	0.87	0.16	65,65,65,65	0
57	MG	2Q	203	1/1	0.87	0.21	50,50,50,50	0
57	MG	1a	1659	1/1	0.87	0.20	47,47,47,47	0
57	MG	2a	3011	1/1	0.87	0.31	65,65,65,65	0
57	MG	2A	3116	1/1	0.87	0.12	66,66,66,66	0
57	MG	1A	3272	1/1	0.87	0.29	67,67,67,67	0
57	MG	2a	3059	1/1	0.87	0.25	67,67,67,67	0
57	MG	1A	3972	1/1	0.87	0.11	58,58,58,58	0
57	MG	2A	3475	1/1	0.87	0.17	70,70,70,70	0
57	MG	1A	3983	1/1	0.87	0.13	39,39,39,39	0
57	MG	1a	1778	1/1	0.87	0.11	82,82,82,82	0
57	MG	2a	3071	1/1	0.87	0.20	68,68,68,68	0
57	MG	2a	3078	1/1	0.87	0.17	58,58,58,58	0
57	MG	2a	3080	1/1	0.87	0.13	55,55,55,55	0
57	MG	2A	3487	1/1	0.87	0.12	59,59,59,59	0
57	MG	2a	3102	1/1	0.87	0.17	74,74,74,74	0
57	MG	2a	3116	1/1	0.87	0.15	60,60,60,60	0
57	MG	1D	303	1/1	0.87	0.13	48,48,48,48	0
57	MG	1A	3277	1/1	0.87	0.23	63,63,63,63	0
57	MG	1A	3990	1/1	0.87	0.12	55,55,55,55	0
57	MG	1a	1793	1/1	0.87	0.09	68,68,68,68	0
57	MG	1a	1798	1/1	0.87	0.14	52,52,52,52	0
57	MG	2a	3162	1/1	0.87	0.10	67,67,67,67	0
57	MG	2a	3164	1/1	0.87	0.12	54,54,54,54	0
57	MG	1a	1799	1/1	0.87	0.13	63,63,63,63	0
57	MG	1a	1685	1/1	0.87	0.16	59,59,59,59	0
57	MG	1a	1688	1/1	0.87	0.21	68,68,68,68	0
57	MG	2A	3292	1/1	0.87	0.17	59,59,59,59	0
57	MG	2A	3312	1/1	0.87	0.15	58,58,58,58	0
57	MG	2A	3549	1/1	0.87	0.14	74,74,74,74	0
57	MG	2A	3556	1/1	0.87	0.20	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3152	1/1	0.87	0.14	63,63,63,63	0
57	MG	1A	3892	1/1	0.87	0.12	50,50,50,50	0
57	MG	1a	1836	1/1	0.87	0.12	57,57,57,57	0
57	MG	1a	1833	1/1	0.88	0.12	68,68,68,68	0
57	MG	2A	3610	1/1	0.88	0.15	53,53,53,53	0
57	MG	1a	1834	1/1	0.88	0.11	71,71,71,71	0
57	MG	2A	3625	1/1	0.88	0.13	64,64,64,64	0
57	MG	2A	3341	1/1	0.88	0.09	43,43,43,43	0
57	MG	2A	3346	1/1	0.88	0.16	62,62,62,62	0
57	MG	1B	212	1/1	0.88	0.09	54,54,54,54	0
57	MG	1a	1690	1/1	0.88	0.17	60,60,60,60	0
57	MG	1A	3377	1/1	0.88	0.11	47,47,47,47	0
57	MG	2A	3678	1/1	0.88	0.11	41,41,41,41	0
57	MG	2A	3679	1/1	0.88	0.12	56,56,56,56	0
57	MG	1a	1698	1/1	0.88	0.30	62,62,62,62	0
57	MG	2A	3682	1/1	0.88	0.16	54,54,54,54	0
57	MG	1A	3726	1/1	0.88	0.11	48,48,48,48	0
57	MG	1A	3606	1/1	0.88	0.17	63,63,63,63	0
57	MG	1A	3736	1/1	0.88	0.09	33,33,33,33	0
57	MG	2A	3401	1/1	0.88	0.12	57,57,57,57	0
57	MG	1A	3461	1/1	0.88	0.21	35,35,35,35	0
57	MG	1A	3210	1/1	0.88	0.43	50,50,50,50	0
57	MG	1H	202	1/1	0.88	0.12	58,58,58,58	0
57	MG	1N	204	1/1	0.88	0.07	52,52,52,52	0
57	MG	1i	201	1/1	0.88	0.16	65,65,65,65	0
57	MG	1y	203	1/1	0.88	0.13	73,73,73,73	0
57	MG	2B	210	1/1	0.88	0.28	68,68,68,68	0
57	MG	1A	3763	1/1	0.88	0.18	55,55,55,55	0
57	MG	1A	3621	1/1	0.88	0.15	35,35,35,35	0
57	MG	2A	3444	1/1	0.88	0.11	52,52,52,52	0
57	MG	2A	3076	1/1	0.88	0.23	61,61,61,61	0
57	MG	21	101	1/1	0.88	0.09	59,59,59,59	0
57	MG	1A	3482	1/1	0.88	0.12	59,59,59,59	0
57	MG	1A	3416	1/1	0.88	0.06	18,18,18,18	0
57	MG	2a	3018	1/1	0.88	0.14	63,63,63,63	0
57	MG	1A	3795	1/1	0.88	0.10	33,33,33,33	0
57	MG	10	105	1/1	0.88	0.16	58,58,58,58	0
57	MG	2a	3037	1/1	0.88	0.18	59,59,59,59	0
57	MG	2a	3047	1/1	0.88	0.14	63,63,63,63	0
57	MG	2a	3050	1/1	0.88	0.09	60,60,60,60	0
57	MG	1A	3334	1/1	0.88	0.12	55,55,55,55	0
57	MG	1A	3648	1/1	0.88	0.12	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3651	1/1	0.88	0.29	37,37,37,37	0
57	MG	1A	3660	1/1	0.88	0.13	56,56,56,56	0
57	MG	1A	3502	1/1	0.88	0.08	24,24,24,24	0
57	MG	1A	3336	1/1	0.88	0.29	65,65,65,65	0
57	MG	2A	3493	1/1	0.88	0.09	50,50,50,50	0
57	MG	1A	3691	1/1	0.88	0.11	43,43,43,43	0
57	MG	2A	3507	1/1	0.88	0.13	60,60,60,60	0
57	MG	1A	3218	1/1	0.88	0.21	67,67,67,67	0
57	MG	2A	3198	1/1	0.88	0.16	46,46,46,46	0
57	MG	2A	3520	1/1	0.88	0.15	43,43,43,43	0
57	MG	2a	3132	1/1	0.88	0.14	56,56,56,56	0
57	MG	1A	3871	1/1	0.88	0.11	55,55,55,55	0
57	MG	2a	3138	1/1	0.88	0.08	65,65,65,65	0
57	MG	2A	3525	1/1	0.88	0.20	42,42,42,42	0
57	MG	2A	3200	1/1	0.88	0.24	57,57,57,57	0
57	MG	2A	3222	1/1	0.88	0.14	59,59,59,59	0
57	MG	2A	3530	1/1	0.88	0.19	55,55,55,55	0
57	MG	2a	3163	1/1	0.88	0.11	60,60,60,60	0
57	MG	1A	3884	1/1	0.88	0.07	33,33,33,33	0
57	MG	2A	3240	1/1	0.88	0.11	57,57,57,57	0
57	MG	1A	3189	1/1	0.88	0.19	59,59,59,59	0
57	MG	1a	1807	1/1	0.88	0.21	69,69,69,69	0
57	MG	2A	3272	1/1	0.88	0.28	51,51,51,51	0
57	MG	1A	3888	1/1	0.88	0.15	33,33,33,33	0
57	MG	2a	3181	1/1	0.88	0.15	74,74,74,74	0
57	MG	2a	3183	1/1	0.88	0.15	65,65,65,65	0
57	MG	1A	3591	1/1	0.88	0.14	61,61,61,61	0
57	MG	2a	3189	1/1	0.88	0.15	59,59,59,59	0
57	MG	2A	3573	1/1	0.88	0.12	46,46,46,46	0
57	MG	1a	1826	1/1	0.88	0.21	59,59,59,59	0
57	MG	1a	1828	1/1	0.88	0.12	70,70,70,70	0
57	MG	1a	1829	1/1	0.88	0.17	73,73,73,73	0
57	MG	1A	3408	1/1	0.89	0.11	31,31,31,31	0
57	MG	2A	3624	1/1	0.89	0.12	64,64,64,64	0
57	MG	1A	3607	1/1	0.89	0.15	59,59,59,59	0
57	MG	1G	201	1/1	0.89	0.11	65,65,65,65	0
57	MG	2A	3627	1/1	0.89	0.10	48,48,48,48	0
57	MG	1a	1858	1/1	0.89	0.11	63,63,63,63	0
57	MG	2A	3348	1/1	0.89	0.09	49,49,49,49	0
57	MG	2A	3652	1/1	0.89	0.09	49,49,49,49	0
57	MG	1A	3479	1/1	0.89	0.15	59,59,59,59	0
57	MG	1a	1869	1/1	0.89	0.16	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1a	1872	1/1	0.89	0.14	70,70,70,70	0
57	MG	1a	1717	1/1	0.89	0.11	67,67,67,67	0
57	MG	2A	3374	1/1	0.89	0.10	58,58,58,58	0
57	MG	1A	3959	1/1	0.89	0.09	53,53,53,53	0
57	MG	1A	3757	1/1	0.89	0.07	37,37,37,37	0
57	MG	2A	3395	1/1	0.89	0.15	59,59,59,59	0
57	MG	1A	3346	1/1	0.89	0.09	33,33,33,33	0
57	MG	2A	3712	1/1	0.89	0.17	62,62,62,62	0
57	MG	1A	3156	1/1	0.89	0.10	47,47,47,47	0
57	MG	1Q	205	1/1	0.89	0.10	51,51,51,51	0
57	MG	2A	3727	1/1	0.89	0.10	54,54,54,54	0
57	MG	1A	3430	1/1	0.89	0.08	37,37,37,37	0
57	MG	2A	3003	1/1	0.89	0.12	58,58,58,58	0
57	MG	1A	3973	1/1	0.89	0.12	55,55,55,55	0
57	MG	2A	3428	1/1	0.89	0.24	45,45,45,45	0
57	MG	2A	3429	1/1	0.89	0.16	52,52,52,52	0
57	MG	2A	3430	1/1	0.89	0.18	55,55,55,55	0
57	MG	1A	3497	1/1	0.89	0.13	32,32,32,32	0
57	MG	2A	3061	1/1	0.89	0.23	56,56,56,56	0
57	MG	1a	1771	1/1	0.89	0.17	51,51,51,51	0
57	MG	1a	1772	1/1	0.89	0.19	65,65,65,65	0
57	MG	1A	3632	1/1	0.89	0.12	53,53,53,53	0
57	MG	1a	1775	1/1	0.89	0.14	57,57,57,57	0
57	MG	18	103	1/1	0.89	0.08	53,53,53,53	0
57	MG	1A	3988	1/1	0.89	0.12	50,50,50,50	0
57	MG	2A	3456	1/1	0.89	0.10	61,61,61,61	0
57	MG	1A	3331	1/1	0.89	0.10	59,59,59,59	0
57	MG	2a	3035	1/1	0.89	0.23	69,69,69,69	0
57	MG	1a	1630	1/1	0.89	0.10	52,52,52,52	0
57	MG	2A	3470	1/1	0.89	0.14	62,62,62,62	0
57	MG	2A	3147	1/1	0.89	0.17	50,50,50,50	0
57	MG	2A	3161	1/1	0.89	0.14	55,55,55,55	0
57	MG	2A	3478	1/1	0.89	0.10	34,34,34,34	0
57	MG	2A	3162	1/1	0.89	0.19	63,63,63,63	0
57	MG	1a	1634	1/1	0.89	0.08	47,47,47,47	0
57	MG	1A	3640	1/1	0.89	0.09	21,21,21,21	0
57	MG	1A	3644	1/1	0.89	0.08	42,42,42,42	0
57	MG	2a	3072	1/1	0.89	0.16	62,62,62,62	0
57	MG	1a	1797	1/1	0.89	0.11	61,61,61,61	0
57	MG	1a	1651	1/1	0.89	0.17	55,55,55,55	0
57	MG	2a	3086	1/1	0.89	0.14	65,65,65,65	0
57	MG	2A	3505	1/1	0.89	0.11	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3510	1/1	0.89	0.13	37,37,37,37	0
57	MG	2a	3105	1/1	0.89	0.14	63,63,63,63	0
57	MG	2a	3111	1/1	0.89	0.20	63,63,63,63	0
57	MG	1A	3212	1/1	0.89	0.13	51,51,51,51	0
57	MG	1A	3379	1/1	0.89	0.08	42,42,42,42	0
57	MG	2a	3130	1/1	0.89	0.23	68,68,68,68	0
57	MG	2A	3516	1/1	0.89	0.15	65,65,65,65	0
57	MG	2A	3207	1/1	0.89	0.13	55,55,55,55	0
57	MG	2a	3137	1/1	0.89	0.12	65,65,65,65	0
57	MG	2A	3521	1/1	0.89	0.09	57,57,57,57	0
57	MG	1A	3385	1/1	0.89	0.12	27,27,27,27	0
57	MG	1A	3681	1/1	0.89	0.11	58,58,58,58	0
57	MG	2A	3235	1/1	0.89	0.16	60,60,60,60	0
57	MG	1A	3555	1/1	0.89	0.09	45,45,45,45	0
57	MG	2A	3241	1/1	0.89	0.20	63,63,63,63	0
57	MG	1A	3581	1/1	0.89	0.11	63,63,63,63	0
57	MG	1A	3582	1/1	0.89	0.09	44,44,44,44	0
57	MG	2A	3249	1/1	0.89	0.32	49,49,49,49	0
57	MG	2a	3171	1/1	0.89	0.12	59,59,59,59	0
57	MG	2A	3252	1/1	0.89	0.16	63,63,63,63	0
57	MG	1A	3586	1/1	0.89	0.09	53,53,53,53	0
57	MG	2A	3279	1/1	0.89	0.15	62,62,62,62	0
57	MG	1A	3458	1/1	0.89	0.12	60,60,60,60	0
57	MG	2a	3182	1/1	0.89	0.16	68,68,68,68	0
57	MG	1A	3592	1/1	0.89	0.09	29,29,29,29	0
57	MG	2A	3297	1/1	0.89	0.15	38,38,38,38	0
57	MG	1A	3261	1/1	0.89	0.10	46,46,46,46	0
57	MG	2A	3314	1/1	0.89	0.08	36,36,36,36	0
57	MG	2h	201	1/1	0.89	0.14	73,73,73,73	0
57	MG	2x	101	1/1	0.89	0.10	42,42,42,42	0
58	MPD	1T	205	8/8	0.89	0.17	52,60,64,64	0
58	MPD	1a	1881	8/8	0.89	0.16	54,63,67,70	0
57	MG	1A	3603	1/1	0.89	0.09	48,48,48,48	0
57	MG	1a	1838	1/1	0.89	0.17	65,65,65,65	0
57	MG	2A	3616	1/1	0.89	0.14	66,66,66,66	0
57	MG	1a	1812	1/1	0.90	0.14	63,63,63,63	0
57	MG	1a	1668	1/1	0.90	0.14	62,62,62,62	0
57	MG	2A	3276	1/1	0.90	0.28	59,59,59,59	0
57	MG	1A	3433	1/1	0.90	0.10	28,28,28,28	0
57	MG	2A	3615	1/1	0.90	0.13	48,48,48,48	0
57	MG	1B	206	1/1	0.90	0.21	56,56,56,56	0
57	MG	2A	3621	1/1	0.90	0.13	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1a	1676	1/1	0.90	0.13	56,56,56,56	0
57	MG	1A	3245	1/1	0.90	0.24	61,61,61,61	0
57	MG	2A	3298	1/1	0.90	0.19	61,61,61,61	0
57	MG	1A	3716	1/1	0.90	0.11	38,38,38,38	0
57	MG	1a	1687	1/1	0.90	0.13	64,64,64,64	0
57	MG	1B	226	1/1	0.90	0.11	53,53,53,53	0
57	MG	1a	1839	1/1	0.90	0.14	71,71,71,71	0
57	MG	1a	1689	1/1	0.90	0.20	58,58,58,58	0
57	MG	1A	3186	1/1	0.90	0.13	42,42,42,42	0
57	MG	1a	1695	1/1	0.90	0.09	61,61,61,61	0
57	MG	2A	3667	1/1	0.90	0.11	63,63,63,63	0
57	MG	1A	3444	1/1	0.90	0.10	26,26,26,26	0
57	MG	1A	3446	1/1	0.90	0.14	45,45,45,45	0
57	MG	1A	3738	1/1	0.90	0.12	49,49,49,49	0
57	MG	2A	3359	1/1	0.90	0.12	51,51,51,51	0
57	MG	2A	3684	1/1	0.90	0.15	69,69,69,69	0
57	MG	2A	3360	1/1	0.90	0.10	63,63,63,63	0
57	MG	2A	3699	1/1	0.90	0.10	51,51,51,51	0
57	MG	1A	3932	1/1	0.90	0.08	48,48,48,48	0
57	MG	1A	3934	1/1	0.90	0.11	22,22,22,22	0
57	MG	2A	3368	1/1	0.90	0.10	37,37,37,37	0
57	MG	1a	1878	1/1	0.90	0.13	57,57,57,57	0
57	MG	1A	3629	1/1	0.90	0.18	39,39,39,39	0
57	MG	2A	3381	1/1	0.90	0.08	58,58,58,58	0
57	MG	1d	301	1/1	0.90	0.20	73,73,73,73	0
57	MG	2A	3385	1/1	0.90	0.10	44,44,44,44	0
57	MG	2A	3389	1/1	0.90	0.10	59,59,59,59	0
57	MG	2A	3393	1/1	0.90	0.09	33,33,33,33	0
57	MG	2B	202	1/1	0.90	0.15	59,59,59,59	0
57	MG	2B	204	1/1	0.90	0.15	65,65,65,65	0
57	MG	1d	306	1/1	0.90	0.10	79,79,79,79	0
57	MG	1e	201	1/1	0.90	0.17	62,62,62,62	0
57	MG	1a	1709	1/1	0.90	0.11	53,53,53,53	0
57	MG	2B	214	1/1	0.90	0.07	58,58,58,58	0
57	MG	2B	215	1/1	0.90	0.10	62,62,62,62	0
57	MG	2A	3400	1/1	0.90	0.11	55,55,55,55	0
57	MG	2D	311	1/1	0.90	0.12	55,55,55,55	0
57	MG	1g	3102	1/1	0.90	0.09	54,54,54,54	0
57	MG	1a	1714	1/1	0.90	0.12	58,58,58,58	0
57	MG	2R	202	1/1	0.90	0.14	44,44,44,44	0
57	MG	2V	201	1/1	0.90	0.16	67,67,67,67	0
57	MG	1N	203	1/1	0.90	0.08	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2a	3001	1/1	0.90	0.10	50,50,50,50	0
57	MG	2A	3408	1/1	0.90	0.10	59,59,59,59	0
57	MG	2A	3421	1/1	0.90	0.20	47,47,47,47	0
57	MG	2a	3013	1/1	0.90	0.09	63,63,63,63	0
57	MG	1A	3249	1/1	0.90	0.13	51,51,51,51	0
57	MG	1o	102	1/1	0.90	0.21	57,57,57,57	0
57	MG	1a	1723	1/1	0.90	0.13	52,52,52,52	0
57	MG	1A	3388	1/1	0.90	0.09	49,49,49,49	0
57	MG	2A	3025	1/1	0.90	0.17	54,54,54,54	0
57	MG	2a	3039	1/1	0.90	0.09	71,71,71,71	0
57	MG	2A	3039	1/1	0.90	0.11	48,48,48,48	0
57	MG	1A	3759	1/1	0.90	0.13	50,50,50,50	0
57	MG	2A	3434	1/1	0.90	0.16	58,58,58,58	0
57	MG	1a	1736	1/1	0.90	0.10	66,66,66,66	0
57	MG	1A	3341	1/1	0.90	0.13	36,36,36,36	0
57	MG	2a	3065	1/1	0.90	0.23	62,62,62,62	0
57	MG	2A	3068	1/1	0.90	0.09	52,52,52,52	0
57	MG	2A	3075	1/1	0.90	0.13	46,46,46,46	0
57	MG	1A	3561	1/1	0.90	0.14	46,46,46,46	0
57	MG	2A	3082	1/1	0.90	0.17	64,64,64,64	0
57	MG	1A	3570	1/1	0.90	0.11	51,51,51,51	0
57	MG	1T	204	1/1	0.90	0.09	60,60,60,60	0
57	MG	1a	1759	1/1	0.90	0.12	57,57,57,57	0
57	MG	1A	3774	1/1	0.90	0.12	36,36,36,36	0
57	MG	1a	1765	1/1	0.90	0.11	53,53,53,53	0
57	MG	2A	3124	1/1	0.90	0.17	54,54,54,54	0
57	MG	1a	1769	1/1	0.90	0.21	66,66,66,66	0
57	MG	2A	3136	1/1	0.90	0.12	63,63,63,63	0
57	MG	2A	3481	1/1	0.90	0.12	57,57,57,57	0
57	MG	2a	3127	1/1	0.90	0.13	54,54,54,54	0
57	MG	1A	3645	1/1	0.90	0.12	28,28,28,28	0
57	MG	1o	106	1/1	0.90	0.11	46,46,46,46	0
57	MG	1s	106	1/1	0.90	0.14	38,38,38,38	0
57	MG	1A	3575	1/1	0.90	0.13	59,59,59,59	0
57	MG	1A	3801	1/1	0.90	0.12	52,52,52,52	0
57	MG	1a	1611	1/1	0.90	0.19	51,51,51,51	0
57	MG	1A	3342	1/1	0.90	0.09	41,41,41,41	0
57	MG	1A	3806	1/1	0.90	0.12	57,57,57,57	0
57	MG	2A	3181	1/1	0.90	0.12	57,57,57,57	0
57	MG	2A	3187	1/1	0.90	0.11	57,57,57,57	0
57	MG	2A	3188	1/1	0.90	0.26	67,67,67,67	0
57	MG	1a	1780	1/1	0.90	0.16	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2a	3168	1/1	0.90	0.17	56,56,56,56	0
57	MG	1A	3173	1/1	0.90	0.10	49,49,49,49	0
57	MG	1A	3464	1/1	0.90	0.10	60,60,60,60	0
57	MG	2a	3172	1/1	0.90	0.18	62,62,62,62	0
57	MG	1A	3676	1/1	0.90	0.13	52,52,52,52	0
57	MG	2A	3527	1/1	0.90	0.11	52,52,52,52	0
57	MG	1a	1795	1/1	0.90	0.10	64,64,64,64	0
57	MG	2A	3208	1/1	0.90	0.20	53,53,53,53	0
57	MG	1a	1642	1/1	0.90	0.10	57,57,57,57	0
57	MG	1a	1645	1/1	0.90	0.16	59,59,59,59	0
57	MG	2A	3534	1/1	0.90	0.12	55,55,55,55	0
57	MG	2A	3225	1/1	0.90	0.21	54,54,54,54	0
57	MG	1A	3312	1/1	0.90	0.10	40,40,40,40	0
57	MG	1A	3480	1/1	0.90	0.11	37,37,37,37	0
57	MG	2k	201	1/1	0.90	0.16	61,61,61,61	0
57	MG	2r	101	1/1	0.90	0.12	64,64,64,64	0
57	MG	1A	3423	1/1	0.90	0.07	33,33,33,33	0
57	MG	1A	3700	1/1	0.90	0.08	33,33,33,33	0
57	MG	2A	3570	1/1	0.90	0.11	42,42,42,42	0
57	MG	2A	3571	1/1	0.90	0.09	58,58,58,58	0
57	MG	1A	3484	1/1	0.90	0.11	43,43,43,43	0
57	MG	1A	3313	1/1	0.90	0.13	79,79,79,79	0
57	MG	1A	3733	1/1	0.91	0.08	51,51,51,51	0
57	MG	2A	3319	1/1	0.91	0.12	50,50,50,50	0
57	MG	1a	1877	1/1	0.91	0.12	67,67,67,67	0
57	MG	1A	3894	1/1	0.91	0.12	60,60,60,60	0
57	MG	1D	316	1/1	0.91	0.09	51,51,51,51	0
57	MG	2A	3334	1/1	0.91	0.08	54,54,54,54	0
57	MG	2A	3630	1/1	0.91	0.16	59,59,59,59	0
57	MG	1b	301	1/1	0.91	0.14	67,67,67,67	0
57	MG	2A	3641	1/1	0.91	0.10	49,49,49,49	0
57	MG	1A	3577	1/1	0.91	0.10	51,51,51,51	0
57	MG	1A	3898	1/1	0.91	0.08	34,34,34,34	0
57	MG	1A	3580	1/1	0.91	0.12	47,47,47,47	0
57	MG	1A	3359	1/1	0.91	0.08	30,30,30,30	0
57	MG	1A	3910	1/1	0.91	0.09	45,45,45,45	0
57	MG	2A	3676	1/1	0.91	0.10	63,63,63,63	0
57	MG	1A	3920	1/1	0.91	0.08	25,25,25,25	0
57	MG	1O	201	1/1	0.91	0.09	45,45,45,45	0
57	MG	1A	3404	1/1	0.91	0.06	31,31,31,31	0
57	MG	1l	201	1/1	0.91	0.09	55,55,55,55	0
57	MG	1a	1737	1/1	0.91	0.09	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1y	201	1/1	0.91	0.09	56,56,56,56	0
57	MG	2A	3695	1/1	0.91	0.13	55,55,55,55	0
57	MG	1A	3491	1/1	0.91	0.07	24,24,24,24	0
57	MG	2A	3700	1/1	0.91	0.14	61,61,61,61	0
57	MG	1w	101	1/1	0.91	0.12	54,54,54,54	0
57	MG	2A	3001	1/1	0.91	0.24	66,66,66,66	0
57	MG	1a	1739	1/1	0.91	0.14	56,56,56,56	0
57	MG	2A	3008	1/1	0.91	0.26	45,45,45,45	0
57	MG	2A	3723	1/1	0.91	0.17	56,56,56,56	0
57	MG	1A	3587	1/1	0.91	0.15	36,36,36,36	0
57	MG	2A	3038	1/1	0.91	0.16	52,52,52,52	0
57	MG	2A	3728	1/1	0.91	0.12	52,52,52,52	0
57	MG	1A	3950	1/1	0.91	0.11	43,43,43,43	0
57	MG	2A	3732	1/1	0.91	0.15	71,71,71,71	0
57	MG	1a	1753	1/1	0.91	0.13	60,60,60,60	0
57	MG	1A	3165	1/1	0.91	0.20	50,50,50,50	0
57	MG	2A	3058	1/1	0.91	0.22	56,56,56,56	0
57	MG	2A	3405	1/1	0.91	0.18	61,61,61,61	0
57	MG	2B	203	1/1	0.91	0.11	63,63,63,63	0
57	MG	1A	3664	1/1	0.91	0.11	54,54,54,54	0
57	MG	1V	207	1/1	0.91	0.08	46,46,46,46	0
57	MG	2A	3073	1/1	0.91	0.16	54,54,54,54	0
57	MG	1A	3366	1/1	0.91	0.12	60,60,60,60	0
57	MG	2A	3424	1/1	0.91	0.16	53,53,53,53	0
57	MG	1a	1766	1/1	0.91	0.10	62,62,62,62	0
57	MG	1A	3675	1/1	0.91	0.06	12,12,12,12	0
57	MG	2D	303	1/1	0.91	0.42	55,55,55,55	0
57	MG	2A	3084	1/1	0.91	0.10	53,53,53,53	0
57	MG	2A	3090	1/1	0.91	0.18	70,70,70,70	0
57	MG	2N	201	1/1	0.91	0.13	55,55,55,55	0
57	MG	2P	203	1/1	0.91	0.16	64,64,64,64	0
57	MG	1A	3968	1/1	0.91	0.10	68,68,68,68	0
57	MG	1A	3778	1/1	0.91	0.15	63,63,63,63	0
57	MG	2T	203	1/1	0.91	0.09	55,55,55,55	0
57	MG	1A	3970	1/1	0.91	0.08	48,48,48,48	0
57	MG	2V	202	1/1	0.91	0.14	46,46,46,46	0
57	MG	19	101	1/1	0.91	0.18	46,46,46,46	0
57	MG	28	101	1/1	0.91	0.14	54,54,54,54	0
57	MG	2A	3442	1/1	0.91	0.10	44,44,44,44	0
57	MG	2A	3115	1/1	0.91	0.09	60,60,60,60	0
57	MG	1A	3419	1/1	0.91	0.08	29,29,29,29	0
57	MG	1A	3791	1/1	0.91	0.07	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2a	3015	1/1	0.91	0.17	55,55,55,55	0
57	MG	1a	1614	1/1	0.91	0.11	67,67,67,67	0
57	MG	2A	3455	1/1	0.91	0.13	78,78,78,78	0
57	MG	1a	1616	1/1	0.91	0.16	56,56,56,56	0
57	MG	2a	3028	1/1	0.91	0.13	64,64,64,64	0
57	MG	2a	3030	1/1	0.91	0.14	63,63,63,63	0
57	MG	2A	3141	1/1	0.91	0.12	55,55,55,55	0
57	MG	1A	3982	1/1	0.91	0.12	44,44,44,44	0
57	MG	1a	1787	1/1	0.91	0.09	71,71,71,71	0
57	MG	2a	3040	1/1	0.91	0.17	57,57,57,57	0
57	MG	2A	3154	1/1	0.91	0.08	44,44,44,44	0
57	MG	2a	3048	1/1	0.91	0.26	61,61,61,61	0
57	MG	2A	3160	1/1	0.91	0.16	56,56,56,56	0
57	MG	1a	1628	1/1	0.91	0.16	57,57,57,57	0
57	MG	1A	3680	1/1	0.91	0.12	29,29,29,29	0
57	MG	1A	3598	1/1	0.91	0.15	45,45,45,45	0
57	MG	2A	3483	1/1	0.91	0.13	54,54,54,54	0
57	MG	1a	1794	1/1	0.91	0.12	55,55,55,55	0
57	MG	2a	3067	1/1	0.91	0.12	74,74,74,74	0
57	MG	2A	3172	1/1	0.91	0.15	78,78,78,78	0
57	MG	1A	3683	1/1	0.91	0.08	42,42,42,42	0
57	MG	2A	3490	1/1	0.91	0.13	58,58,58,58	0
57	MG	1A	3373	1/1	0.91	0.07	21,21,21,21	0
57	MG	2A	3495	1/1	0.91	0.10	51,51,51,51	0
57	MG	1A	3809	1/1	0.91	0.12	64,64,64,64	0
57	MG	2a	3088	1/1	0.91	0.15	65,65,65,65	0
57	MG	2A	3498	1/1	0.91	0.08	62,62,62,62	0
57	MG	2a	3094	1/1	0.91	0.11	59,59,59,59	0
57	MG	2a	3100	1/1	0.91	0.10	68,68,68,68	0
57	MG	1A	3811	1/1	0.91	0.10	54,54,54,54	0
57	MG	2a	3103	1/1	0.91	0.11	47,47,47,47	0
57	MG	1a	1647	1/1	0.91	0.12	60,60,60,60	0
57	MG	2a	3107	1/1	0.91	0.15	57,57,57,57	0
57	MG	1A	3293	1/1	0.91	0.10	76,76,76,76	0
57	MG	2a	3112	1/1	0.91	0.08	76,76,76,76	0
57	MG	2a	3113	1/1	0.91	0.14	58,58,58,58	0
57	MG	2A	3197	1/1	0.91	0.19	73,73,73,73	0
57	MG	2a	3119	1/1	0.91	0.09	60,60,60,60	0
57	MG	1A	3698	1/1	0.91	0.11	19,19,19,19	0
57	MG	1A	3833	1/1	0.91	0.12	60,60,60,60	0
57	MG	2a	3129	1/1	0.91	0.14	68,68,68,68	0
57	MG	1A	3834	1/1	0.91	0.08	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3462	1/1	0.91	0.09	44,44,44,44	0
57	MG	2A	3523	1/1	0.91	0.07	41,41,41,41	0
57	MG	1a	1824	1/1	0.91	0.10	68,68,68,68	0
57	MG	2A	3214	1/1	0.91	0.24	71,71,71,71	0
57	MG	2a	3140	1/1	0.91	0.12	61,61,61,61	0
57	MG	2A	3217	1/1	0.91	0.11	60,60,60,60	0
57	MG	2a	3144	1/1	0.91	0.10	60,60,60,60	0
57	MG	2A	3528	1/1	0.91	0.09	54,54,54,54	0
57	MG	2a	3154	1/1	0.91	0.12	67,67,67,67	0
57	MG	1A	3531	1/1	0.91	0.10	60,60,60,60	0
57	MG	2a	3160	1/1	0.91	0.10	48,48,48,48	0
57	MG	1A	3429	1/1	0.91	0.17	59,59,59,59	0
57	MG	1A	3041	1/1	0.91	0.10	47,47,47,47	0
57	MG	1a	1832	1/1	0.91	0.10	61,61,61,61	0
57	MG	1A	4026	1/1	0.91	0.10	46,46,46,46	0
57	MG	1A	3469	1/1	0.91	0.14	64,64,64,64	0
57	MG	2A	3538	1/1	0.91	0.18	68,68,68,68	0
57	MG	2A	3540	1/1	0.91	0.12	64,64,64,64	0
57	MG	1a	1835	1/1	0.91	0.16	57,57,57,57	0
57	MG	1B	203	1/1	0.91	0.17	52,52,52,52	0
57	MG	1a	1683	1/1	0.91	0.16	69,69,69,69	0
57	MG	2A	3564	1/1	0.91	0.17	61,61,61,61	0
57	MG	1A	3478	1/1	0.91	0.15	53,53,53,53	0
57	MG	1B	207	1/1	0.91	0.22	49,49,49,49	0
57	MG	1a	1842	1/1	0.91	0.16	62,62,62,62	0
57	MG	1B	210	1/1	0.91	0.20	54,54,54,54	0
57	MG	2a	3187	1/1	0.91	0.16	68,68,68,68	0
57	MG	1A	3721	1/1	0.91	0.19	51,51,51,51	0
57	MG	2A	3283	1/1	0.91	0.25	58,58,58,58	0
57	MG	1B	219	1/1	0.91	0.08	45,45,45,45	0
57	MG	1B	223	1/1	0.91	0.07	55,55,55,55	0
57	MG	2A	3596	1/1	0.91	0.10	61,61,61,61	0
57	MG	2A	3606	1/1	0.91	0.09	57,57,57,57	0
58	MPD	1A	4029	8/8	0.91	0.17	37,50,57,60	0
57	MG	2A	3608	1/1	0.91	0.10	49,49,49,49	0
57	MG	2A	3609	1/1	0.91	0.11	42,42,42,42	0
57	MG	1A	3352	1/1	0.91	0.10	13,13,13,13	0
57	MG	1A	3179	1/1	0.91	0.22	52,52,52,52	0
57	MG	1A	3731	1/1	0.91	0.09	35,35,35,35	0
57	MG	2A	3366	1/1	0.92	0.08	37,37,37,37	0
57	MG	18	102	1/1	0.92	0.28	42,42,42,42	0
57	MG	1A	3609	1/1	0.92	0.12	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3206	1/1	0.92	0.16	58,58,58,58	0
57	MG	1a	1768	1/1	0.92	0.15	64,64,64,64	0
57	MG	2A	3382	1/1	0.92	0.12	65,65,65,65	0
57	MG	2A	3685	1/1	0.92	0.09	43,43,43,43	0
57	MG	2A	3689	1/1	0.92	0.13	55,55,55,55	0
57	MG	1a	1608	1/1	0.92	0.07	70,70,70,70	0
57	MG	1A	3477	1/1	0.92	0.06	23,23,23,23	0
57	MG	2A	3697	1/1	0.92	0.11	54,54,54,54	0
57	MG	2A	3698	1/1	0.92	0.11	58,58,58,58	0
57	MG	2A	3049	1/1	0.92	0.08	55,55,55,55	0
57	MG	1A	3544	1/1	0.92	0.11	52,52,52,52	0
57	MG	1A	3994	1/1	0.92	0.10	39,39,39,39	0
57	MG	2A	3060	1/1	0.92	0.19	47,47,47,47	0
57	MG	2A	3706	1/1	0.92	0.13	60,60,60,60	0
57	MG	1a	1615	1/1	0.92	0.10	58,58,58,58	0
57	MG	1A	3706	1/1	0.92	0.16	45,45,45,45	0
57	MG	2A	3722	1/1	0.92	0.18	61,61,61,61	0
57	MG	1A	3835	1/1	0.92	0.21	37,37,37,37	0
57	MG	1A	3708	1/1	0.92	0.08	48,48,48,48	0
57	MG	1A	3208	1/1	0.92	0.17	50,50,50,50	0
57	MG	1a	1631	1/1	0.92	0.15	50,50,50,50	0
57	MG	2A	3083	1/1	0.92	0.10	59,59,59,59	0
57	MG	2A	3410	1/1	0.92	0.08	37,37,37,37	0
57	MG	1a	1784	1/1	0.92	0.08	52,52,52,52	0
57	MG	1a	1785	1/1	0.92	0.12	63,63,63,63	0
57	MG	2A	3092	1/1	0.92	0.16	63,63,63,63	0
57	MG	1a	1786	1/1	0.92	0.10	63,63,63,63	0
57	MG	2A	3426	1/1	0.92	0.19	56,56,56,56	0
57	MG	1A	3628	1/1	0.92	0.12	45,45,45,45	0
57	MG	2A	3098	1/1	0.92	0.11	49,49,49,49	0
57	MG	2B	208	1/1	0.92	0.26	59,59,59,59	0
57	MG	2A	3104	1/1	0.92	0.16	63,63,63,63	0
57	MG	1A	3854	1/1	0.92	0.07	38,38,38,38	0
57	MG	2A	3432	1/1	0.92	0.15	47,47,47,47	0
57	MG	1A	4010	1/1	0.92	0.13	55,55,55,55	0
57	MG	1A	3059	1/1	0.92	0.09	52,52,52,52	0
57	MG	2D	302	1/1	0.92	0.18	46,46,46,46	0
57	MG	1A	3438	1/1	0.92	0.16	32,32,32,32	0
57	MG	2A	3438	1/1	0.92	0.15	57,57,57,57	0
57	MG	2A	3121	1/1	0.92	0.23	60,60,60,60	0
57	MG	1A	4022	1/1	0.92	0.07	47,47,47,47	0
57	MG	2P	201	1/1	0.92	0.11	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3725	1/1	0.92	0.09	58,58,58,58	0
57	MG	2A	3134	1/1	0.92	0.22	62,62,62,62	0
57	MG	2A	3135	1/1	0.92	0.11	57,57,57,57	0
57	MG	1a	1652	1/1	0.92	0.13	64,64,64,64	0
57	MG	1a	1653	1/1	0.92	0.08	51,51,51,51	0
57	MG	1A	3877	1/1	0.92	0.12	47,47,47,47	0
57	MG	1a	1804	1/1	0.92	0.11	67,67,67,67	0
57	MG	25	101	1/1	0.92	0.59	51,51,51,51	0
57	MG	2A	3461	1/1	0.92	0.14	60,60,60,60	0
57	MG	1A	3881	1/1	0.92	0.09	34,34,34,34	0
57	MG	2a	3002	1/1	0.92	0.12	52,52,52,52	0
57	MG	2a	3007	1/1	0.92	0.17	62,62,62,62	0
57	MG	1A	3066	1/1	0.92	0.11	40,40,40,40	0
57	MG	1A	3343	1/1	0.92	0.08	44,44,44,44	0
57	MG	1A	3399	1/1	0.92	0.11	47,47,47,47	0
57	MG	1a	1810	1/1	0.92	0.10	60,60,60,60	0
57	MG	2A	3169	1/1	0.92	0.10	56,56,56,56	0
57	MG	2a	3019	1/1	0.92	0.09	44,44,44,44	0
57	MG	2A	3170	1/1	0.92	0.33	68,68,68,68	0
57	MG	1A	3191	1/1	0.92	0.11	56,56,56,56	0
57	MG	1a	1813	1/1	0.92	0.14	61,61,61,61	0
57	MG	1a	1669	1/1	0.92	0.14	45,45,45,45	0
57	MG	2A	3174	1/1	0.92	0.17	58,58,58,58	0
57	MG	1A	3494	1/1	0.92	0.09	27,27,27,27	0
57	MG	2a	3038	1/1	0.92	0.14	58,58,58,58	0
57	MG	1a	1674	1/1	0.92	0.16	56,56,56,56	0
57	MG	2A	3182	1/1	0.92	0.09	61,61,61,61	0
57	MG	2a	3045	1/1	0.92	0.22	65,65,65,65	0
57	MG	2a	3046	1/1	0.92	0.14	65,65,65,65	0
57	MG	1B	215	1/1	0.92	0.10	58,58,58,58	0
57	MG	1A	3647	1/1	0.92	0.07	39,39,39,39	0
57	MG	2a	3049	1/1	0.92	0.21	62,62,62,62	0
57	MG	2A	3504	1/1	0.92	0.10	66,66,66,66	0
57	MG	2a	3051	1/1	0.92	0.16	52,52,52,52	0
57	MG	1a	1678	1/1	0.92	0.14	64,64,64,64	0
57	MG	2A	3506	1/1	0.92	0.10	57,57,57,57	0
57	MG	1A	3223	1/1	0.92	0.10	65,65,65,65	0
57	MG	2A	3510	1/1	0.92	0.09	61,61,61,61	0
57	MG	1A	3752	1/1	0.92	0.11	56,56,56,56	0
57	MG	1A	3295	1/1	0.92	0.09	67,67,67,67	0
57	MG	1B	229	1/1	0.92	0.09	58,58,58,58	0
57	MG	2A	3203	1/1	0.92	0.24	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3588	1/1	0.92	0.12	42,42,42,42	0
57	MG	2a	3074	1/1	0.92	0.15	53,53,53,53	0
57	MG	1A	3499	1/1	0.92	0.07	32,32,32,32	0
57	MG	1A	3915	1/1	0.92	0.07	52,52,52,52	0
57	MG	2A	3524	1/1	0.92	0.15	50,50,50,50	0
57	MG	1a	1843	1/1	0.92	0.15	65,65,65,65	0
57	MG	2A	3221	1/1	0.92	0.11	56,56,56,56	0
57	MG	1D	314	1/1	0.92	0.29	38,38,38,38	0
57	MG	1a	1849	1/1	0.92	0.14	63,63,63,63	0
57	MG	1A	3227	1/1	0.92	0.15	42,42,42,42	0
57	MG	2A	3226	1/1	0.92	0.10	49,49,49,49	0
57	MG	2A	3230	1/1	0.92	0.12	56,56,56,56	0
57	MG	1D	318	1/1	0.92	0.11	51,51,51,51	0
57	MG	1a	1700	1/1	0.92	0.23	65,65,65,65	0
57	MG	1A	3923	1/1	0.92	0.09	26,26,26,26	0
57	MG	2A	3245	1/1	0.92	0.12	60,60,60,60	0
57	MG	2a	3114	1/1	0.92	0.10	63,63,63,63	0
57	MG	1a	1865	1/1	0.92	0.11	66,66,66,66	0
57	MG	1F	308	1/1	0.92	0.10	52,52,52,52	0
57	MG	1a	1871	1/1	0.92	0.15	63,63,63,63	0
57	MG	1A	3668	1/1	0.92	0.11	61,61,61,61	0
57	MG	2A	3559	1/1	0.92	0.09	45,45,45,45	0
57	MG	2A	3253	1/1	0.92	0.27	50,50,50,50	0
57	MG	2A	3565	1/1	0.92	0.10	59,59,59,59	0
57	MG	2A	3254	1/1	0.92	0.13	52,52,52,52	0
57	MG	2A	3269	1/1	0.92	0.15	52,52,52,52	0
57	MG	1a	1873	1/1	0.92	0.10	57,57,57,57	0
57	MG	2A	3274	1/1	0.92	0.14	47,47,47,47	0
57	MG	2A	3577	1/1	0.92	0.11	47,47,47,47	0
57	MG	1A	3669	1/1	0.92	0.13	56,56,56,56	0
57	MG	1A	3769	1/1	0.92	0.07	35,35,35,35	0
57	MG	2a	3153	1/1	0.92	0.11	65,65,65,65	0
57	MG	2A	3584	1/1	0.92	0.10	43,43,43,43	0
57	MG	2A	3588	1/1	0.92	0.09	58,58,58,58	0
57	MG	2a	3158	1/1	0.92	0.12	69,69,69,69	0
57	MG	1A	3947	1/1	0.92	0.07	43,43,43,43	0
57	MG	1A	3504	1/1	0.92	0.08	25,25,25,25	0
57	MG	1A	3597	1/1	0.92	0.17	33,33,33,33	0
57	MG	2A	3603	1/1	0.92	0.12	39,39,39,39	0
57	MG	1A	3232	1/1	0.92	0.13	37,37,37,37	0
57	MG	1d	303	1/1	0.92	0.11	56,56,56,56	0
57	MG	2A	3307	1/1	0.92	0.08	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1d	305	1/1	0.92	0.10	57,57,57,57	0
57	MG	2A	3611	1/1	0.92	0.08	36,36,36,36	0
57	MG	2a	3174	1/1	0.92	0.11	61,61,61,61	0
57	MG	1A	3789	1/1	0.92	0.08	34,34,34,34	0
57	MG	1a	1727	1/1	0.92	0.14	63,63,63,63	0
57	MG	2A	3619	1/1	0.92	0.07	60,60,60,60	0
57	MG	1f	201	1/1	0.92	0.26	68,68,68,68	0
57	MG	1A	3965	1/1	0.92	0.10	47,47,47,47	0
57	MG	1A	3599	1/1	0.92	0.11	50,50,50,50	0
57	MG	1A	3512	1/1	0.92	0.16	40,40,40,40	0
57	MG	1A	3797	1/1	0.92	0.09	38,38,38,38	0
57	MG	2A	3336	1/1	0.92	0.11	48,48,48,48	0
57	MG	1A	3798	1/1	0.92	0.11	44,44,44,44	0
57	MG	1A	3100	1/1	0.92	0.32	36,36,36,36	0
57	MG	2A	3634	1/1	0.92	0.12	59,59,59,59	0
57	MG	1A	3199	1/1	0.92	0.20	56,56,56,56	0
57	MG	1t	202	1/1	0.92	0.11	56,56,56,56	0
57	MG	1A	3692	1/1	0.92	0.10	59,59,59,59	0
57	MG	1a	1756	1/1	0.92	0.13	47,47,47,47	0
57	MG	2A	3661	1/1	0.92	0.10	38,38,38,38	0
58	MPD	2A	3739	8/8	0.92	0.15	46,56,63,64	0
57	MG	1A	3694	1/1	0.92	0.11	58,58,58,58	0
57	MG	2A	3666	1/1	0.92	0.09	48,48,48,48	0
57	MG	15	107	1/1	0.92	0.10	54,54,54,54	0
57	MG	2A	3258	1/1	0.93	0.08	47,47,47,47	0
57	MG	2A	3261	1/1	0.93	0.13	62,62,62,62	0
57	MG	2A	3617	1/1	0.93	0.07	38,38,38,38	0
57	MG	2A	3266	1/1	0.93	0.20	52,52,52,52	0
57	MG	2A	3267	1/1	0.93	0.10	51,51,51,51	0
57	MG	1a	1662	1/1	0.93	0.12	55,55,55,55	0
57	MG	1A	3781	1/1	0.93	0.10	57,57,57,57	0
57	MG	1A	3788	1/1	0.93	0.07	47,47,47,47	0
57	MG	2A	3275	1/1	0.93	0.09	48,48,48,48	0
57	MG	1a	1850	1/1	0.93	0.10	59,59,59,59	0
57	MG	2A	3629	1/1	0.93	0.08	64,64,64,64	0
57	MG	2A	3277	1/1	0.93	0.14	54,54,54,54	0
57	MG	1a	1665	1/1	0.93	0.10	62,62,62,62	0
57	MG	1a	1666	1/1	0.93	0.17	52,52,52,52	0
57	MG	2A	3637	1/1	0.93	0.08	59,59,59,59	0
57	MG	1A	3150	1/1	0.93	0.08	41,41,41,41	0
57	MG	2A	3286	1/1	0.93	0.10	42,42,42,42	0
57	MG	1a	1859	1/1	0.93	0.10	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3654	1/1	0.93	0.08	63,63,63,63	0
57	MG	1A	3413	1/1	0.93	0.05	36,36,36,36	0
57	MG	1a	1861	1/1	0.93	0.15	57,57,57,57	0
57	MG	1A	3999	1/1	0.93	0.07	23,23,23,23	0
57	MG	1A	3503	1/1	0.93	0.07	44,44,44,44	0
57	MG	1a	1673	1/1	0.93	0.09	56,56,56,56	0
57	MG	2A	3672	1/1	0.93	0.06	61,61,61,61	0
57	MG	1A	3197	1/1	0.93	0.13	45,45,45,45	0
57	MG	1A	3639	1/1	0.93	0.12	46,46,46,46	0
57	MG	1A	3508	1/1	0.93	0.08	33,33,33,33	0
57	MG	1a	1677	1/1	0.93	0.18	57,57,57,57	0
57	MG	1A	3088	1/1	0.93	0.10	42,42,42,42	0
57	MG	2A	3332	1/1	0.93	0.09	59,59,59,59	0
57	MG	1A	3421	1/1	0.93	0.10	45,45,45,45	0
57	MG	2A	3688	1/1	0.93	0.11	56,56,56,56	0
57	MG	1A	3646	1/1	0.93	0.15	53,53,53,53	0
57	MG	2A	3691	1/1	0.93	0.07	43,43,43,43	0
57	MG	2A	3339	1/1	0.93	0.08	44,44,44,44	0
57	MG	1A	3514	1/1	0.93	0.06	49,49,49,49	0
57	MG	1A	3516	1/1	0.93	0.12	48,48,48,48	0
57	MG	1A	3817	1/1	0.93	0.09	59,59,59,59	0
57	MG	2A	3351	1/1	0.93	0.12	47,47,47,47	0
57	MG	1A	3022	1/1	0.93	0.14	49,49,49,49	0
57	MG	1A	3828	1/1	0.93	0.11	44,44,44,44	0
57	MG	2A	3704	1/1	0.93	0.12	58,58,58,58	0
57	MG	1a	1693	1/1	0.93	0.14	57,57,57,57	0
57	MG	1A	3832	1/1	0.93	0.09	49,49,49,49	0
57	MG	1A	3522	1/1	0.93	0.05	27,27,27,27	0
57	MG	2A	3713	1/1	0.93	0.12	47,47,47,47	0
57	MG	2A	3365	1/1	0.93	0.10	65,65,65,65	0
57	MG	2A	3717	1/1	0.93	0.10	65,65,65,65	0
57	MG	2A	3718	1/1	0.93	0.10	53,53,53,53	0
57	MG	2A	3721	1/1	0.93	0.12	59,59,59,59	0
57	MG	1A	3523	1/1	0.93	0.12	56,56,56,56	0
57	MG	2A	3367	1/1	0.93	0.09	41,41,41,41	0
57	MG	2A	3725	1/1	0.93	0.12	67,67,67,67	0
57	MG	1a	1699	1/1	0.93	0.18	50,50,50,50	0
57	MG	1A	3259	1/1	0.93	0.13	61,61,61,61	0
57	MG	1a	1701	1/1	0.93	0.23	51,51,51,51	0
57	MG	2A	3730	1/1	0.93	0.09	57,57,57,57	0
57	MG	2A	3378	1/1	0.93	0.12	64,64,64,64	0
57	MG	1l	202	1/1	0.93	0.10	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3202	1/1	0.93	0.08	39,39,39,39	0
57	MG	2A	3734	1/1	0.93	0.11	61,61,61,61	0
57	MG	1A	3842	1/1	0.93	0.10	35,35,35,35	0
57	MG	2A	3737	1/1	0.93	0.11	47,47,47,47	0
57	MG	1B	221	1/1	0.93	0.07	27,27,27,27	0
57	MG	1A	3846	1/1	0.93	0.09	34,34,34,34	0
57	MG	1a	1708	1/1	0.93	0.15	52,52,52,52	0
57	MG	1A	3344	1/1	0.93	0.12	28,28,28,28	0
57	MG	1A	3850	1/1	0.93	0.07	43,43,43,43	0
57	MG	2A	3396	1/1	0.93	0.09	49,49,49,49	0
57	MG	2A	3398	1/1	0.93	0.07	46,46,46,46	0
57	MG	2B	212	1/1	0.93	0.09	58,58,58,58	0
57	MG	2A	3007	1/1	0.93	0.08	45,45,45,45	0
57	MG	1B	228	1/1	0.93	0.07	53,53,53,53	0
57	MG	2A	3011	1/1	0.93	0.15	45,45,45,45	0
57	MG	2A	3014	1/1	0.93	0.14	61,61,61,61	0
57	MG	2A	3403	1/1	0.93	0.08	48,48,48,48	0
57	MG	1a	1721	1/1	0.93	0.08	58,58,58,58	0
57	MG	2D	309	1/1	0.93	0.12	64,64,64,64	0
57	MG	2A	3033	1/1	0.93	0.13	54,54,54,54	0
57	MG	1A	3851	1/1	0.93	0.07	32,32,32,32	0
57	MG	1A	3538	1/1	0.93	0.09	45,45,45,45	0
57	MG	2A	3412	1/1	0.93	0.08	55,55,55,55	0
57	MG	2A	3419	1/1	0.93	0.09	39,39,39,39	0
57	MG	2A	3420	1/1	0.93	0.13	40,40,40,40	0
57	MG	2A	3040	1/1	0.93	0.18	58,58,58,58	0
57	MG	2T	201	1/1	0.93	0.13	56,56,56,56	0
57	MG	2A	3042	1/1	0.93	0.12	53,53,53,53	0
57	MG	1A	3540	1/1	0.93	0.07	48,48,48,48	0
57	MG	2A	3048	1/1	0.93	0.07	53,53,53,53	0
57	MG	1A	3431	1/1	0.93	0.06	37,37,37,37	0
57	MG	2A	3051	1/1	0.93	0.27	57,57,57,57	0
57	MG	26	101	1/1	0.93	0.10	56,56,56,56	0
57	MG	1A	3550	1/1	0.93	0.08	44,44,44,44	0
57	MG	1A	3553	1/1	0.93	0.08	48,48,48,48	0
57	MG	1A	3345	1/1	0.93	0.09	55,55,55,55	0
57	MG	1A	3688	1/1	0.93	0.15	33,33,33,33	0
57	MG	2A	3063	1/1	0.93	0.17	60,60,60,60	0
57	MG	2A	3065	1/1	0.93	0.17	60,60,60,60	0
57	MG	1E	305	1/1	0.93	0.07	52,52,52,52	0
57	MG	2a	3014	1/1	0.93	0.12	54,54,54,54	0
57	MG	1a	1742	1/1	0.93	0.11	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2a	3016	1/1	0.93	0.16	60,60,60,60	0
57	MG	2a	3017	1/1	0.93	0.15	56,56,56,56	0
57	MG	1a	1743	1/1	0.93	0.11	50,50,50,50	0
57	MG	1a	1744	1/1	0.93	0.07	60,60,60,60	0
57	MG	1A	3882	1/1	0.93	0.11	40,40,40,40	0
57	MG	2A	3446	1/1	0.93	0.17	64,64,64,64	0
57	MG	1a	1750	1/1	0.93	0.19	74,74,74,74	0
57	MG	1A	3270	1/1	0.93	0.11	27,27,27,27	0
57	MG	2a	3031	1/1	0.93	0.20	54,54,54,54	0
57	MG	2A	3452	1/1	0.93	0.12	61,61,61,61	0
57	MG	2A	3453	1/1	0.93	0.09	51,51,51,51	0
57	MG	1A	3564	1/1	0.93	0.07	51,51,51,51	0
57	MG	1A	3569	1/1	0.93	0.09	34,34,34,34	0
57	MG	1A	3347	1/1	0.93	0.09	20,20,20,20	0
57	MG	2a	3041	1/1	0.93	0.13	61,61,61,61	0
57	MG	2a	3043	1/1	0.93	0.23	60,60,60,60	0
57	MG	2A	3458	1/1	0.93	0.13	47,47,47,47	0
57	MG	1A	3573	1/1	0.93	0.07	38,38,38,38	0
57	MG	1A	3350	1/1	0.93	0.07	24,24,24,24	0
57	MG	2A	3099	1/1	0.93	0.09	52,52,52,52	0
57	MG	1a	1763	1/1	0.93	0.10	62,62,62,62	0
57	MG	1A	3704	1/1	0.93	0.10	51,51,51,51	0
57	MG	1A	3271	1/1	0.93	0.07	50,50,50,50	0
57	MG	2a	3053	1/1	0.93	0.20	48,48,48,48	0
57	MG	2a	3058	1/1	0.93	0.15	67,67,67,67	0
57	MG	1Q	204	1/1	0.93	0.12	53,53,53,53	0
57	MG	2A	3479	1/1	0.93	0.09	53,53,53,53	0
57	MG	1A	3579	1/1	0.93	0.08	43,43,43,43	0
57	MG	2a	3063	1/1	0.93	0.15	63,63,63,63	0
57	MG	2A	3117	1/1	0.93	0.12	59,59,59,59	0
57	MG	1A	3901	1/1	0.93	0.13	40,40,40,40	0
57	MG	1A	3203	1/1	0.93	0.08	47,47,47,47	0
57	MG	2A	3128	1/1	0.93	0.19	47,47,47,47	0
57	MG	2A	3129	1/1	0.93	0.17	64,64,64,64	0
57	MG	1T	202	1/1	0.93	0.11	55,55,55,55	0
57	MG	1A	3906	1/1	0.93	0.11	42,42,42,42	0
57	MG	1V	204	1/1	0.93	0.11	45,45,45,45	0
57	MG	1A	3273	1/1	0.93	0.11	40,40,40,40	0
57	MG	2a	3082	1/1	0.93	0.13	61,61,61,61	0
57	MG	2a	3083	1/1	0.93	0.23	48,48,48,48	0
57	MG	1W	201	1/1	0.93	0.15	45,45,45,45	0
57	MG	2A	3501	1/1	0.93	0.07	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3144	1/1	0.93	0.11	47,47,47,47	0
57	MG	2a	3093	1/1	0.93	0.24	62,62,62,62	0
57	MG	1W	202	1/1	0.93	0.15	40,40,40,40	0
57	MG	2a	3097	1/1	0.93	0.22	60,60,60,60	0
57	MG	2a	3098	1/1	0.93	0.22	50,50,50,50	0
57	MG	1A	3453	1/1	0.93	0.07	58,58,58,58	0
57	MG	2A	3153	1/1	0.93	0.12	60,60,60,60	0
57	MG	1A	3919	1/1	0.93	0.06	13,13,13,13	0
57	MG	2A	3158	1/1	0.93	0.14	51,51,51,51	0
57	MG	1A	3083	1/1	0.93	0.17	32,32,32,32	0
57	MG	2a	3110	1/1	0.93	0.12	52,52,52,52	0
57	MG	1A	3290	1/1	0.93	0.09	52,52,52,52	0
57	MG	1A	3925	1/1	0.93	0.08	21,21,21,21	0
57	MG	1a	1788	1/1	0.93	0.08	69,69,69,69	0
57	MG	1A	3367	1/1	0.93	0.11	29,29,29,29	0
57	MG	1a	1791	1/1	0.93	0.11	55,55,55,55	0
57	MG	2a	3117	1/1	0.93	0.21	65,65,65,65	0
57	MG	1A	3168	1/1	0.93	0.11	52,52,52,52	0
57	MG	2a	3122	1/1	0.93	0.17	57,57,57,57	0
57	MG	1A	3376	1/1	0.93	0.10	42,42,42,42	0
57	MG	1a	1606	1/1	0.93	0.09	68,68,68,68	0
57	MG	2a	3128	1/1	0.93	0.09	60,60,60,60	0
57	MG	1A	3945	1/1	0.93	0.13	55,55,55,55	0
57	MG	1A	3946	1/1	0.93	0.11	46,46,46,46	0
57	MG	2a	3131	1/1	0.93	0.08	54,54,54,54	0
57	MG	1A	3170	1/1	0.93	0.08	49,49,49,49	0
57	MG	1A	3949	1/1	0.93	0.09	61,61,61,61	0
57	MG	1A	3594	1/1	0.93	0.08	23,23,23,23	0
57	MG	1A	3596	1/1	0.93	0.15	53,53,53,53	0
57	MG	1a	1618	1/1	0.93	0.16	56,56,56,56	0
57	MG	1a	1619	1/1	0.93	0.20	59,59,59,59	0
57	MG	1a	1623	1/1	0.93	0.12	57,57,57,57	0
57	MG	2a	3147	1/1	0.93	0.08	70,70,70,70	0
57	MG	1A	3087	1/1	0.93	0.08	38,38,38,38	0
57	MG	2A	3543	1/1	0.93	0.08	39,39,39,39	0
57	MG	2A	3546	1/1	0.93	0.15	37,37,37,37	0
57	MG	1A	3741	1/1	0.93	0.08	38,38,38,38	0
57	MG	2A	3550	1/1	0.93	0.08	58,58,58,58	0
57	MG	2A	3554	1/1	0.93	0.09	52,52,52,52	0
57	MG	1A	3963	1/1	0.93	0.09	26,26,26,26	0
57	MG	1A	3125	1/1	0.93	0.21	58,58,58,58	0
57	MG	1a	1814	1/1	0.93	0.19	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2a	3165	1/1	0.93	0.08	53,53,53,53	0
57	MG	1a	1816	1/1	0.93	0.09	58,58,58,58	0
57	MG	1a	1819	1/1	0.93	0.09	57,57,57,57	0
57	MG	2A	3218	1/1	0.93	0.10	43,43,43,43	0
57	MG	1a	1822	1/1	0.93	0.07	68,68,68,68	0
57	MG	1A	3387	1/1	0.93	0.13	50,50,50,50	0
57	MG	2A	3572	1/1	0.93	0.14	44,44,44,44	0
57	MG	1A	3132	1/1	0.93	0.32	41,41,41,41	0
57	MG	1a	1827	1/1	0.93	0.11	62,62,62,62	0
57	MG	2A	3580	1/1	0.93	0.07	59,59,59,59	0
57	MG	2A	3581	1/1	0.93	0.07	63,63,63,63	0
57	MG	1A	3389	1/1	0.93	0.11	46,46,46,46	0
57	MG	1A	3390	1/1	0.93	0.09	35,35,35,35	0
57	MG	1A	3392	1/1	0.93	0.09	53,53,53,53	0
57	MG	2A	3587	1/1	0.93	0.12	60,60,60,60	0
57	MG	1A	3393	1/1	0.93	0.10	56,56,56,56	0
57	MG	2a	3191	1/1	0.93	0.10	73,73,73,73	0
57	MG	1a	1648	1/1	0.93	0.21	56,56,56,56	0
57	MG	2A	3591	1/1	0.93	0.10	52,52,52,52	0
57	MG	2A	3242	1/1	0.93	0.18	61,61,61,61	0
57	MG	1A	3139	1/1	0.93	0.09	45,45,45,45	0
57	MG	2t	201	1/1	0.93	0.14	51,51,51,51	0
57	MG	2A	3601	1/1	0.93	0.09	66,66,66,66	0
57	MG	1A	3320	1/1	0.93	0.14	41,41,41,41	0
57	MG	1A	3623	1/1	0.93	0.09	53,53,53,53	0
58	MPD	18	104	8/8	0.93	0.13	25,36,38,39	0
57	MG	2A	3607	1/1	0.93	0.12	56,56,56,56	0
57	MG	1A	3321	1/1	0.93	0.15	27,27,27,27	0
57	MG	1A	3405	1/1	0.93	0.07	41,41,41,41	0
57	MG	1a	1840	1/1	0.93	0.11	62,62,62,62	0
57	MG	1a	1661	1/1	0.93	0.11	62,62,62,62	0
57	MG	2A	3639	1/1	0.94	0.10	50,50,50,50	0
57	MG	2A	3305	1/1	0.94	0.12	47,47,47,47	0
57	MG	1A	3713	1/1	0.94	0.07	32,32,32,32	0
57	MG	2A	3308	1/1	0.94	0.14	38,38,38,38	0
57	MG	1a	1705	1/1	0.94	0.11	59,59,59,59	0
57	MG	2A	3656	1/1	0.94	0.10	65,65,65,65	0
57	MG	2A	3658	1/1	0.94	0.08	49,49,49,49	0
57	MG	1A	3131	1/1	0.94	0.14	49,49,49,49	0
57	MG	2A	3316	1/1	0.94	0.05	34,34,34,34	0
57	MG	1A	3891	1/1	0.94	0.16	55,55,55,55	0
57	MG	1A	3228	1/1	0.94	0.12	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3296	1/1	0.94	0.11	49,49,49,49	0
57	MG	1a	1713	1/1	0.94	0.10	69,69,69,69	0
57	MG	2A	3325	1/1	0.94	0.13	58,58,58,58	0
57	MG	2A	3326	1/1	0.94	0.12	41,41,41,41	0
57	MG	2A	3328	1/1	0.94	0.09	54,54,54,54	0
57	MG	2A	3680	1/1	0.94	0.07	51,51,51,51	0
57	MG	1F	310	1/1	0.94	0.10	31,31,31,31	0
57	MG	1o	101	1/1	0.94	0.15	59,59,59,59	0
57	MG	1a	1715	1/1	0.94	0.07	38,38,38,38	0
57	MG	1F	314	1/1	0.94	0.18	60,60,60,60	0
57	MG	2A	3687	1/1	0.94	0.07	49,49,49,49	0
57	MG	1a	1720	1/1	0.94	0.09	62,62,62,62	0
57	MG	1A	3427	1/1	0.94	0.14	39,39,39,39	0
57	MG	1A	3301	1/1	0.94	0.08	36,36,36,36	0
57	MG	1A	3505	1/1	0.94	0.07	27,27,27,27	0
57	MG	2A	3349	1/1	0.94	0.09	44,44,44,44	0
57	MG	1N	202	1/1	0.94	0.10	42,42,42,42	0
57	MG	2A	3353	1/1	0.94	0.11	48,48,48,48	0
57	MG	2A	3005	1/1	0.94	0.10	57,57,57,57	0
57	MG	1a	1726	1/1	0.94	0.10	62,62,62,62	0
57	MG	2A	3701	1/1	0.94	0.10	50,50,50,50	0
57	MG	1A	3067	1/1	0.94	0.08	40,40,40,40	0
57	MG	2A	3361	1/1	0.94	0.13	47,47,47,47	0
57	MG	1A	3369	1/1	0.94	0.17	60,60,60,60	0
57	MG	1a	1732	1/1	0.94	0.13	64,64,64,64	0
57	MG	2A	3708	1/1	0.94	0.10	51,51,51,51	0
57	MG	2A	3711	1/1	0.94	0.08	53,53,53,53	0
57	MG	2A	3016	1/1	0.94	0.16	54,54,54,54	0
57	MG	2A	3023	1/1	0.94	0.19	60,60,60,60	0
57	MG	2A	3714	1/1	0.94	0.13	42,42,42,42	0
57	MG	1A	3905	1/1	0.94	0.22	35,35,35,35	0
57	MG	2A	3029	1/1	0.94	0.10	63,63,63,63	0
57	MG	2A	3369	1/1	0.94	0.11	51,51,51,51	0
57	MG	1A	3233	1/1	0.94	0.12	34,34,34,34	0
57	MG	2A	3034	1/1	0.94	0.28	64,64,64,64	0
57	MG	1A	3613	1/1	0.94	0.09	57,57,57,57	0
57	MG	2A	3724	1/1	0.94	0.20	59,59,59,59	0
57	MG	1A	3914	1/1	0.94	0.07	50,50,50,50	0
57	MG	1a	1741	1/1	0.94	0.07	52,52,52,52	0
57	MG	1A	3434	1/1	0.94	0.13	33,33,33,33	0
57	MG	1A	3743	1/1	0.94	0.07	38,38,38,38	0
57	MG	2A	3045	1/1	0.94	0.07	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3046	1/1	0.94	0.15	50,50,50,50	0
57	MG	1A	3745	1/1	0.94	0.06	28,28,28,28	0
57	MG	1a	1746	1/1	0.94	0.09	63,63,63,63	0
57	MG	1a	1747	1/1	0.94	0.09	52,52,52,52	0
57	MG	2A	3397	1/1	0.94	0.12	42,42,42,42	0
57	MG	2A	3736	1/1	0.94	0.21	59,59,59,59	0
57	MG	1A	3921	1/1	0.94	0.08	37,37,37,37	0
57	MG	2A	3057	1/1	0.94	0.20	62,62,62,62	0
57	MG	1A	3374	1/1	0.94	0.08	25,25,25,25	0
57	MG	1U	201	1/1	0.94	0.18	27,27,27,27	0
57	MG	1A	3622	1/1	0.94	0.14	30,30,30,30	0
57	MG	1a	1754	1/1	0.94	0.09	66,66,66,66	0
57	MG	2A	3064	1/1	0.94	0.06	37,37,37,37	0
57	MG	1A	3436	1/1	0.94	0.05	26,26,26,26	0
57	MG	2A	3066	1/1	0.94	0.07	53,53,53,53	0
57	MG	2A	3067	1/1	0.94	0.08	49,49,49,49	0
57	MG	1A	3626	1/1	0.94	0.17	35,35,35,35	0
57	MG	2A	3415	1/1	0.94	0.07	56,56,56,56	0
57	MG	2A	3418	1/1	0.94	0.09	62,62,62,62	0
57	MG	1A	3938	1/1	0.94	0.09	50,50,50,50	0
57	MG	1A	3758	1/1	0.94	0.10	42,42,42,42	0
57	MG	2D	308	1/1	0.94	0.13	44,44,44,44	0
57	MG	1A	3234	1/1	0.94	0.17	38,38,38,38	0
57	MG	1A	3762	1/1	0.94	0.23	59,59,59,59	0
57	MG	2E	302	1/1	0.94	0.07	43,43,43,43	0
57	MG	2F	303	1/1	0.94	0.14	44,44,44,44	0
57	MG	10	107	1/1	0.94	0.08	50,50,50,50	0
57	MG	11	102	1/1	0.94	0.21	52,52,52,52	0
57	MG	2A	3425	1/1	0.94	0.07	55,55,55,55	0
57	MG	1A	3235	1/1	0.94	0.11	51,51,51,51	0
57	MG	2A	3091	1/1	0.94	0.09	42,42,42,42	0
57	MG	2Q	204	1/1	0.94	0.07	46,46,46,46	0
57	MG	1A	3526	1/1	0.94	0.06	22,22,22,22	0
57	MG	17	104	1/1	0.94	0.16	46,46,46,46	0
57	MG	2A	3094	1/1	0.94	0.13	45,45,45,45	0
57	MG	1A	3528	1/1	0.94	0.11	29,29,29,29	0
57	MG	2A	3097	1/1	0.94	0.11	68,68,68,68	0
57	MG	2W	201	1/1	0.94	0.18	44,44,44,44	0
57	MG	20	102	1/1	0.94	0.13	58,58,58,58	0
57	MG	1A	3631	1/1	0.94	0.07	24,24,24,24	0
57	MG	1A	3529	1/1	0.94	0.10	22,22,22,22	0
57	MG	25	103	1/1	0.94	0.09	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1a	1604	1/1	0.94	0.12	48,48,48,48	0
57	MG	1a	1605	1/1	0.94	0.10	62,62,62,62	0
57	MG	1A	3776	1/1	0.94	0.13	35,35,35,35	0
57	MG	2A	3109	1/1	0.94	0.10	49,49,49,49	0
57	MG	1A	3962	1/1	0.94	0.07	36,36,36,36	0
57	MG	2a	3008	1/1	0.94	0.11	60,60,60,60	0
57	MG	2a	3009	1/1	0.94	0.16	55,55,55,55	0
57	MG	1a	1781	1/1	0.94	0.10	57,57,57,57	0
57	MG	1A	3634	1/1	0.94	0.07	16,16,16,16	0
57	MG	2A	3118	1/1	0.94	0.17	46,46,46,46	0
57	MG	1a	1610	1/1	0.94	0.09	58,58,58,58	0
57	MG	2A	3123	1/1	0.94	0.21	49,49,49,49	0
57	MG	1A	3441	1/1	0.94	0.11	34,34,34,34	0
57	MG	1a	1612	1/1	0.94	0.17	60,60,60,60	0
57	MG	1A	3027	1/1	0.94	0.09	51,51,51,51	0
57	MG	1A	3383	1/1	0.94	0.11	40,40,40,40	0
57	MG	1A	3384	1/1	0.94	0.06	31,31,31,31	0
57	MG	1A	3790	1/1	0.94	0.10	47,47,47,47	0
57	MG	2a	3027	1/1	0.94	0.31	65,65,65,65	0
57	MG	2A	3465	1/1	0.94	0.09	54,54,54,54	0
57	MG	2A	3469	1/1	0.94	0.10	57,57,57,57	0
57	MG	1A	3449	1/1	0.94	0.08	40,40,40,40	0
57	MG	2a	3032	1/1	0.94	0.16	60,60,60,60	0
57	MG	2a	3033	1/1	0.94	0.14	57,57,57,57	0
57	MG	2A	3471	1/1	0.94	0.11	62,62,62,62	0
57	MG	2A	3137	1/1	0.94	0.18	52,52,52,52	0
57	MG	1a	1622	1/1	0.94	0.07	51,51,51,51	0
57	MG	2A	3476	1/1	0.94	0.07	53,53,53,53	0
57	MG	1A	3450	1/1	0.94	0.08	36,36,36,36	0
57	MG	2A	3145	1/1	0.94	0.09	55,55,55,55	0
57	MG	1A	3977	1/1	0.94	0.09	52,52,52,52	0
57	MG	1A	3978	1/1	0.94	0.08	55,55,55,55	0
57	MG	2A	3482	1/1	0.94	0.14	53,53,53,53	0
57	MG	2A	3151	1/1	0.94	0.07	53,53,53,53	0
57	MG	1a	1629	1/1	0.94	0.08	50,50,50,50	0
57	MG	1a	1800	1/1	0.94	0.13	60,60,60,60	0
57	MG	2A	3488	1/1	0.94	0.09	31,31,31,31	0
57	MG	1A	3330	1/1	0.94	0.07	37,37,37,37	0
57	MG	1A	3551	1/1	0.94	0.07	36,36,36,36	0
57	MG	2a	3054	1/1	0.94	0.07	38,38,38,38	0
57	MG	2a	3055	1/1	0.94	0.11	66,66,66,66	0
57	MG	2a	3056	1/1	0.94	0.10	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3800	1/1	0.94	0.08	31,31,31,31	0
57	MG	1A	3006	1/1	0.94	0.10	35,35,35,35	0
57	MG	1a	1637	1/1	0.94	0.07	43,43,43,43	0
57	MG	2a	3061	1/1	0.94	0.14	54,54,54,54	0
57	MG	1A	3652	1/1	0.94	0.10	41,41,41,41	0
57	MG	2A	3499	1/1	0.94	0.11	53,53,53,53	0
57	MG	2a	3064	1/1	0.94	0.12	42,42,42,42	0
57	MG	1A	3039	1/1	0.94	0.13	41,41,41,41	0
57	MG	1a	1644	1/1	0.94	0.16	49,49,49,49	0
57	MG	1A	3661	1/1	0.94	0.13	40,40,40,40	0
57	MG	1A	3810	1/1	0.94	0.07	73,73,73,73	0
57	MG	2a	3070	1/1	0.94	0.08	56,56,56,56	0
57	MG	1A	3011	1/1	0.94	0.08	50,50,50,50	0
57	MG	2A	3508	1/1	0.94	0.16	56,56,56,56	0
57	MG	2A	3177	1/1	0.94	0.21	50,50,50,50	0
57	MG	2a	3077	1/1	0.94	0.13	64,64,64,64	0
57	MG	1a	1817	1/1	0.94	0.07	78,78,78,78	0
57	MG	1A	3562	1/1	0.94	0.07	38,38,38,38	0
57	MG	1A	3563	1/1	0.94	0.10	40,40,40,40	0
57	MG	2A	3517	1/1	0.94	0.17	59,59,59,59	0
57	MG	2A	3186	1/1	0.94	0.15	62,62,62,62	0
57	MG	2a	3087	1/1	0.94	0.07	60,60,60,60	0
57	MG	1A	3338	1/1	0.94	0.09	42,42,42,42	0
57	MG	2a	3090	1/1	0.94	0.19	50,50,50,50	0
57	MG	1A	3670	1/1	0.94	0.14	52,52,52,52	0
57	MG	2A	3190	1/1	0.94	0.14	59,59,59,59	0
57	MG	1A	3568	1/1	0.94	0.08	52,52,52,52	0
57	MG	1a	1660	1/1	0.94	0.22	61,61,61,61	0
57	MG	1A	3047	1/1	0.94	0.08	37,37,37,37	0
57	MG	1a	1831	1/1	0.94	0.14	59,59,59,59	0
57	MG	1A	3166	1/1	0.94	0.16	49,49,49,49	0
57	MG	2A	3201	1/1	0.94	0.10	54,54,54,54	0
57	MG	1A	3014	1/1	0.94	0.16	55,55,55,55	0
57	MG	2A	3204	1/1	0.94	0.10	51,51,51,51	0
57	MG	2a	3108	1/1	0.94	0.09	45,45,45,45	0
57	MG	2A	3205	1/1	0.94	0.07	52,52,52,52	0
57	MG	1A	4019	1/1	0.94	0.06	24,24,24,24	0
57	MG	1A	4021	1/1	0.94	0.08	39,39,39,39	0
57	MG	2A	3209	1/1	0.94	0.18	56,56,56,56	0
57	MG	2A	3539	1/1	0.94	0.10	60,60,60,60	0
57	MG	2A	3211	1/1	0.94	0.11	41,41,41,41	0
57	MG	1A	3474	1/1	0.94	0.08	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3216	1/1	0.94	0.14	57,57,57,57	0
57	MG	2a	3120	1/1	0.94	0.12	60,60,60,60	0
57	MG	1A	3475	1/1	0.94	0.09	29,29,29,29	0
57	MG	1A	4025	1/1	0.94	0.23	45,45,45,45	0
57	MG	2A	3552	1/1	0.94	0.08	50,50,50,50	0
57	MG	1A	3845	1/1	0.94	0.08	41,41,41,41	0
57	MG	1a	1670	1/1	0.94	0.10	58,58,58,58	0
57	MG	1A	3395	1/1	0.94	0.08	42,42,42,42	0
57	MG	1a	1672	1/1	0.94	0.17	57,57,57,57	0
57	MG	1A	3107	1/1	0.94	0.09	37,37,37,37	0
57	MG	2a	3133	1/1	0.94	0.14	63,63,63,63	0
57	MG	2A	3227	1/1	0.94	0.14	55,55,55,55	0
57	MG	1a	1846	1/1	0.94	0.11	59,59,59,59	0
57	MG	2A	3232	1/1	0.94	0.10	64,64,64,64	0
57	MG	2A	3233	1/1	0.94	0.11	53,53,53,53	0
57	MG	1B	205	1/1	0.94	0.11	50,50,50,50	0
57	MG	1A	3172	1/1	0.94	0.08	41,41,41,41	0
57	MG	2a	3146	1/1	0.94	0.09	56,56,56,56	0
57	MG	2A	3576	1/1	0.94	0.10	51,51,51,51	0
57	MG	1A	3276	1/1	0.94	0.13	58,58,58,58	0
57	MG	2a	3152	1/1	0.94	0.09	69,69,69,69	0
57	MG	1a	1852	1/1	0.94	0.07	60,60,60,60	0
57	MG	2A	3244	1/1	0.94	0.12	55,55,55,55	0
57	MG	1A	3697	1/1	0.94	0.09	75,75,75,75	0
57	MG	2a	3157	1/1	0.94	0.14	63,63,63,63	0
57	MG	1A	3583	1/1	0.94	0.11	40,40,40,40	0
57	MG	1a	1679	1/1	0.94	0.10	52,52,52,52	0
57	MG	2a	3161	1/1	0.94	0.10	47,47,47,47	0
57	MG	1a	1680	1/1	0.94	0.07	48,48,48,48	0
57	MG	1B	213	1/1	0.94	0.09	47,47,47,47	0
57	MG	1a	1864	1/1	0.94	0.08	59,59,59,59	0
57	MG	1A	3855	1/1	0.94	0.09	34,34,34,34	0
57	MG	1B	218	1/1	0.94	0.08	52,52,52,52	0
57	MG	2A	3595	1/1	0.94	0.08	46,46,46,46	0
57	MG	1a	1870	1/1	0.94	0.08	64,64,64,64	0
57	MG	2A	3597	1/1	0.94	0.07	63,63,63,63	0
57	MG	1A	3860	1/1	0.94	0.09	36,36,36,36	0
57	MG	1A	3481	1/1	0.94	0.07	43,43,43,43	0
57	MG	1A	3868	1/1	0.94	0.07	45,45,45,45	0
57	MG	1A	3061	1/1	0.94	0.20	43,43,43,43	0
57	MG	2a	3178	1/1	0.94	0.14	53,53,53,53	0
57	MG	1a	1875	1/1	0.94	0.10	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1a	1691	1/1	0.94	0.09	53,53,53,53	0
57	MG	1A	3412	1/1	0.94	0.05	33,33,33,33	0
57	MG	1a	1879	1/1	0.94	0.13	65,65,65,65	0
57	MG	1A	3874	1/1	0.94	0.07	40,40,40,40	0
57	MG	2A	3281	1/1	0.94	0.18	56,56,56,56	0
57	MG	1A	3348	1/1	0.94	0.12	43,43,43,43	0
57	MG	1A	3002	1/1	0.94	0.10	40,40,40,40	0
57	MG	1A	3418	1/1	0.94	0.08	21,21,21,21	0
57	MG	2e	202	1/1	0.94	0.10	65,65,65,65	0
57	MG	2A	3287	1/1	0.94	0.19	56,56,56,56	0
57	MG	1A	3181	1/1	0.94	0.15	46,46,46,46	0
57	MG	2A	3293	1/1	0.94	0.12	54,54,54,54	0
57	MG	2A	3295	1/1	0.94	0.16	56,56,56,56	0
57	MG	2A	3296	1/1	0.94	0.12	60,60,60,60	0
57	MG	2A	3628	1/1	0.94	0.06	64,64,64,64	0
57	MG	1A	3711	1/1	0.94	0.07	38,38,38,38	0
57	MG	1D	315	1/1	0.94	0.19	63,63,63,63	0
57	MG	2A	3631	1/1	0.94	0.12	53,53,53,53	0
57	MG	2A	3299	1/1	0.94	0.08	38,38,38,38	0
57	MG	2A	3301	1/1	0.94	0.11	21,21,21,21	0
57	MG	2A	3635	1/1	0.94	0.10	55,55,55,55	0
57	MG	2A	3304	1/1	0.94	0.07	49,49,49,49	0
57	MG	1A	3974	1/1	0.95	0.07	45,45,45,45	0
57	MG	2A	3108	1/1	0.95	0.13	58,58,58,58	0
57	MG	1A	3782	1/1	0.95	0.11	36,36,36,36	0
57	MG	2A	3112	1/1	0.95	0.09	47,47,47,47	0
57	MG	2A	3113	1/1	0.95	0.20	45,45,45,45	0
57	MG	1A	3783	1/1	0.95	0.05	27,27,27,27	0
57	MG	2A	3707	1/1	0.95	0.06	73,73,73,73	0
57	MG	1A	3981	1/1	0.95	0.09	46,46,46,46	0
57	MG	2A	3710	1/1	0.95	0.06	53,53,53,53	0
57	MG	1A	3070	1/1	0.95	0.13	22,22,22,22	0
57	MG	1a	1802	1/1	0.95	0.10	55,55,55,55	0
57	MG	2A	3119	1/1	0.95	0.11	43,43,43,43	0
57	MG	1A	3456	1/1	0.95	0.14	51,51,51,51	0
57	MG	2A	3122	1/1	0.95	0.08	41,41,41,41	0
57	MG	2A	3411	1/1	0.95	0.10	56,56,56,56	0
57	MG	1a	1635	1/1	0.95	0.19	63,63,63,63	0
57	MG	2A	3719	1/1	0.95	0.08	58,58,58,58	0
57	MG	1A	3537	1/1	0.95	0.18	40,40,40,40	0
57	MG	1a	1806	1/1	0.95	0.09	66,66,66,66	0
57	MG	1A	3269	1/1	0.95	0.09	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3130	1/1	0.95	0.25	45,45,45,45	0
57	MG	1A	3642	1/1	0.95	0.08	51,51,51,51	0
57	MG	2A	3133	1/1	0.95	0.15	46,46,46,46	0
57	MG	1a	1639	1/1	0.95	0.16	60,60,60,60	0
57	MG	1a	1640	1/1	0.95	0.11	53,53,53,53	0
57	MG	1A	3398	1/1	0.95	0.14	49,49,49,49	0
57	MG	1a	1643	1/1	0.95	0.10	64,64,64,64	0
57	MG	2A	3427	1/1	0.95	0.10	52,52,52,52	0
57	MG	1A	3541	1/1	0.95	0.07	47,47,47,47	0
57	MG	2A	3143	1/1	0.95	0.14	56,56,56,56	0
57	MG	1A	3205	1/1	0.95	0.16	46,46,46,46	0
57	MG	1A	3548	1/1	0.95	0.07	43,43,43,43	0
57	MG	1A	3549	1/1	0.95	0.06	25,25,25,25	0
57	MG	1A	3804	1/1	0.95	0.09	51,51,51,51	0
57	MG	1A	4001	1/1	0.95	0.09	28,28,28,28	0
57	MG	2A	3435	1/1	0.95	0.07	36,36,36,36	0
57	MG	1a	1825	1/1	0.95	0.08	49,49,49,49	0
57	MG	2B	205	1/1	0.95	0.08	49,49,49,49	0
57	MG	2B	206	1/1	0.95	0.06	42,42,42,42	0
57	MG	1A	3075	1/1	0.95	0.10	41,41,41,41	0
57	MG	2A	3439	1/1	0.95	0.12	64,64,64,64	0
57	MG	2A	3156	1/1	0.95	0.09	60,60,60,60	0
57	MG	1A	3031	1/1	0.95	0.08	16,16,16,16	0
57	MG	1A	4006	1/1	0.95	0.10	29,29,29,29	0
57	MG	1A	3655	1/1	0.95	0.11	39,39,39,39	0
57	MG	1A	3656	1/1	0.95	0.12	52,52,52,52	0
57	MG	2B	217	1/1	0.95	0.10	57,57,57,57	0
57	MG	2A	3450	1/1	0.95	0.11	57,57,57,57	0
57	MG	2A	3163	1/1	0.95	0.11	56,56,56,56	0
57	MG	1A	3659	1/1	0.95	0.07	30,30,30,30	0
57	MG	2D	305	1/1	0.95	0.26	46,46,46,46	0
57	MG	1A	3552	1/1	0.95	0.07	47,47,47,47	0
57	MG	1A	4018	1/1	0.95	0.10	41,41,41,41	0
57	MG	1A	3407	1/1	0.95	0.07	35,35,35,35	0
57	MG	1A	3470	1/1	0.95	0.07	60,60,60,60	0
57	MG	2F	301	1/1	0.95	0.13	42,42,42,42	0
57	MG	1A	3831	1/1	0.95	0.07	40,40,40,40	0
57	MG	2G	3301	1/1	0.95	0.06	68,68,68,68	0
57	MG	1A	3471	1/1	0.95	0.11	50,50,50,50	0
57	MG	1A	3176	1/1	0.95	0.10	39,39,39,39	0
57	MG	1A	3211	1/1	0.95	0.24	40,40,40,40	0
57	MG	2P	202	1/1	0.95	0.05	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1B	201	1/1	0.95	0.10	46,46,46,46	0
57	MG	2A	3466	1/1	0.95	0.12	48,48,48,48	0
57	MG	2A	3467	1/1	0.95	0.10	60,60,60,60	0
57	MG	1A	3476	1/1	0.95	0.08	22,22,22,22	0
57	MG	2A	3183	1/1	0.95	0.08	46,46,46,46	0
57	MG	1A	3840	1/1	0.95	0.07	15,15,15,15	0
57	MG	1B	204	1/1	0.95	0.12	53,53,53,53	0
57	MG	2A	3474	1/1	0.95	0.15	46,46,46,46	0
57	MG	1a	1848	1/1	0.95	0.07	52,52,52,52	0
57	MG	2W	202	1/1	0.95	0.12	51,51,51,51	0
57	MG	1A	3672	1/1	0.95	0.06	38,38,38,38	0
57	MG	2A	3477	1/1	0.95	0.07	57,57,57,57	0
57	MG	1A	3140	1/1	0.95	0.09	39,39,39,39	0
57	MG	2A	3196	1/1	0.95	0.11	51,51,51,51	0
57	MG	1A	3351	1/1	0.95	0.06	37,37,37,37	0
57	MG	1A	3677	1/1	0.95	0.07	27,27,27,27	0
57	MG	1a	1853	1/1	0.95	0.06	53,53,53,53	0
57	MG	1A	3847	1/1	0.95	0.07	44,44,44,44	0
57	MG	2a	3003	1/1	0.95	0.19	57,57,57,57	0
57	MG	1a	1857	1/1	0.95	0.12	64,64,64,64	0
57	MG	1A	3679	1/1	0.95	0.16	47,47,47,47	0
57	MG	1A	3417	1/1	0.95	0.10	21,21,21,21	0
57	MG	1A	3572	1/1	0.95	0.06	45,45,45,45	0
57	MG	2A	3206	1/1	0.95	0.07	40,40,40,40	0
57	MG	2a	3012	1/1	0.95	0.22	58,58,58,58	0
57	MG	2A	3492	1/1	0.95	0.07	61,61,61,61	0
57	MG	1A	3280	1/1	0.95	0.08	52,52,52,52	0
57	MG	2A	3494	1/1	0.95	0.08	33,33,33,33	0
57	MG	1a	1863	1/1	0.95	0.14	50,50,50,50	0
57	MG	1A	3685	1/1	0.95	0.12	47,47,47,47	0
57	MG	1A	3282	1/1	0.95	0.08	38,38,38,38	0
57	MG	1A	3857	1/1	0.95	0.21	50,50,50,50	0
57	MG	1A	3284	1/1	0.95	0.07	37,37,37,37	0
57	MG	2a	3023	1/1	0.95	0.09	54,54,54,54	0
57	MG	2a	3024	1/1	0.95	0.06	46,46,46,46	0
57	MG	1B	227	1/1	0.95	0.07	52,52,52,52	0
57	MG	2a	3026	1/1	0.95	0.24	69,69,69,69	0
57	MG	1A	3578	1/1	0.95	0.07	62,62,62,62	0
57	MG	2A	3219	1/1	0.95	0.12	53,53,53,53	0
57	MG	2a	3029	1/1	0.95	0.09	51,51,51,51	0
57	MG	1A	3864	1/1	0.95	0.08	25,25,25,25	0
57	MG	1A	3866	1/1	0.95	0.14	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3509	1/1	0.95	0.06	39,39,39,39	0
57	MG	1A	3483	1/1	0.95	0.07	41,41,41,41	0
57	MG	2a	3034	1/1	0.95	0.17	52,52,52,52	0
57	MG	2A	3224	1/1	0.95	0.09	51,51,51,51	0
57	MG	1a	1876	1/1	0.95	0.11	69,69,69,69	0
57	MG	2A	3514	1/1	0.95	0.09	66,66,66,66	0
57	MG	1A	3360	1/1	0.95	0.09	38,38,38,38	0
57	MG	1A	3488	1/1	0.95	0.11	51,51,51,51	0
57	MG	2A	3229	1/1	0.95	0.09	43,43,43,43	0
57	MG	1A	3489	1/1	0.95	0.08	46,46,46,46	0
57	MG	2a	3044	1/1	0.95	0.18	56,56,56,56	0
57	MG	1A	3875	1/1	0.95	0.08	47,47,47,47	0
57	MG	1A	3214	1/1	0.95	0.21	38,38,38,38	0
57	MG	1A	3584	1/1	0.95	0.07	17,17,17,17	0
57	MG	2A	3238	1/1	0.95	0.19	45,45,45,45	0
57	MG	2A	3239	1/1	0.95	0.21	43,43,43,43	0
57	MG	1A	3585	1/1	0.95	0.11	36,36,36,36	0
57	MG	1d	304	1/1	0.95	0.14	62,62,62,62	0
57	MG	2a	3052	1/1	0.95	0.14	43,43,43,43	0
57	MG	1E	306	1/1	0.95	0.08	38,38,38,38	0
57	MG	1E	308	1/1	0.95	0.09	48,48,48,48	0
57	MG	1A	3425	1/1	0.95	0.05	19,19,19,19	0
57	MG	1a	1710	1/1	0.95	0.17	52,52,52,52	0
57	MG	1A	3426	1/1	0.95	0.19	41,41,41,41	0
57	MG	2A	3248	1/1	0.95	0.08	51,51,51,51	0
57	MG	1F	311	1/1	0.95	0.18	39,39,39,39	0
57	MG	1F	312	1/1	0.95	0.20	42,42,42,42	0
57	MG	1A	3142	1/1	0.95	0.08	39,39,39,39	0
57	MG	1F	316	1/1	0.95	0.11	32,32,32,32	0
57	MG	1A	3889	1/1	0.95	0.06	28,28,28,28	0
57	MG	2A	3259	1/1	0.95	0.18	56,56,56,56	0
57	MG	2A	3260	1/1	0.95	0.17	57,57,57,57	0
57	MG	1A	3590	1/1	0.95	0.16	59,59,59,59	0
57	MG	1A	3185	1/1	0.95	0.23	37,37,37,37	0
57	MG	2a	3069	1/1	0.95	0.09	57,57,57,57	0
57	MG	2A	3555	1/1	0.95	0.06	56,56,56,56	0
57	MG	1A	3058	1/1	0.95	0.07	25,25,25,25	0
57	MG	2A	3268	1/1	0.95	0.11	21,21,21,21	0
57	MG	1A	3500	1/1	0.95	0.15	25,25,25,25	0
57	MG	2A	3562	1/1	0.95	0.13	48,48,48,48	0
57	MG	1A	3188	1/1	0.95	0.09	32,32,32,32	0
57	MG	2a	3079	1/1	0.95	0.08	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3718	1/1	0.95	0.13	60,60,60,60	0
57	MG	2A	3568	1/1	0.95	0.09	52,52,52,52	0
57	MG	1a	1731	1/1	0.95	0.10	55,55,55,55	0
57	MG	2a	3084	1/1	0.95	0.20	54,54,54,54	0
57	MG	1x	101	1/1	0.95	0.07	46,46,46,46	0
57	MG	1A	3719	1/1	0.95	0.19	38,38,38,38	0
57	MG	2A	3002	1/1	0.95	0.08	54,54,54,54	0
57	MG	2a	3089	1/1	0.95	0.08	52,52,52,52	0
57	MG	2A	3280	1/1	0.95	0.09	47,47,47,47	0
57	MG	1a	1733	1/1	0.95	0.09	65,65,65,65	0
57	MG	1A	3432	1/1	0.95	0.05	33,33,33,33	0
57	MG	1A	3724	1/1	0.95	0.11	25,25,25,25	0
57	MG	2A	3285	1/1	0.95	0.07	53,53,53,53	0
57	MG	1A	3086	1/1	0.95	0.10	43,43,43,43	0
57	MG	1A	3190	1/1	0.95	0.09	53,53,53,53	0
57	MG	2A	3289	1/1	0.95	0.09	46,46,46,46	0
57	MG	2A	3585	1/1	0.95	0.09	46,46,46,46	0
57	MG	1A	3117	1/1	0.95	0.06	31,31,31,31	0
57	MG	1T	201	1/1	0.95	0.07	36,36,36,36	0
57	MG	2A	3017	1/1	0.95	0.11	52,52,52,52	0
57	MG	1A	3600	1/1	0.95	0.11	35,35,35,35	0
57	MG	1A	3601	1/1	0.95	0.07	40,40,40,40	0
57	MG	2A	3028	1/1	0.95	0.08	38,38,38,38	0
57	MG	1A	3602	1/1	0.95	0.07	35,35,35,35	0
57	MG	1U	203	1/1	0.95	0.26	55,55,55,55	0
57	MG	1A	3195	1/1	0.95	0.15	60,60,60,60	0
57	MG	2A	3602	1/1	0.95	0.07	35,35,35,35	0
57	MG	2a	3118	1/1	0.95	0.18	60,60,60,60	0
57	MG	1A	3739	1/1	0.95	0.07	31,31,31,31	0
57	MG	2A	3605	1/1	0.95	0.07	64,64,64,64	0
57	MG	2A	3306	1/1	0.95	0.15	37,37,37,37	0
57	MG	2a	3123	1/1	0.95	0.07	61,61,61,61	0
57	MG	2a	3124	1/1	0.95	0.11	73,73,73,73	0
57	MG	1A	3511	1/1	0.95	0.10	48,48,48,48	0
57	MG	1A	3437	1/1	0.95	0.08	45,45,45,45	0
57	MG	1X	101	1/1	0.95	0.07	40,40,40,40	0
57	MG	1A	3239	1/1	0.95	0.33	39,39,39,39	0
57	MG	1A	3933	1/1	0.95	0.09	48,48,48,48	0
57	MG	2A	3612	1/1	0.95	0.06	50,50,50,50	0
57	MG	1A	3748	1/1	0.95	0.13	43,43,43,43	0
57	MG	2A	3047	1/1	0.95	0.17	51,51,51,51	0
57	MG	1a	1760	1/1	0.95	0.11	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1a	1761	1/1	0.95	0.08	61,61,61,61	0
57	MG	2A	3324	1/1	0.95	0.17	64,64,64,64	0
57	MG	2A	3622	1/1	0.95	0.09	43,43,43,43	0
57	MG	1A	3936	1/1	0.95	0.08	55,55,55,55	0
57	MG	1A	3610	1/1	0.95	0.07	43,43,43,43	0
57	MG	2a	3145	1/1	0.95	0.07	56,56,56,56	0
57	MG	1A	3244	1/1	0.95	0.08	63,63,63,63	0
57	MG	1A	3517	1/1	0.95	0.07	46,46,46,46	0
57	MG	1a	1767	1/1	0.95	0.10	56,56,56,56	0
57	MG	15	108	1/1	0.95	0.10	47,47,47,47	0
57	MG	1A	3520	1/1	0.95	0.06	44,44,44,44	0
57	MG	1A	3618	1/1	0.95	0.10	33,33,33,33	0
57	MG	1A	3948	1/1	0.95	0.13	53,53,53,53	0
57	MG	1A	3324	1/1	0.95	0.08	40,40,40,40	0
57	MG	2A	3633	1/1	0.95	0.07	67,67,67,67	0
57	MG	1A	3761	1/1	0.95	0.15	47,47,47,47	0
57	MG	1A	3159	1/1	0.95	0.05	35,35,35,35	0
57	MG	2A	3070	1/1	0.95	0.08	49,49,49,49	0
57	MG	2A	3638	1/1	0.95	0.06	63,63,63,63	0
57	MG	2A	3352	1/1	0.95	0.10	57,57,57,57	0
57	MG	1A	3952	1/1	0.95	0.09	55,55,55,55	0
57	MG	2A	3354	1/1	0.95	0.10	39,39,39,39	0
57	MG	2A	3647	1/1	0.95	0.10	60,60,60,60	0
57	MG	2A	3650	1/1	0.95	0.07	49,49,49,49	0
57	MG	1A	3955	1/1	0.95	0.05	20,20,20,20	0
57	MG	1A	3015	1/1	0.95	0.14	33,33,33,33	0
57	MG	2A	3078	1/1	0.95	0.15	57,57,57,57	0
57	MG	2A	3079	1/1	0.95	0.09	51,51,51,51	0
57	MG	2A	3362	1/1	0.95	0.07	40,40,40,40	0
57	MG	2A	3081	1/1	0.95	0.16	66,66,66,66	0
57	MG	2A	3662	1/1	0.95	0.10	44,44,44,44	0
57	MG	1A	3625	1/1	0.95	0.14	29,29,29,29	0
57	MG	1A	3524	1/1	0.95	0.09	39,39,39,39	0
57	MG	1a	1783	1/1	0.95	0.08	55,55,55,55	0
57	MG	2A	3671	1/1	0.95	0.07	59,59,59,59	0
57	MG	2a	3186	1/1	0.95	0.07	52,52,52,52	0
57	MG	1A	3525	1/1	0.95	0.07	42,42,42,42	0
57	MG	1A	3770	1/1	0.95	0.15	44,44,44,44	0
57	MG	2a	3190	1/1	0.95	0.14	58,58,58,58	0
57	MG	1A	3772	1/1	0.95	0.05	50,50,50,50	0
57	MG	2A	3371	1/1	0.95	0.08	49,49,49,49	0
57	MG	1A	3127	1/1	0.95	0.10	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1a	1617	1/1	0.95	0.13	54,54,54,54	0
57	MG	2j	3201	1/1	0.95	0.09	60,60,60,60	0
57	MG	2A	3375	1/1	0.95	0.06	59,59,59,59	0
57	MG	1A	3253	1/1	0.95	0.19	30,30,30,30	0
57	MG	1a	1790	1/1	0.95	0.13	62,62,62,62	0
57	MG	1A	3255	1/1	0.95	0.19	43,43,43,43	0
57	MG	1a	1621	1/1	0.95	0.20	52,52,52,52	0
57	MG	2A	3100	1/1	0.95	0.07	53,53,53,53	0
57	MG	2A	3101	1/1	0.95	0.06	50,50,50,50	0
57	MG	2A	3391	1/1	0.95	0.08	58,58,58,58	0
57	MG	2A	3392	1/1	0.95	0.07	40,40,40,40	0
57	MG	1A	3130	1/1	0.95	0.06	33,33,33,33	0
59	ARG	1B	231	12/12	0.95	0.09	24,39,48,53	0
57	MG	2A	3105	1/1	0.95	0.14	45,45,45,45	0
60	ZN	24	501	1/1	0.95	0.13	122,122,122,122	0
57	MG	1A	3532	1/1	0.95	0.10	25,25,25,25	0
57	MG	1a	1625	1/1	0.96	0.07	42,42,42,42	0
57	MG	1A	3942	1/1	0.96	0.12	49,49,49,49	0
57	MG	1A	3267	1/1	0.96	0.07	43,43,43,43	0
57	MG	1a	1867	1/1	0.96	0.06	52,52,52,52	0
57	MG	1A	3382	1/1	0.96	0.15	67,67,67,67	0
57	MG	1A	3734	1/1	0.96	0.29	40,40,40,40	0
57	MG	2A	3640	1/1	0.96	0.12	68,68,68,68	0
57	MG	2A	3278	1/1	0.96	0.06	55,55,55,55	0
57	MG	1A	3735	1/1	0.96	0.14	34,34,34,34	0
57	MG	1A	3268	1/1	0.96	0.06	31,31,31,31	0
57	MG	1A	3007	1/1	0.96	0.06	28,28,28,28	0
57	MG	1A	3032	1/1	0.96	0.09	44,44,44,44	0
57	MG	1A	3010	1/1	0.96	0.07	39,39,39,39	0
57	MG	2A	3284	1/1	0.96	0.06	45,45,45,45	0
57	MG	1A	3742	1/1	0.96	0.09	39,39,39,39	0
57	MG	1A	3953	1/1	0.96	0.14	53,53,53,53	0
57	MG	2A	3660	1/1	0.96	0.12	50,50,50,50	0
57	MG	1A	3071	1/1	0.96	0.11	27,27,27,27	0
57	MG	1a	1641	1/1	0.96	0.10	68,68,68,68	0
57	MG	2A	3290	1/1	0.96	0.28	48,48,48,48	0
57	MG	1A	3956	1/1	0.96	0.09	41,41,41,41	0
57	MG	1A	3957	1/1	0.96	0.15	61,61,61,61	0
57	MG	1A	3016	1/1	0.96	0.13	32,32,32,32	0
57	MG	1d	302	1/1	0.96	0.11	57,57,57,57	0
57	MG	2A	3673	1/1	0.96	0.10	66,66,66,66	0
57	MG	1A	3746	1/1	0.96	0.07	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3677	1/1	0.96	0.09	65,65,65,65	0
57	MG	1a	1646	1/1	0.96	0.31	64,64,64,64	0
57	MG	1A	3194	1/1	0.96	0.10	46,46,46,46	0
57	MG	1A	3134	1/1	0.96	0.16	34,34,34,34	0
57	MG	2A	3303	1/1	0.96	0.07	37,37,37,37	0
57	MG	1A	3196	1/1	0.96	0.08	44,44,44,44	0
57	MG	2A	3683	1/1	0.96	0.07	55,55,55,55	0
57	MG	1e	202	1/1	0.96	0.07	48,48,48,48	0
57	MG	1e	203	1/1	0.96	0.13	49,49,49,49	0
57	MG	1A	3135	1/1	0.96	0.06	32,32,32,32	0
57	MG	1A	3498	1/1	0.96	0.06	42,42,42,42	0
57	MG	2A	3309	1/1	0.96	0.10	51,51,51,51	0
57	MG	2A	3690	1/1	0.96	0.07	51,51,51,51	0
57	MG	2A	3310	1/1	0.96	0.07	52,52,52,52	0
57	MG	2A	3692	1/1	0.96	0.06	54,54,54,54	0
57	MG	1g	3101	1/1	0.96	0.14	52,52,52,52	0
57	MG	2A	3313	1/1	0.96	0.06	44,44,44,44	0
57	MG	1a	1654	1/1	0.96	0.06	42,42,42,42	0
57	MG	1a	1655	1/1	0.96	0.12	60,60,60,60	0
57	MG	2A	3317	1/1	0.96	0.07	37,37,37,37	0
57	MG	1A	3138	1/1	0.96	0.13	31,31,31,31	0
57	MG	1A	3611	1/1	0.96	0.05	41,41,41,41	0
57	MG	1A	3396	1/1	0.96	0.06	40,40,40,40	0
57	MG	1A	3397	1/1	0.96	0.07	38,38,38,38	0
57	MG	1m	201	1/1	0.96	0.07	65,65,65,65	0
57	MG	1n	101	1/1	0.96	0.07	58,58,58,58	0
57	MG	1A	3614	1/1	0.96	0.07	51,51,51,51	0
57	MG	1A	3766	1/1	0.96	0.09	34,34,34,34	0
57	MG	1A	3615	1/1	0.96	0.15	41,41,41,41	0
57	MG	1A	3980	1/1	0.96	0.05	21,21,21,21	0
57	MG	1A	3616	1/1	0.96	0.04	40,40,40,40	0
57	MG	2A	3335	1/1	0.96	0.10	34,34,34,34	0
57	MG	1A	3288	1/1	0.96	0.07	23,23,23,23	0
57	MG	2A	3337	1/1	0.96	0.06	45,45,45,45	0
57	MG	1A	3020	1/1	0.96	0.22	31,31,31,31	0
57	MG	1x	102	1/1	0.96	0.06	26,26,26,26	0
57	MG	2A	3342	1/1	0.96	0.06	53,53,53,53	0
57	MG	2A	3720	1/1	0.96	0.05	40,40,40,40	0
57	MG	1A	3985	1/1	0.96	0.06	32,32,32,32	0
57	MG	1A	3986	1/1	0.96	0.18	46,46,46,46	0
57	MG	1A	3620	1/1	0.96	0.07	48,48,48,48	0
57	MG	2A	3350	1/1	0.96	0.09	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3403	1/1	0.96	0.05	23,23,23,23	0
57	MG	1A	3989	1/1	0.96	0.07	41,41,41,41	0
57	MG	1A	3506	1/1	0.96	0.07	42,42,42,42	0
57	MG	1A	3777	1/1	0.96	0.06	39,39,39,39	0
57	MG	1A	3507	1/1	0.96	0.06	49,49,49,49	0
57	MG	1A	3201	1/1	0.96	0.19	46,46,46,46	0
57	MG	1A	3780	1/1	0.96	0.07	32,32,32,32	0
57	MG	2A	3018	1/1	0.96	0.18	37,37,37,37	0
57	MG	2A	3021	1/1	0.96	0.06	37,37,37,37	0
57	MG	1A	3080	1/1	0.96	0.14	35,35,35,35	0
57	MG	2A	3024	1/1	0.96	0.08	63,63,63,63	0
57	MG	1A	3082	1/1	0.96	0.09	41,41,41,41	0
57	MG	2A	3026	1/1	0.96	0.10	46,46,46,46	0
57	MG	1A	3144	1/1	0.96	0.07	35,35,35,35	0
57	MG	1A	3785	1/1	0.96	0.07	52,52,52,52	0
57	MG	2A	3032	1/1	0.96	0.14	51,51,51,51	0
57	MG	2A	3370	1/1	0.96	0.12	60,60,60,60	0
57	MG	1A	3787	1/1	0.96	0.06	35,35,35,35	0
57	MG	1a	1686	1/1	0.96	0.16	52,52,52,52	0
57	MG	2A	3035	1/1	0.96	0.07	49,49,49,49	0
57	MG	2B	209	1/1	0.96	0.19	60,60,60,60	0
57	MG	2A	3037	1/1	0.96	0.07	39,39,39,39	0
57	MG	2B	211	1/1	0.96	0.11	57,57,57,57	0
57	MG	1A	4004	1/1	0.96	0.13	47,47,47,47	0
57	MG	1A	3299	1/1	0.96	0.22	31,31,31,31	0
57	MG	1A	3515	1/1	0.96	0.06	31,31,31,31	0
57	MG	1A	3046	1/1	0.96	0.07	12,12,12,12	0
57	MG	2A	3384	1/1	0.96	0.10	58,58,58,58	0
57	MG	1A	3302	1/1	0.96	0.10	33,33,33,33	0
57	MG	2D	301	1/1	0.96	0.10	42,42,42,42	0
57	MG	2A	3387	1/1	0.96	0.06	46,46,46,46	0
57	MG	1a	1692	1/1	0.96	0.07	49,49,49,49	0
57	MG	1A	4012	1/1	0.96	0.11	15,15,15,15	0
57	MG	1a	1694	1/1	0.96	0.12	39,39,39,39	0
57	MG	1A	3792	1/1	0.96	0.07	17,17,17,17	0
57	MG	2D	310	1/1	0.96	0.07	42,42,42,42	0
57	MG	1A	4016	1/1	0.96	0.07	42,42,42,42	0
57	MG	2E	301	1/1	0.96	0.13	59,59,59,59	0
57	MG	1A	4017	1/1	0.96	0.06	51,51,51,51	0
57	MG	2E	304	1/1	0.96	0.08	57,57,57,57	0
57	MG	2A	3053	1/1	0.96	0.07	42,42,42,42	0
57	MG	2A	3055	1/1	0.96	0.10	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3633	1/1	0.96	0.05	39,39,39,39	0
57	MG	1A	3518	1/1	0.96	0.08	53,53,53,53	0
57	MG	1A	3635	1/1	0.96	0.06	20,20,20,20	0
57	MG	2A	3059	1/1	0.96	0.07	41,41,41,41	0
57	MG	1A	3799	1/1	0.96	0.09	43,43,43,43	0
57	MG	1A	4023	1/1	0.96	0.06	53,53,53,53	0
57	MG	2Q	202	1/1	0.96	0.24	55,55,55,55	0
57	MG	2A	3062	1/1	0.96	0.07	48,48,48,48	0
57	MG	1A	3303	1/1	0.96	0.05	31,31,31,31	0
57	MG	1A	3309	1/1	0.96	0.12	33,33,33,33	0
57	MG	1A	3310	1/1	0.96	0.14	34,34,34,34	0
57	MG	2T	202	1/1	0.96	0.09	65,65,65,65	0
57	MG	1A	4028	1/1	0.96	0.10	46,46,46,46	0
57	MG	2T	204	1/1	0.96	0.08	45,45,45,45	0
57	MG	1A	3084	1/1	0.96	0.10	41,41,41,41	0
57	MG	1A	3805	1/1	0.96	0.12	22,22,22,22	0
57	MG	2A	3417	1/1	0.96	0.06	33,33,33,33	0
57	MG	1a	1711	1/1	0.96	0.05	44,44,44,44	0
57	MG	2A	3071	1/1	0.96	0.12	56,56,56,56	0
57	MG	1A	3153	1/1	0.96	0.09	54,54,54,54	0
57	MG	1A	3021	1/1	0.96	0.13	36,36,36,36	0
57	MG	1A	3315	1/1	0.96	0.08	46,46,46,46	0
57	MG	2A	3077	1/1	0.96	0.09	47,47,47,47	0
57	MG	27	101	1/1	0.96	0.19	40,40,40,40	0
57	MG	1A	3316	1/1	0.96	0.10	33,33,33,33	0
57	MG	1a	1718	1/1	0.96	0.05	48,48,48,48	0
57	MG	2A	3080	1/1	0.96	0.07	50,50,50,50	0
57	MG	1a	1719	1/1	0.96	0.05	42,42,42,42	0
57	MG	2a	3004	1/1	0.96	0.16	60,60,60,60	0
57	MG	2a	3006	1/1	0.96	0.07	51,51,51,51	0
57	MG	1A	3158	1/1	0.96	0.19	34,34,34,34	0
57	MG	1B	209	1/1	0.96	0.07	48,48,48,48	0
57	MG	1A	3814	1/1	0.96	0.05	50,50,50,50	0
57	MG	2A	3085	1/1	0.96	0.15	49,49,49,49	0
57	MG	2A	3086	1/1	0.96	0.10	50,50,50,50	0
57	MG	1A	3213	1/1	0.96	0.07	36,36,36,36	0
57	MG	1a	1724	1/1	0.96	0.07	55,55,55,55	0
57	MG	1A	3819	1/1	0.96	0.14	46,46,46,46	0
57	MG	1A	3049	1/1	0.96	0.12	36,36,36,36	0
57	MG	1B	216	1/1	0.96	0.13	45,45,45,45	0
57	MG	1B	217	1/1	0.96	0.08	56,56,56,56	0
57	MG	1a	1730	1/1	0.96	0.08	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3653	1/1	0.96	0.11	28,28,28,28	0
57	MG	2a	3020	1/1	0.96	0.11	46,46,46,46	0
57	MG	2A	3443	1/1	0.96	0.07	39,39,39,39	0
57	MG	2a	3022	1/1	0.96	0.07	49,49,49,49	0
57	MG	1A	3654	1/1	0.96	0.06	28,28,28,28	0
57	MG	1B	220	1/1	0.96	0.07	37,37,37,37	0
57	MG	1A	3160	1/1	0.96	0.10	37,37,37,37	0
57	MG	2A	3448	1/1	0.96	0.06	51,51,51,51	0
57	MG	2A	3103	1/1	0.96	0.08	42,42,42,42	0
57	MG	1B	222	1/1	0.96	0.08	35,35,35,35	0
57	MG	1A	3219	1/1	0.96	0.14	25,25,25,25	0
57	MG	1B	224	1/1	0.96	0.06	44,44,44,44	0
57	MG	1A	3657	1/1	0.96	0.07	50,50,50,50	0
57	MG	1A	3220	1/1	0.96	0.05	43,43,43,43	0
57	MG	1A	3839	1/1	0.96	0.08	59,59,59,59	0
57	MG	2A	3457	1/1	0.96	0.09	48,48,48,48	0
57	MG	1A	3162	1/1	0.96	0.20	32,32,32,32	0
57	MG	1a	1745	1/1	0.96	0.10	59,59,59,59	0
57	MG	2A	3114	1/1	0.96	0.21	55,55,55,55	0
57	MG	2A	3462	1/1	0.96	0.10	62,62,62,62	0
57	MG	1A	3224	1/1	0.96	0.07	53,53,53,53	0
57	MG	1A	3662	1/1	0.96	0.06	34,34,34,34	0
57	MG	2a	3042	1/1	0.96	0.25	60,60,60,60	0
57	MG	1A	3844	1/1	0.96	0.06	43,43,43,43	0
57	MG	1D	304	1/1	0.96	0.09	49,49,49,49	0
57	MG	1D	306	1/1	0.96	0.07	38,38,38,38	0
57	MG	2A	3120	1/1	0.96	0.16	57,57,57,57	0
57	MG	1A	3663	1/1	0.96	0.07	44,44,44,44	0
57	MG	1A	3057	1/1	0.96	0.12	47,47,47,47	0
57	MG	1a	1755	1/1	0.96	0.10	64,64,64,64	0
57	MG	1A	3543	1/1	0.96	0.15	31,31,31,31	0
57	MG	2A	3125	1/1	0.96	0.07	53,53,53,53	0
57	MG	2A	3126	1/1	0.96	0.18	45,45,45,45	0
57	MG	1A	3848	1/1	0.96	0.04	32,32,32,32	0
57	MG	1A	3091	1/1	0.96	0.10	35,35,35,35	0
57	MG	1A	3547	1/1	0.96	0.08	47,47,47,47	0
57	MG	1A	3230	1/1	0.96	0.06	29,29,29,29	0
57	MG	1A	3231	1/1	0.96	0.19	40,40,40,40	0
57	MG	1E	307	1/1	0.96	0.11	25,25,25,25	0
57	MG	1A	3853	1/1	0.96	0.04	36,36,36,36	0
57	MG	2A	3486	1/1	0.96	0.08	53,53,53,53	0
57	MG	1E	309	1/1	0.96	0.09	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1E	310	1/1	0.96	0.07	40,40,40,40	0
57	MG	1A	3673	1/1	0.96	0.06	20,20,20,20	0
57	MG	1A	3674	1/1	0.96	0.20	55,55,55,55	0
57	MG	1A	3167	1/1	0.96	0.09	30,30,30,30	0
57	MG	1A	3858	1/1	0.96	0.07	49,49,49,49	0
57	MG	1A	3859	1/1	0.96	0.04	15,15,15,15	0
57	MG	1A	3442	1/1	0.96	0.06	21,21,21,21	0
57	MG	2A	3148	1/1	0.96	0.10	42,42,42,42	0
57	MG	2A	3497	1/1	0.96	0.05	41,41,41,41	0
57	MG	2A	3149	1/1	0.96	0.20	53,53,53,53	0
57	MG	2a	3073	1/1	0.96	0.05	44,44,44,44	0
57	MG	1A	3861	1/1	0.96	0.11	53,53,53,53	0
57	MG	2a	3075	1/1	0.96	0.20	48,48,48,48	0
57	MG	2a	3076	1/1	0.96	0.14	54,54,54,54	0
57	MG	1A	3443	1/1	0.96	0.05	28,28,28,28	0
57	MG	1A	3093	1/1	0.96	0.11	34,34,34,34	0
57	MG	2A	3155	1/1	0.96	0.05	37,37,37,37	0
57	MG	1A	3003	1/1	0.96	0.04	28,28,28,28	0
57	MG	2a	3081	1/1	0.96	0.09	54,54,54,54	0
57	MG	2A	3157	1/1	0.96	0.09	55,55,55,55	0
57	MG	1A	3558	1/1	0.96	0.06	20,20,20,20	0
57	MG	1A	3682	1/1	0.96	0.07	52,52,52,52	0
57	MG	2a	3085	1/1	0.96	0.26	53,53,53,53	0
57	MG	1a	1782	1/1	0.96	0.10	54,54,54,54	0
57	MG	1A	3171	1/1	0.96	0.12	24,24,24,24	0
57	MG	1A	3872	1/1	0.96	0.12	36,36,36,36	0
57	MG	2A	3164	1/1	0.96	0.12	39,39,39,39	0
57	MG	2A	3515	1/1	0.96	0.09	42,42,42,42	0
57	MG	1A	3684	1/1	0.96	0.06	34,34,34,34	0
57	MG	1Q	202	1/1	0.96	0.11	43,43,43,43	0
57	MG	1Q	203	1/1	0.96	0.07	27,27,27,27	0
57	MG	2a	3095	1/1	0.96	0.24	64,64,64,64	0
57	MG	2a	3096	1/1	0.96	0.27	48,48,48,48	0
57	MG	1A	3237	1/1	0.96	0.11	31,31,31,31	0
57	MG	1A	3686	1/1	0.96	0.11	36,36,36,36	0
57	MG	1R	201	1/1	0.96	0.14	32,32,32,32	0
57	MG	2a	3101	1/1	0.96	0.06	65,65,65,65	0
57	MG	1A	3878	1/1	0.96	0.09	31,31,31,31	0
57	MG	2A	3176	1/1	0.96	0.11	44,44,44,44	0
57	MG	1A	3879	1/1	0.96	0.08	37,37,37,37	0
57	MG	1A	3012	1/1	0.96	0.22	40,40,40,40	0
57	MG	2A	3180	1/1	0.96	0.05	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3451	1/1	0.96	0.07	57,57,57,57	0
57	MG	1T	203	1/1	0.96	0.05	43,43,43,43	0
57	MG	1A	3689	1/1	0.96	0.07	54,54,54,54	0
57	MG	2A	3184	1/1	0.96	0.05	41,41,41,41	0
57	MG	1A	3567	1/1	0.96	0.05	30,30,30,30	0
57	MG	1U	202	1/1	0.96	0.17	27,27,27,27	0
57	MG	2A	3537	1/1	0.96	0.16	52,52,52,52	0
57	MG	1A	3886	1/1	0.96	0.08	22,22,22,22	0
57	MG	1U	206	1/1	0.96	0.10	28,28,28,28	0
57	MG	2A	3191	1/1	0.96	0.08	55,55,55,55	0
57	MG	2a	3121	1/1	0.96	0.11	60,60,60,60	0
57	MG	2A	3542	1/1	0.96	0.10	54,54,54,54	0
57	MG	1A	3452	1/1	0.96	0.10	30,30,30,30	0
57	MG	1V	205	1/1	0.96	0.08	46,46,46,46	0
57	MG	1V	206	1/1	0.96	0.14	56,56,56,56	0
57	MG	1A	3693	1/1	0.96	0.16	57,57,57,57	0
57	MG	2A	3551	1/1	0.96	0.05	63,63,63,63	0
57	MG	1A	3030	1/1	0.96	0.06	21,21,21,21	0
57	MG	2A	3553	1/1	0.96	0.06	63,63,63,63	0
57	MG	1A	3696	1/1	0.96	0.05	55,55,55,55	0
57	MG	1A	3353	1/1	0.96	0.08	37,37,37,37	0
57	MG	2A	3202	1/1	0.96	0.21	56,56,56,56	0
57	MG	1A	3893	1/1	0.96	0.08	35,35,35,35	0
57	MG	1a	1811	1/1	0.96	0.06	68,68,68,68	0
57	MG	10	101	1/1	0.96	0.11	31,31,31,31	0
57	MG	10	103	1/1	0.96	0.07	36,36,36,36	0
57	MG	1A	3174	1/1	0.96	0.13	38,38,38,38	0
57	MG	2a	3142	1/1	0.96	0.06	55,55,55,55	0
57	MG	2A	3567	1/1	0.96	0.06	55,55,55,55	0
57	MG	1a	1815	1/1	0.96	0.14	55,55,55,55	0
57	MG	1A	3895	1/1	0.96	0.05	43,43,43,43	0
57	MG	1A	3356	1/1	0.96	0.06	29,29,29,29	0
57	MG	1a	1818	1/1	0.96	0.08	45,45,45,45	0
57	MG	2a	3150	1/1	0.96	0.12	60,60,60,60	0
57	MG	2A	3215	1/1	0.96	0.07	53,53,53,53	0
57	MG	1A	3574	1/1	0.96	0.08	47,47,47,47	0
57	MG	1a	1821	1/1	0.96	0.06	73,73,73,73	0
57	MG	2a	3155	1/1	0.96	0.09	60,60,60,60	0
57	MG	11	104	1/1	0.96	0.09	47,47,47,47	0
57	MG	1a	1823	1/1	0.96	0.13	64,64,64,64	0
57	MG	2A	3220	1/1	0.96	0.07	47,47,47,47	0
57	MG	2a	3159	1/1	0.96	0.10	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	15	102	1/1	0.96	0.10	27,27,27,27	0
57	MG	1A	3459	1/1	0.96	0.09	50,50,50,50	0
57	MG	1A	3064	1/1	0.96	0.06	35,35,35,35	0
57	MG	1A	3113	1/1	0.96	0.09	26,26,26,26	0
57	MG	2A	3586	1/1	0.96	0.06	48,48,48,48	0
57	MG	1A	3251	1/1	0.96	0.17	38,38,38,38	0
57	MG	17	105	1/1	0.96	0.06	34,34,34,34	0
57	MG	18	101	1/1	0.96	0.09	31,31,31,31	0
57	MG	2a	3169	1/1	0.96	0.06	65,65,65,65	0
57	MG	1A	3252	1/1	0.96	0.08	44,44,44,44	0
57	MG	1A	3909	1/1	0.96	0.07	39,39,39,39	0
57	MG	2A	3593	1/1	0.96	0.08	48,48,48,48	0
57	MG	2A	3231	1/1	0.96	0.15	53,53,53,53	0
57	MG	1A	3465	1/1	0.96	0.04	36,36,36,36	0
57	MG	2a	3176	1/1	0.96	0.09	51,51,51,51	0
57	MG	19	102	1/1	0.96	0.18	46,46,46,46	0
57	MG	2A	3599	1/1	0.96	0.07	49,49,49,49	0
57	MG	2A	3600	1/1	0.96	0.06	41,41,41,41	0
57	MG	19	103	1/1	0.96	0.06	55,55,55,55	0
57	MG	2A	3236	1/1	0.96	0.08	39,39,39,39	0
57	MG	1a	1602	1/1	0.96	0.09	41,41,41,41	0
57	MG	1a	1603	1/1	0.96	0.07	66,66,66,66	0
57	MG	1A	3466	1/1	0.96	0.07	39,39,39,39	0
57	MG	1A	3065	1/1	0.96	0.06	53,53,53,53	0
57	MG	2a	3188	1/1	0.96	0.10	58,58,58,58	0
57	MG	1A	3918	1/1	0.96	0.09	21,21,21,21	0
57	MG	2A	3243	1/1	0.96	0.08	49,49,49,49	0
57	MG	1A	3368	1/1	0.96	0.05	32,32,32,32	0
57	MG	1a	1844	1/1	0.96	0.06	64,64,64,64	0
57	MG	1A	3254	1/1	0.96	0.14	33,33,33,33	0
57	MG	1A	3370	1/1	0.96	0.07	27,27,27,27	0
57	MG	1A	3372	1/1	0.96	0.05	28,28,28,28	0
57	MG	1A	3722	1/1	0.96	0.05	38,38,38,38	0
57	MG	2p	101	1/1	0.96	0.06	37,37,37,37	0
57	MG	2A	3250	1/1	0.96	0.20	55,55,55,55	0
57	MG	1A	3928	1/1	0.96	0.08	45,45,45,45	0
57	MG	1A	3931	1/1	0.96	0.13	33,33,33,33	0
57	MG	1A	3723	1/1	0.96	0.06	39,39,39,39	0
57	MG	2A	3256	1/1	0.96	0.10	54,54,54,54	0
57	MG	1A	3182	1/1	0.96	0.26	36,36,36,36	0
57	MG	1A	3183	1/1	0.96	0.07	31,31,31,31	0
57	MG	1A	3260	1/1	0.96	0.13	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3121	1/1	0.96	0.05	25,25,25,25	0
57	MG	2A	3262	1/1	0.96	0.29	49,49,49,49	0
57	MG	1A	3939	1/1	0.96	0.05	47,47,47,47	0
57	MG	1A	3940	1/1	0.96	0.08	50,50,50,50	0
57	MG	1a	1624	1/1	0.96	0.07	41,41,41,41	0
57	MG	2A	3390	1/1	0.97	0.06	52,52,52,52	0
57	MG	1A	3755	1/1	0.97	0.10	38,38,38,38	0
57	MG	2A	3111	1/1	0.97	0.09	63,63,63,63	0
57	MG	1A	3305	1/1	0.97	0.07	39,39,39,39	0
57	MG	1A	3115	1/1	0.97	0.13	41,41,41,41	0
57	MG	1A	3935	1/1	0.97	0.10	30,30,30,30	0
57	MG	1A	3226	1/1	0.97	0.14	31,31,31,31	0
57	MG	1A	3116	1/1	0.97	0.12	32,32,32,32	0
57	MG	1A	3411	1/1	0.97	0.14	25,25,25,25	0
57	MG	1A	3079	1/1	0.97	0.14	41,41,41,41	0
57	MG	11	101	1/1	0.97	0.12	37,37,37,37	0
57	MG	1A	3764	1/1	0.97	0.07	64,64,64,64	0
57	MG	11	103	1/1	0.97	0.08	37,37,37,37	0
57	MG	1A	3943	1/1	0.97	0.05	29,29,29,29	0
57	MG	11	105	1/1	0.97	0.07	28,28,28,28	0
57	MG	13	102	1/1	0.97	0.08	58,58,58,58	0
57	MG	15	101	1/1	0.97	0.07	29,29,29,29	0
57	MG	1A	3765	1/1	0.97	0.08	21,21,21,21	0
57	MG	1a	1801	1/1	0.97	0.06	52,52,52,52	0
57	MG	1A	3119	1/1	0.97	0.06	28,28,28,28	0
57	MG	2A	3413	1/1	0.97	0.04	42,42,42,42	0
57	MG	1A	3414	1/1	0.97	0.06	17,17,17,17	0
57	MG	1A	3314	1/1	0.97	0.24	33,33,33,33	0
57	MG	17	101	1/1	0.97	0.10	38,38,38,38	0
57	MG	17	103	1/1	0.97	0.15	33,33,33,33	0
57	MG	1A	3040	1/1	0.97	0.08	33,33,33,33	0
57	MG	1A	3519	1/1	0.97	0.06	39,39,39,39	0
57	MG	1A	3771	1/1	0.97	0.10	36,36,36,36	0
57	MG	2A	3140	1/1	0.97	0.19	47,47,47,47	0
57	MG	1A	3175	1/1	0.97	0.10	19,19,19,19	0
57	MG	1A	3773	1/1	0.97	0.05	32,32,32,32	0
57	MG	1A	3317	1/1	0.97	0.09	31,31,31,31	0
57	MG	1A	3954	1/1	0.97	0.05	47,47,47,47	0
57	MG	1A	3775	1/1	0.97	0.04	42,42,42,42	0
57	MG	1a	1601	1/1	0.97	0.06	46,46,46,46	0
57	MG	1A	3124	1/1	0.97	0.08	36,36,36,36	0
57	MG	1A	3081	1/1	0.97	0.10	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3958	1/1	0.97	0.05	48,48,48,48	0
57	MG	2A	3152	1/1	0.97	0.16	46,46,46,46	0
57	MG	1A	3004	1/1	0.97	0.10	45,45,45,45	0
57	MG	1a	1820	1/1	0.97	0.12	62,62,62,62	0
57	MG	2A	3436	1/1	0.97	0.12	58,58,58,58	0
57	MG	1A	3424	1/1	0.97	0.08	55,55,55,55	0
57	MG	1a	1607	1/1	0.97	0.08	50,50,50,50	0
57	MG	1A	3326	1/1	0.97	0.06	35,35,35,35	0
57	MG	1A	3328	1/1	0.97	0.10	34,34,34,34	0
57	MG	2A	3159	1/1	0.97	0.07	33,33,33,33	0
57	MG	1A	3964	1/1	0.97	0.05	50,50,50,50	0
57	MG	1A	3329	1/1	0.97	0.06	43,43,43,43	0
57	MG	2A	3445	1/1	0.97	0.04	48,48,48,48	0
57	MG	1A	3966	1/1	0.97	0.12	47,47,47,47	0
57	MG	2D	306	1/1	0.97	0.11	38,38,38,38	0
57	MG	2D	307	1/1	0.97	0.12	42,42,42,42	0
57	MG	1a	1613	1/1	0.97	0.14	37,37,37,37	0
57	MG	1A	3530	1/1	0.97	0.07	37,37,37,37	0
57	MG	1A	3784	1/1	0.97	0.08	40,40,40,40	0
57	MG	2A	3167	1/1	0.97	0.25	43,43,43,43	0
57	MG	1A	3236	1/1	0.97	0.20	27,27,27,27	0
57	MG	1A	3786	1/1	0.97	0.04	24,24,24,24	0
57	MG	2E	303	1/1	0.97	0.06	45,45,45,45	0
57	MG	1A	3971	1/1	0.97	0.07	65,65,65,65	0
57	MG	1A	3044	1/1	0.97	0.07	22,22,22,22	0
57	MG	2F	302	1/1	0.97	0.06	43,43,43,43	0
57	MG	1a	1620	1/1	0.97	0.06	56,56,56,56	0
57	MG	2F	304	1/1	0.97	0.18	49,49,49,49	0
57	MG	1A	3062	1/1	0.97	0.06	33,33,33,33	0
57	MG	1A	3649	1/1	0.97	0.10	41,41,41,41	0
57	MG	2I	201	1/1	0.97	0.09	52,52,52,52	0
57	MG	1A	3976	1/1	0.97	0.10	32,32,32,32	0
57	MG	2O	201	1/1	0.97	0.08	47,47,47,47	0
57	MG	1A	3650	1/1	0.97	0.10	37,37,37,37	0
57	MG	2A	3179	1/1	0.97	0.07	49,49,49,49	0
57	MG	2A	3463	1/1	0.97	0.05	32,32,32,32	0
57	MG	2Q	201	1/1	0.97	0.05	46,46,46,46	0
57	MG	1A	3534	1/1	0.97	0.04	44,44,44,44	0
57	MG	1A	3979	1/1	0.97	0.20	41,41,41,41	0
57	MG	1A	3240	1/1	0.97	0.19	36,36,36,36	0
57	MG	1A	3793	1/1	0.97	0.09	44,44,44,44	0
57	MG	2R	203	1/1	0.97	0.13	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3468	1/1	0.97	0.06	61,61,61,61	0
57	MG	1A	3794	1/1	0.97	0.09	35,35,35,35	0
57	MG	2A	3185	1/1	0.97	0.18	53,53,53,53	0
57	MG	1a	1847	1/1	0.97	0.07	64,64,64,64	0
57	MG	1A	3241	1/1	0.97	0.09	31,31,31,31	0
57	MG	1A	3984	1/1	0.97	0.07	25,25,25,25	0
57	MG	2V	203	1/1	0.97	0.08	53,53,53,53	0
57	MG	1A	3796	1/1	0.97	0.07	43,43,43,43	0
57	MG	1A	3340	1/1	0.97	0.04	32,32,32,32	0
57	MG	2Y	201	1/1	0.97	0.11	45,45,45,45	0
57	MG	20	101	1/1	0.97	0.06	46,46,46,46	0
57	MG	2A	3192	1/1	0.97	0.07	45,45,45,45	0
57	MG	1A	3539	1/1	0.97	0.05	19,19,19,19	0
57	MG	1A	3013	1/1	0.97	0.09	18,18,18,18	0
57	MG	25	102	1/1	0.97	0.11	41,41,41,41	0
57	MG	1A	3036	1/1	0.97	0.07	28,28,28,28	0
57	MG	1A	3658	1/1	0.97	0.05	46,46,46,46	0
57	MG	1A	3991	1/1	0.97	0.07	52,52,52,52	0
57	MG	1A	3802	1/1	0.97	0.04	25,25,25,25	0
57	MG	1A	3542	1/1	0.97	0.05	24,24,24,24	0
57	MG	1A	3187	1/1	0.97	0.06	31,31,31,31	0
57	MG	1a	1862	1/1	0.97	0.07	46,46,46,46	0
57	MG	1A	3996	1/1	0.97	0.07	38,38,38,38	0
57	MG	2a	3005	1/1	0.97	0.07	52,52,52,52	0
57	MG	1A	3048	1/1	0.97	0.03	23,23,23,23	0
57	MG	1A	3998	1/1	0.97	0.04	38,38,38,38	0
57	MG	1A	3545	1/1	0.97	0.14	45,45,45,45	0
57	MG	1a	1868	1/1	0.97	0.08	46,46,46,46	0
57	MG	1A	3808	1/1	0.97	0.10	48,48,48,48	0
57	MG	1A	3250	1/1	0.97	0.21	35,35,35,35	0
57	MG	2A	3212	1/1	0.97	0.10	47,47,47,47	0
57	MG	2A	3213	1/1	0.97	0.05	38,38,38,38	0
57	MG	1A	3137	1/1	0.97	0.15	30,30,30,30	0
57	MG	1A	3665	1/1	0.97	0.06	28,28,28,28	0
57	MG	2A	3500	1/1	0.97	0.06	31,31,31,31	0
57	MG	1A	3089	1/1	0.97	0.06	34,34,34,34	0
57	MG	1a	1656	1/1	0.97	0.06	45,45,45,45	0
57	MG	1A	4005	1/1	0.97	0.05	45,45,45,45	0
57	MG	1A	3813	1/1	0.97	0.05	61,61,61,61	0
57	MG	1A	3090	1/1	0.97	0.07	42,42,42,42	0
57	MG	1A	3815	1/1	0.97	0.05	32,32,32,32	0
57	MG	1A	3349	1/1	0.97	0.05	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3192	1/1	0.97	0.12	32,32,32,32	0
57	MG	1A	4013	1/1	0.97	0.12	44,44,44,44	0
57	MG	2A	3512	1/1	0.97	0.07	47,47,47,47	0
57	MG	1A	3820	1/1	0.97	0.05	52,52,52,52	0
57	MG	1A	4015	1/1	0.97	0.04	29,29,29,29	0
57	MG	1A	3447	1/1	0.97	0.07	49,49,49,49	0
57	MG	2A	3228	1/1	0.97	0.07	54,54,54,54	0
57	MG	1A	3825	1/1	0.97	0.11	24,24,24,24	0
57	MG	2A	3519	1/1	0.97	0.06	46,46,46,46	0
57	MG	1A	3193	1/1	0.97	0.09	30,30,30,30	0
57	MG	1A	3829	1/1	0.97	0.12	37,37,37,37	0
57	MG	1A	3556	1/1	0.97	0.06	17,17,17,17	0
57	MG	1A	3557	1/1	0.97	0.04	31,31,31,31	0
57	MG	2A	3234	1/1	0.97	0.20	50,50,50,50	0
57	MG	1A	3258	1/1	0.97	0.10	42,42,42,42	0
57	MG	1A	3038	1/1	0.97	0.08	34,34,34,34	0
57	MG	2A	3237	1/1	0.97	0.16	48,48,48,48	0
57	MG	1A	3678	1/1	0.97	0.04	40,40,40,40	0
57	MG	1A	3836	1/1	0.97	0.05	33,33,33,33	0
57	MG	1A	3354	1/1	0.97	0.06	25,25,25,25	0
57	MG	2A	3531	1/1	0.97	0.07	48,48,48,48	0
57	MG	1A	3092	1/1	0.97	0.16	28,28,28,28	0
57	MG	1A	3050	1/1	0.97	0.06	38,38,38,38	0
57	MG	1A	3566	1/1	0.97	0.11	18,18,18,18	0
57	MG	1a	1681	1/1	0.97	0.07	48,48,48,48	0
57	MG	1A	3262	1/1	0.97	0.15	28,28,28,28	0
57	MG	1A	3455	1/1	0.97	0.04	14,14,14,14	0
57	MG	1A	3263	1/1	0.97	0.05	33,33,33,33	0
57	MG	1A	3457	1/1	0.97	0.08	34,34,34,34	0
57	MG	1B	208	1/1	0.97	0.05	41,41,41,41	0
57	MG	1A	3571	1/1	0.97	0.09	41,41,41,41	0
57	MG	2A	3544	1/1	0.97	0.11	43,43,43,43	0
57	MG	2A	3545	1/1	0.97	0.08	34,34,34,34	0
57	MG	1A	3265	1/1	0.97	0.05	54,54,54,54	0
57	MG	1y	202	1/1	0.97	0.07	51,51,51,51	0
57	MG	1B	211	1/1	0.97	0.09	42,42,42,42	0
57	MG	1A	3362	1/1	0.97	0.06	41,41,41,41	0
57	MG	2A	3257	1/1	0.97	0.08	41,41,41,41	0
57	MG	1A	3690	1/1	0.97	0.06	42,42,42,42	0
57	MG	1A	3364	1/1	0.97	0.06	20,20,20,20	0
57	MG	1A	3266	1/1	0.97	0.14	34,34,34,34	0
57	MG	1A	3145	1/1	0.97	0.05	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3557	1/1	0.97	0.08	41,41,41,41	0
57	MG	1A	3147	1/1	0.97	0.12	49,49,49,49	0
57	MG	2A	3264	1/1	0.97	0.07	48,48,48,48	0
57	MG	1A	3094	1/1	0.97	0.05	25,25,25,25	0
57	MG	2A	3563	1/1	0.97	0.06	49,49,49,49	0
57	MG	2A	3006	1/1	0.97	0.06	43,43,43,43	0
57	MG	1A	3096	1/1	0.97	0.08	46,46,46,46	0
57	MG	1A	3051	1/1	0.97	0.16	35,35,35,35	0
57	MG	2A	3010	1/1	0.97	0.07	52,52,52,52	0
57	MG	1A	3154	1/1	0.97	0.20	28,28,28,28	0
57	MG	2A	3013	1/1	0.97	0.05	27,27,27,27	0
57	MG	1A	3701	1/1	0.97	0.05	37,37,37,37	0
57	MG	2A	3015	1/1	0.97	0.09	34,34,34,34	0
57	MG	1A	3204	1/1	0.97	0.06	40,40,40,40	0
57	MG	1A	3472	1/1	0.97	0.05	42,42,42,42	0
57	MG	1A	3473	1/1	0.97	0.06	51,51,51,51	0
57	MG	2A	3578	1/1	0.97	0.05	55,55,55,55	0
57	MG	2A	3020	1/1	0.97	0.10	45,45,45,45	0
57	MG	1A	3375	1/1	0.97	0.04	16,16,16,16	0
57	MG	1A	3707	1/1	0.97	0.06	45,45,45,45	0
57	MG	1A	3274	1/1	0.97	0.15	26,26,26,26	0
57	MG	1A	3709	1/1	0.97	0.11	42,42,42,42	0
57	MG	1A	3155	1/1	0.97	0.07	31,31,31,31	0
57	MG	1a	1712	1/1	0.97	0.10	44,44,44,44	0
57	MG	2a	3092	1/1	0.97	0.09	53,53,53,53	0
57	MG	1A	3589	1/1	0.97	0.15	30,30,30,30	0
57	MG	2A	3030	1/1	0.97	0.06	38,38,38,38	0
57	MG	2A	3589	1/1	0.97	0.04	48,48,48,48	0
57	MG	2A	3291	1/1	0.97	0.06	37,37,37,37	0
57	MG	1A	3876	1/1	0.97	0.06	45,45,45,45	0
57	MG	1D	312	1/1	0.97	0.14	23,23,23,23	0
57	MG	1A	3072	1/1	0.97	0.05	30,30,30,30	0
57	MG	1A	3380	1/1	0.97	0.05	22,22,22,22	0
57	MG	2A	3036	1/1	0.97	0.12	41,41,41,41	0
57	MG	1A	3715	1/1	0.97	0.12	47,47,47,47	0
57	MG	2a	3104	1/1	0.97	0.05	55,55,55,55	0
57	MG	2A	3598	1/1	0.97	0.04	48,48,48,48	0
57	MG	1A	3278	1/1	0.97	0.10	42,42,42,42	0
57	MG	2A	3300	1/1	0.97	0.05	40,40,40,40	0
57	MG	1D	317	1/1	0.97	0.04	38,38,38,38	0
57	MG	1A	3717	1/1	0.97	0.12	38,38,38,38	0
57	MG	2A	3041	1/1	0.97	0.14	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3604	1/1	0.97	0.06	41,41,41,41	0
57	MG	1A	3883	1/1	0.97	0.07	39,39,39,39	0
57	MG	2a	3115	1/1	0.97	0.07	51,51,51,51	0
57	MG	1A	3207	1/1	0.97	0.13	39,39,39,39	0
57	MG	1A	3281	1/1	0.97	0.08	48,48,48,48	0
57	MG	1A	3102	1/1	0.97	0.06	46,46,46,46	0
57	MG	1A	3386	1/1	0.97	0.04	24,24,24,24	0
57	MG	1A	3105	1/1	0.97	0.05	29,29,29,29	0
57	MG	2A	3311	1/1	0.97	0.14	52,52,52,52	0
57	MG	1A	3486	1/1	0.97	0.05	19,19,19,19	0
57	MG	2A	3614	1/1	0.97	0.06	26,26,26,26	0
57	MG	2A	3050	1/1	0.97	0.04	43,43,43,43	0
57	MG	1F	301	1/1	0.97	0.05	26,26,26,26	0
57	MG	2A	3052	1/1	0.97	0.10	51,51,51,51	0
57	MG	1A	3106	1/1	0.97	0.06	30,30,30,30	0
57	MG	2A	3054	1/1	0.97	0.04	38,38,38,38	0
57	MG	1F	309	1/1	0.97	0.06	35,35,35,35	0
57	MG	1a	1734	1/1	0.97	0.15	47,47,47,47	0
57	MG	2A	3321	1/1	0.97	0.08	47,47,47,47	0
57	MG	1a	1735	1/1	0.97	0.04	49,49,49,49	0
57	MG	2a	3134	1/1	0.97	0.10	66,66,66,66	0
57	MG	1A	3056	1/1	0.97	0.07	41,41,41,41	0
57	MG	1A	3727	1/1	0.97	0.07	39,39,39,39	0
57	MG	1A	3490	1/1	0.97	0.12	45,45,45,45	0
57	MG	2A	3327	1/1	0.97	0.08	56,56,56,56	0
57	MG	1F	313	1/1	0.97	0.07	31,31,31,31	0
57	MG	2A	3329	1/1	0.97	0.10	53,53,53,53	0
57	MG	1A	3291	1/1	0.97	0.08	49,49,49,49	0
57	MG	1F	315	1/1	0.97	0.09	46,46,46,46	0
57	MG	1A	3732	1/1	0.97	0.18	28,28,28,28	0
57	MG	1A	3897	1/1	0.97	0.05	47,47,47,47	0
57	MG	2A	3636	1/1	0.97	0.08	64,64,64,64	0
57	MG	1A	3604	1/1	0.97	0.07	44,44,44,44	0
57	MG	2a	3151	1/1	0.97	0.06	68,68,68,68	0
57	MG	1G	204	1/1	0.97	0.07	45,45,45,45	0
57	MG	2A	3338	1/1	0.97	0.08	46,46,46,46	0
57	MG	1A	3899	1/1	0.97	0.09	37,37,37,37	0
57	MG	2A	3340	1/1	0.97	0.07	59,59,59,59	0
57	MG	1A	3605	1/1	0.97	0.06	44,44,44,44	0
57	MG	1A	3391	1/1	0.97	0.05	37,37,37,37	0
57	MG	2A	3649	1/1	0.97	0.16	49,49,49,49	0
57	MG	2A	3344	1/1	0.97	0.09	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3345	1/1	0.97	0.06	35,35,35,35	0
57	MG	2A	3072	1/1	0.97	0.10	32,32,32,32	0
57	MG	1A	3163	1/1	0.97	0.11	36,36,36,36	0
57	MG	2A	3657	1/1	0.97	0.07	51,51,51,51	0
57	MG	1A	3903	1/1	0.97	0.06	45,45,45,45	0
57	MG	1P	202	1/1	0.97	0.07	25,25,25,25	0
57	MG	1A	3904	1/1	0.97	0.12	33,33,33,33	0
57	MG	1A	3164	1/1	0.97	0.08	29,29,29,29	0
57	MG	1a	1757	1/1	0.97	0.07	57,57,57,57	0
57	MG	2A	3663	1/1	0.97	0.07	38,38,38,38	0
57	MG	2A	3664	1/1	0.97	0.08	38,38,38,38	0
57	MG	1Q	201	1/1	0.97	0.05	29,29,29,29	0
57	MG	2a	3173	1/1	0.97	0.06	63,63,63,63	0
57	MG	2A	3356	1/1	0.97	0.07	46,46,46,46	0
57	MG	1A	3215	1/1	0.97	0.06	27,27,27,27	0
57	MG	2A	3668	1/1	0.97	0.06	63,63,63,63	0
57	MG	2A	3670	1/1	0.97	0.05	41,41,41,41	0
57	MG	1A	3908	1/1	0.97	0.04	41,41,41,41	0
57	MG	1A	3740	1/1	0.97	0.06	38,38,38,38	0
57	MG	1A	3217	1/1	0.97	0.18	30,30,30,30	0
57	MG	2A	3674	1/1	0.97	0.05	44,44,44,44	0
57	MG	2A	3675	1/1	0.97	0.05	42,42,42,42	0
57	MG	1A	3077	1/1	0.97	0.14	28,28,28,28	0
57	MG	1A	3300	1/1	0.97	0.11	32,32,32,32	0
57	MG	2A	3087	1/1	0.97	0.10	41,41,41,41	0
57	MG	2A	3089	1/1	0.97	0.14	48,48,48,48	0
57	MG	1R	203	1/1	0.97	0.09	45,45,45,45	0
57	MG	1A	3917	1/1	0.97	0.05	39,39,39,39	0
57	MG	1A	3744	1/1	0.97	0.06	41,41,41,41	0
57	MG	1A	3110	1/1	0.97	0.09	25,25,25,25	0
57	MG	1a	1770	1/1	0.97	0.08	51,51,51,51	0
57	MG	1A	3023	1/1	0.97	0.10	33,33,33,33	0
57	MG	1A	3400	1/1	0.97	0.07	27,27,27,27	0
57	MG	1A	3922	1/1	0.97	0.06	37,37,37,37	0
57	MG	2k	202	1/1	0.97	0.06	58,58,58,58	0
57	MG	1A	3402	1/1	0.97	0.06	18,18,18,18	0
57	MG	1A	3924	1/1	0.97	0.05	28,28,28,28	0
57	MG	2A	3379	1/1	0.97	0.08	40,40,40,40	0
57	MG	2A	3380	1/1	0.97	0.14	60,60,60,60	0
57	MG	1A	3750	1/1	0.97	0.05	49,49,49,49	0
57	MG	1U	208	1/1	0.97	0.10	30,30,30,30	0
57	MG	1A	3926	1/1	0.97	0.07	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3927	1/1	0.97	0.11	22,22,22,22	0
57	MG	1A	3114	1/1	0.97	0.07	30,30,30,30	0
57	MG	2A	3386	1/1	0.97	0.06	35,35,35,35	0
57	MG	1A	3930	1/1	0.97	0.12	38,38,38,38	0
57	MG	2A	3702	1/1	0.97	0.07	53,53,53,53	0
60	ZN	14	501	1/1	0.97	0.12	101,101,101,101	0
57	MG	2A	3388	1/1	0.97	0.09	46,46,46,46	0
57	MG	1A	3619	1/1	0.97	0.13	52,52,52,52	0
57	MG	2A	3265	1/1	0.98	0.12	27,27,27,27	0
57	MG	1A	3136	1/1	0.98	0.04	33,33,33,33	0
57	MG	1A	3243	1/1	0.98	0.06	24,24,24,24	0
57	MG	1A	3608	1/1	0.98	0.04	21,21,21,21	0
57	MG	1A	3095	1/1	0.98	0.03	14,14,14,14	0
57	MG	2A	3503	1/1	0.98	0.08	52,52,52,52	0
57	MG	2A	3270	1/1	0.98	0.17	44,44,44,44	0
57	MG	2A	3271	1/1	0.98	0.05	26,26,26,26	0
57	MG	1A	4008	1/1	0.98	0.05	55,55,55,55	0
57	MG	1A	4009	1/1	0.98	0.06	43,43,43,43	0
57	MG	1A	3033	1/1	0.98	0.07	29,29,29,29	0
57	MG	1A	3406	1/1	0.98	0.07	52,52,52,52	0
57	MG	1A	3865	1/1	0.98	0.07	28,28,28,28	0
57	MG	1A	3730	1/1	0.98	0.20	26,26,26,26	0
57	MG	1A	3867	1/1	0.98	0.07	40,40,40,40	0
57	MG	1A	3318	1/1	0.98	0.03	16,16,16,16	0
57	MG	2A	3069	1/1	0.98	0.05	38,38,38,38	0
57	MG	1A	3869	1/1	0.98	0.05	34,34,34,34	0
57	MG	1A	3319	1/1	0.98	0.26	29,29,29,29	0
57	MG	1A	3409	1/1	0.98	0.06	20,20,20,20	0
57	MG	1A	3410	1/1	0.98	0.07	26,26,26,26	0
57	MG	2A	3074	1/1	0.98	0.07	30,30,30,30	0
57	MG	1A	4020	1/1	0.98	0.04	54,54,54,54	0
57	MG	2A	3288	1/1	0.98	0.11	52,52,52,52	0
57	MG	1A	3509	1/1	0.98	0.04	29,29,29,29	0
57	MG	1A	3017	1/1	0.98	0.12	28,28,28,28	0
57	MG	1a	1796	1/1	0.98	0.05	45,45,45,45	0
57	MG	1A	3737	1/1	0.98	0.04	27,27,27,27	0
57	MG	1A	3247	1/1	0.98	0.11	25,25,25,25	0
57	MG	2A	3294	1/1	0.98	0.05	34,34,34,34	0
57	MG	2R	201	1/1	0.98	0.09	46,46,46,46	0
57	MG	1A	3322	1/1	0.98	0.05	27,27,27,27	0
57	MG	1A	3513	1/1	0.98	0.10	20,20,20,20	0
57	MG	1A	4027	1/1	0.98	0.15	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3248	1/1	0.98	0.11	39,39,39,39	0
57	MG	1A	3415	1/1	0.98	0.05	26,26,26,26	0
57	MG	1A	3099	1/1	0.98	0.05	43,43,43,43	0
57	MG	2U	201	1/1	0.98	0.22	48,48,48,48	0
57	MG	2A	3535	1/1	0.98	0.07	55,55,55,55	0
57	MG	1A	3624	1/1	0.98	0.08	55,55,55,55	0
57	MG	2A	3302	1/1	0.98	0.05	50,50,50,50	0
57	MG	1A	3327	1/1	0.98	0.10	42,42,42,42	0
57	MG	1a	1627	1/1	0.98	0.06	50,50,50,50	0
57	MG	1A	3141	1/1	0.98	0.17	35,35,35,35	0
57	MG	1A	3887	1/1	0.98	0.03	38,38,38,38	0
57	MG	1A	3747	1/1	0.98	0.05	34,34,34,34	0
57	MG	1A	3073	1/1	0.98	0.04	32,32,32,32	0
57	MG	2A	3095	1/1	0.98	0.06	51,51,51,51	0
57	MG	1a	1632	1/1	0.98	0.13	47,47,47,47	0
57	MG	2A	3548	1/1	0.98	0.05	44,44,44,44	0
57	MG	1A	3420	1/1	0.98	0.04	32,32,32,32	0
57	MG	1A	3143	1/1	0.98	0.05	18,18,18,18	0
57	MG	1A	3751	1/1	0.98	0.05	30,30,30,30	0
57	MG	1A	3074	1/1	0.98	0.04	32,32,32,32	0
57	MG	2A	3315	1/1	0.98	0.05	36,36,36,36	0
57	MG	1A	3332	1/1	0.98	0.04	37,37,37,37	0
57	MG	2A	3102	1/1	0.98	0.14	50,50,50,50	0
57	MG	1B	214	1/1	0.98	0.06	37,37,37,37	0
57	MG	1A	3333	1/1	0.98	0.07	19,19,19,19	0
57	MG	1A	3035	1/1	0.98	0.11	44,44,44,44	0
57	MG	1A	3335	1/1	0.98	0.06	23,23,23,23	0
57	MG	2A	3560	1/1	0.98	0.04	60,60,60,60	0
57	MG	2A	3561	1/1	0.98	0.04	26,26,26,26	0
57	MG	2A	3322	1/1	0.98	0.06	36,36,36,36	0
57	MG	1A	3076	1/1	0.98	0.10	29,29,29,29	0
57	MG	1A	3760	1/1	0.98	0.10	42,42,42,42	0
57	MG	1A	3428	1/1	0.98	0.04	26,26,26,26	0
57	MG	2A	3566	1/1	0.98	0.07	66,66,66,66	0
57	MG	1A	3256	1/1	0.98	0.12	35,35,35,35	0
57	MG	1A	3339	1/1	0.98	0.10	23,23,23,23	0
57	MG	1A	3641	1/1	0.98	0.06	42,42,42,42	0
57	MG	1a	1650	1/1	0.98	0.13	53,53,53,53	0
57	MG	2A	3330	1/1	0.98	0.12	51,51,51,51	0
57	MG	1A	3257	1/1	0.98	0.08	40,40,40,40	0
57	MG	1a	1830	1/1	0.98	0.08	57,57,57,57	0
57	MG	2A	3575	1/1	0.98	0.10	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3643	1/1	0.98	0.07	32,32,32,32	0
57	MG	1A	3149	1/1	0.98	0.09	33,33,33,33	0
57	MG	1A	3052	1/1	0.98	0.07	26,26,26,26	0
57	MG	2A	3579	1/1	0.98	0.06	44,44,44,44	0
57	MG	1A	3151	1/1	0.98	0.05	33,33,33,33	0
57	MG	1A	3536	1/1	0.98	0.05	23,23,23,23	0
57	MG	1a	1657	1/1	0.98	0.07	51,51,51,51	0
57	MG	1A	3911	1/1	0.98	0.06	44,44,44,44	0
57	MG	1D	302	1/1	0.98	0.06	32,32,32,32	0
57	MG	1A	3912	1/1	0.98	0.04	31,31,31,31	0
57	MG	2A	3343	1/1	0.98	0.11	37,37,37,37	0
57	MG	1A	3108	1/1	0.98	0.08	29,29,29,29	0
57	MG	2a	3036	1/1	0.98	0.08	46,46,46,46	0
57	MG	2A	3127	1/1	0.98	0.07	42,42,42,42	0
57	MG	1a	1841	1/1	0.98	0.05	54,54,54,54	0
57	MG	1D	305	1/1	0.98	0.10	28,28,28,28	0
57	MG	1A	3053	1/1	0.98	0.12	29,29,29,29	0
57	MG	1D	307	1/1	0.98	0.10	41,41,41,41	0
57	MG	1D	309	1/1	0.98	0.05	36,36,36,36	0
57	MG	1D	310	1/1	0.98	0.10	31,31,31,31	0
57	MG	1D	311	1/1	0.98	0.13	42,42,42,42	0
57	MG	1A	3916	1/1	0.98	0.06	54,54,54,54	0
57	MG	1A	3054	1/1	0.98	0.12	33,33,33,33	0
57	MG	2A	3139	1/1	0.98	0.10	53,53,53,53	0
57	MG	2A	3358	1/1	0.98	0.05	38,38,38,38	0
57	MG	1A	3264	1/1	0.98	0.08	32,32,32,32	0
57	MG	1A	3439	1/1	0.98	0.07	37,37,37,37	0
57	MG	2A	3142	1/1	0.98	0.05	40,40,40,40	0
57	MG	1A	3112	1/1	0.98	0.10	29,29,29,29	0
57	MG	1A	3024	1/1	0.98	0.03	14,14,14,14	0
57	MG	1a	1854	1/1	0.98	0.06	49,49,49,49	0
57	MG	1A	3157	1/1	0.98	0.15	37,37,37,37	0
57	MG	1E	301	1/1	0.98	0.05	42,42,42,42	0
57	MG	2a	3057	1/1	0.98	0.08	57,57,57,57	0
57	MG	1E	302	1/1	0.98	0.11	36,36,36,36	0
57	MG	1E	303	1/1	0.98	0.05	32,32,32,32	0
57	MG	2A	3150	1/1	0.98	0.04	52,52,52,52	0
57	MG	1A	3037	1/1	0.98	0.04	34,34,34,34	0
57	MG	2A	3613	1/1	0.98	0.08	50,50,50,50	0
57	MG	1A	3546	1/1	0.98	0.04	25,25,25,25	0
57	MG	1A	3025	1/1	0.98	0.10	35,35,35,35	0
57	MG	2A	3373	1/1	0.98	0.04	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3445	1/1	0.98	0.04	12,12,12,12	0
57	MG	2A	3618	1/1	0.98	0.06	60,60,60,60	0
57	MG	1A	3209	1/1	0.98	0.11	44,44,44,44	0
57	MG	2A	3620	1/1	0.98	0.06	46,46,46,46	0
57	MG	2A	3376	1/1	0.98	0.05	47,47,47,47	0
57	MG	1A	3026	1/1	0.98	0.18	25,25,25,25	0
57	MG	1a	1684	1/1	0.98	0.05	48,48,48,48	0
57	MG	1A	3161	1/1	0.98	0.09	22,22,22,22	0
57	MG	1A	3019	1/1	0.98	0.10	20,20,20,20	0
57	MG	1F	304	1/1	0.98	0.07	36,36,36,36	0
57	MG	1F	306	1/1	0.98	0.10	24,24,24,24	0
57	MG	1A	3357	1/1	0.98	0.06	37,37,37,37	0
57	MG	1A	3554	1/1	0.98	0.21	21,21,21,21	0
57	MG	1A	3358	1/1	0.98	0.04	23,23,23,23	0
57	MG	1A	3667	1/1	0.98	0.12	42,42,42,42	0
57	MG	1A	3118	1/1	0.98	0.14	21,21,21,21	0
57	MG	2A	3168	1/1	0.98	0.15	36,36,36,36	0
57	MG	1A	3937	1/1	0.98	0.10	53,53,53,53	0
57	MG	1A	3275	1/1	0.98	0.16	25,25,25,25	0
57	MG	1A	3085	1/1	0.98	0.17	29,29,29,29	0
57	MG	1a	1697	1/1	0.98	0.10	55,55,55,55	0
57	MG	1A	3671	1/1	0.98	0.08	29,29,29,29	0
57	MG	1A	3560	1/1	0.98	0.03	32,32,32,32	0
57	MG	2A	3175	1/1	0.98	0.09	43,43,43,43	0
57	MG	1A	3120	1/1	0.98	0.08	17,17,17,17	0
57	MG	2A	3642	1/1	0.98	0.04	49,49,49,49	0
57	MG	1G	203	1/1	0.98	0.06	58,58,58,58	0
57	MG	2A	3644	1/1	0.98	0.06	54,54,54,54	0
57	MG	1a	1702	1/1	0.98	0.10	48,48,48,48	0
57	MG	2A	3648	1/1	0.98	0.05	51,51,51,51	0
57	MG	1A	3363	1/1	0.98	0.07	38,38,38,38	0
57	MG	1H	201	1/1	0.98	0.06	34,34,34,34	0
57	MG	2A	3651	1/1	0.98	0.06	50,50,50,50	0
57	MG	1A	3216	1/1	0.98	0.10	38,38,38,38	0
57	MG	2A	3653	1/1	0.98	0.04	44,44,44,44	0
57	MG	1A	3365	1/1	0.98	0.04	33,33,33,33	0
57	MG	2A	3655	1/1	0.98	0.05	49,49,49,49	0
57	MG	1A	3565	1/1	0.98	0.08	41,41,41,41	0
57	MG	1A	3279	1/1	0.98	0.09	38,38,38,38	0
57	MG	2a	3106	1/1	0.98	0.06	53,53,53,53	0
57	MG	2A	3406	1/1	0.98	0.09	39,39,39,39	0
57	MG	2A	3407	1/1	0.98	0.06	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2a	3109	1/1	0.98	0.07	52,52,52,52	0
57	MG	1A	3460	1/1	0.98	0.03	23,23,23,23	0
57	MG	2A	3409	1/1	0.98	0.16	53,53,53,53	0
57	MG	1P	201	1/1	0.98	0.14	29,29,29,29	0
57	MG	1A	3028	1/1	0.98	0.18	22,22,22,22	0
57	MG	1A	3122	1/1	0.98	0.10	27,27,27,27	0
57	MG	2A	3189	1/1	0.98	0.04	49,49,49,49	0
57	MG	2A	3414	1/1	0.98	0.05	52,52,52,52	0
57	MG	1A	3123	1/1	0.98	0.10	36,36,36,36	0
57	MG	2A	3416	1/1	0.98	0.12	50,50,50,50	0
57	MG	2A	3669	1/1	0.98	0.04	52,52,52,52	0
57	MG	1A	3283	1/1	0.98	0.11	38,38,38,38	0
57	MG	1A	3807	1/1	0.98	0.05	29,29,29,29	0
57	MG	1a	1716	1/1	0.98	0.07	41,41,41,41	0
57	MG	2A	3194	1/1	0.98	0.07	40,40,40,40	0
57	MG	2A	3195	1/1	0.98	0.07	48,48,48,48	0
57	MG	1A	3169	1/1	0.98	0.04	25,25,25,25	0
57	MG	2a	3126	1/1	0.98	0.06	60,60,60,60	0
57	MG	1A	3285	1/1	0.98	0.13	39,39,39,39	0
57	MG	1A	3467	1/1	0.98	0.07	24,24,24,24	0
57	MG	1A	3286	1/1	0.98	0.05	25,25,25,25	0
57	MG	1A	3576	1/1	0.98	0.07	43,43,43,43	0
57	MG	1A	3287	1/1	0.98	0.15	27,27,27,27	0
57	MG	1A	3221	1/1	0.98	0.08	29,29,29,29	0
57	MG	1A	3289	1/1	0.98	0.14	33,33,33,33	0
57	MG	1A	3063	1/1	0.98	0.11	44,44,44,44	0
57	MG	1A	3818	1/1	0.98	0.04	36,36,36,36	0
57	MG	2a	3136	1/1	0.98	0.07	50,50,50,50	0
57	MG	1A	3043	1/1	0.98	0.04	13,13,13,13	0
57	MG	1a	1728	1/1	0.98	0.05	39,39,39,39	0
57	MG	2a	3139	1/1	0.98	0.09	59,59,59,59	0
57	MG	1A	3225	1/1	0.98	0.04	20,20,20,20	0
57	MG	1A	3822	1/1	0.98	0.04	32,32,32,32	0
57	MG	2A	3210	1/1	0.98	0.10	52,52,52,52	0
57	MG	2a	3143	1/1	0.98	0.07	47,47,47,47	0
57	MG	1A	3823	1/1	0.98	0.05	43,43,43,43	0
57	MG	1A	3695	1/1	0.98	0.04	57,57,57,57	0
57	MG	2A	3693	1/1	0.98	0.03	35,35,35,35	0
57	MG	1U	207	1/1	0.98	0.07	32,32,32,32	0
57	MG	2A	3440	1/1	0.98	0.04	34,34,34,34	0
57	MG	2A	3696	1/1	0.98	0.05	53,53,53,53	0
57	MG	1A	3126	1/1	0.98	0.05	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3009	1/1	0.98	0.12	41,41,41,41	0
57	MG	1V	201	1/1	0.98	0.14	28,28,28,28	0
57	MG	1A	3029	1/1	0.98	0.06	30,30,30,30	0
57	MG	1A	3128	1/1	0.98	0.09	62,62,62,62	0
57	MG	1A	3830	1/1	0.98	0.05	26,26,26,26	0
57	MG	1A	3298	1/1	0.98	0.03	14,14,14,14	0
57	MG	1a	1740	1/1	0.98	0.03	55,55,55,55	0
57	MG	2A	3449	1/1	0.98	0.05	49,49,49,49	0
57	MG	1A	3229	1/1	0.98	0.08	27,27,27,27	0
57	MG	1A	3702	1/1	0.98	0.03	41,41,41,41	0
57	MG	2A	3019	1/1	0.98	0.06	40,40,40,40	0
57	MG	1A	3129	1/1	0.98	0.07	31,31,31,31	0
57	MG	1A	3005	1/1	0.98	0.10	21,21,21,21	0
57	MG	2A	3022	1/1	0.98	0.11	42,42,42,42	0
57	MG	1A	3178	1/1	0.98	0.12	19,19,19,19	0
57	MG	10	102	1/1	0.98	0.04	34,34,34,34	0
57	MG	1A	3837	1/1	0.98	0.23	34,34,34,34	0
57	MG	2A	3716	1/1	0.98	0.05	55,55,55,55	0
57	MG	2A	3459	1/1	0.98	0.07	48,48,48,48	0
57	MG	10	104	1/1	0.98	0.08	39,39,39,39	0
57	MG	2A	3027	1/1	0.98	0.06	50,50,50,50	0
57	MG	1a	1749	1/1	0.98	0.05	68,68,68,68	0
57	MG	1A	3838	1/1	0.98	0.15	26,26,26,26	0
57	MG	1A	3008	1/1	0.98	0.06	29,29,29,29	0
57	MG	2A	3031	1/1	0.98	0.09	36,36,36,36	0
57	MG	1A	3485	1/1	0.98	0.05	44,44,44,44	0
57	MG	10	108	1/1	0.98	0.15	32,32,32,32	0
57	MG	2a	3180	1/1	0.98	0.04	63,63,63,63	0
57	MG	1A	3304	1/1	0.98	0.04	37,37,37,37	0
57	MG	1A	3487	1/1	0.98	0.04	25,25,25,25	0
57	MG	1A	3843	1/1	0.98	0.06	21,21,21,21	0
57	MG	2a	3184	1/1	0.98	0.04	47,47,47,47	0
57	MG	1A	3595	1/1	0.98	0.06	29,29,29,29	0
57	MG	1A	3180	1/1	0.98	0.12	28,28,28,28	0
57	MG	2A	3473	1/1	0.98	0.09	54,54,54,54	0
57	MG	1A	3712	1/1	0.98	0.17	31,31,31,31	0
57	MG	1A	3992	1/1	0.98	0.04	45,45,45,45	0
57	MG	1A	3306	1/1	0.98	0.18	40,40,40,40	0
57	MG	15	104	1/1	0.98	0.05	33,33,33,33	0
57	MG	2A	3043	1/1	0.98	0.04	24,24,24,24	0
57	MG	1a	1764	1/1	0.98	0.03	41,41,41,41	0
57	MG	2f	201	1/1	0.98	0.05	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3307	1/1	0.98	0.11	34,34,34,34	0
57	MG	2A	3251	1/1	0.98	0.06	41,41,41,41	0
57	MG	1A	3068	1/1	0.98	0.10	33,33,33,33	0
57	MG	1A	3133	1/1	0.98	0.08	28,28,28,28	0
57	MG	1A	3069	1/1	0.98	0.19	32,32,32,32	0
57	MG	2A	3255	1/1	0.98	0.11	39,39,39,39	0
57	MG	17	102	1/1	0.98	0.04	28,28,28,28	0
57	MG	1A	3495	1/1	0.98	0.04	24,24,24,24	0
57	MG	1A	3184	1/1	0.98	0.08	28,28,28,28	0
57	MG	1A	3720	1/1	0.98	0.04	38,38,38,38	0
57	MG	2A	3491	1/1	0.98	0.04	56,56,56,56	0
57	MG	1a	1773	1/1	0.98	0.06	63,63,63,63	0
57	MG	1A	3001	1/1	0.98	0.04	25,25,25,25	0
57	MG	1A	3856	1/1	0.98	0.06	41,41,41,41	0
57	MG	2B	216	1/1	0.98	0.09	54,54,54,54	0
57	MG	2A	3263	1/1	0.98	0.04	38,38,38,38	0
57	MG	1A	3401	1/1	0.98	0.04	31,31,31,31	0
60	ZN	2Y	202	1/1	0.98	0.04	75,75,75,75	0
57	MG	2B	219	1/1	0.98	0.06	59,59,59,59	0
60	ZN	2n	501	1/1	0.98	0.05	85,85,85,85	0
61	SF4	2d	501	8/8	0.98	0.06	65,72,77,83	0
57	MG	2B	220	1/1	0.98	0.09	43,43,43,43	0
57	MG	1a	1855	1/1	0.99	0.04	51,51,51,51	0
57	MG	1D	301	1/1	0.99	0.14	27,27,27,27	0
57	MG	2A	3088	1/1	0.99	0.19	38,38,38,38	0
57	MG	1A	3325	1/1	0.99	0.04	32,32,32,32	0
57	MG	1A	3101	1/1	0.99	0.17	26,26,26,26	0
57	MG	2A	3166	1/1	0.99	0.12	42,42,42,42	0
57	MG	1A	3754	1/1	0.99	0.04	31,31,31,31	0
57	MG	1A	3200	1/1	0.99	0.06	27,27,27,27	0
57	MG	1A	3873	1/1	0.99	0.04	36,36,36,36	0
57	MG	1A	3756	1/1	0.99	0.04	17,17,17,17	0
57	MG	1D	308	1/1	0.99	0.05	14,14,14,14	0
57	MG	1A	3146	1/1	0.99	0.05	35,35,35,35	0
57	MG	1A	3045	1/1	0.99	0.08	34,34,34,34	0
57	MG	1a	1866	1/1	0.99	0.08	46,46,46,46	0
57	MG	1A	3308	1/1	0.99	0.08	29,29,29,29	0
57	MG	1A	3148	1/1	0.99	0.05	28,28,28,28	0
57	MG	1A	3103	1/1	0.99	0.07	32,32,32,32	0
57	MG	1A	3880	1/1	0.99	0.04	28,28,28,28	0
57	MG	1A	3381	1/1	0.99	0.06	13,13,13,13	0
57	MG	2D	304	1/1	0.99	0.11	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3333	1/1	0.99	0.04	42,42,42,42	0
57	MG	1A	3104	1/1	0.99	0.22	29,29,29,29	0
57	MG	1A	3728	1/1	0.99	0.04	28,28,28,28	0
57	MG	1A	3929	1/1	0.99	0.02	12,12,12,12	0
57	MG	1A	3177	1/1	0.99	0.12	18,18,18,18	0
57	MG	1A	3238	1/1	0.99	0.11	35,35,35,35	0
57	MG	2A	3502	1/1	0.99	0.03	39,39,39,39	0
57	MG	1U	204	1/1	0.99	0.14	32,32,32,32	0
57	MG	2A	3110	1/1	0.99	0.03	31,31,31,31	0
57	MG	1U	205	1/1	0.99	0.09	35,35,35,35	0
57	MG	2a	3149	1/1	0.99	0.09	52,52,52,52	0
57	MG	1A	3222	1/1	0.99	0.07	22,22,22,22	0
57	MG	2E	305	1/1	0.99	0.06	36,36,36,36	0
57	MG	2E	306	1/1	0.99	0.11	44,44,44,44	0
57	MG	1A	3337	1/1	0.99	0.07	22,22,22,22	0
57	MG	2A	3594	1/1	0.99	0.05	34,34,34,34	0
57	MG	1A	3699	1/1	0.99	0.03	37,37,37,37	0
57	MG	1A	3294	1/1	0.99	0.03	31,31,31,31	0
57	MG	1V	202	1/1	0.99	0.06	29,29,29,29	0
57	MG	2A	3686	1/1	0.99	0.03	41,41,41,41	0
57	MG	2A	3347	1/1	0.99	0.07	37,37,37,37	0
57	MG	1V	203	1/1	0.99	0.03	35,35,35,35	0
57	MG	1A	3636	1/1	0.99	0.09	38,38,38,38	0
57	MG	1a	1752	1/1	0.99	0.04	47,47,47,47	0
57	MG	1A	3042	1/1	0.99	0.05	29,29,29,29	0
57	MG	2A	3273	1/1	0.99	0.03	31,31,31,31	0
57	MG	1A	3638	1/1	0.99	0.06	33,33,33,33	0
57	MG	2A	3518	1/1	0.99	0.04	49,49,49,49	0
57	MG	2a	3167	1/1	0.99	0.05	63,63,63,63	0
57	MG	1A	3060	1/1	0.99	0.07	36,36,36,36	0
57	MG	2A	3355	1/1	0.99	0.03	35,35,35,35	0
57	MG	1A	3242	1/1	0.99	0.05	26,26,26,26	0
57	MG	1F	302	1/1	0.99	0.04	23,23,23,23	0
57	MG	1F	303	1/1	0.99	0.20	27,27,27,27	0
57	MG	1A	3941	1/1	0.99	0.03	46,46,46,46	0
57	MG	1F	305	1/1	0.99	0.05	29,29,29,29	0
57	MG	1A	3492	1/1	0.99	0.06	45,45,45,45	0
57	MG	1F	307	1/1	0.99	0.03	25,25,25,25	0
57	MG	1A	3055	1/1	0.99	0.07	27,27,27,27	0
57	MG	2A	3131	1/1	0.99	0.06	45,45,45,45	0
57	MG	1a	1633	1/1	0.99	0.03	32,32,32,32	0
57	MG	1A	3098	1/1	0.99	0.05	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3468	1/1	0.99	0.06	18,18,18,18	0
57	MG	2A	3709	1/1	0.99	0.03	49,49,49,49	0
57	MG	1A	3816	1/1	0.99	0.10	36,36,36,36	0
57	MG	1A	3018	1/1	0.99	0.05	23,23,23,23	0
57	MG	1A	3009	1/1	0.99	0.03	22,22,22,22	0
57	MG	2A	3138	1/1	0.99	0.05	29,29,29,29	0
57	MG	23	101	1/1	0.99	0.07	48,48,48,48	0
57	MG	1t	201	1/1	0.99	0.04	56,56,56,56	0
57	MG	1A	3323	1/1	0.99	0.06	16,16,16,16	0
57	MG	1A	3527	1/1	0.99	0.10	22,22,22,22	0
57	MG	1A	3821	1/1	0.99	0.04	41,41,41,41	0
57	MG	2A	3541	1/1	0.99	0.03	49,49,49,49	0
57	MG	1A	3862	1/1	0.99	0.04	40,40,40,40	0
57	MG	2A	3377	1/1	0.99	0.03	36,36,36,36	0
57	MG	13	101	1/1	0.99	0.10	26,26,26,26	0
57	MG	1A	3111	1/1	0.99	0.14	26,26,26,26	0
57	MG	2a	3099	1/1	0.99	0.02	63,63,63,63	0
57	MG	13	103	1/1	0.99	0.04	41,41,41,41	0
57	MG	2A	3547	1/1	0.99	0.07	44,44,44,44	0
57	MG	1A	3907	1/1	0.99	0.03	34,34,34,34	0
57	MG	1A	3371	1/1	0.99	0.08	27,27,27,27	0
57	MG	15	103	1/1	0.99	0.05	29,29,29,29	0
57	MG	2A	3004	1/1	0.99	0.05	38,38,38,38	0
57	MG	2A	3729	1/1	0.99	0.08	38,38,38,38	0
57	MG	1a	1649	1/1	0.99	0.06	35,35,35,35	0
57	MG	1A	3559	1/1	0.99	0.03	29,29,29,29	0
57	MG	15	105	1/1	0.99	0.14	28,28,28,28	0
57	MG	1A	3501	1/1	0.99	0.03	23,23,23,23	0
57	MG	1N	201	1/1	0.99	0.03	43,43,43,43	0
57	MG	1A	3826	1/1	0.99	0.04	32,32,32,32	0
60	ZN	1Y	501	1/1	0.99	0.03	55,55,55,55	0
57	MG	2A	3645	1/1	0.99	0.02	34,34,34,34	0
60	ZN	15	109	1/1	0.99	0.02	38,38,38,38	0
60	ZN	16	501	1/1	0.99	0.04	39,39,39,39	0
60	ZN	1n	102	1/1	0.99	0.03	68,68,68,68	0
57	MG	2A	3646	1/1	0.99	0.06	35,35,35,35	0
57	MG	1A	3827	1/1	0.99	0.06	23,23,23,23	0
60	ZN	25	104	1/1	0.99	0.03	51,51,51,51	0
60	ZN	29	501	1/1	0.99	0.03	57,57,57,57	0
57	MG	2A	3012	1/1	0.99	0.07	55,55,55,55	0
61	SF4	1d	307	8/8	0.99	0.05	58,62,71,72	0
57	MG	1A	3913	1/1	0.99	0.03	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3961	1/1	0.99	0.05	22,22,22,22	0
57	MG	1A	3378	1/1	1.00	0.01	11,11,11,11	0
60	ZN	26	102	1/1	1.00	0.02	52,52,52,52	0
57	MG	2A	3485	1/1	1.00	0.04	33,33,33,33	0
60	ZN	19	104	1/1	1.00	0.02	38,38,38,38	0
57	MG	2A	3574	1/1	1.00	0.03	58,58,58,58	0
57	MG	1A	3975	1/1	1.00	0.02	39,39,39,39	0
57	MG	1A	3297	1/1	1.00	0.06	23,23,23,23	0

6.5 Other polymers (i)

There are no such residues in this entry.