wwPDB X-ray Structure Validation Summary Report (i)

Aug 6, 2026 – 09:15 AM EDT

PDB ID	:	8VTY / pdb_00008vty
Title	:	Crystal structure of the wild-type Thermus thermophilus 70S ribosome in complex with ciprofloxacin and protein Y at 2.60A resolution
Authors	:	Aleksandrova, E.V.; Ma, C.-X.; Klepacki, D.; Alizadeh, F.; Vazquez-Laslop, N.; Liang, J.-H.; Polikanov, Y.S.; Mankin, A.S.
Deposited on	:	2024-01-27
Resolution	:	2.60 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 (1)) were used in the production of this report:

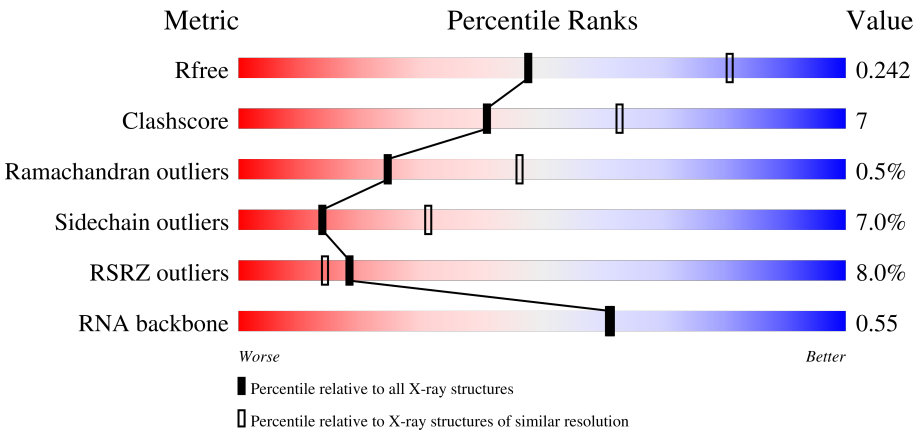
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
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 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)
RNA backbone	3983	1014 (2.84-2.36)

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	5% 69% 25% • •
1	2A	2915	6% 66% 27% 6% •
2	1B	121	2% 80% 18% ••

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Mol	Chain	Length	Quality of chain
2	2B	121	5% 59% 37%
3	1D	276	% 83% 15%
3	2D	276	% 83% 13%
4	1E	206	% 78% 17%
4	2E	206	% 76% 19%
5	1F	210	% 77% 16%
5	2F	210	73% 20%
6	1G	182	7% 74% 22%
6	2G	182	25% 52% 44%
7	1H	180	4% 76% 21%
7	2H	180	18% 61% 33%
8	1I	148	7% 78% 17%
8	2I	148	3% 77% 20%
9	1N	140	% 83% 13%
9	2N	140	2% 78% 21%
10	1O	122	84% 16%
10	2O	122	84% 16%
11	1P	150	% 81% 17%
11	2P	150	% 82% 13%
12	1Q	141	87% 11%
12	2Q	141	4% 82% 16%
13	1R	118	80% 19%
13	2R	118	79% 19%
14	1S	112	% 78% 18%
14	2S	112	19% 69% 28%

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Mol	Chain	Length	Quality of chain
15	1T	146	3% 66% 22% 10%
15	2T	146	% 71% 18% 10%
16	1U	118	87% 10%
16	2U	118	81% 17%
17	1V	101	85% 14%
17	2V	101	3% 74% 23%
18	1W	113	2% 85% 13%
18	2W	113	2% 84% 12%
19	1X	96	2% 80% 16%
19	2X	96	6% 85% 14%
20	1Y	110	% 75% 22%
20	2Y	110	5% 79% 16%
21	1Z	206	2% 80% 17%
21	2Z	206	8% 78% 17%
22	10	85	% 82% 8% 9%
22	20	85	7% 81% 9% 9%
23	11	98	% 78% 20%
23	21	98	5% 72% 24%
24	12	72	% 81% 17%
24	22	72	% 69% 24%
25	13	60	73% 23%
25	23	60	5% 82% 15%
26	14	71	28% 61% 31%
26	24	71	35% 51% 41% 6%
27	15	60	2% 87% 12%

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Mol	Chain	Length	Quality of chain
27	25	60	80% 18%
28	16	54	89% 9%
28	26	54	76% 19%
29	17	49	8% 82% 14%
29	27	49	10% 82% 12%
30	18	65	2% 72% 25%
30	28	65	3% 82% 17%
31	19	37	3% 84% 16%
31	29	37	8% 62% 38%
32	1a	1521	4% 61% 32% 6%
32	2a	1521	8% 60% 33% 6%
33	1b	256	21% 55% 30% 5% 10%
33	2b	256	27% 53% 33% 5% 10%
34	1c	239	9% 67% 18% 14%
34	2c	239	28% 61% 22% 14%
35	1d	209	10% 65% 31%
35	2d	209	11% 74% 23%
36	1e	162	2% 66% 22% 9%
36	2e	162	5% 64% 26% 9%
37	1f	101	2% 76% 22%
37	2f	101	81% 18%
38	1g	156	3% 78% 21%
38	2g	156	17% 72% 26%
39	1h	138	4% 71% 27%
39	2h	138	4% 68% 28%

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Mol	Chain	Length	Quality of chain
40	1i	128	28% 63% 29% 7%
40	2i	128	66% 58% 37%
41	1j	105	27% 70% 21% 8%
41	2j	105	67% 52% 36% 9%
42	1k	129	3% 79% 9% 12%
42	2k	129	8% 71% 16% 12%
43	1l	132	4% 80% 13% 8%
43	2l	132	5% 68% 23% 8%
44	1m	126	15% 59% 29% 8%
44	2m	126	29% 52% 35% 10%
45	1n	61	8% 57% 38%
45	2n	61	62% 66% 30%
46	1o	89	3% 75% 20%
46	2o	89	8% 67% 27%
47	1p	88	24% 57% 35% 7%
47	2p	88	6% 65% 25% 7%
48	1q	105	5% 68% 25% 6%
48	2q	105	3% 70% 22% 6%
49	1r	88	2% 64% 14% 23%
49	2r	88	2% 57% 19% 23%
50	1s	93	11% 56% 30% 11%
50	2s	93	47% 49% 35% 11%
51	1t	106	19% 66% 19% 6% 9%
51	2t	106	7% 74% 18% 8%
52	1u	27	22% 67% 15% 15%

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Mol	Chain	Length	Quality of chain
52	2u	27	70% 59% 26% 15%
53	1y	113	5% 72% 12% • 14%
53	2y	113	29% 61% 20% • 15%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
54	MG	1A	3641	-	-	-	X
54	MG	1A	3996	-	-	-	X
54	MG	1a	1794	-	-	-	X
54	MG	2A	3190	-	-	-	X
54	MG	2A	3409	-	-	-	X
54	MG	2a	3079	-	-	-	X
54	MG	2a	3160	-	-	-	X

2 Entry composition (i)

There are 60 unique types of molecules in this entry. The entry contains 297563 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	77	608	375	129	103	1	0	0	0
22	20	77	608	375	129	103	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
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
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
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
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
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
			Total	C	N	O	S			
53	2y	96	749	468	141	137	3	0	0	0

- Molecule 54 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
54	1A	1056	1056	1056	0	0
			Total	Mg		
54	1B	29	29	29	0	0
			Total	Mg		
54	1D	18	18	18	0	0
			Total	Mg		
54	1E	9	9	9	0	0
			Total	Mg		
54	1F	19	19	19	0	0
			Total	Mg		
54	1G	4	4	4	0	0
			Total	Mg		
54	1H	3	3	3	0	0
			Total	Mg		
54	1N	5	5	5	0	0
			Total	Mg		
54	1O	1	1	1	0	0
			Total	Mg		
54	1P	6	6	6	0	0
			Total	Mg		
54	1Q	5	5	5	0	0
			Total	Mg		
54	1R	6	6	6	0	0
			Total	Mg		
54	1T	5	5	5	0	0
			Total	Mg		
54	1U	7	7	7	0	0
			Total	Mg		
54	1V	6	6	6	0	0
			Total	Mg		
54	1W	3	3	3	0	0
			Total	Mg		
54	1Z	1	1	1	0	0
			Total	Mg		
54	10	7	7	7	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
54	11	5	5	5	0	0
54	13	4	4	4	0	0
54	14	1	1	1	0	0
54	15	8	8	8	0	0
54	17	7	7	7	0	0
54	18	3	3	3	0	0
54	19	2	2	2	0	0
54	1a	277	277	277	0	0
54	1b	1	1	1	0	0
54	1d	5	5	5	0	0
54	1e	2	2	2	0	0
54	1f	2	2	2	0	0
54	1g	3	3	3	0	0
54	1h	2	2	2	0	0
54	1i	1	1	1	0	0
54	1k	1	1	1	0	0
54	1l	2	2	2	0	0
54	1m	1	1	1	0	0
54	1n	3	3	3	0	0
54	1o	1	1	1	0	0
54	1t	1	1	1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
54	1y	4	4	4	0	0
54	2A	741	741	741	0	0
54	2B	18	18	18	0	0
54	2D	12	12	12	0	0
54	2E	7	7	7	0	0
54	2F	4	4	4	0	0
54	2G	3	3	3	0	0
54	2N	1	1	1	0	0
54	2O	2	2	2	0	0
54	2Q	3	3	3	0	0
54	2R	3	3	3	0	0
54	2T	3	3	3	0	0
54	2V	3	3	3	0	0
54	2W	3	3	3	0	0
54	2X	1	1	1	0	0
54	2Y	1	1	1	0	0
54	20	3	3	3	0	0
54	21	1	1	1	0	0
54	23	2	2	2	0	0
54	25	1	1	1	0	0
54	27	1	1	1	0	0

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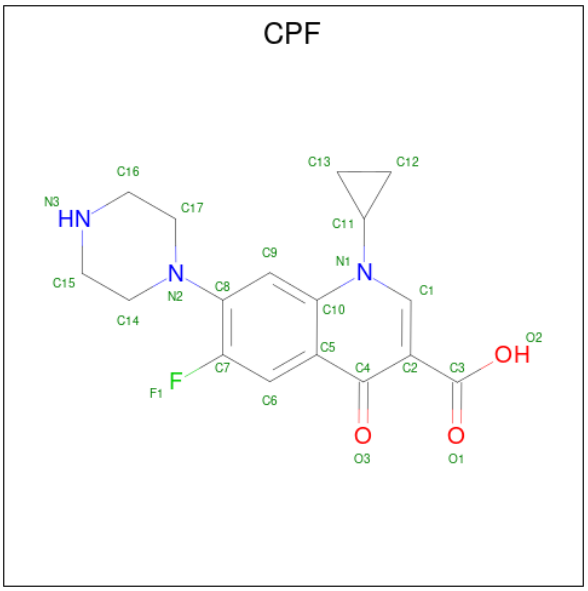
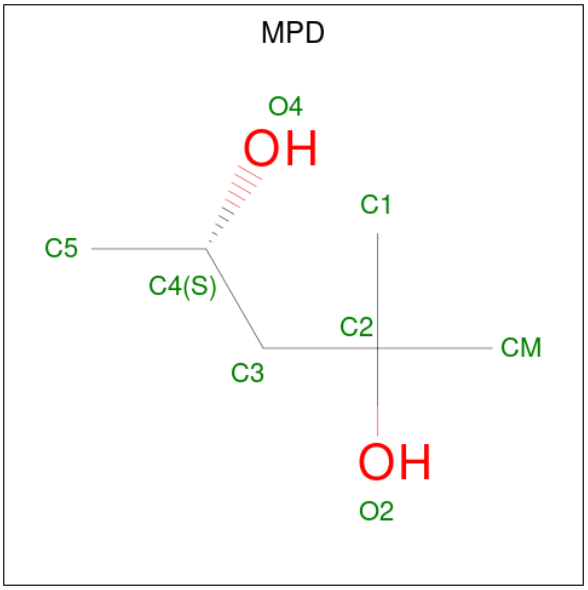
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
54	28	2	Total Mg 2 2	0	0
54	2a	195	Total Mg 195 195	0	0
54	2d	1	Total Mg 1 1	0	0
54	2e	1	Total Mg 1 1	0	0
54	2f	2	Total Mg 2 2	0	0
54	2j	1	Total Mg 1 1	0	0
54	2k	1	Total Mg 1 1	0	0
54	2n	1	Total Mg 1 1	0	0
54	2o	1	Total Mg 1 1	0	0
54	2p	1	Total Mg 1 1	0	0
54	2r	1	Total Mg 1 1	0	0
54	2t	1	Total Mg 1 1	0	0

- Molecule 55 is 1-CYCLOPROPYL-6-FLUORO-4-OXO-7-PIPERAZIN-1-YL-1,4-DIHYDROQUINOLINE-3-CARBOXYLIC ACID (CCD ID: CPF) (formula: $C_{17}H_{18}FN_3O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
55	1A	1	Total	C	F	N	O	0	0
			24	17	1	3	3		
55	2A	1	Total	C	F	N	O	0	0
			24	17	1	3	3		

- Molecule 56 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
56	1A	1	Total	C	O	0	0
			8	6	2		
56	1O	1	Total	C	O	0	0
			8	6	2		

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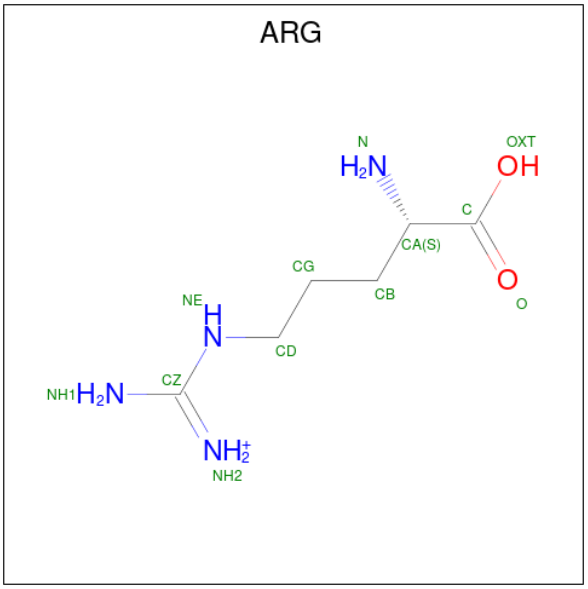
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
56	18	1	8	6	2		0	0
			Total	C	O			
56	1a	1	8	6	2		0	0
			Total	C	O			
56	2A	1	8	6	2		0	0
			Total	C	O			
56	2A	1	8	6	2		0	0
			Total	C	O			
56	2B	1	8	6	2		0	0

- Molecule 57 is ARGININE (CCD ID: ARG) (formula: $C_6H_{15}N_4O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
57	1B	1	12	6	4	2	0	0
			Total	C	N	O		
57	1F	1	12	6	4	2	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
58	1Y	1	1	1	0	0
			Total	Zn		
58	14	1	1	1	0	0

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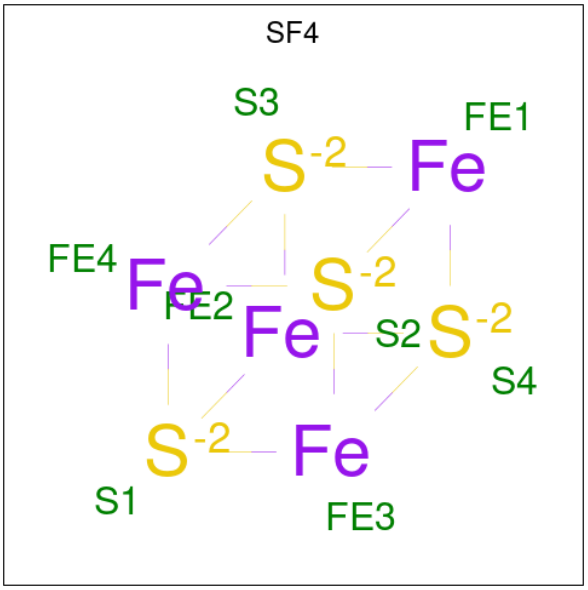
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
58	15	1	1	1	0	0
58	16	1	1	1	0	0
58	19	1	1	1	0	0
58	1n	1	1	1	0	0
58	2Y	1	1	1	0	0
58	24	1	1	1	0	0
58	25	1	1	1	0	0
58	26	1	1	1	0	0
58	29	1	1	1	0	0
58	2n	1	1	1	0	0

- Molecule 59 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
59	1d	1	8	4	4	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
59	2d	1	8	4	4	0	0

- Molecule 60 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
60	1A	3927	3927	3927	0	0
			Total	O		
60	1B	89	89	89	0	0
			Total	O		
60	1D	110	110	110	0	0
			Total	O		
60	1E	72	72	72	0	0
			Total	O		
60	1F	67	67	67	0	0
			Total	O		
60	1G	16	16	16	0	0
			Total	O		
60	1H	14	14	14	0	0
			Total	O		
60	1I	5	5	5	0	0
			Total	O		
60	1N	52	52	52	0	0
			Total	O		
60	1O	25	25	25	0	0
			Total	O		
60	1P	65	65	65	0	0
			Total	O		
60	1Q	41	41	41	0	0
			Total	O		
60	1R	32	32	32	0	0
			Total	O		
60	1S	8	8	8	0	0
			Total	O		
60	1T	36	36	36	0	0
			Total	O		
60	1U	43	43	43	0	0
			Total	O		
60	1V	36	36	36	0	0
			Total	O		
60	1W	28	28	28	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	1X	26	Total O 26 26	0	0
60	1Y	17	Total O 17 17	0	0
60	1Z	11	Total O 11 11	0	0
60	10	25	Total O 25 25	0	0
60	11	28	Total O 28 28	0	0
60	12	13	Total O 13 13	0	0
60	13	25	Total O 25 25	0	0
60	14	3	Total O 3 3	0	0
60	15	28	Total O 28 28	0	0
60	16	20	Total O 20 20	0	0
60	17	13	Total O 13 13	0	0
60	18	28	Total O 28 28	0	0
60	19	8	Total O 8 8	0	0
60	1a	496	Total O 496 496	0	0
60	1b	1	Total O 1 1	0	0
60	1c	1	Total O 1 1	0	0
60	1d	9	Total O 9 9	0	0
60	1e	10	Total O 10 10	0	0
60	1f	1	Total O 1 1	0	0
60	1h	1	Total O 1 1	0	0
60	1j	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	1k	1	Total O 1 1	0	0
60	1l	4	Total O 4 4	0	0
60	1o	4	Total O 4 4	0	0
60	1p	1	Total O 1 1	0	0
60	1y	5	Total O 5 5	0	0
60	2A	2249	Total O 2249 2249	0	0
60	2B	42	Total O 42 42	0	0
60	2D	47	Total O 47 47	0	0
60	2E	28	Total O 28 28	0	0
60	2F	23	Total O 23 23	0	0
60	2G	4	Total O 4 4	0	0
60	2H	1	Total O 1 1	0	0
60	2N	6	Total O 6 6	0	0
60	2O	15	Total O 15 15	0	0
60	2P	21	Total O 21 21	0	0
60	2Q	18	Total O 18 18	0	0
60	2R	22	Total O 22 22	0	0
60	2S	2	Total O 2 2	0	0
60	2T	12	Total O 12 12	0	0
60	2U	16	Total O 16 16	0	0
60	2V	8	Total O 8 8	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	2W	19	Total O 19 19	0	0
60	2X	8	Total O 8 8	0	0
60	2Y	4	Total O 4 4	0	0
60	2Z	8	Total O 8 8	0	0
60	20	10	Total O 10 10	0	0
60	21	17	Total O 17 17	0	0
60	22	2	Total O 2 2	0	0
60	23	2	Total O 2 2	0	0
60	25	7	Total O 7 7	0	0
60	26	6	Total O 6 6	0	0
60	27	9	Total O 9 9	0	0
60	28	15	Total O 15 15	0	0
60	2a	404	Total O 404 404	0	0
60	2d	3	Total O 3 3	0	0
60	2e	3	Total O 3 3	0	0
60	2f	3	Total O 3 3	0	0
60	2j	2	Total O 2 2	0	0
60	2l	5	Total O 5 5	0	0
60	2o	2	Total O 2 2	0	0
60	2p	1	Total O 1 1	0	0
60	2q	1	Total O 1 1	0	0

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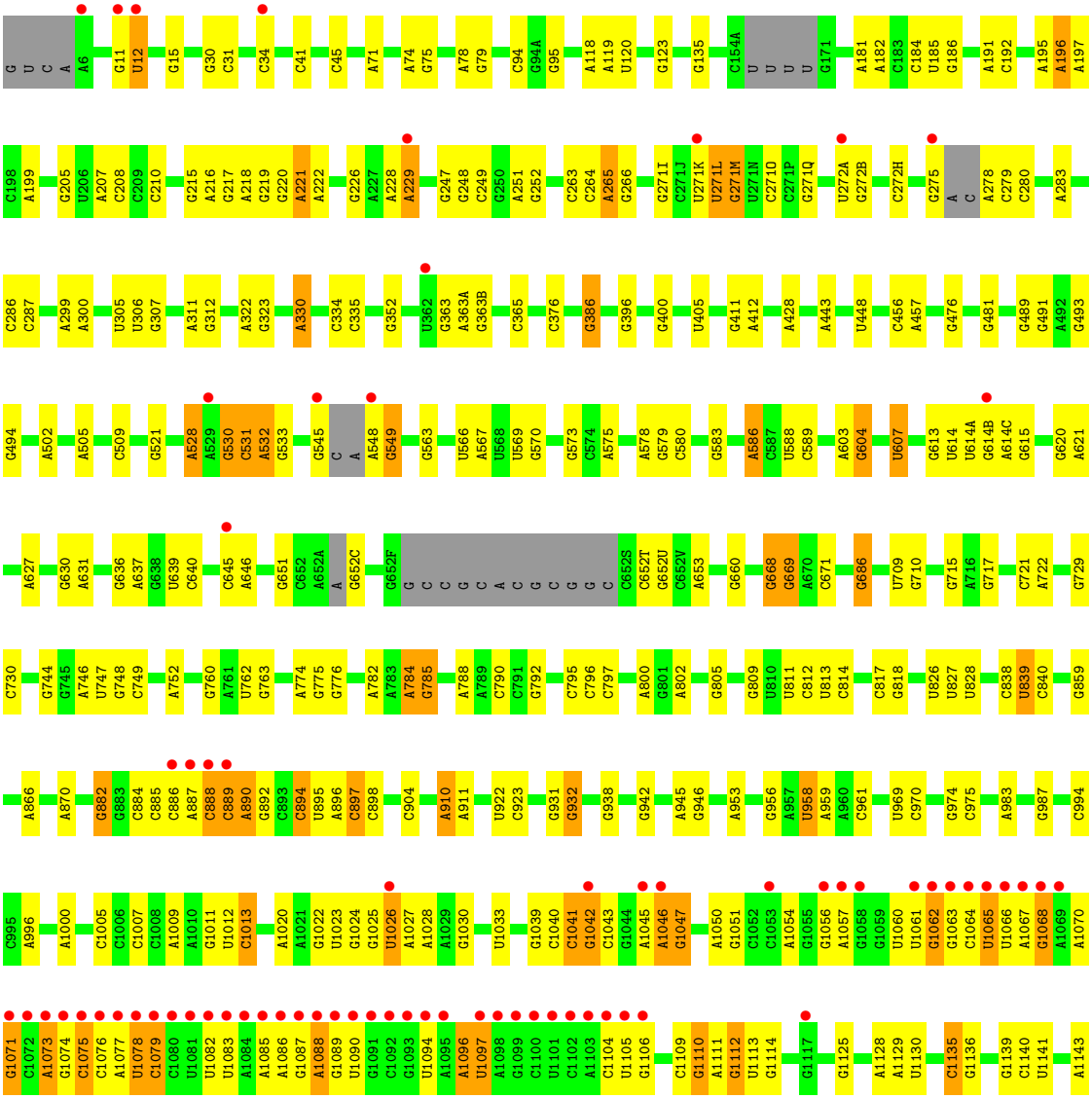
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	2r	3	Total O 3 3	0	0
60	2t	3	Total O 3 3	0	0
60	2u	1	Total O 1 1	0	0
60	2y	1	Total O 1 1	0	0

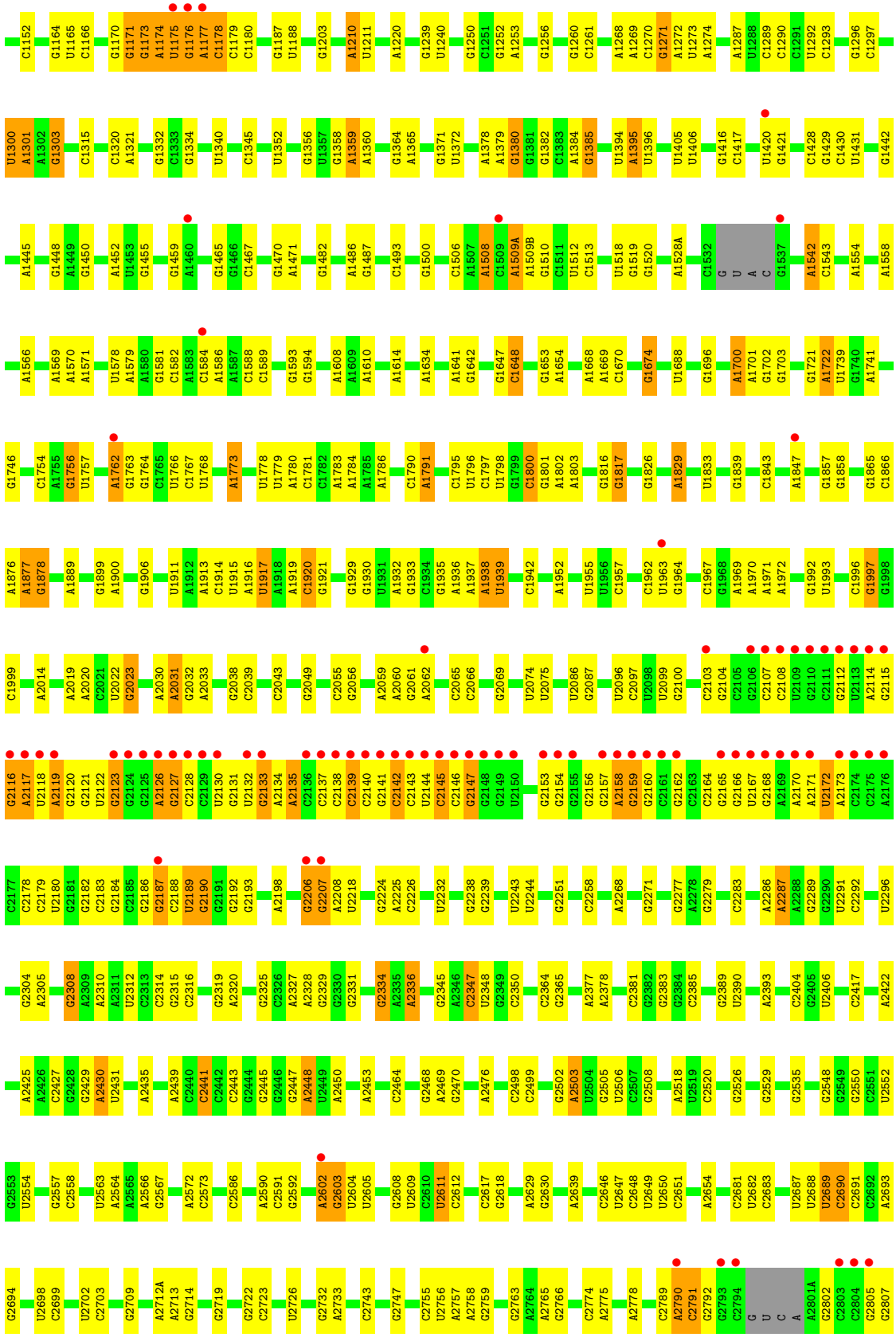
3 Residue-property plots (i)

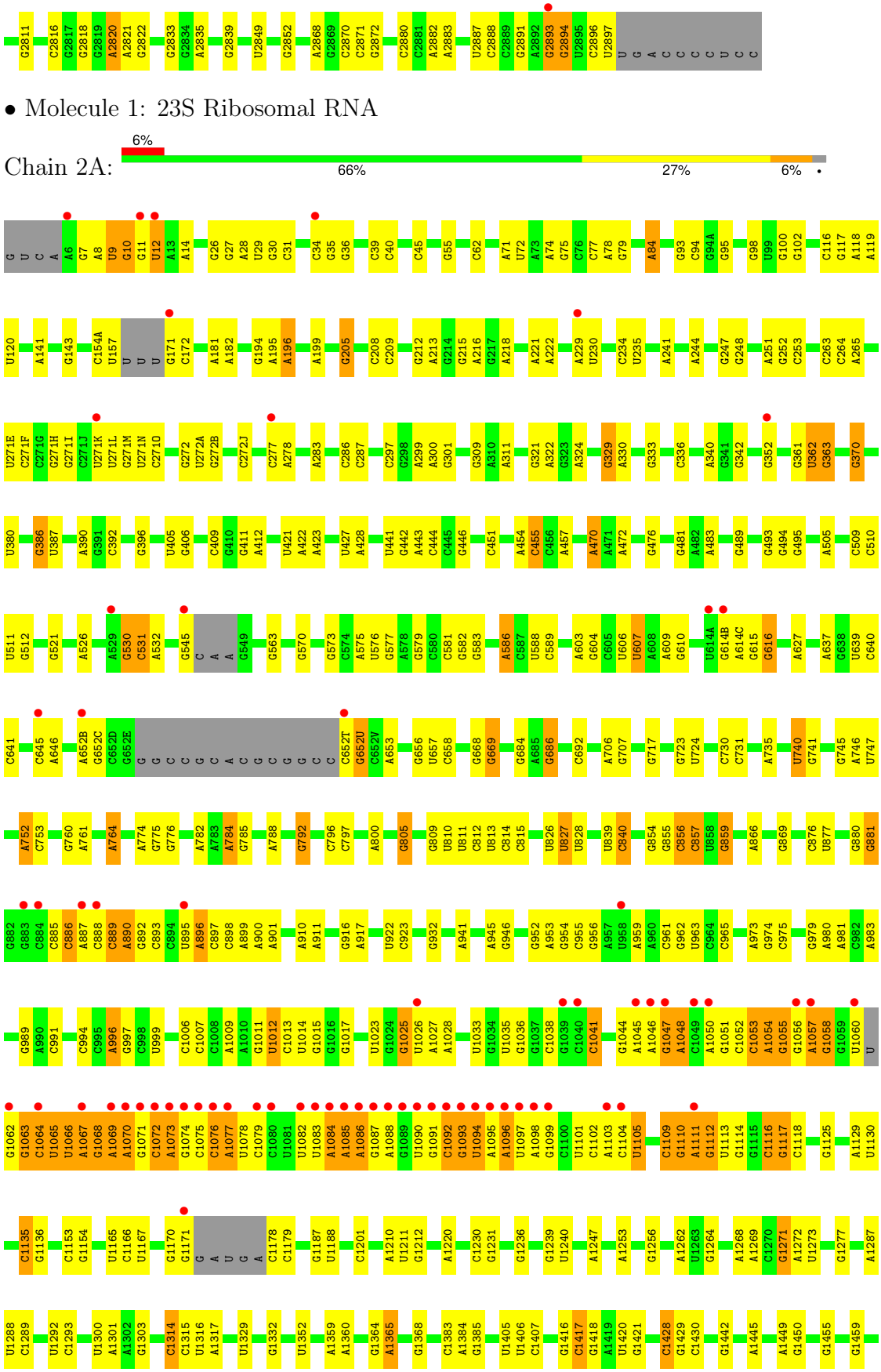
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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




C1152 G1164 U1165 C1166 G1170 G1171 G1173 A1174 U1175 G1176 A1177 C1178 C1179 C1180 G1187 U1188 G1203 A1210 U1211 A1220 G1239 U1240 G1250 C1251 G1252 A1253 G1256 G1260 C1261 A1268 A1269 C1270 G1271 A1272 U1273 A1274 A1287 U1288 C1289 C1290 C1291 U1292 C1293 G1296 C1297
U1300 A1301 A1302 G1303 C1315 C1320 A1321 G1332 C1333 G1334 U1340 C1345 U1352 G1356 U1357 G1358 A1359 A1360 G1364 A1365 G1371 U1372 A1378 A1379 G1380 G1381 G1382 C1383 A1384 G1385 U1394 A1395 U1396 U1405 U1406 G1416 C1417 U1420 G1421 C1428 G1429 C1430 U1431 G1442
A1445 G1448 A1449 G1450 A1452 U1453 G1455 G1459 A1460 G1465 G1466 C1467 G1470 A1471 G1482 A1486 G1487 C1493 G1500 C1506 A1507 A1508 C1509 A1509A A1509B G1510 C1511 U1512 C1513 U1518 G1519 G1520 A1528A C1532 G U A C G1537 A1542 C1543 A1554 A1558
A1566 A1569 A1570 A1571 U1578 A1579 A1580 G1581 C1582 A1583 C1584 A1586 A1587 C1588 C1589 G1593 G1594 A1608 A1609 A1610 A1614 A1634 A1641 G1642 G1647 C1648 G1653 A1654 A1668 A1669 C1670 G1674 U1688 G1696 A1700 A1701 G1702 G1703 G1721 A1722 U1739 G1740 A1741
G1746 C1754 A1755 G1756 U1757 A1762 G1763 G1764 C1765 U1766 C1767 U1768 A1773 U1778 U1779 A1780 C1781 C1782 A1783 A1784 A1785 A1786 C1790 A1791 C1795 U1796 C1797 U1798 G1799 C1800 G1801 A1802 A1803 G1816 G1817 G1826 A1829 U1833 G1839 C1843 A1847 G1857 G1858 G1865 C1866
A1876 A1877 G1878 A1889 G1899 A1900 G1906 U1911 A1912 A1913 C1914 U1915 A1916 U1917 A1918 A1919 C1920 G1921 G1929 G1930 U1931 A1932 G1933 C1934 G1935 A1936 A1937 A1938 U1939 C1942 A1952 U1955 U1956 C1957 C1962 U1963 G1964 C1967 G1968 A1969 A1970 A1971 A1972 G1992 U1993 C1996 G1997 G1998
C1999 A2014 A2019 A2020 C2021 U2022 G2023 A2030 A2031 G2032 A2033 G2038 C2039 C2043 G2049 C2055 G2056 A2059 A2060 G2061 A2062 C2065 C2066 G2069 U2074 U2075 U2086 G2087 U2096 C2097 U2098 U2099 G2100 C2103 G2104 C2105 G2106 C2107 C2108 U2109 G2110 C2111 G2112 U2113 A2114 G2115
G2116 A2117 U2118 A2119 G2120 C2121 U2122 G2123 G2124 G2125 A2126 G2127 C2128 G2129 U2130 G2131 U2132 G2133 A2134 A2135 C2136 C2137 C2138 C2139 C2140 G2141 C2142 C2143 U2144 C2145 C2146 G2147 G2148 G2149 U2150 G2153 G2154 G2155 G2156 G2157 A2158 G2159 G2160 C2161 G2162 C2163 C2164 G2165 G2166 U2167 G2168 A2169 A2170 A2171 U2172 A2173 C2174 C2175 A2176
C2177 C2178 C2179 U2180 G2181 G2182 C2183 G2184 C2185 G2186 G2187 C2188 U2189 G2190 G2191 G2192 G2193 A2198 G2206 A2207 A2208 U2218 G2224 A2225 C2226 U2232 G2238 G2239 U2243 U2244 G2251 C2258 A2268 G2271 G2277 A2278 G2279 C2283 A2286 A2287 A2288 G2289 G2290 U2291 C2292 U2296
G2304 A2305 G2308 A2309 A2310 A2311 U2312 C2313 C2314 C2315 C2316 G2319 A2320 G2325 C2326 A2327 A2328 G2329 G2330 G2331 G2334 A2335 A2336 G2345 A2346 C2347 U2348 G2349 C2350 C2364 G2365 A2377 A2378 C2381 G2382 G2383 G2384 C2385 G2389 U2390 A2393 C2404 G2405 U2406 C2417 A2422
A2425 A2426 C2427 G2428 G2429 A2430 U2431 A2435 A2439 C2440 C2441 C2442 C2443 G2444 G2445 G2446 A2447 A2448 U2449 A2450 A2453 C2464 G2468 A2469 G2470 A2476 C2498 C2499 G2502 A2503 U2504 G2505 U2506 C2507 G2508 A2518 U2519 C2520 G2526 G2529 G2535 G2548 G2549 G2550 C2551 U2552
G2553 U2554 G2557 C2558 U2563 A2564 A2565 A2566 G2567 A2572 C2573 C2586 A2590 C2591 G2592 A2602 G2603 U2604 U2605 G2608 U2609 C2610 U2611 C2612 C2617 G2618 A2629 G2630 A2639 C2646 U2647 C2648 U2649 U2650 C2651 A2654 C2681 U2682 C2683 U2687 U2688 U2689 C2690 C2691 C2692 A2693
G2694 U2698 C2699 U2702 C2703 G2709 A2712A A2713 G2714 G2719 G2722 C2723 U2726 G2732 A2733 C2743 G2747 C2755 U2756 A2757 A2758 G2759 G2763 A2764 A2765 G2766 C2774 A2775 A2778 C2789 A2790 C2791 G2792 G2793 C2794 G U C A A2801A G2802 C2803 C2804 G2805 G2807


G2811 C2816 G2817 G2818 G2819 A2820 A2821 G2822 G2833 G2834 A2835 G2839 U2849 G2852 A2868 G2869 C2870 C2871 G2872 C2880 C2881 A2882 A2883 U2887 C2888 C2889 G2891 A2892 G2893 G2894 U2895 C2896 U2897 U G A C C C C U C C
• Molecule 1: 23S Ribosomal RNA
Chain 2A:
6%
66%
27%
6%
G U C A A6 G7 A8 U9 G10 G11 U12 A13 A14 G26 G27 A28 U29 G30 C31 C34 G35 G36 C39 C40 C45 G55 C62 A71 U72 A73 A74 G75 C76 C77 A78 G79 A84 G93 C94 G94A G95 G98 U99 G100 G102 C116 G117 A118 A119
U120 A141 G143 C154A U157 U U U G171 C172 A181 A182 G194 A195 A196 A199 G205 C208 C209 G212 A213 G214 G215 A216 G217 A218 A221 A222 A229 U230 C234 U235 A241 A244 G247 G248 A251 G252 C253 C263 C264 A265
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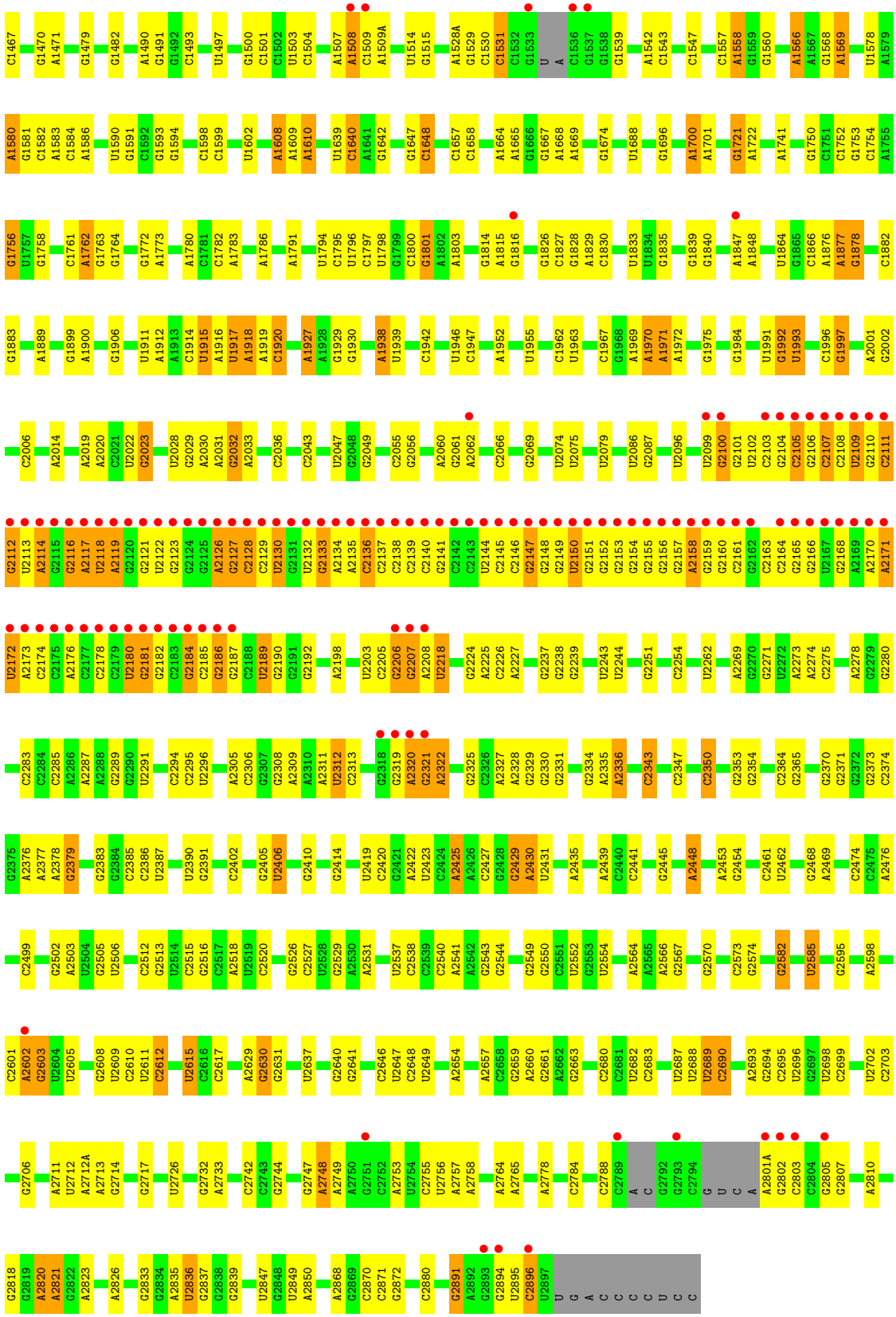
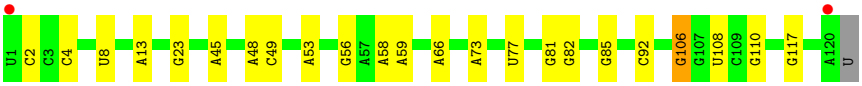


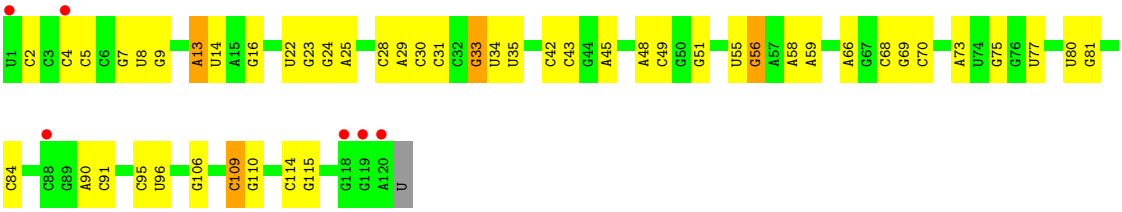
• Molecule 2: 5S Ribosomal RNA

Chain 1B:



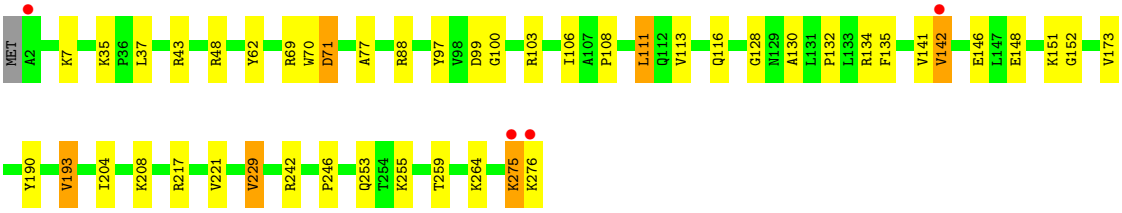
- Molecule 2: 5S Ribosomal RNA

Chain 2B:



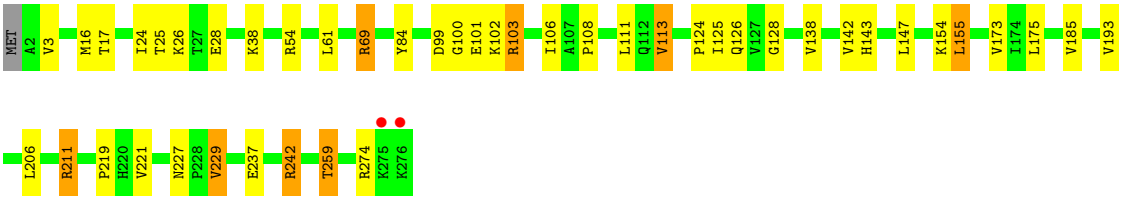
- Molecule 3: 50S ribosomal protein L2

Chain 1D:



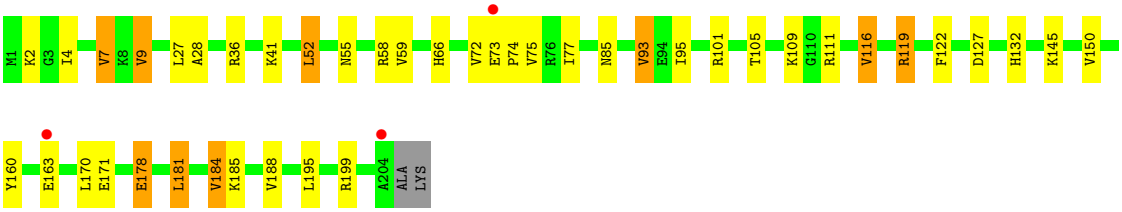
- Molecule 3: 50S ribosomal protein L2

Chain 2D:



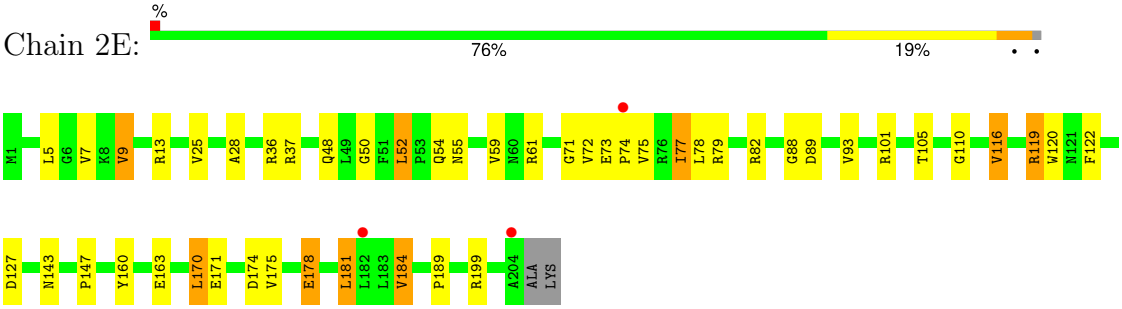
- Molecule 4: 50S ribosomal protein L3

Chain 1E:



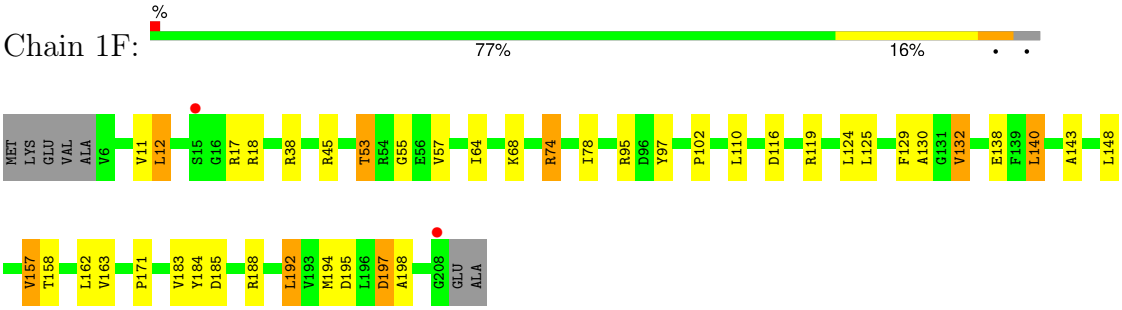
- Molecule 4: 50S ribosomal protein L3

Chain 2E:



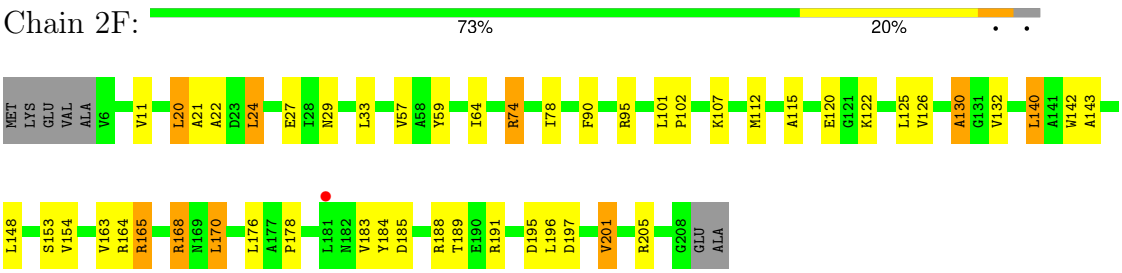
- Molecule 5: 50S ribosomal protein L4

Chain 1F:



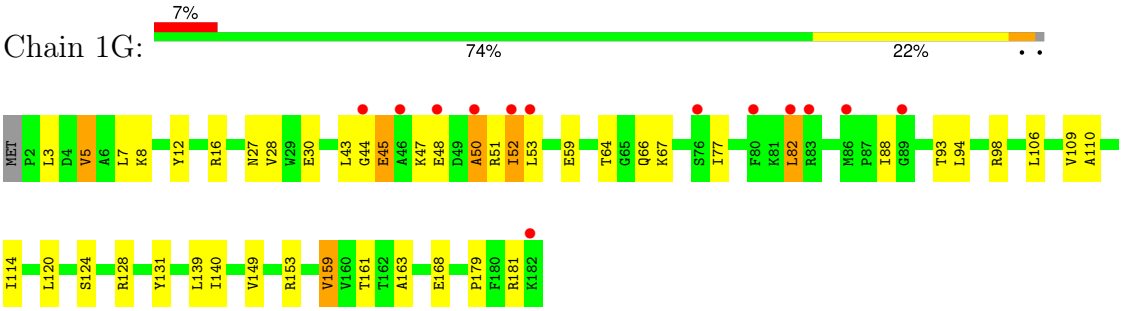
- Molecule 5: 50S ribosomal protein L4

Chain 2F:



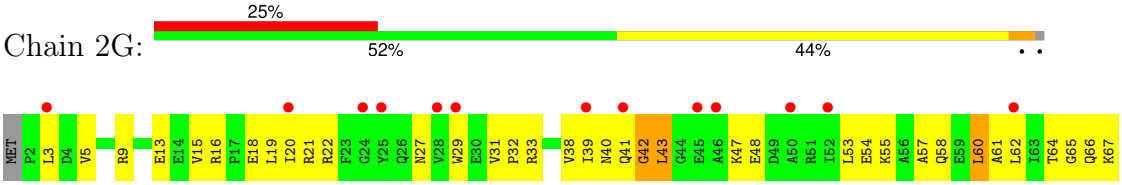
- Molecule 6: 50S ribosomal protein L5

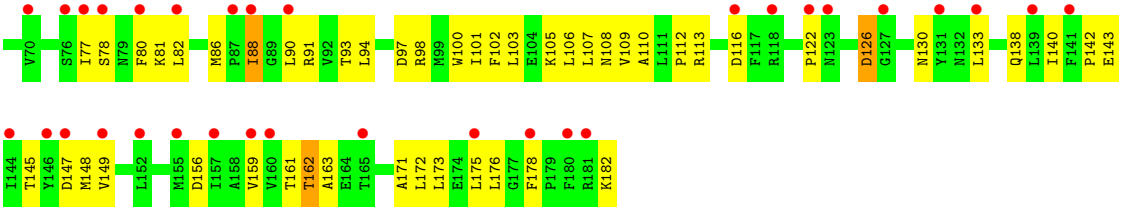
Chain 1G:



- Molecule 6: 50S ribosomal protein L5

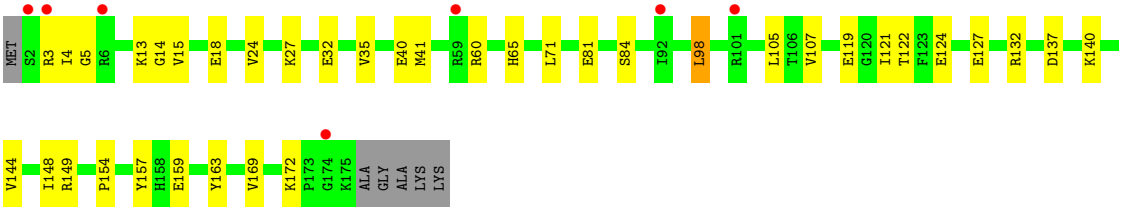
Chain 2G:





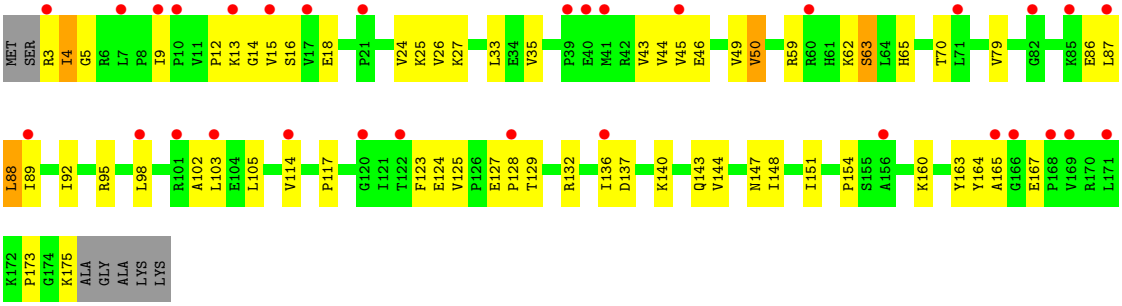
- Molecule 7: 50S ribosomal protein L6

Chain 1H:



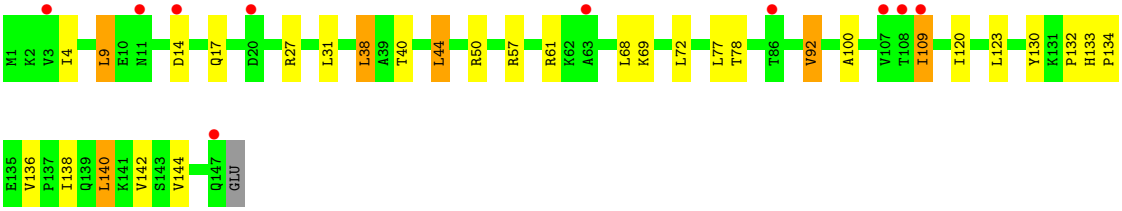
- Molecule 7: 50S ribosomal protein L6

Chain 2H:



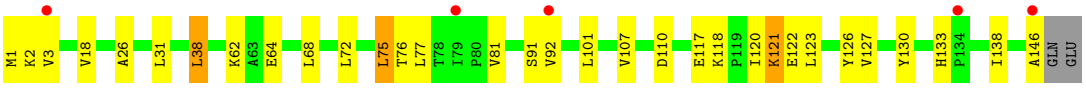
- Molecule 8: 50S ribosomal protein L9

Chain 1I:



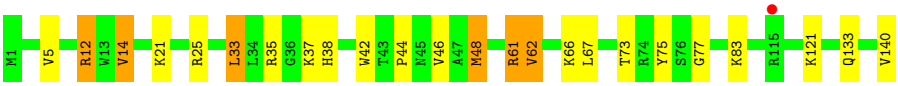
- Molecule 8: 50S ribosomal protein L9

Chain 2I:



• Molecule 9: 50S ribosomal protein L13

Chain 1N:



• Molecule 9: 50S ribosomal protein L13

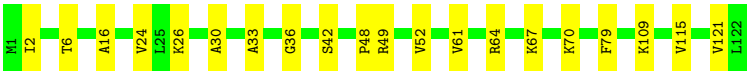
Chain 2N:

• Molecule 10: 50S ribosomal protein L14

Chain 1O:

• Molecule 10: 50S ribosomal protein L14

Chain 2O:

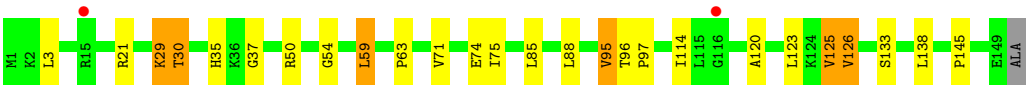


• Molecule 11: 50S ribosomal protein L15

Chain 1P:

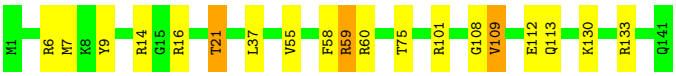
• Molecule 11: 50S ribosomal protein L15

Chain 2P:



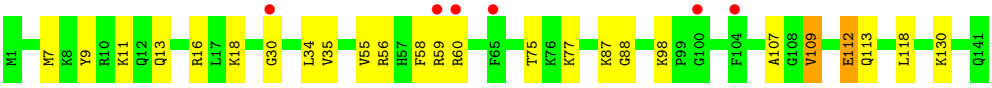
• Molecule 12: 50S ribosomal protein L16

Chain 1Q:



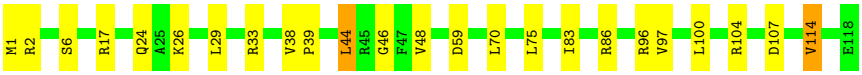
- Molecule 12: 50S ribosomal protein L16

Chain 2Q:



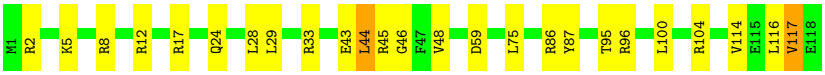
- Molecule 13: 50S ribosomal protein L17

Chain 1R:



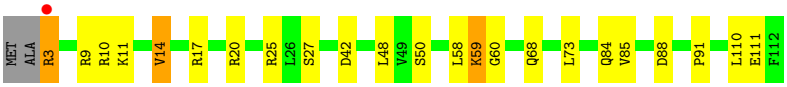
- Molecule 13: 50S ribosomal protein L17

Chain 2R:



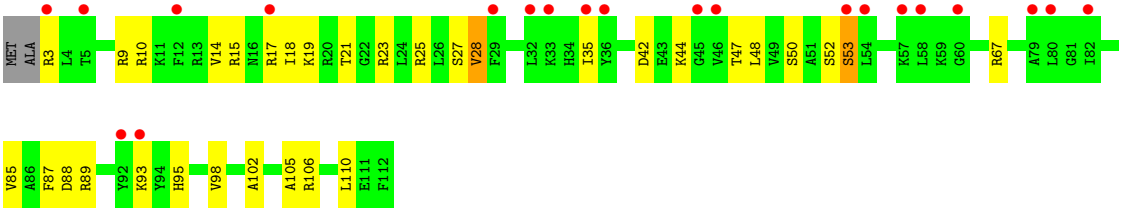
- Molecule 14: 50S ribosomal protein L18

Chain 1S:



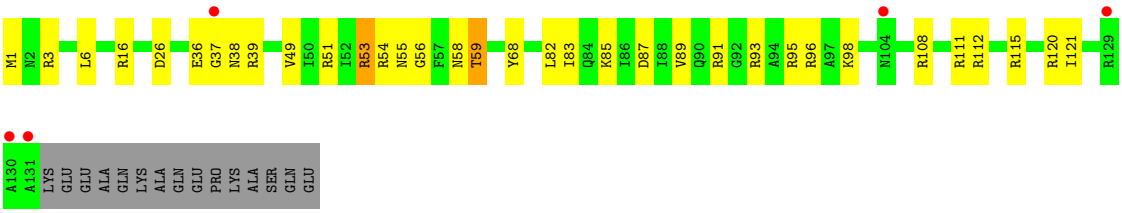
- Molecule 14: 50S ribosomal protein L18

Chain 2S:



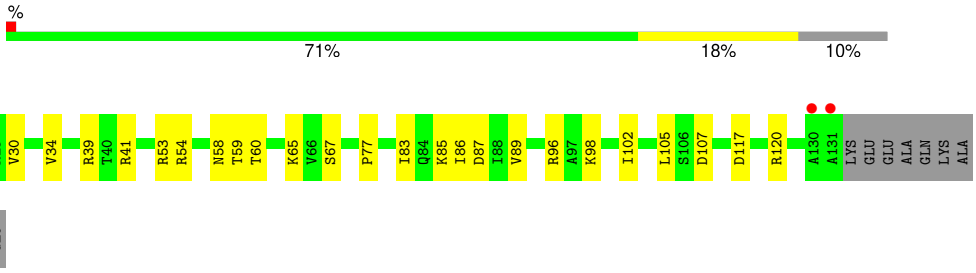
- Molecule 15: 50S ribosomal protein L19

Chain 1T:



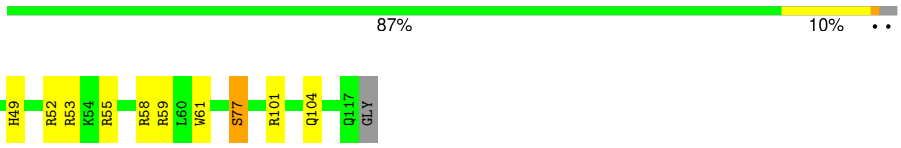
• Molecule 15: 50S ribosomal protein L19

Chain 2T:



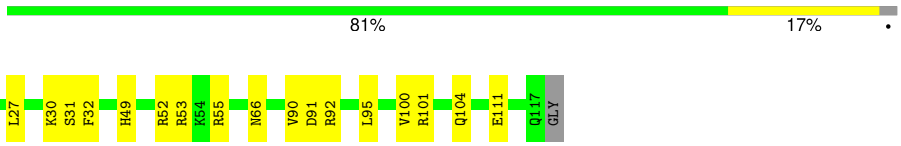
• Molecule 16: 50S ribosomal protein L20

Chain 1U:



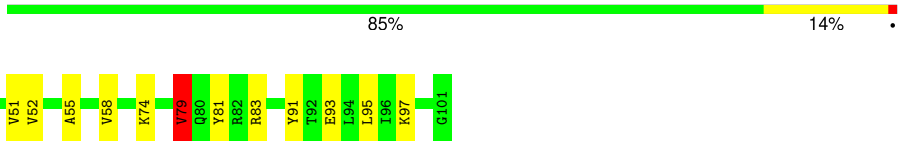
• Molecule 16: 50S ribosomal protein L20

Chain 2U:



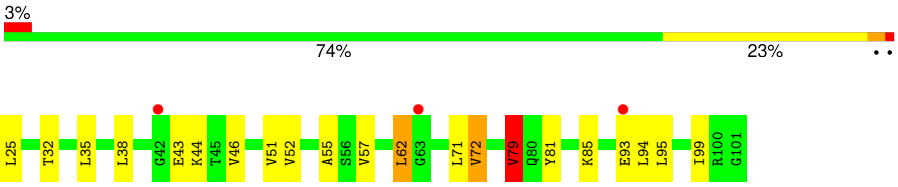
• Molecule 17: 50S ribosomal protein L21

Chain 1V:



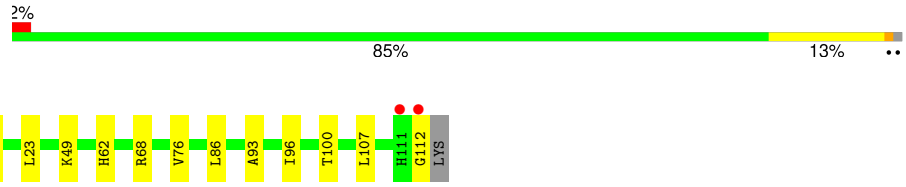
• Molecule 17: 50S ribosomal protein L21

Chain 2V:



• Molecule 18: 50S ribosomal protein L22

Chain 1W:

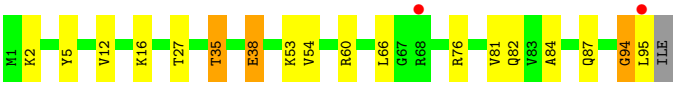


• Molecule 18: 50S ribosomal protein L22

Chain 2W:

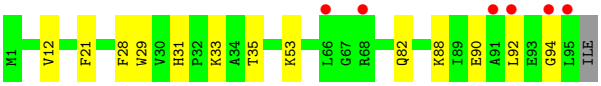
• Molecule 19: 50S ribosomal protein L23

Chain 1X:



• Molecule 19: 50S ribosomal protein L23

Chain 2X:



• Molecule 20: 50S ribosomal protein L24

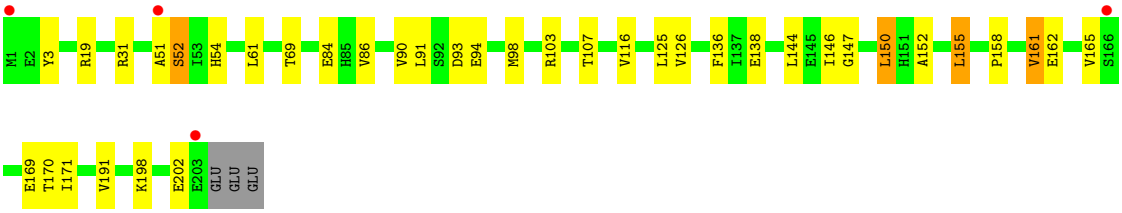
Chain 1Y:

• Molecule 20: 50S ribosomal protein L24

Chain 2Y:

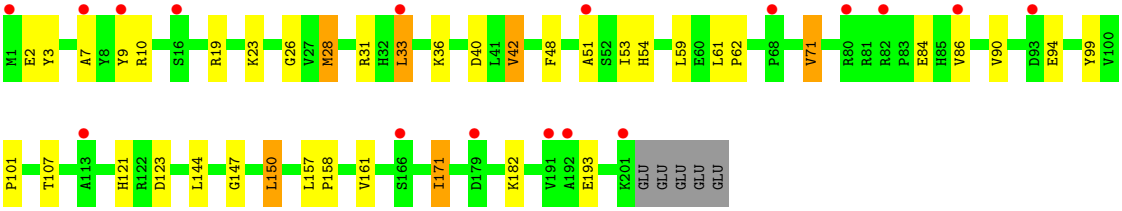
• Molecule 21: 50S ribosomal protein L25

Chain 1Z:



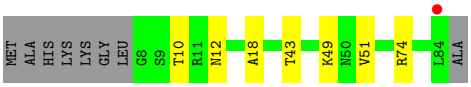
• Molecule 21: 50S ribosomal protein L25

Chain 2Z:



• Molecule 22: 50S ribosomal protein L27

Chain 10:

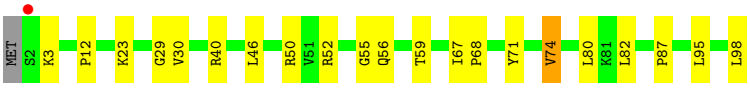


• Molecule 22: 50S ribosomal protein L27

Chain 20:

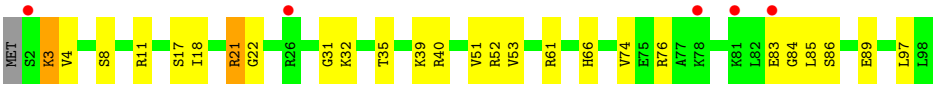
• Molecule 23: 50S ribosomal protein L28

Chain 11:



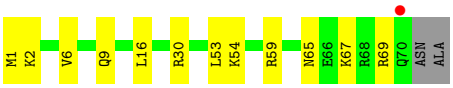
• Molecule 23: 50S ribosomal protein L28

Chain 21:



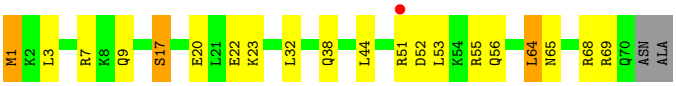
• Molecule 24: 50S ribosomal protein L29

Chain 12:



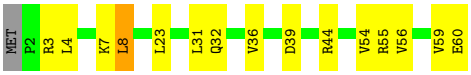
• Molecule 24: 50S ribosomal protein L29

Chain 22:



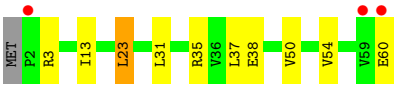
• Molecule 25: 50S ribosomal protein L30

Chain 13:



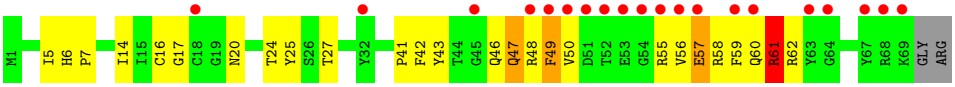
• Molecule 25: 50S ribosomal protein L30

Chain 23:



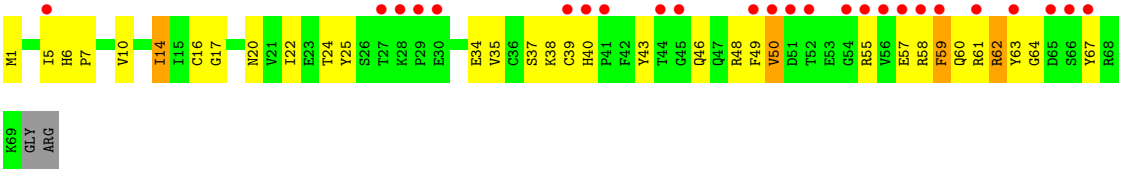
• Molecule 26: 50S ribosomal protein L31

Chain 14:



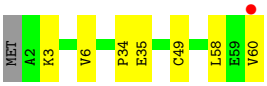
• Molecule 26: 50S ribosomal protein L31

Chain 24:



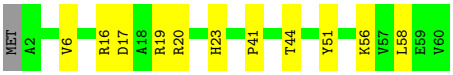
• Molecule 27: 50S ribosomal protein L32

Chain 15:



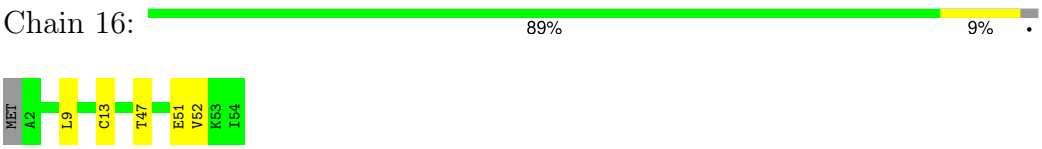
• Molecule 27: 50S ribosomal protein L32

Chain 25:



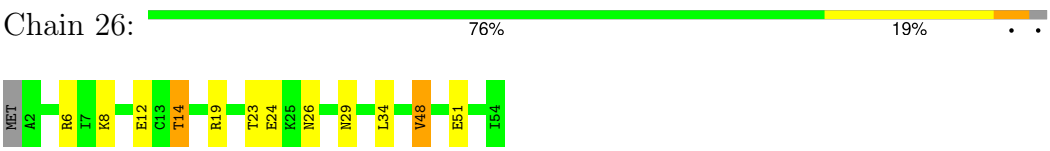
- Molecule 28: 50S ribosomal protein L33

Chain 16:



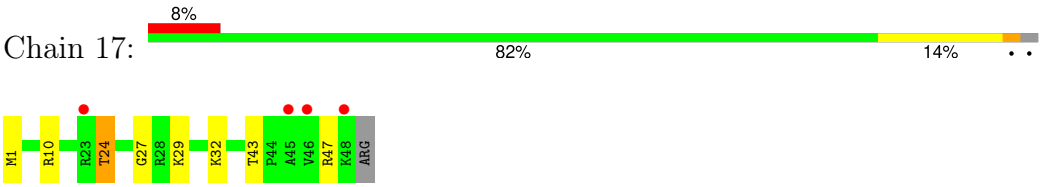
- Molecule 28: 50S ribosomal protein L33

Chain 26:



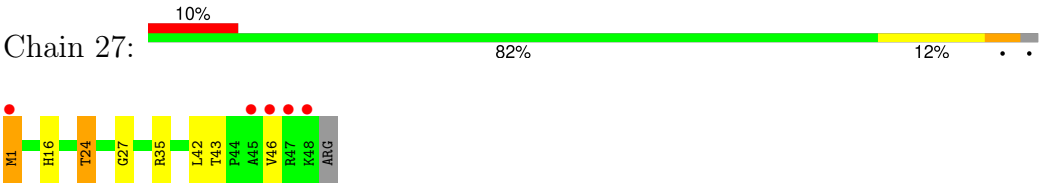
- Molecule 29: 50S ribosomal protein L34

Chain 17:



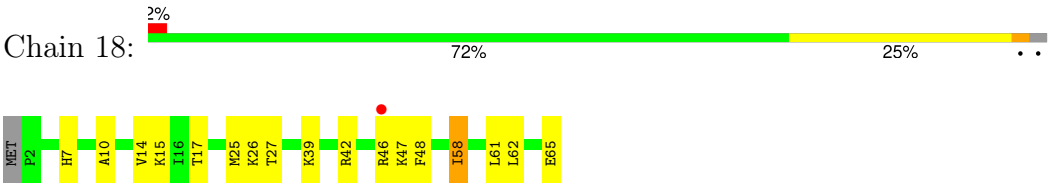
- Molecule 29: 50S ribosomal protein L34

Chain 27:



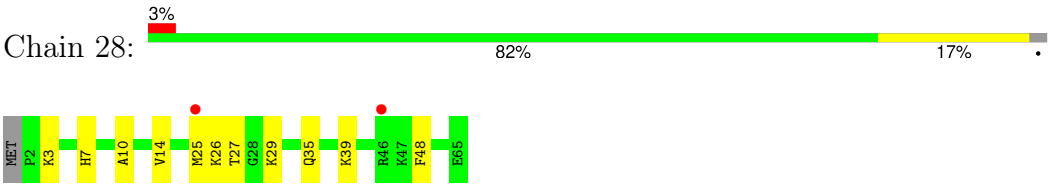
- Molecule 30: 50S ribosomal protein L35

Chain 18:



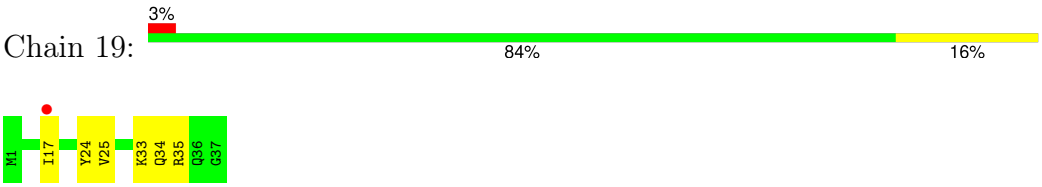
- Molecule 30: 50S ribosomal protein L35

Chain 28:



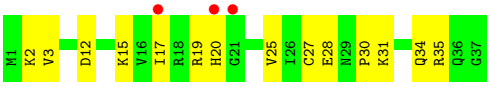
- Molecule 31: 50S ribosomal protein L36

Chain 19:



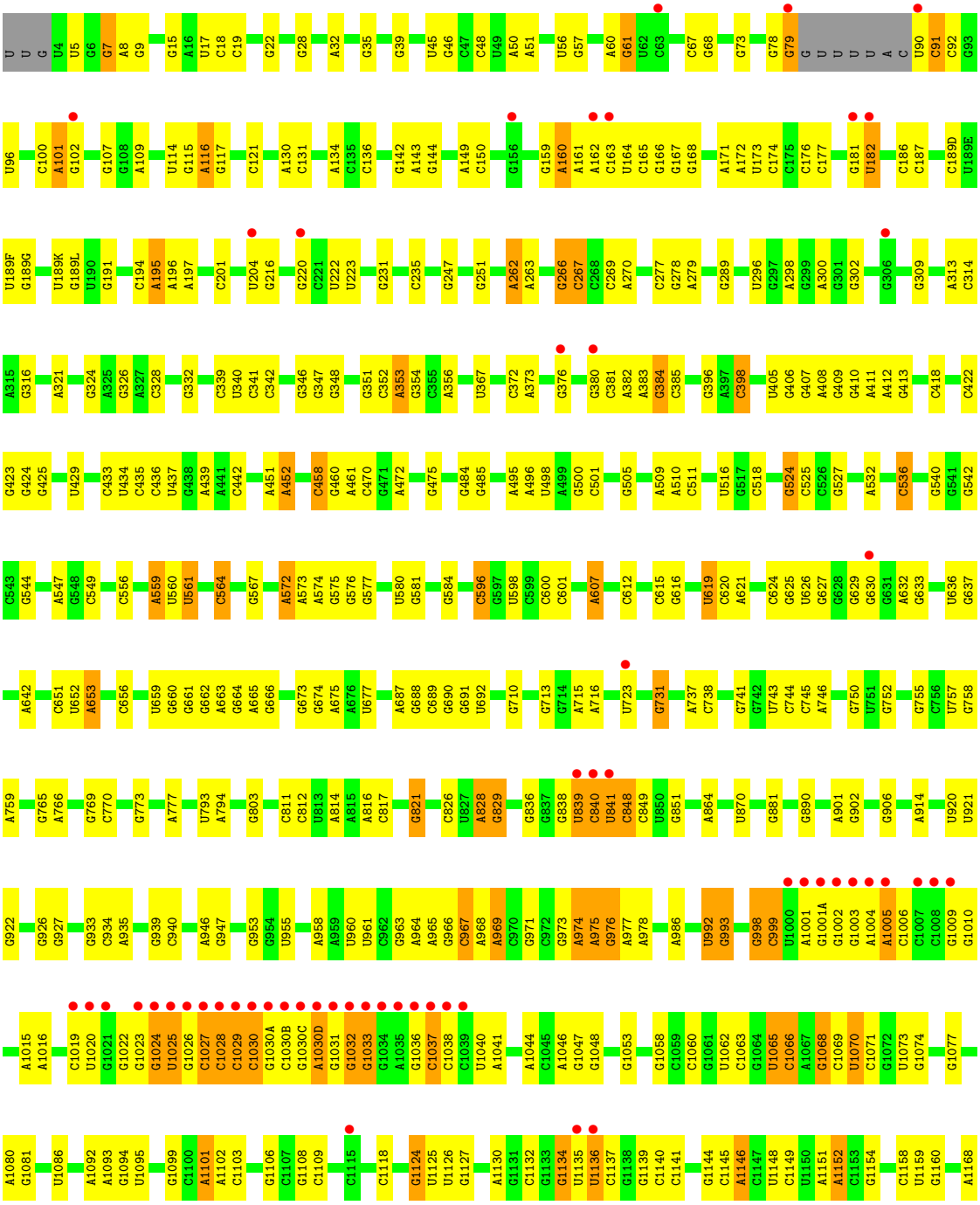
- Molecule 31: 50S ribosomal protein L36

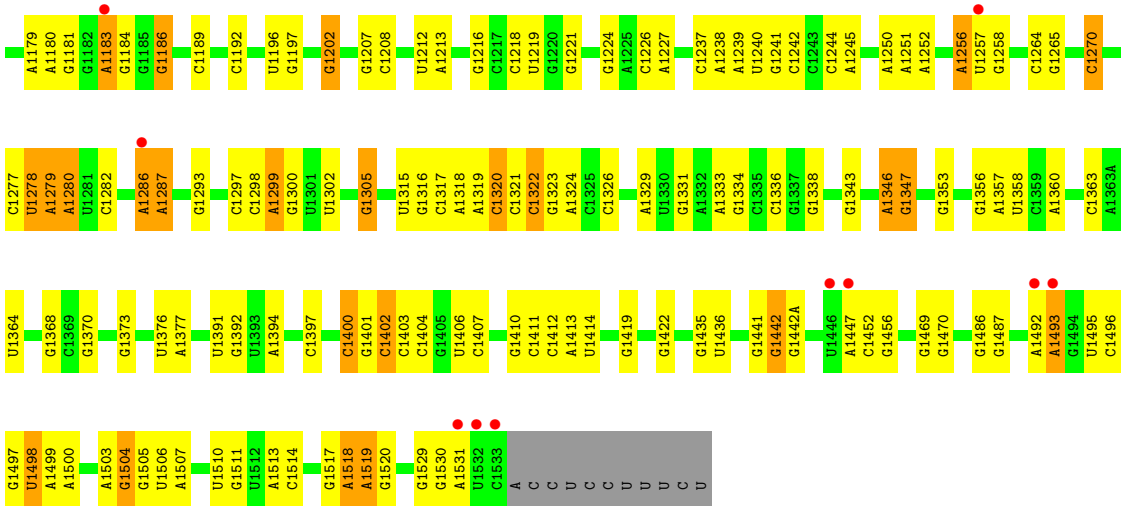
Chain 29:



- Molecule 32: 16S Ribosomal RNA

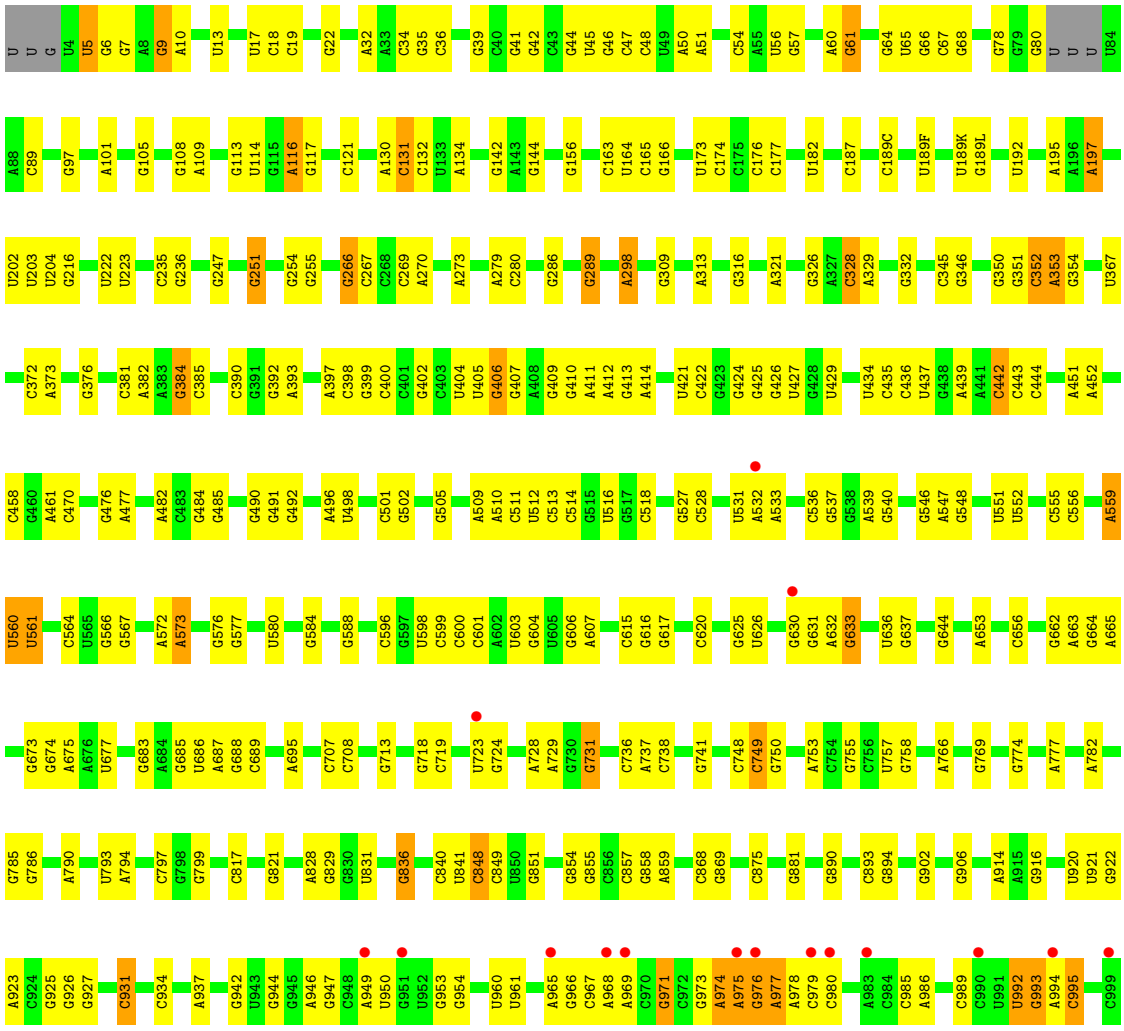
Chain 1a:

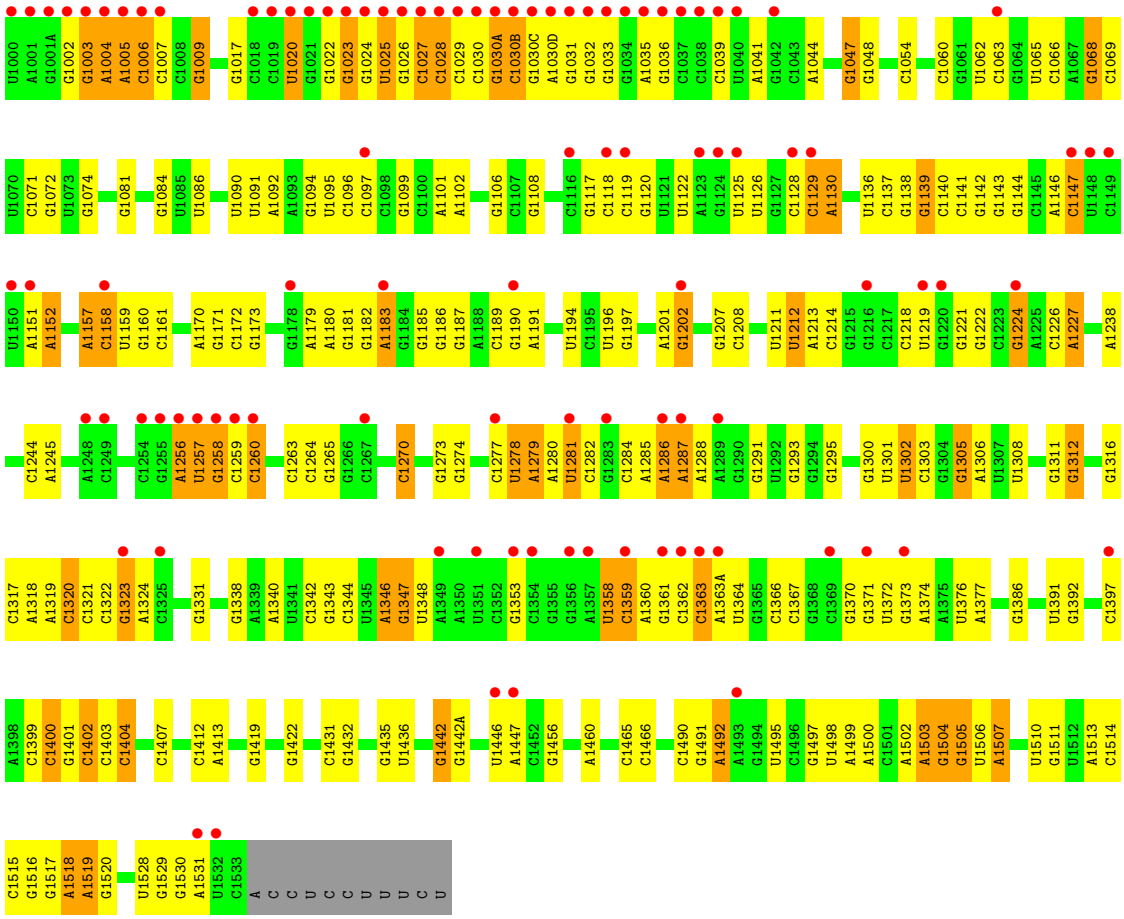




- Molecule 32: 16S Ribosomal RNA

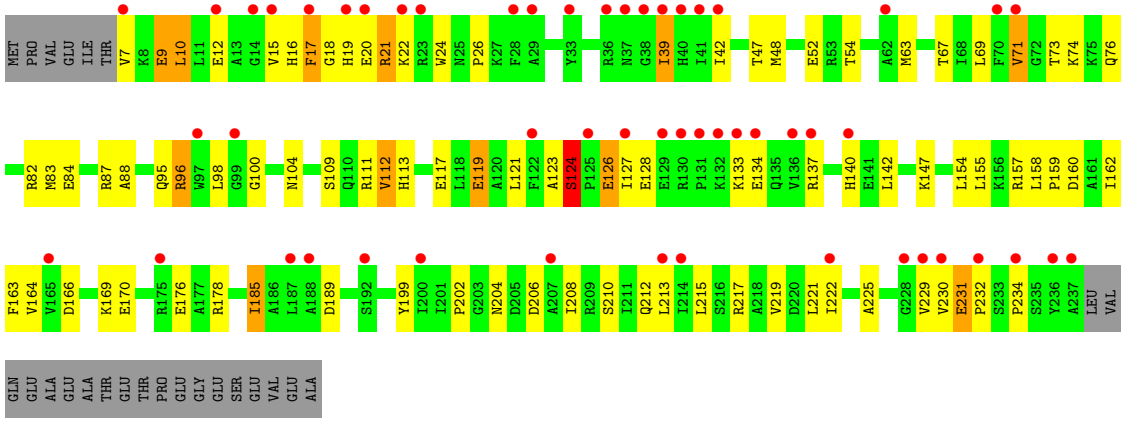
Chain 2a:





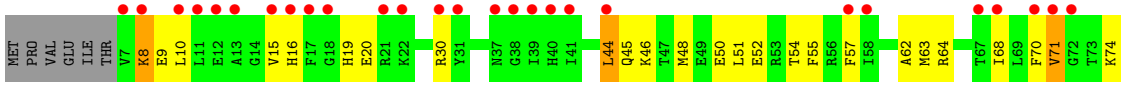
- Molecule 33: 30S ribosomal protein S2

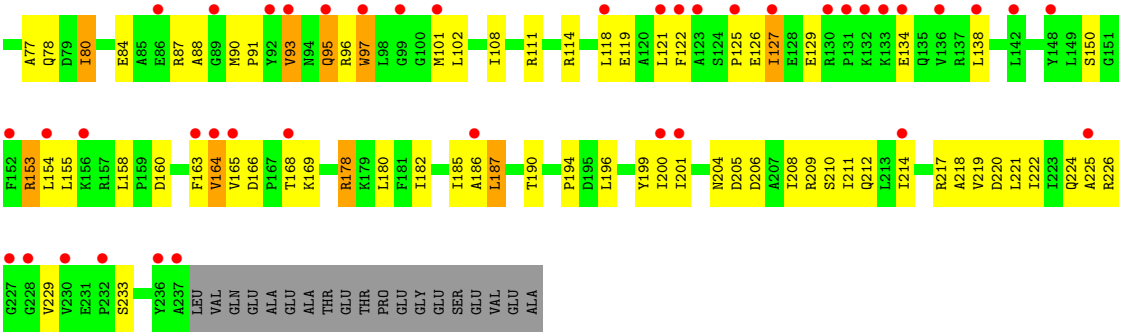
Chain 1b:



- Molecule 33: 30S ribosomal protein S2

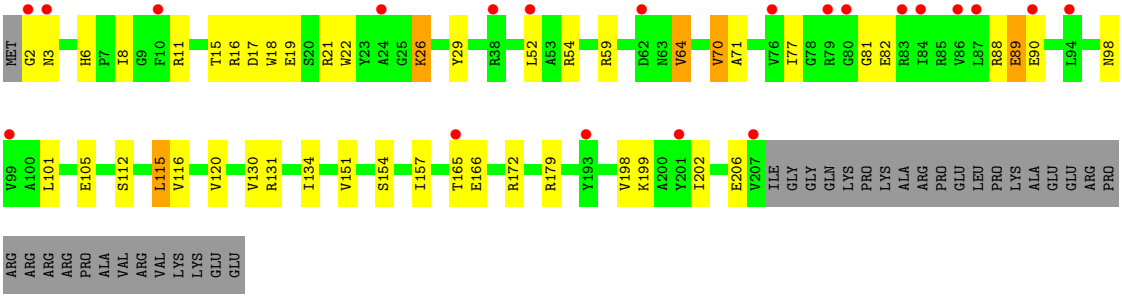
Chain 2b:





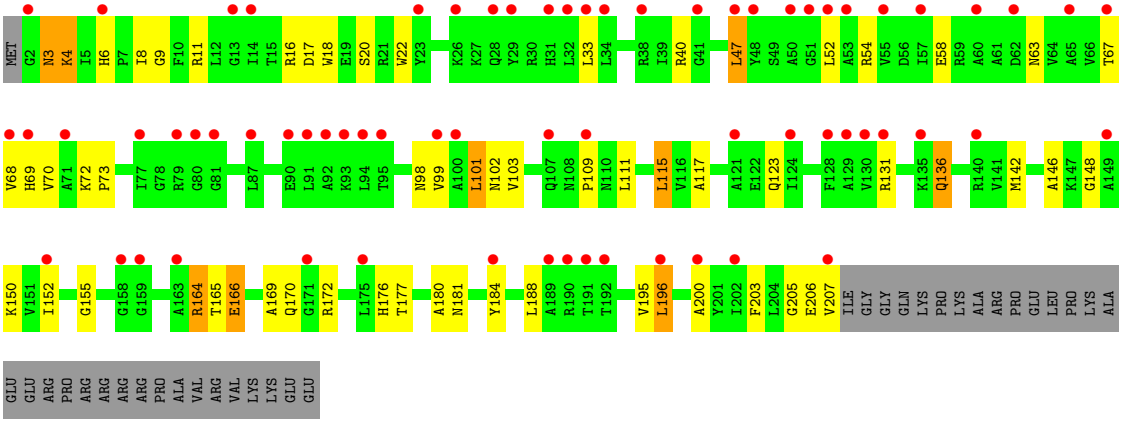
- Molecule 34: 30S ribosomal protein S3

Chain 1c:



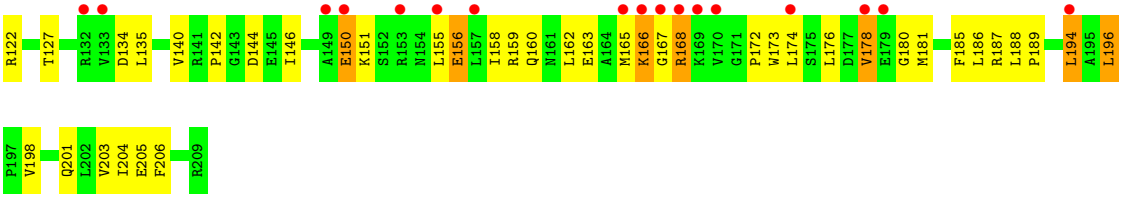
- Molecule 34: 30S ribosomal protein S3

Chain 2c:



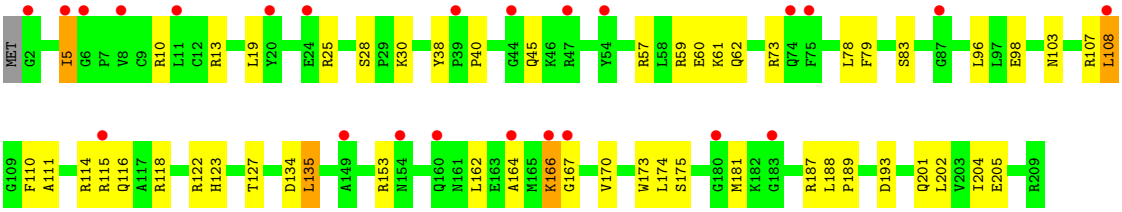
- Molecule 35: 30S ribosomal protein S4

Chain 1d:



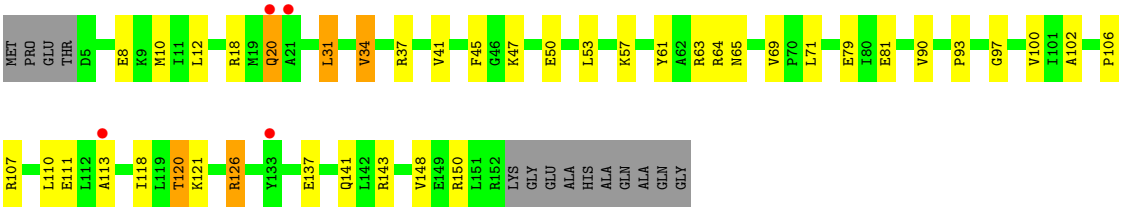
• Molecule 35: 30S ribosomal protein S4

Chain 2d:



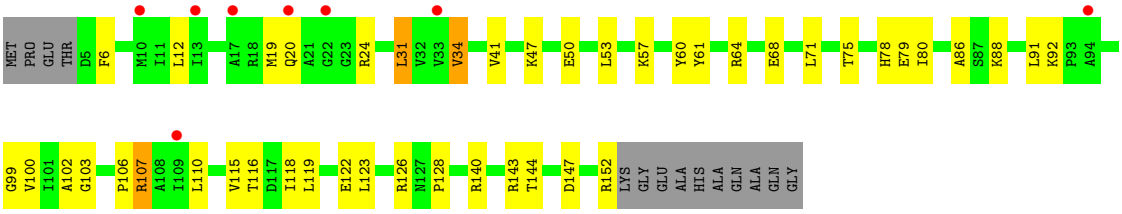
• Molecule 36: 30S ribosomal protein S5

Chain 1e:



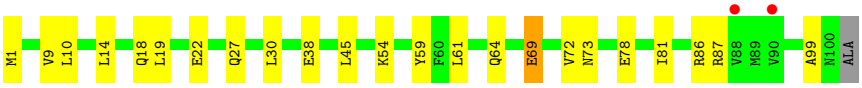
• Molecule 36: 30S ribosomal protein S5

Chain 2e:



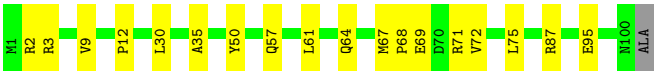
• Molecule 37: 30S ribosomal protein S6

Chain 1f:



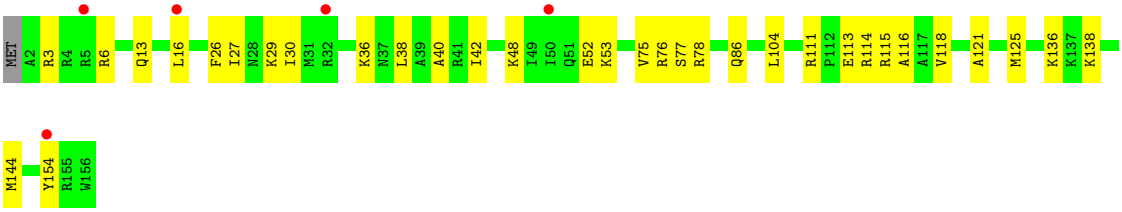
• Molecule 37: 30S ribosomal protein S6

Chain 2f:



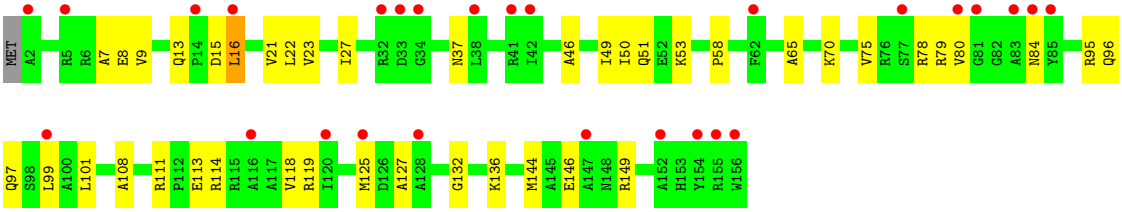
• Molecule 38: 30S ribosomal protein S7

Chain 1g:



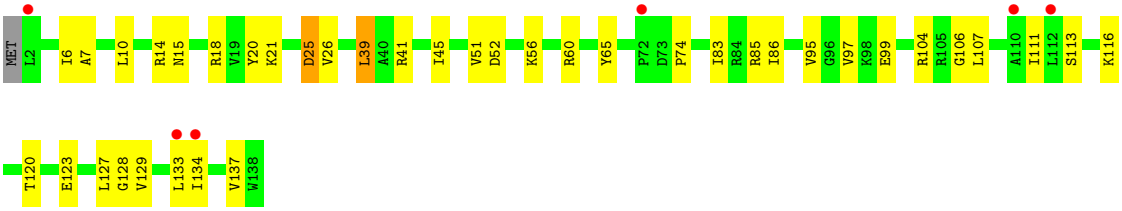
• Molecule 38: 30S ribosomal protein S7

Chain 2g:



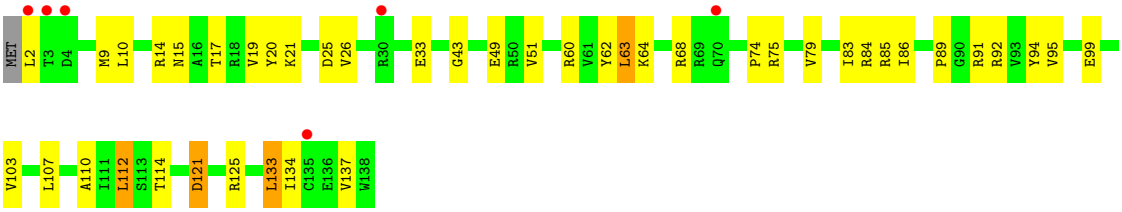
• Molecule 39: 30S ribosomal protein S8

Chain 1h:



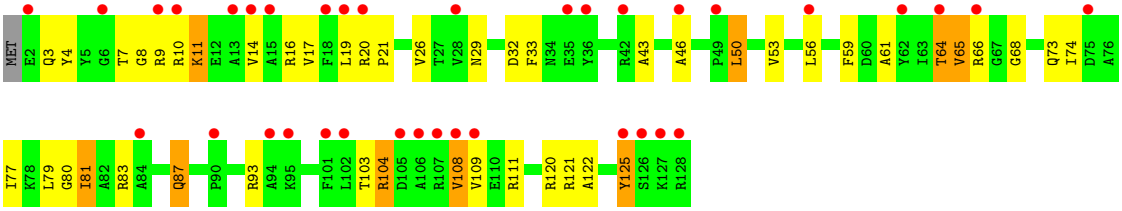
• Molecule 39: 30S ribosomal protein S8

Chain 2h:



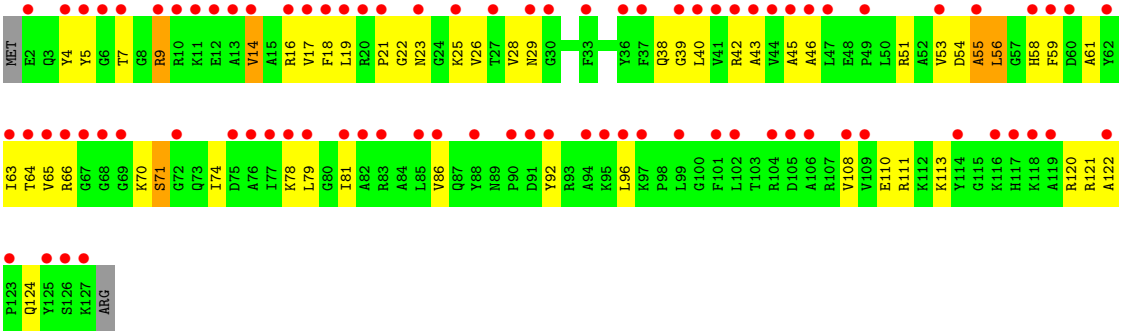
• Molecule 40: 30S ribosomal protein S9

Chain 1i:



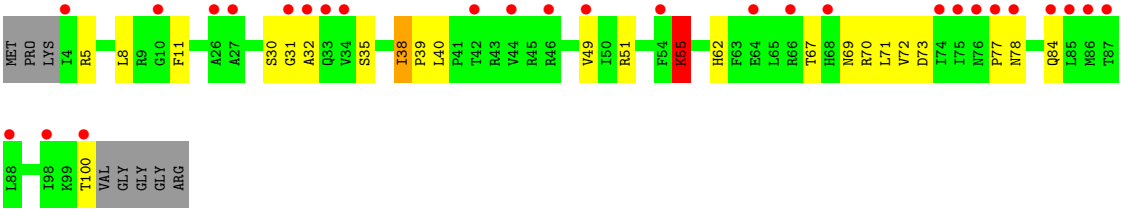
• Molecule 40: 30S ribosomal protein S9

Chain 2i:



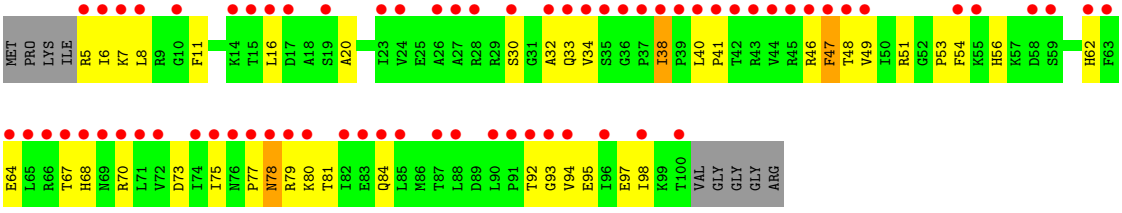
• Molecule 41: 30S ribosomal protein S10

Chain 1j:



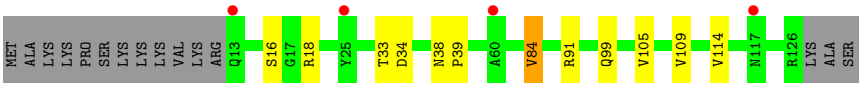
• Molecule 41: 30S ribosomal protein S10

Chain 2j:



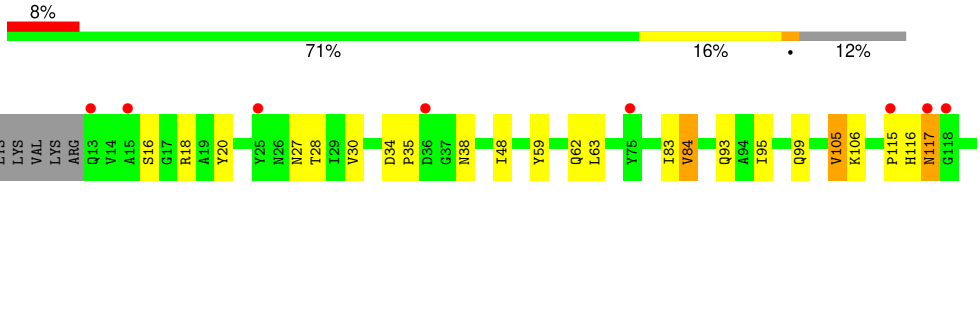
• Molecule 42: 30S ribosomal protein S11

Chain 1k:



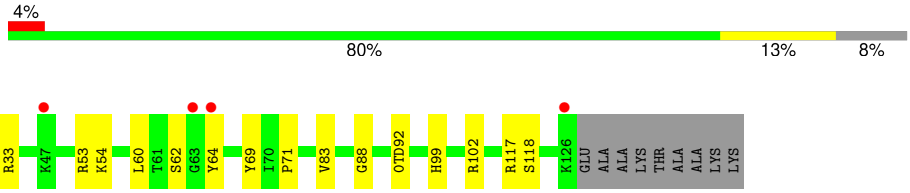
- Molecule 42: 30S ribosomal protein S11

Chain 2k:



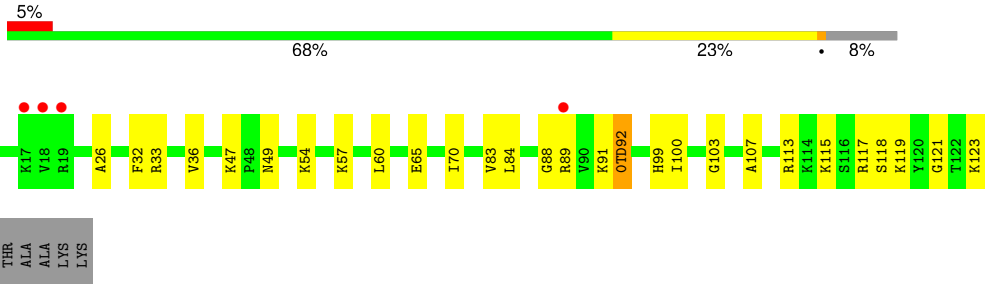
- Molecule 43: 30S ribosomal protein S12

Chain 1l:



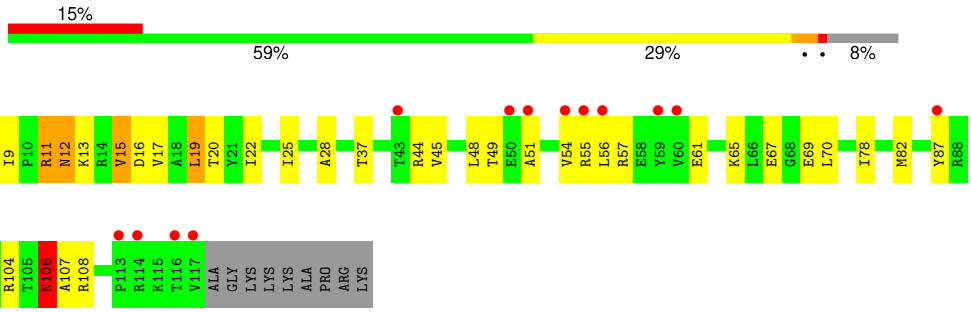
- Molecule 43: 30S ribosomal protein S12

Chain 2l:



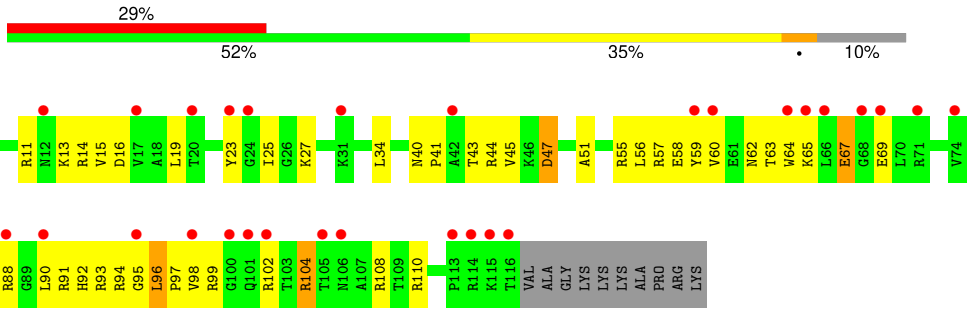
- Molecule 44: 30S ribosomal protein S13

Chain 1m:



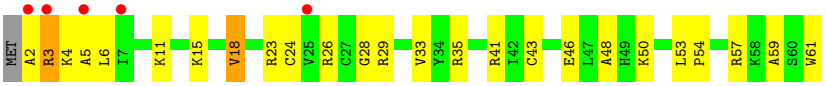
- Molecule 44: 30S ribosomal protein S13

Chain 2m:



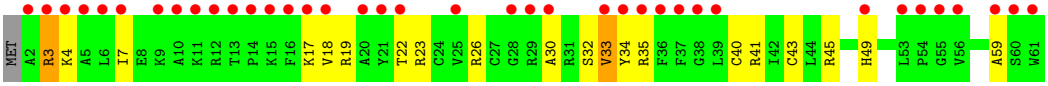
• Molecule 45: 30S ribosomal protein S14 type Z

Chain 1n:



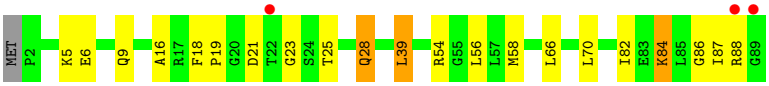
• Molecule 45: 30S ribosomal protein S14 type Z

Chain 2n:



• Molecule 46: 30S ribosomal protein S15

Chain 1o:

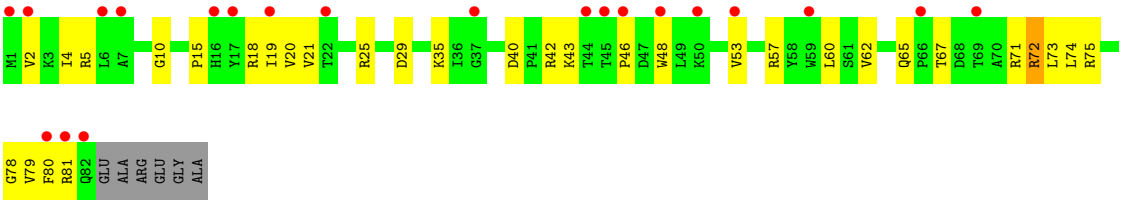


• Molecule 46: 30S ribosomal protein S15

Chain 2o:

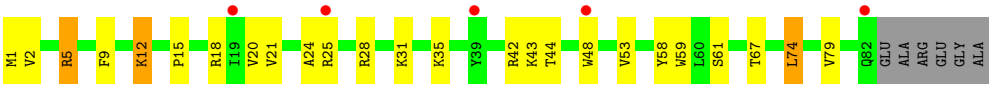
• Molecule 47: 30S ribosomal protein S16

Chain 1p:



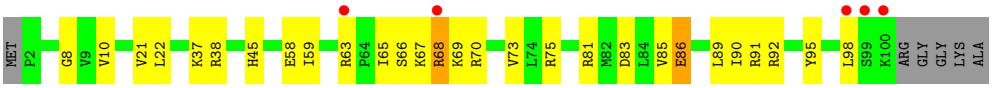
• Molecule 47: 30S ribosomal protein S16

Chain 2p:



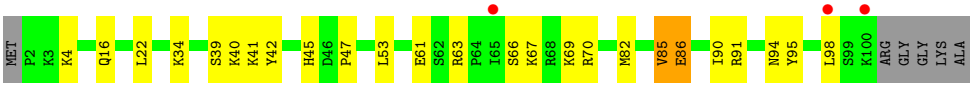
• Molecule 48: 30S ribosomal protein S17

Chain 1q: 5% 68% 25% • 6%



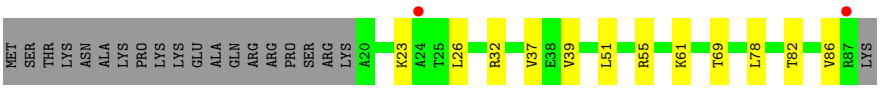
• Molecule 48: 30S ribosomal protein S17

Chain 2q: 3% 70% 22% • 6%



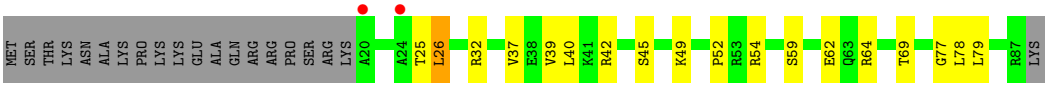
• Molecule 49: 30S ribosomal protein S18

Chain 1r: 2% 64% 14% 23%



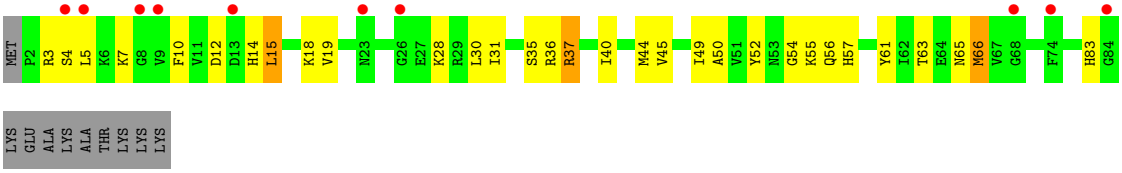
• Molecule 49: 30S ribosomal protein S18

Chain 2r: 2% 57% 19% • 23%



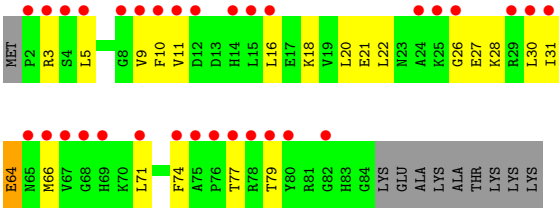
• Molecule 50: 30S ribosomal protein S19

Chain 1s: 11% 56% 30% • 11%



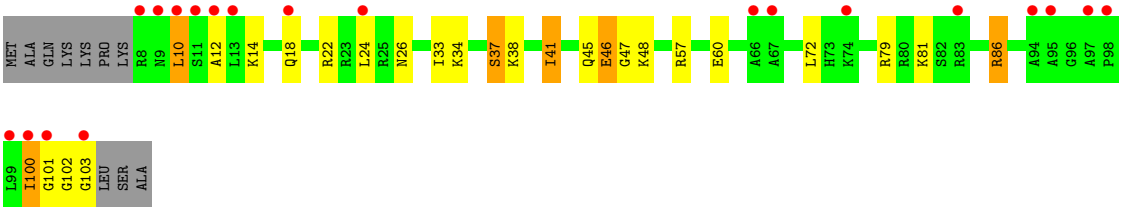
• Molecule 50: 30S ribosomal protein S19

Chain 2s: 47% 49% 35% • 11%



• Molecule 51: 30S ribosomal protein S20

Chain 1t:

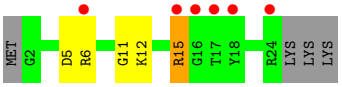


- Molecule 51: 30S ribosomal protein S20

Chain 2t:

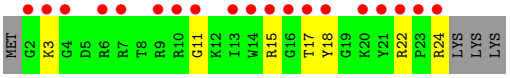
- Molecule 52: 30S ribosomal protein Thx

Chain 1u:



- Molecule 52: 30S ribosomal protein Thx

Chain 2u:

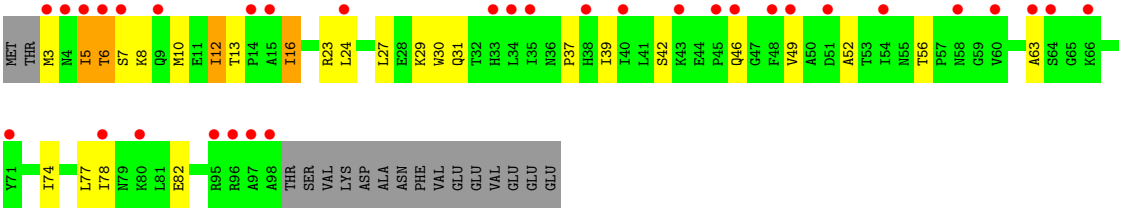


- Molecule 53: Ribosome-associated inhibitor A

Chain 1y:

- Molecule 53: Ribosome-associated inhibitor A

Chain 2y:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	209.90Å 449.76Å 620.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	122.00 – 2.60 122.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (122.00-2.60) 99.8 (122.00-2.60)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.21 (at 2.62Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.203 , 0.241 0.205 , 0.242	Depositor DCC
R_{free} test set	88927 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	53.0	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 49.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	297563	wwPDB-VP
Average B, all atoms (Å^2)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.55% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, OMC, PSU, OMG, G7M, CPF, 5MU, 2MA, 5MC, M2G, 0TD, MPD, SF4, ZN, UR3, MA6, 2MG, OMU, 4OC

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	0.19	0/69031	0.36	0/107754
1	2A	0.16	0/68903	0.34	0/107552
2	1B	0.15	0/2876	0.31	0/4486
2	2B	0.13	0/2878	0.27	0/4490
3	1D	0.19	0/2181	0.43	0/2940
3	2D	0.15	0/2186	0.41	0/2944
4	1E	0.17	0/1592	0.41	0/2149
4	2E	0.16	0/1592	0.39	0/2149
5	1F	0.17	0/1619	0.38	0/2193
5	2F	0.15	0/1615	0.41	0/2188
6	1G	0.14	0/1451	0.37	0/1961
6	2G	0.14	0/1449	0.35	0/1957
7	1H	0.15	0/1356	0.36	0/1834
7	2H	0.14	0/1350	0.37	0/1826
8	1I	0.15	0/1109	0.38	0/1512
8	2I	0.13	0/1091	0.36	0/1490
9	1N	0.16	0/1148	0.37	0/1547
9	2N	0.13	0/1144	0.33	0/1543
10	1O	0.17	0/943	0.40	0/1269
10	2O	0.15	0/943	0.37	0/1269
11	1P	0.18	0/1152	0.41	0/1533
11	2P	0.15	0/1152	0.42	0/1533
12	1Q	0.17	0/1143	0.40	0/1527
12	2Q	0.13	0/1143	0.35	0/1527
13	1R	0.17	0/982	0.40	0/1312
13	2R	0.15	0/982	0.39	0/1312
14	1S	0.15	0/887	0.37	0/1180
14	2S	0.14	0/880	0.38	0/1172
15	1T	0.17	0/1105	0.43	0/1477
15	2T	0.15	0/1097	0.39	0/1468
16	1U	0.18	0/977	0.38	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
16	2U	0.13	0/977	0.34	0/1301
17	1V	0.16	0/786	0.38	0/1053
17	2V	0.14	0/782	0.34	0/1049
18	1W	0.18	0/897	0.38	0/1205
18	2W	0.15	0/897	0.35	0/1205
19	1X	0.17	0/764	0.41	0/1025
19	2X	0.14	0/764	0.39	0/1025
20	1Y	0.17	0/823	0.44	0/1099
20	2Y	0.13	0/823	0.37	0/1100
21	1Z	0.14	0/1620	0.34	0/2200
21	2Z	0.13	0/1590	0.36	0/2162
22	10	0.18	0/616	0.45	0/821
22	20	0.15	0/616	0.41	0/821
23	11	0.17	0/761	0.38	0/1013
23	21	0.16	0/766	0.36	0/1018
24	12	0.15	0/590	0.37	0/781
24	22	0.14	0/594	0.38	0/785
25	13	0.17	0/474	0.41	0/635
25	23	0.13	0/469	0.34	0/630
26	14	0.18	0/559	0.54	0/754
26	24	0.22	0/549	0.58	2/741 (0.3%)
27	15	0.17	0/473	0.44	0/639
27	25	0.18	0/469	0.42	0/635
28	16	0.17	0/460	0.40	0/613
28	26	0.15	0/456	0.35	0/608
29	17	0.20	0/426	0.43	0/561
29	27	0.19	0/426	0.45	0/561
30	18	0.17	0/525	0.39	0/691
30	28	0.14	0/525	0.35	0/691
31	19	0.17	0/310	0.41	0/407
31	29	0.15	0/310	0.36	0/407
32	1a	0.14	0/35795	0.31	0/55864
32	2a	0.14	0/35890	0.31	0/56012
33	1b	0.15	0/1876	0.41	0/2533
33	2b	0.17	0/1860	0.41	0/2518
34	1c	0.14	0/1582	0.37	0/2137
34	2c	0.15	0/1566	0.36	0/2119
35	1d	0.14	0/1695	0.38	0/2274
35	2d	0.14	0/1698	0.37	0/2277
36	1e	0.15	0/1149	0.39	0/1548
36	2e	0.14	0/1149	0.37	0/1548
37	1f	0.14	0/827	0.35	0/1120
37	2f	0.13	0/829	0.35	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
38	1g	0.13	0/1254	0.33	0/1683
38	2g	0.13	0/1248	0.32	0/1676
39	1h	0.13	0/1118	0.36	0/1506
39	2h	0.13	0/1108	0.36	0/1494
40	1i	0.14	0/1005	0.39	0/1351
40	2i	0.15	0/985	0.39	0/1329
41	1j	0.14	0/732	0.35	0/993
41	2j	0.16	0/723	0.40	0/984
42	1k	0.14	0/849	0.36	0/1150
42	2k	0.14	0/848	0.38	0/1149
43	1l	0.14	0/937	0.37	0/1260
43	2l	0.14	0/937	0.37	0/1260
44	1m	0.15	0/924	0.41	0/1242
44	2m	0.16	0/905	0.47	1/1217 (0.1%)
45	1n	0.13	0/501	0.36	0/664
45	2n	0.14	0/501	0.36	0/664
46	1o	0.14	0/739	0.33	0/985
46	2o	0.14	0/739	0.36	0/985
47	1p	0.15	0/697	0.44	0/939
47	2p	0.13	0/693	0.39	0/935
48	1q	0.14	0/836	0.36	0/1117
48	2q	0.14	0/836	0.37	0/1117
49	1r	0.13	0/560	0.35	0/746
49	2r	0.14	0/560	0.34	0/746
50	1s	0.13	0/663	0.40	0/895
50	2s	0.13	0/660	0.35	0/893
51	1t	0.15	0/734	0.43	0/969
51	2t	0.14	0/736	0.36	0/976
52	1u	0.13	0/203	0.36	0/266
52	2u	0.21	0/203	0.47	0/266
53	1y	0.17	0/776	0.31	0/1048
53	2y	0.12	0/761	0.29	0/1030
All	All	0.16	0/309941	0.35	3/463239 (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
11	1P	0	1
11	2P	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
33	1b	0	1
All	All	0	3

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	24	59	PHE	CA-C-N	5.29	131.22	121.70
26	24	59	PHE	C-N-CA	5.29	131.22	121.70
44	2m	84	ILE	N-CA-C	-5.06	106.66	112.98

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	1P	35	HIS	Peptide
33	1b	231	GLU	Peptide
11	2P	35	HIS	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	31207	449	0
1	2A	61758	0	31153	518	0
2	1B	2572	0	1305	12	0
2	2B	2573	0	1306	29	0
3	1D	2131	0	2207	36	0
3	2D	2136	0	2218	34	0
4	1E	1559	0	1618	26	0
4	2E	1559	0	1618	28	0
5	1F	1584	0	1625	26	0
5	2F	1580	0	1619	33	0
6	1G	1426	0	1445	31	0
6	2G	1424	0	1441	54	0
7	1H	1330	0	1407	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	2H	1324	0	1402	39	0
8	1I	1094	0	1127	21	0
8	2I	1076	0	1094	16	0
9	1N	1121	0	1195	15	0
9	2N	1117	0	1184	19	0
10	1O	933	0	996	16	0
10	2O	933	0	996	12	0
11	1P	1135	0	1212	25	0
11	2P	1135	0	1212	17	0
12	1Q	1122	0	1179	10	0
12	2Q	1122	0	1179	17	0
13	1R	968	0	1033	15	0
13	2R	968	0	1033	14	0
14	1S	877	0	938	17	0
14	2S	870	0	923	27	0
15	1T	1091	0	1151	25	0
15	2T	1083	0	1136	17	0
16	1U	959	0	1019	12	0
16	2U	959	0	1019	15	0
17	1V	775	0	841	12	0
17	2V	771	0	830	13	0
18	1W	886	0	940	9	0
18	2W	886	0	940	10	0
19	1X	750	0	814	13	0
19	2X	750	0	814	6	0
20	1Y	810	0	892	13	0
20	2Y	810	0	887	12	0
21	1Z	1587	0	1598	21	0
21	2Z	1557	0	1564	28	0
22	10	608	0	622	6	0
22	20	608	0	622	5	0
23	11	754	0	823	14	0
23	21	759	0	837	17	0
24	12	588	0	643	8	0
24	22	592	0	654	10	0
25	13	469	0	518	8	0
25	23	464	0	514	6	0
26	14	546	0	522	15	0
26	24	536	0	514	25	0
27	15	459	0	476	4	0
27	25	455	0	465	5	0
28	16	453	0	473	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	26	449	0	469	9	0
29	17	418	0	467	9	0
29	27	418	0	467	4	0
30	18	517	0	582	14	0
30	28	517	0	582	8	0
31	19	307	0	335	3	0
31	29	307	0	335	8	0
32	1a	32246	0	16295	335	0
32	2a	32331	0	16338	352	0
33	1b	1842	0	1862	47	0
33	2b	1825	0	1828	61	0
34	1c	1558	0	1557	28	0
34	2c	1542	0	1517	40	0
35	1d	1665	0	1687	56	0
35	2d	1668	0	1703	37	0
36	1e	1133	0	1191	30	0
36	2e	1133	0	1191	27	0
37	1f	814	0	808	14	0
37	2f	816	0	808	13	0
38	1g	1235	0	1249	18	0
38	2g	1229	0	1238	20	0
39	1h	1098	0	1143	24	0
39	2h	1088	0	1126	24	0
40	1i	986	0	990	34	0
40	2i	966	0	953	33	0
41	1j	719	0	672	15	0
41	2j	710	0	661	34	0
42	1k	834	0	838	6	0
42	2k	833	0	836	16	0
43	1l	932	0	981	10	0
43	2l	932	0	981	20	0
44	1m	914	0	954	27	0
44	2m	895	0	920	31	0
45	1n	492	0	529	21	0
45	2n	492	0	529	17	0
46	1o	728	0	760	13	0
46	2o	728	0	760	15	0
47	1p	681	0	697	18	0
47	2p	677	0	686	15	0
48	1q	823	0	891	19	0
48	2q	823	0	891	22	0
49	1r	555	0	618	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
49	2r	555	0	618	11	0
50	1s	648	0	658	24	0
50	2s	645	0	635	31	0
51	1t	732	0	809	15	0
51	2t	733	0	795	13	0
52	1u	199	0	208	3	0
52	2u	199	0	208	3	0
53	1y	764	0	786	16	0
53	2y	749	0	757	20	0
54	10	7	0	0	0	0
54	11	5	0	0	0	0
54	13	4	0	0	0	0
54	14	1	0	0	0	0
54	15	8	0	0	0	0
54	17	7	0	0	0	0
54	18	3	0	0	0	0
54	19	2	0	0	0	0
54	1A	1056	0	0	0	0
54	1B	29	0	0	0	0
54	1D	18	0	0	0	0
54	1E	9	0	0	0	0
54	1F	19	0	0	0	0
54	1G	4	0	0	0	0
54	1H	3	0	0	0	0
54	1N	5	0	0	0	0
54	1O	1	0	0	0	0
54	1P	6	0	0	0	0
54	1Q	5	0	0	0	0
54	1R	6	0	0	0	0
54	1T	5	0	0	0	0
54	1U	7	0	0	0	0
54	1V	6	0	0	0	0
54	1W	3	0	0	0	0
54	1Z	1	0	0	0	0
54	1a	277	0	0	0	0
54	1b	1	0	0	0	0
54	1d	5	0	0	0	0
54	1e	2	0	0	0	0
54	1f	2	0	0	0	0
54	1g	3	0	0	0	0
54	1h	2	0	0	0	0
54	1i	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	1k	1	0	0	0	0
54	1l	2	0	0	0	0
54	1m	1	0	0	0	0
54	1n	3	0	0	0	0
54	1o	1	0	0	0	0
54	1t	1	0	0	0	0
54	1y	4	0	0	0	0
54	20	3	0	0	0	0
54	21	1	0	0	0	0
54	23	2	0	0	0	0
54	25	1	0	0	0	0
54	27	1	0	0	0	0
54	28	2	0	0	0	0
54	2A	741	0	0	0	0
54	2B	18	0	0	0	0
54	2D	12	0	0	0	0
54	2E	7	0	0	0	0
54	2F	4	0	0	0	0
54	2G	3	0	0	0	0
54	2N	1	0	0	0	0
54	2O	2	0	0	0	0
54	2Q	3	0	0	0	0
54	2R	3	0	0	0	0
54	2T	3	0	0	0	0
54	2V	3	0	0	0	0
54	2W	3	0	0	0	0
54	2X	1	0	0	0	0
54	2Y	1	0	0	0	0
54	2a	195	0	0	0	0
54	2d	1	0	0	0	0
54	2e	1	0	0	0	0
54	2f	2	0	0	0	0
54	2j	1	0	0	0	0
54	2k	1	0	0	0	0
54	2n	1	0	0	0	0
54	2o	1	0	0	0	0
54	2p	1	0	0	0	0
54	2r	1	0	0	0	0
54	2t	1	0	0	0	0
55	1A	24	0	17	1	0
55	2A	24	0	17	3	0
56	18	8	0	14	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	1A	8	0	14	1	0
56	1O	8	0	14	1	0
56	1a	8	0	14	4	0
56	2A	16	0	28	1	0
56	2B	8	0	14	0	0
57	1B	12	0	12	1	0
57	1F	12	0	12	2	0
58	14	1	0	0	0	0
58	15	1	0	0	0	0
58	16	1	0	0	0	0
58	19	1	0	0	0	0
58	1Y	1	0	0	0	0
58	1n	1	0	0	0	0
58	24	1	0	0	0	0
58	25	1	0	0	0	0
58	26	1	0	0	0	0
58	29	1	0	0	0	0
58	2Y	1	0	0	0	0
58	2n	1	0	0	0	0
59	1d	8	0	0	0	0
59	2d	8	0	0	0	0
60	10	25	0	0	0	0
60	11	28	0	0	0	0
60	12	13	0	0	3	0
60	13	25	0	0	2	0
60	14	3	0	0	0	0
60	15	28	0	0	0	0
60	16	20	0	0	0	0
60	17	13	0	0	0	0
60	18	28	0	0	1	0
60	19	8	0	0	0	0
60	1A	3927	0	0	79	0
60	1B	89	0	0	5	0
60	1D	110	0	0	3	0
60	1E	72	0	0	3	0
60	1F	67	0	0	1	0
60	1G	16	0	0	0	0
60	1H	14	0	0	0	0
60	1I	5	0	0	0	0
60	1N	52	0	0	0	0
60	1O	25	0	0	1	0
60	1P	65	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	1Q	41	0	0	1	0
60	1R	32	0	0	1	0
60	1S	8	0	0	1	0
60	1T	36	0	0	2	0
60	1U	43	0	0	3	0
60	1V	36	0	0	0	0
60	1W	28	0	0	1	0
60	1X	26	0	0	1	0
60	1Y	17	0	0	2	0
60	1Z	11	0	0	0	0
60	1a	496	0	0	22	0
60	1b	1	0	0	0	0
60	1c	1	0	0	0	0
60	1d	9	0	0	1	0
60	1e	10	0	0	1	0
60	1f	1	0	0	0	0
60	1h	1	0	0	0	0
60	1j	1	0	0	0	0
60	1k	1	0	0	0	0
60	1l	4	0	0	0	0
60	1o	4	0	0	0	0
60	1p	1	0	0	0	0
60	1y	5	0	0	0	0
60	20	10	0	0	0	0
60	21	17	0	0	2	0
60	22	2	0	0	0	0
60	23	2	0	0	1	0
60	25	7	0	0	0	0
60	26	6	0	0	1	0
60	27	9	0	0	0	0
60	28	15	0	0	0	0
60	2A	2249	0	0	87	0
60	2B	42	0	0	3	0
60	2D	47	0	0	1	0
60	2E	28	0	0	1	0
60	2F	23	0	0	0	0
60	2G	4	0	0	0	0
60	2H	1	0	0	1	0
60	2N	6	0	0	1	0
60	2O	15	0	0	0	0
60	2P	21	0	0	1	0
60	2Q	18	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	2R	22	0	0	2	0
60	2S	2	0	0	0	0
60	2T	12	0	0	0	0
60	2U	16	0	0	3	0
60	2V	8	0	0	0	0
60	2W	19	0	0	0	0
60	2X	8	0	0	0	0
60	2Y	4	0	0	0	0
60	2Z	8	0	0	0	0
60	2a	404	0	0	22	0
60	2d	3	0	0	1	0
60	2e	3	0	0	0	0
60	2f	3	0	0	0	0
60	2j	2	0	0	1	0
60	2l	5	0	0	1	0
60	2o	2	0	0	1	0
60	2p	1	0	0	0	0
60	2q	1	0	0	0	0
60	2r	3	0	0	0	0
60	2t	3	0	0	0	0
60	2u	1	0	0	0	0
60	2y	1	0	0	0	0
All	All	297563	0	194555	3101	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 7.

The worst 5 of 3101 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1082:U:H3	1:1A:1086:A:N6	1.39	1.19
1:1A:1082:U:O4	1:1A:1086:A:N1	1.97	0.97
32:1a:1086:U:H3	32:1a:1099:G:H22	1.16	0.94
15:1T:55:ASN:H	15:1T:59:THR:HG22	1.35	0.90
1:2A:2319:G:H22	14:2S:3:ARG:HD3	1.37	0.87

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%)	261 (96%)	12 (4%)	0	100	100
3	2D	273/276 (99%)	262 (96%)	10 (4%)	1 (0%)	30	51
4	1E	202/206 (98%)	195 (96%)	6 (3%)	1 (0%)	24	46
4	2E	202/206 (98%)	193 (96%)	7 (4%)	2 (1%)	12	28
5	1F	201/210 (96%)	197 (98%)	3 (2%)	1 (0%)	24	46
5	2F	201/210 (96%)	195 (97%)	5 (2%)	1 (0%)	24	46
6	1G	179/182 (98%)	171 (96%)	4 (2%)	4 (2%)	5	10
6	2G	179/182 (98%)	164 (92%)	12 (7%)	3 (2%)	7	15
7	1H	172/180 (96%)	161 (94%)	11 (6%)	0	100	100
7	2H	171/180 (95%)	155 (91%)	16 (9%)	0	100	100
8	1I	145/148 (98%)	132 (91%)	13 (9%)	0	100	100
8	2I	144/148 (97%)	134 (93%)	10 (7%)	0	100	100
9	1N	138/140 (99%)	135 (98%)	3 (2%)	0	100	100
9	2N	138/140 (99%)	133 (96%)	5 (4%)	0	100	100
10	1O	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
10	2O	120/122 (98%)	116 (97%)	4 (3%)	0	100	100
11	1P	147/150 (98%)	137 (93%)	9 (6%)	1 (1%)	18	38
11	2P	147/150 (98%)	141 (96%)	6 (4%)	0	100	100
12	1Q	139/141 (99%)	134 (96%)	4 (3%)	1 (1%)	18	38
12	2Q	139/141 (99%)	134 (96%)	5 (4%)	0	100	100
13	1R	116/118 (98%)	112 (97%)	4 (3%)	0	100	100
13	2R	116/118 (98%)	113 (97%)	3 (3%)	0	100	100
14	1S	108/112 (96%)	101 (94%)	7 (6%)	0	100	100
14	2S	108/112 (96%)	101 (94%)	7 (6%)	0	100	100
15	1T	129/146 (88%)	121 (94%)	8 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	2T	129/146 (88%)	123 (95%)	6 (5%)	0	100	100
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%)	96 (97%)	2 (2%)	1 (1%)	12	28
17	2V	99/101 (98%)	92 (93%)	6 (6%)	1 (1%)	12	28
18	1W	110/113 (97%)	109 (99%)	1 (1%)	0	100	100
18	2W	110/113 (97%)	109 (99%)	1 (1%)	0	100	100
19	1X	93/96 (97%)	91 (98%)	1 (1%)	1 (1%)	11	25
19	2X	93/96 (97%)	91 (98%)	1 (1%)	1 (1%)	11	25
20	1Y	105/110 (96%)	99 (94%)	6 (6%)	0	100	100
20	2Y	105/110 (96%)	102 (97%)	3 (3%)	0	100	100
21	1Z	201/206 (98%)	191 (95%)	9 (4%)	1 (0%)	24	46
21	2Z	199/206 (97%)	186 (94%)	13 (6%)	0	100	100
22	10	75/85 (88%)	73 (97%)	2 (3%)	0	100	100
22	20	75/85 (88%)	73 (97%)	2 (3%)	0	100	100
23	11	95/98 (97%)	93 (98%)	2 (2%)	0	100	100
23	21	95/98 (97%)	92 (97%)	2 (2%)	1 (1%)	11	25
24	12	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
24	22	68/72 (94%)	65 (96%)	3 (4%)	0	100	100
25	13	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
25	23	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
26	14	67/71 (94%)	54 (81%)	9 (13%)	4 (6%)	1	1
26	24	67/71 (94%)	51 (76%)	13 (19%)	3 (4%)	2	2
27	15	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
27	25	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
28	16	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
28	26	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
29	17	46/49 (94%)	46 (100%)	0	0	100	100
29	27	46/49 (94%)	46 (100%)	0	0	100	100
30	18	62/65 (95%)	62 (100%)	0	0	100	100
30	28	62/65 (95%)	62 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	19	35/37 (95%)	35 (100%)	0	0	100	100
31	29	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
33	1b	229/256 (90%)	198 (86%)	26 (11%)	5 (2%)	5	10
33	2b	229/256 (90%)	201 (88%)	22 (10%)	6 (3%)	4	7
34	1c	204/239 (85%)	190 (93%)	14 (7%)	0	100	100
34	2c	204/239 (85%)	175 (86%)	28 (14%)	1 (0%)	24	46
35	1d	206/209 (99%)	198 (96%)	8 (4%)	0	100	100
35	2d	206/209 (99%)	198 (96%)	8 (4%)	0	100	100
36	1e	146/162 (90%)	139 (95%)	7 (5%)	0	100	100
36	2e	146/162 (90%)	142 (97%)	4 (3%)	0	100	100
37	1f	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
37	2f	98/101 (97%)	95 (97%)	3 (3%)	0	100	100
38	1g	153/156 (98%)	148 (97%)	5 (3%)	0	100	100
38	2g	153/156 (98%)	146 (95%)	6 (4%)	1 (1%)	18	38
39	1h	135/138 (98%)	129 (96%)	6 (4%)	0	100	100
39	2h	135/138 (98%)	127 (94%)	8 (6%)	0	100	100
40	1i	125/128 (98%)	114 (91%)	10 (8%)	1 (1%)	16	34
40	2i	124/128 (97%)	109 (88%)	12 (10%)	3 (2%)	4	9
41	1j	95/105 (90%)	81 (85%)	11 (12%)	3 (3%)	3	5
41	2j	94/105 (90%)	82 (87%)	9 (10%)	3 (3%)	3	5
42	1k	112/129 (87%)	105 (94%)	7 (6%)	0	100	100
42	2k	112/129 (87%)	106 (95%)	5 (4%)	1 (1%)	14	30
43	1l	119/132 (90%)	117 (98%)	2 (2%)	0	100	100
43	2l	119/132 (90%)	113 (95%)	6 (5%)	0	100	100
44	1m	114/126 (90%)	104 (91%)	8 (7%)	2 (2%)	6	14
44	2m	112/126 (89%)	97 (87%)	12 (11%)	3 (3%)	4	7
45	1n	58/61 (95%)	55 (95%)	3 (5%)	0	100	100
45	2n	58/61 (95%)	53 (91%)	5 (9%)	0	100	100
46	1o	86/89 (97%)	79 (92%)	6 (7%)	1 (1%)	10	23
46	2o	86/89 (97%)	79 (92%)	5 (6%)	2 (2%)	5	9
47	1p	80/88 (91%)	74 (92%)	5 (6%)	1 (1%)	9	21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	2p	80/88 (91%)	74 (92%)	6 (8%)	0	100	100
48	1q	97/105 (92%)	91 (94%)	5 (5%)	1 (1%)	12	28
48	2q	97/105 (92%)	90 (93%)	7 (7%)	0	100	100
49	1r	66/88 (75%)	64 (97%)	2 (3%)	0	100	100
49	2r	66/88 (75%)	65 (98%)	1 (2%)	0	100	100
50	1s	81/93 (87%)	74 (91%)	7 (9%)	0	100	100
50	2s	81/93 (87%)	69 (85%)	12 (15%)	0	100	100
51	1t	94/106 (89%)	88 (94%)	6 (6%)	0	100	100
51	2t	96/106 (91%)	91 (95%)	5 (5%)	0	100	100
52	1u	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
52	2u	21/27 (78%)	18 (86%)	2 (10%)	1 (5%)	2	2
53	1y	95/113 (84%)	95 (100%)	0	0	100	100
53	2y	94/113 (83%)	92 (98%)	2 (2%)	0	100	100
All	All	11629/12354 (94%)	10978 (94%)	588 (5%)	63 (0%)	24	46

5 of 63 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
33	1b	21	ARG
33	1b	124	SER
44	1m	67	GLU
44	1m	106	ASN
5	2F	130	ALA

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%)	199 (93%)	15 (7%)	14	31
3	2D	215/218 (99%)	199 (93%)	16 (7%)	13	29
4	1E	164/166 (99%)	150 (92%)	14 (8%)	10	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	2E	164/166 (99%)	152 (93%)	12 (7%)	13	29
5	1F	160/166 (96%)	145 (91%)	15 (9%)	8	18
5	2F	159/166 (96%)	144 (91%)	15 (9%)	8	18
6	1G	144/156 (92%)	134 (93%)	10 (7%)	14	32
6	2G	142/156 (91%)	128 (90%)	14 (10%)	7	16
7	1H	144/148 (97%)	134 (93%)	10 (7%)	14	32
7	2H	143/148 (97%)	129 (90%)	14 (10%)	7	17
8	1I	111/124 (90%)	104 (94%)	7 (6%)	16	36
8	2I	108/124 (87%)	100 (93%)	8 (7%)	13	29
9	1N	119/119 (100%)	109 (92%)	10 (8%)	10	23
9	2N	118/119 (99%)	109 (92%)	9 (8%)	12	27
10	1O	100/100 (100%)	99 (99%)	1 (1%)	68	86
10	2O	100/100 (100%)	98 (98%)	2 (2%)	48	74
11	1P	115/116 (99%)	110 (96%)	5 (4%)	26	51
11	2P	115/116 (99%)	104 (90%)	11 (10%)	8	17
12	1Q	111/111 (100%)	103 (93%)	8 (7%)	13	30
12	2Q	111/111 (100%)	104 (94%)	7 (6%)	16	36
13	1R	101/101 (100%)	94 (93%)	7 (7%)	14	32
13	2R	101/101 (100%)	92 (91%)	9 (9%)	9	20
14	1S	87/88 (99%)	79 (91%)	8 (9%)	8	19
14	2S	85/88 (97%)	79 (93%)	6 (7%)	13	31
15	1T	115/127 (91%)	110 (96%)	5 (4%)	26	51
15	2T	113/127 (89%)	109 (96%)	4 (4%)	32	59
16	1U	93/94 (99%)	90 (97%)	3 (3%)	34	62
16	2U	93/94 (99%)	90 (97%)	3 (3%)	34	62
17	1V	81/82 (99%)	78 (96%)	3 (4%)	30	57
17	2V	80/82 (98%)	72 (90%)	8 (10%)	7	16
18	1W	90/92 (98%)	85 (94%)	5 (6%)	19	40
18	2W	90/92 (98%)	84 (93%)	6 (7%)	15	33
19	1X	77/78 (99%)	74 (96%)	3 (4%)	28	55
19	2X	77/78 (99%)	75 (97%)	2 (3%)	40	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	1Y	86/91 (94%)	80 (93%)	6 (7%)	14	31
20	2Y	86/91 (94%)	81 (94%)	5 (6%)	18	39
21	1Z	169/179 (94%)	155 (92%)	14 (8%)	10	23
21	2Z	165/179 (92%)	152 (92%)	13 (8%)	11	26
22	10	61/67 (91%)	59 (97%)	2 (3%)	33	61
22	20	61/67 (91%)	60 (98%)	1 (2%)	55	79
23	11	79/83 (95%)	74 (94%)	5 (6%)	16	36
23	21	81/83 (98%)	76 (94%)	5 (6%)	16	36
24	12	65/67 (97%)	63 (97%)	2 (3%)	35	63
24	22	66/67 (98%)	60 (91%)	6 (9%)	9	19
25	13	51/52 (98%)	47 (92%)	4 (8%)	11	26
25	23	50/52 (96%)	47 (94%)	3 (6%)	17	37
26	14	58/63 (92%)	54 (93%)	4 (7%)	14	32
26	24	54/63 (86%)	48 (89%)	6 (11%)	6	12
27	15	51/52 (98%)	49 (96%)	2 (4%)	28	55
27	25	50/52 (96%)	48 (96%)	2 (4%)	28	55
28	16	51/52 (98%)	50 (98%)	1 (2%)	48	74
28	26	50/52 (96%)	48 (96%)	2 (4%)	28	55
29	17	41/42 (98%)	39 (95%)	2 (5%)	22	47
29	27	41/42 (98%)	37 (90%)	4 (10%)	7	17
30	18	54/55 (98%)	51 (94%)	3 (6%)	19	40
30	28	54/55 (98%)	51 (94%)	3 (6%)	19	40
31	19	34/34 (100%)	33 (97%)	1 (3%)	37	65
31	29	34/34 (100%)	33 (97%)	1 (3%)	37	65
33	1b	191/220 (87%)	164 (86%)	27 (14%)	3	6
33	2b	187/220 (85%)	163 (87%)	24 (13%)	4	8
34	1c	144/188 (77%)	135 (94%)	9 (6%)	16	36
34	2c	140/188 (74%)	127 (91%)	13 (9%)	8	18
35	1d	171/181 (94%)	155 (91%)	16 (9%)	8	18
35	2d	172/181 (95%)	160 (93%)	12 (7%)	14	31
36	1e	114/123 (93%)	107 (94%)	7 (6%)	17	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	2e	114/123 (93%)	106 (93%)	8 (7%)	14	31
37	1f	85/90 (94%)	79 (93%)	6 (7%)	13	31
37	2f	85/90 (94%)	82 (96%)	3 (4%)	32	59
38	1g	120/127 (94%)	112 (93%)	8 (7%)	15	33
38	2g	119/127 (94%)	109 (92%)	10 (8%)	10	23
39	1h	116/119 (98%)	110 (95%)	6 (5%)	21	44
39	2h	114/119 (96%)	103 (90%)	11 (10%)	8	17
40	1i	91/99 (92%)	81 (89%)	10 (11%)	6	13
40	2i	88/99 (89%)	77 (88%)	11 (12%)	4	9
41	1j	68/92 (74%)	64 (94%)	4 (6%)	18	38
41	2j	68/92 (74%)	63 (93%)	5 (7%)	13	29
42	1k	83/99 (84%)	80 (96%)	3 (4%)	31	58
42	2k	83/99 (84%)	79 (95%)	4 (5%)	23	47
43	1l	96/108 (89%)	94 (98%)	2 (2%)	47	73
43	2l	96/108 (89%)	93 (97%)	3 (3%)	35	63
44	1m	90/101 (89%)	82 (91%)	8 (9%)	9	20
44	2m	87/101 (86%)	82 (94%)	5 (6%)	18	40
45	1n	49/50 (98%)	45 (92%)	4 (8%)	10	24
45	2n	49/50 (98%)	45 (92%)	4 (8%)	10	24
46	1o	78/80 (98%)	74 (95%)	4 (5%)	21	45
46	2o	78/80 (98%)	70 (90%)	8 (10%)	7	15
47	1p	69/74 (93%)	60 (87%)	9 (13%)	4	8
47	2p	68/74 (92%)	61 (90%)	7 (10%)	7	15
48	1q	94/97 (97%)	92 (98%)	2 (2%)	47	73
48	2q	94/97 (97%)	91 (97%)	3 (3%)	34	62
49	1r	59/77 (77%)	58 (98%)	1 (2%)	53	78
49	2r	59/77 (77%)	57 (97%)	2 (3%)	32	60
50	1s	68/80 (85%)	61 (90%)	7 (10%)	7	15
50	2s	67/80 (84%)	60 (90%)	7 (10%)	7	14
51	1t	71/82 (87%)	62 (87%)	9 (13%)	4	9
51	2t	70/82 (85%)	65 (93%)	5 (7%)	13	31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
52	1u	18/22 (82%)	17 (94%)	1 (6%)	19 40
52	2u	18/22 (82%)	18 (100%)	0	100 100
53	1y	82/98 (84%)	80 (98%)	2 (2%)	43 70
53	2y	79/98 (81%)	71 (90%)	8 (10%)	7 15
All	All	9524/10260 (93%)	8854 (93%)	670 (7%)	14 31

5 of 670 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
18	2W	107	LEU
36	2e	107	ARG
21	2Z	86	VAL
18	2W	100	THR
33	2b	52	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 140 such sidechains are listed below:

Mol	Chain	Res	Type
35	2d	160	GLN
38	2g	13	GLN
44	2m	62	ASN
38	1g	64	GLN
38	1g	28	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2865/2915 (98%)	396 (13%)	27 (0%)
1	2A	2858/2915 (98%)	460 (16%)	32 (1%)
2	1B	119/121 (98%)	9 (7%)	0
2	2B	119/121 (98%)	15 (12%)	0
32	1a	1497/1521 (98%)	241 (16%)	0
32	2a	1501/1521 (98%)	254 (16%)	0
All	All	8959/9114 (98%)	1375 (15%)	59 (0%)

5 of 1375 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	12	U
1	1A	15	G
1	1A	34	C
1	1A	45	C
1	1A	71	A

5 of 59 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2A	195	A
1	2A	2601	C
1	2A	827	U
1	2A	2406	U
1	2A	1992	G

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

48 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	$\#\|Z\| > 2$
1	OMU	2A	2552	54,1	19,22,23	1.18	3 (15%)	25,31,34	1.87	5 (20%)
32	2MG	1a	1207	32,54	23,26,27	1.24	2 (8%)	33,38,41	2.36	9 (27%)
32	5MC	2a	1404	32	19,22,23	1.69	3 (15%)	26,32,35	1.12	3 (11%)
1	5MC	1A	1942	54,1	19,22,23	1.59	3 (15%)	26,32,35	1.10	2 (7%)
32	5MC	2a	967	32	19,22,23	1.79	3 (15%)	26,32,35	1.10	2 (7%)
32	PSU	2a	516	32,54	18,21,22	1.36	2 (11%)	21,30,33	2.09	5 (23%)
43	0TD	2l	92	43	8,9,10	4.37	1 (12%)	6,11,13	1.27	1 (16%)
43	0TD	1l	92	43	8,9,10	4.52	1 (12%)	6,11,13	6.96	2 (33%)
32	UR3	2a	1498	32	19,22,23	1.00	2 (10%)	26,32,35	1.73	3 (11%)
1	OMU	1A	2552	54,1	19,22,23	1.24	2 (10%)	25,31,34	1.77	5 (20%)
32	G7M	1a	527	32,54	23,26,27	1.52	3 (13%)	34,39,42	1.71	5 (14%)
1	5MU	2A	1915	1	19,22,23	1.45	4 (21%)	27,32,35	2.20	8 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	PSU	1A	1917	54,1	18,21,22	1.36	2 (11%)	21,30,33	1.98	3 (14%)
32	5MC	1a	1407	32	19,22,23	1.71	3 (15%)	26,32,35	1.14	3 (11%)
1	5MC	2A	1962	54,1	19,22,23	1.61	3 (15%)	26,32,35	1.14	2 (7%)
32	4OC	1a	1402	32	20,23,24	0.75	0	25,32,35	0.99	1 (4%)
1	5MU	1A	1939	54,1	19,22,23	1.43	6 (31%)	27,32,35	2.10	6 (22%)
32	M2G	1a	966	32	24,27,28	1.29	4 (16%)	33,40,43	1.85	6 (18%)
32	UR3	1a	1498	32	19,22,23	0.99	1 (5%)	26,32,35	1.74	3 (11%)
32	5MC	2a	1400	32	19,22,23	1.66	3 (15%)	26,32,35	1.17	3 (11%)
32	5MC	1a	1404	32	19,22,23	1.63	3 (15%)	26,32,35	1.09	2 (7%)
1	PSU	1A	1911	1	18,21,22	1.34	2 (11%)	21,30,33	2.05	5 (23%)
32	MA6	1a	1518	32	23,26,27	0.41	0	33,38,41	1.98	9 (27%)
32	PSU	1a	516	32,54	18,21,22	1.38	2 (11%)	21,30,33	1.97	4 (19%)
32	MA6	1a	1519	32	23,26,27	0.42	0	33,38,41	2.03	9 (27%)
32	G7M	2a	527	32,54	23,26,27	1.52	3 (13%)	34,39,42	1.73	5 (14%)
32	M2G	2a	966	32	24,27,28	1.29	3 (12%)	33,40,43	1.85	6 (18%)
1	5MU	2A	1939	1	19,22,23	1.41	5 (26%)	27,32,35	2.16	6 (22%)
32	4OC	2a	1402	32	20,23,24	0.77	0	25,32,35	1.01	1 (4%)
1	5MC	2A	1942	1	19,22,23	1.72	3 (15%)	26,32,35	1.13	2 (7%)
1	2MA	1A	2503	54,1	22,25,26	1.50	4 (18%)	32,37,40	2.34	7 (21%)
1	OMG	2A	2251	54,1	23,26,27	1.18	3 (13%)	32,38,41	2.02	6 (18%)
32	5MC	1a	1400	32	19,22,23	1.76	3 (15%)	26,32,35	1.14	2 (7%)
1	PSU	1A	2605	1	18,21,22	1.37	3 (16%)	21,30,33	2.03	4 (19%)
1	2MA	2A	2503	54,1	22,25,26	1.50	4 (18%)	32,37,40	2.34	8 (25%)
1	PSU	2A	2605	1	18,21,22	1.32	2 (11%)	21,30,33	2.09	4 (19%)
1	OMC	1A	1920	1	19,22,23	0.78	0	25,31,34	0.85	1 (4%)
32	MA6	2a	1518	32	23,26,27	0.40	0	33,38,41	2.03	9 (27%)
32	MA6	2a	1519	32	23,26,27	0.41	0	33,38,41	2.09	9 (27%)
1	OMG	1A	2251	54,1	23,26,27	1.20	3 (13%)	32,38,41	2.00	6 (18%)
1	5MC	1A	1962	54,1	19,22,23	1.78	3 (15%)	26,32,35	1.20	3 (11%)
1	OMC	2A	1920	1	19,22,23	0.80	0	25,31,34	0.98	1 (4%)
32	2MG	2a	1207	32	23,26,27	1.21	2 (8%)	33,38,41	2.21	7 (21%)
1	5MU	1A	1915	54,1	19,22,23	1.47	6 (31%)	27,32,35	2.18	8 (29%)
1	PSU	2A	1911	1	18,21,22	1.37	2 (11%)	21,30,33	2.02	4 (19%)
32	5MC	2a	1407	32	19,22,23	1.64	2 (10%)	26,32,35	1.16	3 (11%)
32	5MC	1a	967	32	19,22,23	1.67	3 (15%)	26,32,35	1.12	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	PSU	2A	1917	1	18,21,22	1.37	2 (11%)	21,30,33	1.97	3 (14%)

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
1	OMU	2A	2552	54,1	-	0/9/27/28	0/2/2/2
32	2MG	1a	1207	32,54	-	0/9/27/28	0/3/3/3
32	5MC	2a	1404	32	-	0/7/25/26	0/2/2/2
1	5MC	1A	1942	54,1	-	0/7/25/26	0/2/2/2
32	5MC	2a	967	32	-	0/7/25/26	0/2/2/2
32	PSU	2a	516	32,54	-	0/7/25/26	0/2/2/2
43	0TD	2l	92	43	-	3/7/12/14	-
43	0TD	1l	92	43	-	2/7/12/14	-
32	UR3	2a	1498	32	-	0/7/25/26	0/2/2/2
1	OMU	1A	2552	54,1	-	0/9/27/28	0/2/2/2
32	G7M	1a	527	32,54	-	1/7/25/26	0/3/3/3
1	5MU	2A	1915	1	-	2/7/25/26	0/2/2/2
1	PSU	1A	1917	54,1	-	0/7/25/26	0/2/2/2
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
1	5MC	2A	1962	54,1	-	0/7/25/26	0/2/2/2
32	4OC	1a	1402	32	-	2/9/29/30	0/2/2/2
1	5MU	1A	1939	54,1	-	0/7/25/26	0/2/2/2
32	M2G	1a	966	32	-	0/11/29/30	0/3/3/3
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
32	5MC	2a	1400	32	-	1/7/25/26	0/2/2/2
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
32	MA6	1a	1518	32	-	0/11/29/30	0/3/3/3
32	PSU	1a	516	32,54	-	0/7/25/26	0/2/2/2
32	MA6	1a	1519	32	-	2/11/29/30	0/3/3/3
32	G7M	2a	527	32,54	-	3/7/25/26	0/3/3/3
32	M2G	2a	966	32	-	0/11/29/30	0/3/3/3
1	5MU	2A	1939	1	-	0/7/25/26	0/2/2/2
32	4OC	2a	1402	32	-	1/9/29/30	0/2/2/2
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
1	2MA	1A	2503	54,1	-	1/7/25/26	0/3/3/3
1	OMG	2A	2251	54,1	-	0/9/27/28	0/3/3/3
32	5MC	1a	1400	32	-	2/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	1A	2605	1	-	0/7/25/26	0/2/2/2
1	2MA	2A	2503	54,1	-	2/7/25/26	0/3/3/3
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
1	OMC	1A	1920	1	-	0/9/27/28	0/2/2/2
32	MA6	2a	1518	32	-	0/11/29/30	0/3/3/3
32	MA6	2a	1519	32	-	2/11/29/30	0/3/3/3
1	OMG	1A	2251	54,1	-	0/9/27/28	0/3/3/3
1	5MC	1A	1962	54,1	-	0/7/25/26	0/2/2/2
1	OMC	2A	1920	1	-	0/9/27/28	0/2/2/2
32	2MG	2a	1207	32	-	0/9/27/28	0/3/3/3
1	5MU	1A	1915	54,1	-	2/7/25/26	0/2/2/2
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
32	5MC	2a	1407	32	-	0/7/25/26	0/2/2/2
32	5MC	1a	967	32	-	0/7/25/26	0/2/2/2
1	PSU	2A	1917	1	-	1/7/25/26	0/2/2/2

The worst 5 of 114 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	1l	92	0TD	CB-SB	-12.42	1.69	1.82
43	2l	92	0TD	CB-SB	-12.02	1.70	1.82
32	2a	967	5MC	C5-C4	6.61	1.49	1.44
1	1A	1962	5MC	C5-C4	6.61	1.49	1.44
32	1a	1400	5MC	C5-C4	6.47	1.49	1.44

The worst 5 of 213 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	1l	92	0TD	CSB-SB-CB	-16.76	72.24	102.36
1	1A	2503	2MA	C5-C4-N3	-8.42	118.31	127.18
1	2A	2503	2MA	C5-C4-N3	-8.20	118.55	127.18
32	1a	1207	2MG	C2-N3-C4	7.28	121.11	112.00
32	1a	1498	UR3	C4-N3-C2	-7.03	118.92	124.58

There are no chirality outliers.

5 of 27 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	2A	1915	5MU	O4'-C1'-N1-C2

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Mol	Chain	Res	Type	Atoms
1	2A	1915	5MU	O4'-C1'-N1-C6
43	2l	92	0TD	O-C-CA-CB

There are no ring outliers.

19 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	2a	1404	5MC	2	0
43	2l	92	0TD	1	0
1	2A	1915	5MU	1	0
1	1A	1917	PSU	1	0
32	1a	1402	4OC	1	0
1	1A	1939	5MU	1	0
32	1a	1498	UR3	1	0
32	2a	1400	5MC	1	0
32	1a	1518	MA6	1	0
32	1a	1519	MA6	2	0
32	2a	1402	4OC	2	0
1	1A	2503	2MA	1	0
32	1a	1400	5MC	2	0
1	1A	1920	OMC	1	0
32	2a	1518	MA6	2	0
32	2a	1519	MA6	2	0
1	2A	1920	OMC	1	0
32	1a	967	5MC	1	0
1	2A	1917	PSU	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2572 ligands modelled in this entry, 2559 are monoatomic - leaving 13 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	$\#\|Z\| > 2$
55	CPF	1A	4056	54	27,27,27	2.11	6 (22%)	40,40,40	1.79	11 (27%)
56	MPD	1a	1878	-	7,7,7	0.40	0	9,10,10	0.40	0
56	MPD	18	104	-	7,7,7	0.30	0	9,10,10	0.25	0
59	SF4	1d	306	35	0,12,12	-	-	-		
56	MPD	2A	3744	-	7,7,7	0.31	0	9,10,10	0.17	0
56	MPD	1O	202	-	7,7,7	0.31	0	9,10,10	0.19	0
56	MPD	2A	3743	-	7,7,7	0.33	0	9,10,10	0.30	0
55	CPF	2A	3741	54	27,27,27	2.09	6 (22%)	40,40,40	2.22	13 (32%)
56	MPD	2B	219	-	7,7,7	0.31	0	9,10,10	0.23	0
57	ARG	1F	320	-	10,11,11	0.75	1 (10%)	9,13,13	0.87	1 (11%)
57	ARG	1B	230	54	10,11,11	0.76	1 (10%)	9,13,13	0.99	1 (11%)
59	SF4	2d	302	35	0,12,12	-	-	-		
56	MPD	1A	4058	-	7,7,7	0.35	0	9,10,10	0.34	0

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
55	CPF	1A	4056	54	-	9/12/22/22	0/4/4/4
56	MPD	1a	1878	-	-	5/5/5/5	-
56	MPD	18	104	-	-	4/5/5/5	-
59	SF4	1d	306	35	-	-	0/6/5/5
56	MPD	2A	3744	-	-	4/5/5/5	-
56	MPD	1O	202	-	-	2/5/5/5	-
56	MPD	2A	3743	-	-	0/5/5/5	-
55	CPF	2A	3741	54	-	6/12/22/22	0/4/4/4
56	MPD	2B	219	-	-	3/5/5/5	-
57	ARG	1F	320	-	-	3/11/11/11	-
57	ARG	1B	230	54	-	2/11/11/11	-
59	SF4	2d	302	35	-	-	0/6/5/5
56	MPD	1A	4058	-	-	2/5/5/5	-

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	1A	4056	CPF	C2-C3	-5.59	1.39	1.48
55	2A	3741	CPF	C2-C3	-5.56	1.40	1.48
55	2A	3741	CPF	C5-C4	-4.88	1.38	1.48
55	1A	4056	CPF	C10-N1	-4.71	1.34	1.40
55	1A	4056	CPF	C5-C4	-4.62	1.39	1.48

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	2A	3741	CPF	F1-C7-C8	6.06	124.15	118.37
55	2A	3741	CPF	C9-C8-N2	-4.45	116.11	122.59
55	2A	3741	CPF	C6-C7-C8	-4.44	119.43	123.35
55	2A	3741	CPF	C7-C8-N2	4.16	125.28	120.42
55	1A	4056	CPF	C2-C1-N1	-4.07	119.54	124.42

There are no chirality outliers.

5 of 40 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
55	1A	4056	CPF	C1-C2-C3-O2
55	1A	4056	CPF	C4-C2-C3-O2
55	1A	4056	CPF	C1-C2-C3-O1
55	1A	4056	CPF	C4-C2-C3-O1
55	1A	4056	CPF	C7-C8-N2-C17

There are no ring outliers.

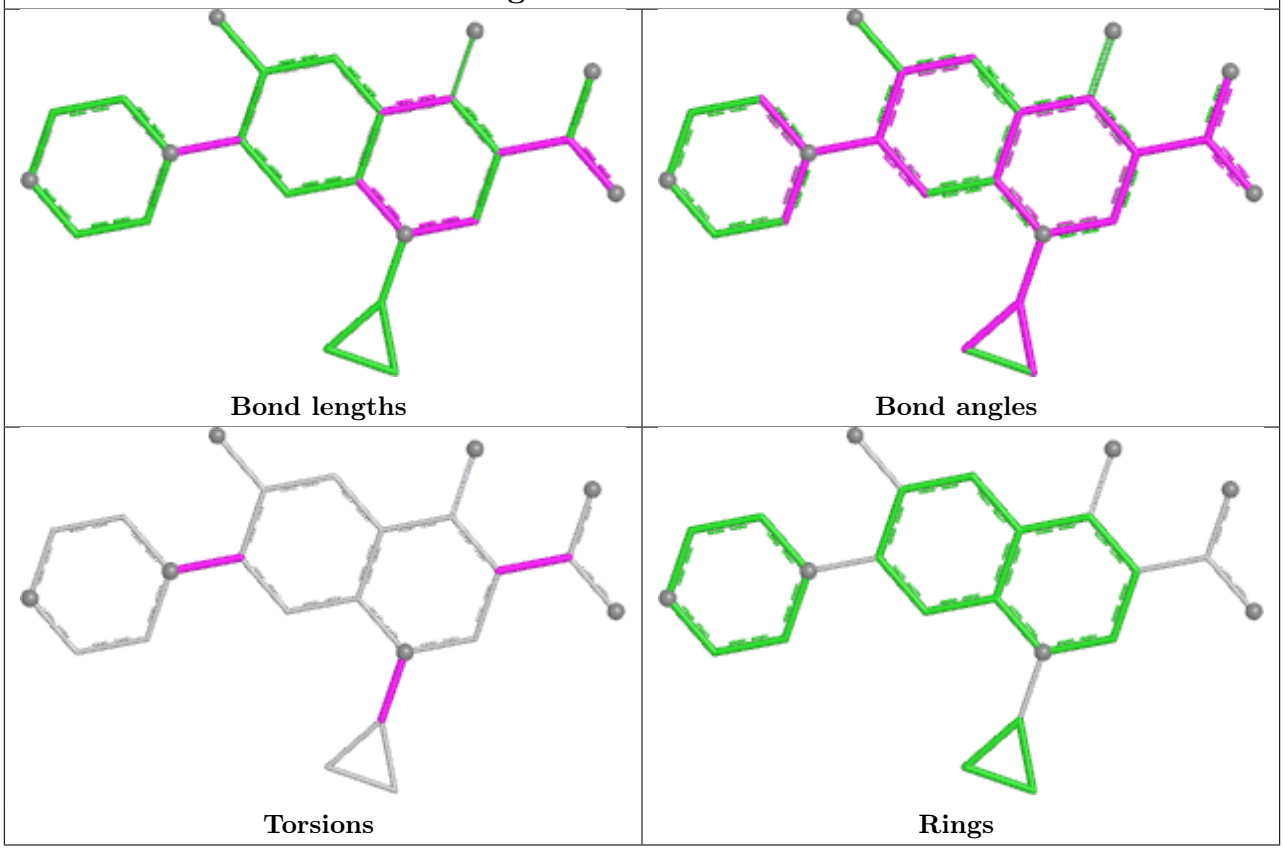
9 monomers are involved in 15 short contacts:

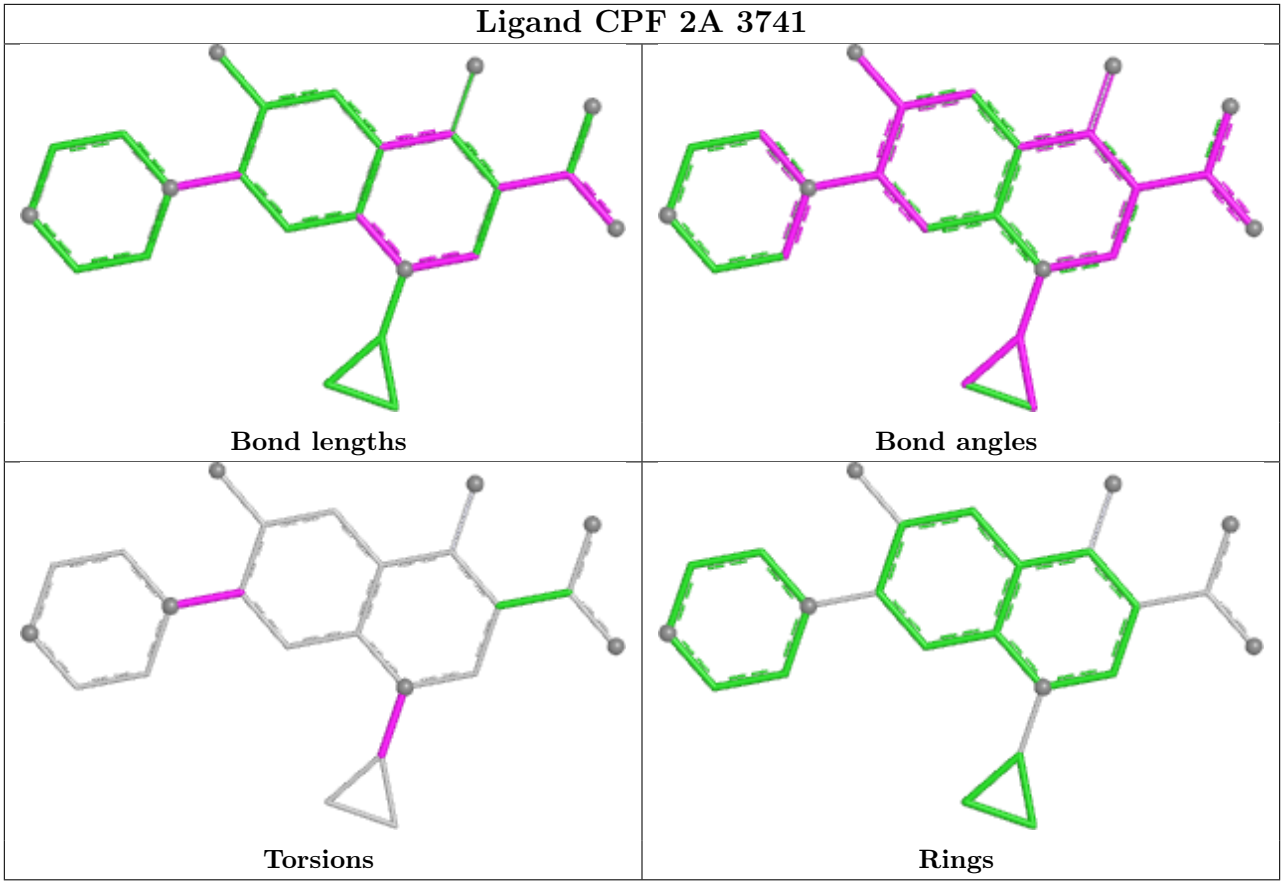
Mol	Chain	Res	Type	Clashes	Symm-Clashes
55	1A	4056	CPF	1	0
56	1a	1878	MPD	4	0
56	18	104	MPD	1	0
56	1O	202	MPD	1	0
56	2A	3743	MPD	1	0
55	2A	3741	CPF	3	0
57	1F	320	ARG	2	0
57	1B	230	ARG	1	0
56	1A	4058	MPD	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand CPF 1A 4056





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%)	-0.39	154 (5%)	31	26	24, 40, 97, 109	0
1	2A	2856/2915 (97%)	0.06	181 (6%)	26	20	31, 57, 100, 110	0
2	1B	120/121 (99%)	-0.17	2 (1%)	69	64	38, 56, 70, 88	0
2	2B	120/121 (99%)	0.81	6 (5%)	34	28	62, 82, 89, 98	0
3	1D	275/276 (99%)	-0.11	4 (1%)	72	68	25, 39, 55, 76	0
3	2D	275/276 (99%)	0.16	2 (0%)	84	82	32, 50, 63, 78	0
4	1E	204/206 (99%)	-0.07	3 (1%)	72	68	23, 42, 64, 78	0
4	2E	204/206 (99%)	0.18	3 (1%)	72	68	36, 57, 73, 81	0
5	1F	203/210 (96%)	-0.01	2 (0%)	79	76	22, 45, 71, 89	0
5	2F	203/210 (96%)	0.38	1 (0%)	87	85	35, 64, 79, 89	0
6	1G	181/182 (99%)	0.69	13 (7%)	21	17	53, 70, 82, 91	0
6	2G	181/182 (99%)	1.55	45 (24%)	2	1	77, 87, 94, 98	0
7	1H	174/180 (96%)	0.33	7 (4%)	42	37	41, 56, 69, 74	0
7	2H	173/180 (96%)	1.42	32 (18%)	3	3	72, 84, 90, 95	0
8	1I	147/148 (99%)	0.85	10 (6%)	23	19	45, 71, 83, 86	0
8	2I	146/148 (98%)	0.86	5 (3%)	48	42	53, 75, 86, 91	0
9	1N	140/140 (100%)	-0.13	1 (0%)	84	82	30, 43, 64, 79	0
9	2N	140/140 (100%)	0.48	3 (2%)	63	58	48, 64, 78, 86	0
10	1O	122/122 (100%)	-0.11	0	100	100	31, 43, 62, 68	0
10	2O	122/122 (100%)	0.12	0	100	100	46, 55, 68, 75	0
11	1P	149/150 (99%)	-0.00	1 (0%)	84	82	24, 48, 68, 81	0
11	2P	149/150 (99%)	0.52	2 (1%)	75	71	39, 66, 83, 88	0
12	1Q	141/141 (100%)	-0.16	0	100	100	31, 43, 57, 71	0
12	2Q	141/141 (100%)	0.69	6 (4%)	40	34	47, 65, 76, 83	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
13	1R	118/118 (100%)	-0.15	0	100	100	29, 41, 55, 63	0
13	2R	118/118 (100%)	0.19	0	100	100	40, 54, 64, 70	0
14	1S	110/112 (98%)	0.27	1 (0%)	81	78	43, 55, 67, 72	0
14	2S	110/112 (98%)	1.29	21 (19%)	3	2	67, 76, 82, 89	0
15	1T	131/146 (89%)	0.09	5 (3%)	44	38	38, 47, 70, 81	0
15	2T	131/146 (89%)	0.37	2 (1%)	72	68	47, 59, 76, 86	0
16	1U	116/118 (98%)	-0.29	0	100	100	28, 35, 49, 65	0
16	2U	116/118 (98%)	0.36	0	100	100	42, 59, 72, 80	0
17	1V	101/101 (100%)	-0.17	0	100	100	27, 46, 63, 71	0
17	2V	101/101 (100%)	0.71	3 (2%)	52	47	41, 69, 77, 84	0
18	1W	112/113 (99%)	-0.18	2 (1%)	67	63	28, 36, 54, 84	0
18	2W	112/113 (99%)	0.13	2 (1%)	67	63	41, 50, 66, 91	0
19	1X	95/96 (98%)	-0.00	2 (2%)	63	58	31, 42, 66, 77	0
19	2X	95/96 (98%)	0.53	6 (6%)	26	20	45, 60, 77, 86	0
20	1Y	107/110 (97%)	0.18	1 (0%)	81	78	37, 51, 68, 78	0
20	2Y	107/110 (97%)	0.93	6 (5%)	30	24	59, 70, 79, 90	0
21	1Z	203/206 (98%)	0.42	4 (1%)	65	60	44, 62, 75, 86	0
21	2Z	201/206 (97%)	1.14	17 (8%)	16	13	68, 79, 85, 92	0
22	10	77/85 (90%)	0.08	1 (1%)	75	71	32, 41, 60, 65	0
22	20	77/85 (90%)	0.80	6 (7%)	19	15	50, 65, 74, 77	0
23	11	97/98 (98%)	0.14	1 (1%)	79	76	32, 45, 69, 75	0
23	21	97/98 (98%)	0.55	5 (5%)	33	27	41, 55, 76, 80	0
24	12	70/72 (97%)	0.18	1 (1%)	73	69	40, 51, 62, 83	0
24	22	70/72 (97%)	0.65	1 (1%)	73	69	61, 70, 77, 79	0
25	13	59/60 (98%)	-0.09	0	100	100	31, 42, 66, 72	0
25	23	59/60 (98%)	0.47	3 (5%)	33	28	51, 62, 80, 84	0
26	14	69/71 (97%)	1.32	20 (28%)	1	1	64, 83, 95, 98	0
26	24	69/71 (97%)	1.93	25 (36%)	1	0	85, 92, 99, 103	0
27	15	59/60 (98%)	-0.15	1 (1%)	69	64	26, 40, 63, 74	0
27	25	59/60 (98%)	0.10	0	100	100	35, 52, 69, 79	0
28	16	53/54 (98%)	-0.21	0	100	100	38, 46, 60, 64	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
28	26	53/54 (98%)	0.52	0 100 100	53, 62, 71, 74	0
29	17	48/49 (97%)	-0.11	4 (8%) 17 13	25, 32, 61, 66	0
29	27	48/49 (97%)	0.14	5 (10%) 11 9	34, 41, 69, 77	0
30	18	64/65 (98%)	-0.23	1 (1%) 70 66	29, 37, 46, 54	0
30	28	64/65 (98%)	0.43	2 (3%) 51 45	48, 56, 63, 72	0
31	19	37/37 (100%)	0.05	1 (2%) 56 50	35, 45, 60, 63	0
31	29	37/37 (100%)	1.18	3 (8%) 18 14	61, 70, 79, 81	0
32	1a	1488/1521 (97%)	0.45	66 (4%) 39 33	39, 73, 96, 110	0
32	2a	1492/1521 (98%)	0.71	115 (7%) 19 15	47, 77, 98, 109	0
33	1b	231/256 (90%)	1.39	53 (22%) 2 2	69, 81, 90, 96	0
33	2b	231/256 (90%)	1.62	68 (29%) 1 1	74, 85, 93, 98	0
34	1c	206/239 (86%)	1.06	21 (10%) 12 9	65, 76, 87, 89	0
34	2c	206/239 (86%)	1.79	68 (33%) 1 1	78, 86, 91, 96	0
35	1d	208/209 (99%)	1.04	21 (10%) 12 9	59, 74, 82, 89	0
35	2d	208/209 (99%)	1.13	24 (11%) 9 7	62, 72, 81, 84	0
36	1e	148/162 (91%)	0.63	4 (2%) 56 50	49, 68, 77, 90	0
36	2e	148/162 (91%)	0.96	8 (5%) 31 26	57, 73, 82, 93	0
37	1f	100/101 (99%)	0.47	2 (2%) 65 60	51, 68, 78, 82	0
37	2f	100/101 (99%)	0.59	0 100 100	56, 69, 78, 84	0
38	1g	155/156 (99%)	0.67	5 (3%) 50 44	68, 75, 83, 90	0
38	2g	155/156 (99%)	1.31	27 (17%) 4 3	76, 84, 89, 92	0
39	1h	137/138 (99%)	0.75	6 (4%) 39 33	58, 70, 78, 80	0
39	2h	137/138 (99%)	0.89	6 (4%) 39 33	62, 74, 81, 83	0
40	1i	127/128 (99%)	1.65	36 (28%) 1 1	66, 81, 87, 89	0
40	2i	126/128 (98%)	2.53	85 (67%) 0 0	77, 88, 93, 94	0
41	1j	97/105 (92%)	1.60	28 (28%) 1 1	65, 81, 90, 94	0
41	2j	96/105 (91%)	2.63	70 (72%) 0 0	79, 89, 93, 97	0
42	1k	114/129 (88%)	0.48	4 (3%) 47 41	46, 66, 76, 81	0
42	2k	114/129 (88%)	0.97	10 (8%) 15 12	60, 73, 82, 86	0
43	1l	121/132 (91%)	0.61	5 (4%) 41 36	51, 62, 73, 79	0
43	2l	121/132 (91%)	0.70	6 (4%) 34 28	56, 67, 76, 80	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
44	1m	116/126 (92%)	1.36	19 (16%)	4	3	68, 79, 84, 90	0
44	2m	114/126 (90%)	1.73	36 (31%)	1	1	80, 88, 93, 95	0
45	1n	60/61 (98%)	1.23	5 (8%)	17	13	67, 76, 83, 86	0
45	2n	60/61 (98%)	2.59	38 (63%)	0	0	80, 87, 93, 97	0
46	1o	88/89 (98%)	0.61	3 (3%)	48	42	47, 69, 80, 82	0
46	2o	88/89 (98%)	0.88	7 (7%)	18	14	58, 73, 81, 86	0
47	1p	82/88 (93%)	1.69	21 (25%)	1	1	62, 74, 83, 88	0
47	2p	82/88 (93%)	1.10	5 (6%)	27	22	62, 70, 80, 83	0
48	1q	99/105 (94%)	1.00	5 (5%)	33	28	57, 71, 80, 84	0
48	2q	99/105 (94%)	0.81	3 (3%)	52	47	55, 72, 79, 82	0
49	1r	68/88 (77%)	0.51	2 (2%)	53	48	58, 67, 80, 86	0
49	2r	68/88 (77%)	0.70	2 (2%)	53	48	62, 71, 82, 84	0
50	1s	83/93 (89%)	1.11	10 (12%)	9	7	71, 81, 87, 90	0
50	2s	83/93 (89%)	2.12	44 (53%)	0	0	79, 91, 95, 96	0
51	1t	96/106 (90%)	1.31	20 (20%)	2	2	64, 75, 86, 90	0
51	2t	98/106 (92%)	0.96	7 (7%)	22	17	60, 73, 84, 87	0
52	1u	23/27 (85%)	1.50	6 (26%)	1	1	72, 77, 81, 81	0
52	2u	23/27 (85%)	2.95	19 (82%)	0	0	80, 86, 89, 90	0
53	1y	97/113 (85%)	0.79	6 (6%)	26	21	59, 69, 78, 84	0
53	2y	96/113 (84%)	1.82	33 (34%)	1	1	73, 83, 88, 91	0
All	All	20766/21468 (96%)	0.45	1664 (8%)	18	14	22, 65, 92, 110	0

The worst 5 of 1664 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1A	1076	C	8.4
45	2n	2	ALA	7.8
41	2j	37	PRO	7.2
7	1H	2	SER	7.1
1	1A	1087	G	6.9

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	0.84	0.11	80,89,96,109	0
1	PSU	2A	1917	20/21	0.86	0.10	78,83,98,100	0
32	2MG	2a	1207	24/25	0.86	0.13	89,94,98,101	0
43	0TD	2l	92	10/11	0.86	0.16	65,71,73,93	0
32	M2G	2a	966	25/26	0.87	0.16	65,72,87,92	0
1	PSU	2A	1911	20/21	0.88	0.09	69,77,90,92	0
1	5MU	1A	1915	21/22	0.88	0.12	73,81,86,90	0
43	0TD	1l	92	10/11	0.89	0.13	56,60,66,80	0
32	5MC	2a	967	21/22	0.89	0.14	71,78,88,88	0
1	PSU	1A	1917	20/21	0.90	0.10	70,75,86,86	0
32	2MG	1a	1207	24/25	0.90	0.12	72,78,83,86	0
1	PSU	1A	1911	20/21	0.92	0.09	63,70,72,72	0
32	PSU	2a	516	20/21	0.93	0.09	79,81,87,87	0
32	5MC	2a	1404	21/22	0.93	0.10	58,64,70,70	0
32	5MC	2a	1407	21/22	0.93	0.11	62,68,74,77	0
32	G7M	2a	527	24/25	0.93	0.12	68,73,75,77	0
1	OMC	2A	1920	21/22	0.94	0.09	63,73,78,82	0
32	5MC	1a	967	21/22	0.94	0.11	66,72,80,82	0
32	UR3	2a	1498	21/22	0.94	0.10	58,65,71,74	0
32	MA6	2a	1518	24/25	0.94	0.12	57,67,73,75	0
32	4OC	2a	1402	22/23	0.94	0.11	61,69,73,74	0
32	M2G	1a	966	25/26	0.95	0.11	60,66,73,78	0
32	5MC	2a	1400	21/22	0.95	0.13	72,76,80,83	0
32	PSU	1a	516	20/21	0.95	0.08	63,68,74,75	0
32	MA6	2a	1519	24/25	0.95	0.12	61,67,71,74	0
32	G7M	1a	527	24/25	0.95	0.11	49,58,62,67	0
32	5MC	1a	1404	21/22	0.96	0.09	51,54,60,64	0
32	5MC	1a	1407	21/22	0.96	0.10	48,56,61,63	0
1	5MC	2A	1942	21/22	0.96	0.08	46,56,60,61	0
32	UR3	1a	1498	21/22	0.96	0.09	48,54,60,70	0
32	MA6	1a	1519	24/25	0.96	0.10	44,52,58,60	0
1	OMC	1A	1920	21/22	0.96	0.10	53,58,63,66	0
32	5MC	1a	1400	21/22	0.96	0.10	53,60,64,67	0
32	4OC	1a	1402	22/23	0.96	0.09	48,57,60,64	0
1	OMG	2A	2251	24/25	0.97	0.09	37,41,44,48	0
1	2MA	2A	2503	23/24	0.97	0.08	30,38,42,44	0
1	OMU	2A	2552	21/22	0.97	0.08	36,42,46,50	0
32	MA6	1a	1518	24/25	0.97	0.10	46,52,57,59	0
1	5MC	1A	1962	21/22	0.97	0.07	29,37,43,45	0
1	2MA	1A	2503	23/24	0.97	0.08	20,28,31,31	0
1	5MC	1A	1942	21/22	0.97	0.08	34,38,42,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	5MC	2A	1962	21/22	0.97	0.09	44,50,54,63	0
1	OMU	1A	2552	21/22	0.98	0.06	27,33,35,38	0
1	PSU	1A	2605	20/21	0.98	0.07	26,30,36,37	0
1	OMG	1A	2251	24/25	0.98	0.06	26,30,33,35	0
1	5MU	2A	1939	21/22	0.98	0.07	36,41,45,46	0
1	PSU	2A	2605	20/21	0.98	0.07	35,41,44,44	0
1	5MU	1A	1939	21/22	0.98	0.07	26,32,36,37	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
54	MG	1A	3986	1/1	0.48	0.27	43,43,43,43	0
54	MG	2a	3041	1/1	0.59	0.24	86,86,86,86	0
54	MG	1a	1743	1/1	0.60	0.21	87,87,87,87	0
54	MG	1a	1836	1/1	0.60	0.20	84,84,84,84	0
54	MG	2A	3380	1/1	0.60	0.23	59,59,59,59	0
54	MG	1A	3872	1/1	0.60	0.20	75,75,75,75	0
54	MG	1A	3213	1/1	0.62	0.26	73,73,73,73	0
54	MG	2A	3208	1/1	0.63	0.28	77,77,77,77	0
54	MG	2A	3034	1/1	0.65	0.29	87,87,87,87	0
54	MG	1A	3581	1/1	0.65	0.20	53,53,53,53	0
54	MG	2A	3343	1/1	0.65	0.25	85,85,85,85	0
54	MG	1a	1676	1/1	0.65	0.20	85,85,85,85	0
54	MG	2G	202	1/1	0.65	0.23	80,80,80,80	0
54	MG	1a	1874	1/1	0.65	0.39	84,84,84,84	0
54	MG	2A	3116	1/1	0.66	0.21	82,82,82,82	0
54	MG	1G	202	1/1	0.67	0.20	71,71,71,71	0
54	MG	1a	1855	1/1	0.67	0.25	86,86,86,86	0
54	MG	2A	3461	1/1	0.67	0.25	72,72,72,72	0
54	MG	1a	1796	1/1	0.67	0.21	86,86,86,86	0
54	MG	2A	3235	1/1	0.67	0.24	83,83,83,83	0
54	MG	2A	3604	1/1	0.68	0.19	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3835	1/1	0.68	0.17	63,63,63,63	0
54	MG	2A	3579	1/1	0.68	0.18	62,62,62,62	0
54	MG	2a	3097	1/1	0.68	0.36	86,86,86,86	0
54	MG	2a	3174	1/1	0.68	0.20	86,86,86,86	0
54	MG	2A	3421	1/1	0.69	0.16	69,69,69,69	0
54	MG	1A	3781	1/1	0.69	0.18	33,33,33,33	0
54	MG	14	101	1/1	0.69	0.14	81,81,81,81	0
54	MG	1A	3812	1/1	0.69	0.17	78,78,78,78	0
54	MG	2A	3736	1/1	0.69	0.24	86,86,86,86	0
54	MG	1A	3261	1/1	0.69	0.30	86,86,86,86	0
54	MG	1A	3641	1/1	0.69	0.41	48,48,48,48	0
54	MG	1A	3983	1/1	0.69	0.18	81,81,81,81	0
54	MG	1A	3699	1/1	0.69	0.22	73,73,73,73	0
54	MG	1a	1795	1/1	0.70	0.16	84,84,84,84	0
54	MG	1A	3849	1/1	0.70	0.18	71,71,71,71	0
54	MG	2A	3610	1/1	0.70	0.17	82,82,82,82	0
54	MG	1a	1865	1/1	0.70	0.20	76,76,76,76	0
56	MPD	1O	202	8/8	0.70	0.24	67,75,81,81	0
54	MG	1A	3756	1/1	0.71	0.23	67,67,67,67	0
54	MG	1A	3891	1/1	0.71	0.23	60,60,60,60	0
54	MG	1a	1818	1/1	0.71	0.24	86,86,86,86	0
54	MG	1a	1754	1/1	0.71	0.20	90,90,90,90	0
54	MG	2a	3194	1/1	0.71	0.20	86,86,86,86	0
54	MG	1a	1837	1/1	0.71	0.22	89,89,89,89	0
54	MG	1A	3796	1/1	0.72	0.31	74,74,74,74	0
54	MG	2A	3364	1/1	0.72	0.21	84,84,84,84	0
54	MG	1A	3924	1/1	0.72	0.20	37,37,37,37	0
54	MG	1a	1671	1/1	0.72	0.17	73,73,73,73	0
54	MG	1a	1765	1/1	0.72	0.20	81,81,81,81	0
54	MG	2a	3062	1/1	0.73	0.21	85,85,85,85	0
54	MG	2a	3092	1/1	0.73	0.15	80,80,80,80	0
54	MG	1a	1794	1/1	0.73	0.44	92,92,92,92	0
54	MG	2A	3420	1/1	0.73	0.28	76,76,76,76	0
54	MG	2a	3002	1/1	0.73	0.19	81,81,81,81	0
54	MG	2j	201	1/1	0.73	0.13	82,82,82,82	0
54	MG	2A	3525	1/1	0.73	0.16	63,63,63,63	0
54	MG	1g	202	1/1	0.74	0.14	73,73,73,73	0
54	MG	2B	201	1/1	0.74	0.15	85,85,85,85	0
54	MG	1A	3686	1/1	0.74	0.15	77,77,77,77	0
54	MG	2O	202	1/1	0.74	0.19	80,80,80,80	0
54	MG	1A	3930	1/1	0.74	0.21	63,63,63,63	0
54	MG	2a	3016	1/1	0.74	0.18	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3441	1/1	0.74	0.19	67,67,67,67	0
54	MG	1A	4034	1/1	0.74	0.28	59,59,59,59	0
54	MG	2A	3507	1/1	0.74	0.20	42,42,42,42	0
54	MG	1a	1675	1/1	0.74	0.31	84,84,84,84	0
54	MG	2A	3558	1/1	0.74	0.17	45,45,45,45	0
54	MG	2A	3266	1/1	0.74	0.35	74,74,74,74	0
54	MG	1A	4040	1/1	0.74	0.20	63,63,63,63	0
54	MG	1a	1684	1/1	0.74	0.36	78,78,78,78	0
54	MG	1a	1857	1/1	0.75	0.25	81,81,81,81	0
54	MG	1A	3703	1/1	0.75	0.24	59,59,59,59	0
54	MG	2A	3729	1/1	0.75	0.33	82,82,82,82	0
54	MG	1A	4037	1/1	0.75	0.27	71,71,71,71	0
54	MG	2A	3409	1/1	0.75	0.40	84,84,84,84	0
54	MG	1A	3860	1/1	0.75	0.18	85,85,85,85	0
54	MG	1a	1808	1/1	0.75	0.17	92,92,92,92	0
54	MG	1A	3964	1/1	0.75	0.25	66,66,66,66	0
54	MG	2A	3460	1/1	0.75	0.22	64,64,64,64	0
54	MG	2A	3193	1/1	0.75	0.20	68,68,68,68	0
54	MG	2A	3474	1/1	0.75	0.19	58,58,58,58	0
54	MG	1A	3362	1/1	0.75	0.18	70,70,70,70	0
54	MG	1a	1761	1/1	0.75	0.20	70,70,70,70	0
54	MG	2A	3540	1/1	0.75	0.17	85,85,85,85	0
54	MG	1A	3520	1/1	0.75	0.14	61,61,61,61	0
54	MG	2A	3561	1/1	0.75	0.24	54,54,54,54	0
54	MG	2A	3300	1/1	0.75	0.21	71,71,71,71	0
56	MPD	2B	219	8/8	0.75	0.30	66,74,79,84	0
54	MG	1A	3531	1/1	0.76	0.23	68,68,68,68	0
54	MG	1A	3996	1/1	0.76	0.43	62,62,62,62	0
54	MG	1a	1860	1/1	0.76	0.17	79,79,79,79	0
54	MG	15	105	1/1	0.76	0.17	56,56,56,56	0
54	MG	15	107	1/1	0.76	0.19	77,77,77,77	0
54	MG	2A	3433	1/1	0.76	0.20	62,62,62,62	0
54	MG	1A	3565	1/1	0.76	0.26	63,63,63,63	0
54	MG	1A	3511	1/1	0.76	0.22	54,54,54,54	0
54	MG	2a	3040	1/1	0.76	0.37	78,78,78,78	0
54	MG	1a	1800	1/1	0.76	0.23	71,71,71,71	0
54	MG	2a	3052	1/1	0.76	0.32	87,87,87,87	0
54	MG	2A	3185	1/1	0.76	0.31	86,86,86,86	0
54	MG	1a	1802	1/1	0.76	0.25	90,90,90,90	0
54	MG	1A	3483	1/1	0.76	0.14	31,31,31,31	0
54	MG	1B	220	1/1	0.76	0.18	50,50,50,50	0
54	MG	1a	1826	1/1	0.76	0.20	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3272	1/1	0.76	0.26	76,76,76,76	0
54	MG	1a	1690	1/1	0.76	0.30	73,73,73,73	0
54	MG	1E	306	1/1	0.76	0.30	70,70,70,70	0
54	MG	2A	3299	1/1	0.77	0.26	70,70,70,70	0
54	MG	2G	201	1/1	0.77	0.14	84,84,84,84	0
54	MG	1a	1828	1/1	0.77	0.21	84,84,84,84	0
54	MG	2A	3493	1/1	0.77	0.21	73,73,73,73	0
54	MG	1A	3984	1/1	0.77	0.20	65,65,65,65	0
54	MG	2A	3509	1/1	0.77	0.23	65,65,65,65	0
54	MG	2a	3035	1/1	0.77	0.30	72,72,72,72	0
54	MG	2A	3053	1/1	0.77	0.28	77,77,77,77	0
54	MG	1B	217	1/1	0.77	0.17	67,67,67,67	0
54	MG	1A	3437	1/1	0.77	0.20	59,59,59,59	0
54	MG	1A	3677	1/1	0.77	0.21	67,67,67,67	0
54	MG	1A	3683	1/1	0.77	0.16	68,68,68,68	0
54	MG	2A	3584	1/1	0.77	0.23	69,69,69,69	0
54	MG	2a	3156	1/1	0.77	0.21	73,73,73,73	0
54	MG	2a	3173	1/1	0.77	0.21	83,83,83,83	0
54	MG	2A	3426	1/1	0.77	0.23	59,59,59,59	0
54	MG	1a	1783	1/1	0.77	0.18	80,80,80,80	0
54	MG	2f	202	1/1	0.77	0.13	69,69,69,69	0
54	MG	2A	3698	1/1	0.77	0.26	62,62,62,62	0
54	MG	1a	1866	1/1	0.77	0.18	80,80,80,80	0
54	MG	1A	3892	1/1	0.77	0.18	59,59,59,59	0
54	MG	2A	3276	1/1	0.78	0.20	87,87,87,87	0
54	MG	2B	214	1/1	0.78	0.15	70,70,70,70	0
54	MG	1a	1820	1/1	0.78	0.19	68,68,68,68	0
54	MG	2A	3489	1/1	0.78	0.20	72,72,72,72	0
54	MG	1a	1825	1/1	0.78	0.18	51,51,51,51	0
54	MG	1a	1777	1/1	0.78	0.18	82,82,82,82	0
54	MG	2A	3345	1/1	0.78	0.16	80,80,80,80	0
54	MG	2a	3019	1/1	0.78	0.18	78,78,78,78	0
54	MG	2A	3515	1/1	0.78	0.26	75,75,75,75	0
54	MG	1A	3878	1/1	0.78	0.22	40,40,40,40	0
54	MG	1A	3624	1/1	0.78	0.20	34,34,34,34	0
54	MG	2a	3049	1/1	0.78	0.26	84,84,84,84	0
54	MG	2A	3153	1/1	0.78	0.14	71,71,71,71	0
54	MG	2A	3410	1/1	0.78	0.23	71,71,71,71	0
54	MG	2a	3074	1/1	0.78	0.24	70,70,70,70	0
54	MG	2a	3077	1/1	0.78	0.21	75,75,75,75	0
54	MG	1a	1715	1/1	0.78	0.22	86,86,86,86	0
54	MG	1A	4017	1/1	0.78	0.24	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2a	3149	1/1	0.78	0.21	71,71,71,71	0
54	MG	2A	3598	1/1	0.78	0.24	62,62,62,62	0
54	MG	1A	3505	1/1	0.78	0.15	63,63,63,63	0
54	MG	1A	3357	1/1	0.78	0.14	49,49,49,49	0
54	MG	2A	3614	1/1	0.78	0.13	71,71,71,71	0
54	MG	1T	204	1/1	0.78	0.11	81,81,81,81	0
54	MG	2A	3707	1/1	0.78	0.36	56,56,56,56	0
54	MG	2A	3442	1/1	0.78	0.13	69,69,69,69	0
54	MG	1a	1771	1/1	0.78	0.18	77,77,77,77	0
57	ARG	1F	320	12/12	0.78	0.20	58,76,81,84	0
54	MG	2A	3400	1/1	0.79	0.17	83,83,83,83	0
54	MG	1a	1641	1/1	0.79	0.25	81,81,81,81	0
54	MG	1a	1833	1/1	0.79	0.27	72,72,72,72	0
54	MG	2a	3038	1/1	0.79	0.18	89,89,89,89	0
54	MG	1A	3910	1/1	0.79	0.15	27,27,27,27	0
54	MG	1A	3611	1/1	0.79	0.16	72,72,72,72	0
54	MG	1A	3441	1/1	0.79	0.22	71,71,71,71	0
54	MG	1A	3284	1/1	0.79	0.21	77,77,77,77	0
54	MG	1A	3859	1/1	0.79	0.17	34,34,34,34	0
54	MG	2A	3270	1/1	0.79	0.30	83,83,83,83	0
54	MG	2A	3657	1/1	0.79	0.17	45,45,45,45	0
54	MG	2a	3079	1/1	0.79	0.56	85,85,85,85	0
54	MG	2A	3693	1/1	0.79	0.27	60,60,60,60	0
54	MG	1a	1863	1/1	0.79	0.16	78,78,78,78	0
54	MG	1A	3704	1/1	0.79	0.22	53,53,53,53	0
54	MG	1A	3738	1/1	0.79	0.12	54,54,54,54	0
54	MG	2a	3160	1/1	0.79	0.47	82,82,82,82	0
54	MG	1A	3646	1/1	0.79	0.15	78,78,78,78	0
54	MG	1A	3497	1/1	0.79	0.18	48,48,48,48	0
54	MG	1A	3591	1/1	0.79	0.19	53,53,53,53	0
54	MG	2A	3052	1/1	0.79	0.28	72,72,72,72	0
54	MG	2A	3368	1/1	0.79	0.23	79,79,79,79	0
54	MG	2A	3524	1/1	0.79	0.16	85,85,85,85	0
54	MG	21	101	1/1	0.79	0.33	84,84,84,84	0
54	MG	19	102	1/1	0.79	0.17	79,79,79,79	0
54	MG	2A	3557	1/1	0.80	0.20	43,43,43,43	0
54	MG	2A	3190	1/1	0.80	0.43	75,75,75,75	0
54	MG	1a	1780	1/1	0.80	0.21	85,85,85,85	0
54	MG	2A	3565	1/1	0.80	0.20	72,72,72,72	0
54	MG	1a	1655	1/1	0.80	0.12	76,76,76,76	0
54	MG	1A	3870	1/1	0.80	0.14	46,46,46,46	0
54	MG	1A	3305	1/1	0.80	0.16	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3600	1/1	0.80	0.15	44,44,44,44	0
54	MG	1A	3456	1/1	0.80	0.19	64,64,64,64	0
54	MG	2a	3050	1/1	0.80	0.28	69,69,69,69	0
54	MG	2A	3606	1/1	0.80	0.20	62,62,62,62	0
54	MG	1D	309	1/1	0.80	0.40	57,57,57,57	0
54	MG	2A	3611	1/1	0.80	0.20	37,37,37,37	0
54	MG	2A	3273	1/1	0.80	0.21	61,61,61,61	0
54	MG	2A	3618	1/1	0.80	0.09	88,88,88,88	0
54	MG	1A	3888	1/1	0.80	0.12	38,38,38,38	0
54	MG	1A	3480	1/1	0.80	0.13	25,25,25,25	0
54	MG	1A	3379	1/1	0.80	0.18	74,74,74,74	0
54	MG	1a	1746	1/1	0.80	0.17	80,80,80,80	0
54	MG	2A	3501	1/1	0.80	0.12	85,85,85,85	0
54	MG	1A	3909	1/1	0.80	0.12	19,19,19,19	0
54	MG	1A	4026	1/1	0.80	0.17	56,56,56,56	0
54	MG	2B	202	1/1	0.80	0.13	82,82,82,82	0
54	MG	2B	213	1/1	0.80	0.19	78,78,78,78	0
54	MG	2A	3093	1/1	0.80	0.18	76,76,76,76	0
54	MG	1A	4033	1/1	0.80	0.22	75,75,75,75	0
54	MG	1A	3188	1/1	0.80	0.17	68,68,68,68	0
54	MG	1A	3790	1/1	0.80	0.24	61,61,61,61	0
54	MG	1a	1867	1/1	0.81	0.27	73,73,73,73	0
54	MG	1a	1694	1/1	0.81	0.17	69,69,69,69	0
54	MG	1d	305	1/1	0.81	0.12	94,94,94,94	0
54	MG	1A	3537	1/1	0.81	0.15	51,51,51,51	0
54	MG	1a	1726	1/1	0.81	0.12	82,82,82,82	0
54	MG	2A	3366	1/1	0.81	0.14	43,43,43,43	0
54	MG	1a	1813	1/1	0.81	0.19	69,69,69,69	0
54	MG	2A	3379	1/1	0.81	0.20	58,58,58,58	0
54	MG	1a	1735	1/1	0.81	0.22	70,70,70,70	0
54	MG	2A	3072	1/1	0.81	0.23	70,70,70,70	0
54	MG	2A	3089	1/1	0.81	0.22	70,70,70,70	0
54	MG	2A	3090	1/1	0.81	0.16	72,72,72,72	0
54	MG	1A	3235	1/1	0.81	0.17	79,79,79,79	0
54	MG	1A	3364	1/1	0.81	0.12	48,48,48,48	0
54	MG	1A	3585	1/1	0.81	0.25	45,45,45,45	0
54	MG	1a	1611	1/1	0.81	0.27	69,69,69,69	0
54	MG	1A	3516	1/1	0.81	0.14	29,29,29,29	0
54	MG	1A	3367	1/1	0.81	0.13	26,26,26,26	0
54	MG	2A	3443	1/1	0.81	0.27	61,61,61,61	0
54	MG	2A	3677	1/1	0.81	0.24	74,74,74,74	0
54	MG	1A	3840	1/1	0.81	0.12	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3450	1/1	0.81	0.19	74,74,74,74	0
54	MG	2A	3253	1/1	0.81	0.21	72,72,72,72	0
54	MG	2A	3486	1/1	0.81	0.23	70,70,70,70	0
54	MG	1a	1781	1/1	0.81	0.14	90,90,90,90	0
54	MG	1A	4024	1/1	0.81	0.16	65,65,65,65	0
54	MG	2A	3499	1/1	0.81	0.12	78,78,78,78	0
54	MG	2n	101	1/1	0.81	0.32	81,81,81,81	0
54	MG	1A	3534	1/1	0.81	0.15	55,55,55,55	0
54	MG	1a	1689	1/1	0.81	0.26	70,70,70,70	0
54	MG	10	106	1/1	0.81	0.11	60,60,60,60	0
54	MG	2E	304	1/1	0.82	0.17	41,41,41,41	0
54	MG	1A	3320	1/1	0.82	0.29	77,77,77,77	0
54	MG	2A	3538	1/1	0.82	0.12	58,58,58,58	0
54	MG	1a	1696	1/1	0.82	0.23	66,66,66,66	0
54	MG	1A	3471	1/1	0.82	0.16	58,58,58,58	0
54	MG	1A	4044	1/1	0.82	0.39	46,46,46,46	0
54	MG	1B	205	1/1	0.82	0.10	59,59,59,59	0
54	MG	1A	3642	1/1	0.82	0.17	67,67,67,67	0
54	MG	2a	3031	1/1	0.82	0.11	80,80,80,80	0
54	MG	2A	3416	1/1	0.82	0.18	58,58,58,58	0
54	MG	1A	3555	1/1	0.82	0.12	44,44,44,44	0
54	MG	2A	3250	1/1	0.82	0.27	73,73,73,73	0
54	MG	1a	1749	1/1	0.82	0.11	61,61,61,61	0
54	MG	1A	3671	1/1	0.82	0.14	65,65,65,65	0
54	MG	1D	318	1/1	0.82	0.19	59,59,59,59	0
54	MG	2A	3608	1/1	0.82	0.26	84,84,84,84	0
54	MG	1a	1764	1/1	0.82	0.14	82,82,82,82	0
54	MG	2a	3064	1/1	0.82	0.35	78,78,78,78	0
54	MG	2A	3036	1/1	0.82	0.26	78,78,78,78	0
54	MG	2A	3046	1/1	0.82	0.14	65,65,65,65	0
54	MG	2A	3297	1/1	0.82	0.13	49,49,49,49	0
54	MG	1A	3489	1/1	0.82	0.11	26,26,26,26	0
54	MG	2A	3675	1/1	0.82	0.12	60,60,60,60	0
54	MG	2a	3119	1/1	0.82	0.18	86,86,86,86	0
54	MG	2A	3477	1/1	0.82	0.14	75,75,75,75	0
54	MG	2A	3684	1/1	0.82	0.15	51,51,51,51	0
54	MG	1A	3940	1/1	0.82	0.18	54,54,54,54	0
54	MG	2A	3301	1/1	0.82	0.14	60,60,60,60	0
54	MG	2A	3333	1/1	0.82	0.24	62,62,62,62	0
54	MG	2A	3339	1/1	0.82	0.13	37,37,37,37	0
54	MG	2a	3195	1/1	0.82	0.18	81,81,81,81	0
54	MG	1Q	204	1/1	0.82	0.18	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3962	1/1	0.82	0.15	53,53,53,53	0
54	MG	2A	3354	1/1	0.82	0.23	78,78,78,78	0
54	MG	1A	3749	1/1	0.82	0.17	68,68,68,68	0
54	MG	1a	1850	1/1	0.82	0.15	66,66,66,66	0
54	MG	2D	308	1/1	0.82	0.20	77,77,77,77	0
54	MG	1A	3389	1/1	0.83	0.12	33,33,33,33	0
54	MG	1A	4000	1/1	0.83	0.20	84,84,84,84	0
54	MG	1A	3785	1/1	0.83	0.13	41,41,41,41	0
54	MG	1A	3688	1/1	0.83	0.26	70,70,70,70	0
54	MG	1A	3435	1/1	0.83	0.13	39,39,39,39	0
54	MG	1A	3900	1/1	0.83	0.13	59,59,59,59	0
54	MG	1A	3543	1/1	0.83	0.17	65,65,65,65	0
54	MG	1a	1774	1/1	0.83	0.18	78,78,78,78	0
54	MG	1A	3833	1/1	0.83	0.24	63,63,63,63	0
54	MG	1A	3667	1/1	0.83	0.14	31,31,31,31	0
54	MG	1a	1657	1/1	0.83	0.41	77,77,77,77	0
54	MG	1a	1871	1/1	0.83	0.18	78,78,78,78	0
54	MG	1a	1669	1/1	0.83	0.32	66,66,66,66	0
54	MG	1A	3722	1/1	0.83	0.12	40,40,40,40	0
54	MG	1A	4047	1/1	0.83	0.14	55,55,55,55	0
54	MG	2A	3316	1/1	0.83	0.14	53,53,53,53	0
54	MG	2A	3328	1/1	0.83	0.13	50,50,50,50	0
54	MG	1i	201	1/1	0.83	0.20	77,77,77,77	0
54	MG	2A	3012	1/1	0.83	0.20	68,68,68,68	0
54	MG	2a	3039	1/1	0.83	0.25	70,70,70,70	0
54	MG	1A	4051	1/1	0.83	0.27	49,49,49,49	0
54	MG	1a	1799	1/1	0.83	0.15	67,67,67,67	0
54	MG	2A	3350	1/1	0.83	0.22	55,55,55,55	0
54	MG	1A	4057	1/1	0.83	0.16	44,44,44,44	0
54	MG	2A	3570	1/1	0.83	0.13	56,56,56,56	0
54	MG	2a	3054	1/1	0.83	0.26	83,83,83,83	0
54	MG	1a	1801	1/1	0.83	0.19	71,71,71,71	0
54	MG	1A	3735	1/1	0.83	0.13	63,63,63,63	0
54	MG	1A	3593	1/1	0.83	0.18	66,66,66,66	0
54	MG	2A	3086	1/1	0.83	0.31	80,80,80,80	0
54	MG	1A	3216	1/1	0.83	0.29	50,50,50,50	0
54	MG	2A	3384	1/1	0.83	0.16	60,60,60,60	0
54	MG	1A	3975	1/1	0.83	0.18	56,56,56,56	0
54	MG	2A	3405	1/1	0.83	0.13	49,49,49,49	0
54	MG	2a	3142	1/1	0.83	0.17	66,66,66,66	0
54	MG	1A	3282	1/1	0.83	0.08	84,84,84,84	0
54	MG	2A	3109	1/1	0.83	0.09	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3615	1/1	0.83	0.20	71,71,71,71	0
54	MG	1A	3778	1/1	0.83	0.13	28,28,28,28	0
54	MG	2A	3619	1/1	0.83	0.34	53,53,53,53	0
54	MG	1A	3874	1/1	0.83	0.13	53,53,53,53	0
54	MG	2A	3162	1/1	0.83	0.17	68,68,68,68	0
54	MG	2A	3182	1/1	0.83	0.20	60,60,60,60	0
54	MG	2A	3681	1/1	0.83	0.12	78,78,78,78	0
54	MG	2A	3683	1/1	0.83	0.16	78,78,78,78	0
54	MG	2A	3429	1/1	0.83	0.22	43,43,43,43	0
54	MG	1A	3988	1/1	0.83	0.09	75,75,75,75	0
54	MG	2A	3440	1/1	0.83	0.14	68,68,68,68	0
54	MG	1A	4008	1/1	0.84	0.16	49,49,49,49	0
54	MG	1A	3782	1/1	0.84	0.15	45,45,45,45	0
54	MG	2A	3503	1/1	0.84	0.18	73,73,73,73	0
54	MG	2A	3042	1/1	0.84	0.31	81,81,81,81	0
54	MG	10	105	1/1	0.84	0.14	57,57,57,57	0
54	MG	1a	1741	1/1	0.84	0.25	68,68,68,68	0
54	MG	2A	3517	1/1	0.84	0.18	70,70,70,70	0
54	MG	2G	203	1/1	0.84	0.17	78,78,78,78	0
54	MG	2A	3521	1/1	0.84	0.16	74,74,74,74	0
54	MG	1a	1821	1/1	0.84	0.14	78,78,78,78	0
54	MG	2A	3061	1/1	0.84	0.27	61,61,61,61	0
54	MG	1A	3647	1/1	0.84	0.29	68,68,68,68	0
54	MG	1A	3662	1/1	0.84	0.12	45,45,45,45	0
54	MG	1a	1827	1/1	0.84	0.18	86,86,86,86	0
54	MG	1A	3182	1/1	0.84	0.19	76,76,76,76	0
54	MG	1A	3803	1/1	0.84	0.22	63,63,63,63	0
54	MG	2A	3098	1/1	0.84	0.26	67,67,67,67	0
54	MG	1A	3719	1/1	0.84	0.13	74,74,74,74	0
54	MG	2A	3574	1/1	0.84	0.14	60,60,60,60	0
54	MG	2A	3577	1/1	0.84	0.19	59,59,59,59	0
54	MG	1A	3821	1/1	0.84	0.18	77,77,77,77	0
54	MG	2A	3391	1/1	0.84	0.29	75,75,75,75	0
54	MG	1a	1637	1/1	0.84	0.24	72,72,72,72	0
54	MG	1A	3670	1/1	0.84	0.29	37,37,37,37	0
54	MG	2A	3406	1/1	0.84	0.15	66,66,66,66	0
54	MG	1A	3478	1/1	0.84	0.14	32,32,32,32	0
54	MG	1a	1859	1/1	0.84	0.19	78,78,78,78	0
54	MG	1A	3673	1/1	0.84	0.12	65,65,65,65	0
54	MG	1a	1664	1/1	0.84	0.15	83,83,83,83	0
54	MG	2A	3202	1/1	0.84	0.24	74,74,74,74	0
54	MG	1A	3739	1/1	0.84	0.16	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2a	3134	1/1	0.84	0.17	69,69,69,69	0
54	MG	2A	3216	1/1	0.84	0.13	67,67,67,67	0
54	MG	1A	3271	1/1	0.84	0.11	48,48,48,48	0
54	MG	2a	3154	1/1	0.84	0.12	67,67,67,67	0
54	MG	1B	210	1/1	0.84	0.38	84,84,84,84	0
54	MG	1A	3753	1/1	0.84	0.12	27,27,27,27	0
54	MG	1A	3404	1/1	0.84	0.15	30,30,30,30	0
54	MG	1a	1876	1/1	0.84	0.24	74,74,74,74	0
54	MG	2a	3181	1/1	0.84	0.20	78,78,78,78	0
54	MG	2A	3457	1/1	0.84	0.10	84,84,84,84	0
54	MG	1A	3760	1/1	0.84	0.17	63,63,63,63	0
54	MG	1A	3645	1/1	0.84	0.28	49,49,49,49	0
54	MG	2A	3275	1/1	0.84	0.15	59,59,59,59	0
54	MG	1A	3374	1/1	0.84	0.12	67,67,67,67	0
54	MG	1l	202	1/1	0.84	0.18	83,83,83,83	0
54	MG	1A	3882	1/1	0.84	0.11	40,40,40,40	0
54	MG	2A	3024	1/1	0.84	0.20	67,67,67,67	0
54	MG	1a	1699	1/1	0.85	0.13	64,64,64,64	0
54	MG	1a	1712	1/1	0.85	0.14	64,64,64,64	0
54	MG	1P	206	1/1	0.85	0.12	48,48,48,48	0
54	MG	1A	3082	1/1	0.85	0.15	57,57,57,57	0
54	MG	1A	3764	1/1	0.85	0.19	59,59,59,59	0
54	MG	2A	3688	1/1	0.85	0.11	75,75,75,75	0
54	MG	1A	3131	1/1	0.85	0.14	59,59,59,59	0
54	MG	1A	3947	1/1	0.85	0.15	52,52,52,52	0
54	MG	2A	3148	1/1	0.85	0.25	66,66,66,66	0
54	MG	1A	3959	1/1	0.85	0.12	59,59,59,59	0
54	MG	2A	3161	1/1	0.85	0.22	84,84,84,84	0
54	MG	2A	3737	1/1	0.85	0.30	72,72,72,72	0
54	MG	1A	3536	1/1	0.85	0.16	44,44,44,44	0
54	MG	1A	3416	1/1	0.85	0.16	68,68,68,68	0
54	MG	2B	204	1/1	0.85	0.11	75,75,75,75	0
54	MG	2B	207	1/1	0.85	0.16	81,81,81,81	0
54	MG	1a	1755	1/1	0.85	0.22	74,74,74,74	0
54	MG	1A	3967	1/1	0.85	0.18	75,75,75,75	0
54	MG	2B	217	1/1	0.85	0.11	83,83,83,83	0
54	MG	1A	3297	1/1	0.85	0.11	53,53,53,53	0
54	MG	2A	3444	1/1	0.85	0.17	66,66,66,66	0
54	MG	2A	3451	1/1	0.85	0.17	70,70,70,70	0
54	MG	2A	3196	1/1	0.85	0.15	63,63,63,63	0
54	MG	1A	3979	1/1	0.85	0.11	50,50,50,50	0
54	MG	1a	1861	1/1	0.85	0.16	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3210	1/1	0.85	0.15	62,62,62,62	0
54	MG	1a	1766	1/1	0.85	0.25	84,84,84,84	0
54	MG	2A	3227	1/1	0.85	0.14	65,65,65,65	0
54	MG	2A	3229	1/1	0.85	0.21	67,67,67,67	0
54	MG	1a	1638	1/1	0.85	0.41	80,80,80,80	0
54	MG	1A	3202	1/1	0.85	0.18	66,66,66,66	0
54	MG	2a	3037	1/1	0.85	0.21	74,74,74,74	0
54	MG	1a	1775	1/1	0.85	0.12	86,86,86,86	0
54	MG	1a	1870	1/1	0.85	0.29	72,72,72,72	0
54	MG	1a	1654	1/1	0.85	0.14	80,80,80,80	0
54	MG	1A	3370	1/1	0.85	0.11	47,47,47,47	0
54	MG	1A	3157	1/1	0.85	0.35	73,73,73,73	0
54	MG	1A	3376	1/1	0.85	0.10	43,43,43,43	0
54	MG	2a	3051	1/1	0.85	0.30	77,77,77,77	0
54	MG	1a	1787	1/1	0.85	0.15	72,72,72,72	0
54	MG	2A	3277	1/1	0.85	0.14	34,34,34,34	0
54	MG	2a	3056	1/1	0.85	0.23	76,76,76,76	0
54	MG	2a	3058	1/1	0.85	0.23	77,77,77,77	0
54	MG	1h	201	1/1	0.85	0.27	59,59,59,59	0
54	MG	1B	224	1/1	0.85	0.20	72,72,72,72	0
54	MG	1B	226	1/1	0.85	0.11	73,73,73,73	0
54	MG	1n	101	1/1	0.85	0.46	78,78,78,78	0
54	MG	2A	3313	1/1	0.85	0.23	63,63,63,63	0
54	MG	1t	201	1/1	0.85	0.13	74,74,74,74	0
54	MG	2a	3093	1/1	0.85	0.19	76,76,76,76	0
54	MG	1A	3587	1/1	0.85	0.18	64,64,64,64	0
54	MG	2A	3023	1/1	0.85	0.19	69,69,69,69	0
54	MG	1D	315	1/1	0.85	0.17	73,73,73,73	0
54	MG	2A	3028	1/1	0.85	0.15	61,61,61,61	0
54	MG	1A	3519	1/1	0.85	0.12	27,27,27,27	0
54	MG	1E	303	1/1	0.85	0.13	29,29,29,29	0
54	MG	1A	3332	1/1	0.85	0.14	29,29,29,29	0
54	MG	2A	3356	1/1	0.85	0.14	72,72,72,72	0
54	MG	2A	3361	1/1	0.85	0.22	63,63,63,63	0
54	MG	2A	3363	1/1	0.85	0.20	71,71,71,71	0
54	MG	1a	1805	1/1	0.85	0.12	70,70,70,70	0
54	MG	1a	1691	1/1	0.85	0.15	59,59,59,59	0
54	MG	1a	1810	1/1	0.85	0.19	76,76,76,76	0
54	MG	2A	3054	1/1	0.85	0.32	76,76,76,76	0
54	MG	2A	3056	1/1	0.85	0.30	59,59,59,59	0
54	MG	2A	3383	1/1	0.85	0.17	52,52,52,52	0
54	MG	1F	312	1/1	0.85	0.15	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MPD	1a	1878	8/8	0.85	0.15	55,70,73,73	0
56	MPD	2A	3743	8/8	0.85	0.28	46,57,62,63	0
56	MPD	2A	3744	8/8	0.85	0.25	63,68,74,74	0
54	MG	2A	3623	1/1	0.85	0.21	62,62,62,62	0
54	MG	1A	3522	1/1	0.85	0.13	58,58,58,58	0
54	MG	1a	1811	1/1	0.86	0.11	71,71,71,71	0
54	MG	2A	3385	1/1	0.86	0.20	65,65,65,65	0
54	MG	2A	3682	1/1	0.86	0.10	74,74,74,74	0
54	MG	1A	3281	1/1	0.86	0.09	77,77,77,77	0
54	MG	2A	3091	1/1	0.86	0.27	68,68,68,68	0
54	MG	1A	3452	1/1	0.86	0.12	53,53,53,53	0
54	MG	1A	3605	1/1	0.86	0.10	42,42,42,42	0
54	MG	2A	3695	1/1	0.86	0.12	53,53,53,53	0
54	MG	1A	3823	1/1	0.86	0.20	42,42,42,42	0
54	MG	2A	3706	1/1	0.86	0.17	65,65,65,65	0
54	MG	1A	3702	1/1	0.86	0.20	43,43,43,43	0
54	MG	2A	3724	1/1	0.86	0.26	71,71,71,71	0
54	MG	1A	3340	1/1	0.86	0.11	65,65,65,65	0
54	MG	1A	3837	1/1	0.86	0.13	44,44,44,44	0
54	MG	2A	3160	1/1	0.86	0.20	75,75,75,75	0
54	MG	2A	3742	1/1	0.86	0.14	50,50,50,50	0
54	MG	1A	3380	1/1	0.86	0.13	63,63,63,63	0
54	MG	1a	1829	1/1	0.86	0.14	83,83,83,83	0
54	MG	1A	3627	1/1	0.86	0.17	39,39,39,39	0
54	MG	1A	3628	1/1	0.86	0.12	65,65,65,65	0
54	MG	2B	208	1/1	0.86	0.26	66,66,66,66	0
54	MG	2B	209	1/1	0.86	0.19	70,70,70,70	0
54	MG	1E	309	1/1	0.86	0.22	58,58,58,58	0
54	MG	1a	1730	1/1	0.86	0.27	75,75,75,75	0
54	MG	2B	215	1/1	0.86	0.09	75,75,75,75	0
54	MG	1A	3987	1/1	0.86	0.14	53,53,53,53	0
54	MG	1a	1740	1/1	0.86	0.14	65,65,65,65	0
54	MG	2A	3450	1/1	0.86	0.13	70,70,70,70	0
54	MG	2A	3207	1/1	0.86	0.17	74,74,74,74	0
54	MG	2A	3453	1/1	0.86	0.12	74,74,74,74	0
54	MG	1G	201	1/1	0.86	0.11	77,77,77,77	0
54	MG	1A	3636	1/1	0.86	0.18	68,68,68,68	0
54	MG	20	103	1/1	0.86	0.19	72,72,72,72	0
54	MG	1A	3993	1/1	0.86	0.28	52,52,52,52	0
54	MG	1A	3036	1/1	0.86	0.30	62,62,62,62	0
54	MG	2a	3003	1/1	0.86	0.15	70,70,70,70	0
54	MG	1a	1752	1/1	0.86	0.19	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3230	1/1	0.86	0.33	68,68,68,68	0
54	MG	2a	3026	1/1	0.86	0.20	78,78,78,78	0
54	MG	2A	3234	1/1	0.86	0.18	75,75,75,75	0
54	MG	1A	3027	1/1	0.86	0.16	65,65,65,65	0
54	MG	2A	3249	1/1	0.86	0.27	68,68,68,68	0
54	MG	1Z	301	1/1	0.86	0.18	69,69,69,69	0
54	MG	1a	1868	1/1	0.86	0.21	65,65,65,65	0
54	MG	2A	3261	1/1	0.86	0.18	62,62,62,62	0
54	MG	1a	1759	1/1	0.86	0.13	76,76,76,76	0
54	MG	1A	4004	1/1	0.86	0.16	86,86,86,86	0
54	MG	1a	1763	1/1	0.86	0.15	68,68,68,68	0
54	MG	1A	3034	1/1	0.86	0.12	63,63,63,63	0
54	MG	1A	3486	1/1	0.86	0.10	32,32,32,32	0
54	MG	1A	3550	1/1	0.86	0.11	47,47,47,47	0
54	MG	1A	3886	1/1	0.86	0.10	31,31,31,31	0
54	MG	2A	3290	1/1	0.86	0.12	62,62,62,62	0
54	MG	2A	3554	1/1	0.86	0.11	77,77,77,77	0
54	MG	18	101	1/1	0.86	0.21	77,77,77,77	0
54	MG	2a	3072	1/1	0.86	0.16	82,82,82,82	0
54	MG	1A	3654	1/1	0.86	0.14	69,69,69,69	0
54	MG	1A	3554	1/1	0.86	0.24	44,44,44,44	0
54	MG	1a	1778	1/1	0.86	0.20	76,76,76,76	0
54	MG	2A	3567	1/1	0.86	0.15	54,54,54,54	0
54	MG	1a	1630	1/1	0.86	0.23	68,68,68,68	0
54	MG	1a	1632	1/1	0.86	0.08	42,42,42,42	0
54	MG	1a	1635	1/1	0.86	0.37	65,65,65,65	0
54	MG	1A	3768	1/1	0.86	0.20	55,55,55,55	0
54	MG	2A	3031	1/1	0.86	0.19	77,77,77,77	0
54	MG	2a	3145	1/1	0.86	0.11	82,82,82,82	0
54	MG	2A	3595	1/1	0.86	0.12	65,65,65,65	0
54	MG	1a	1791	1/1	0.86	0.18	75,75,75,75	0
54	MG	1A	3426	1/1	0.86	0.15	40,40,40,40	0
54	MG	1A	3434	1/1	0.86	0.20	65,65,65,65	0
54	MG	2a	3164	1/1	0.86	0.11	69,69,69,69	0
54	MG	2A	3043	1/1	0.86	0.15	56,56,56,56	0
54	MG	1A	3576	1/1	0.86	0.18	52,52,52,52	0
54	MG	1A	3189	1/1	0.86	0.13	68,68,68,68	0
54	MG	2a	3186	1/1	0.86	0.23	78,78,78,78	0
54	MG	1A	4053	1/1	0.86	0.13	53,53,53,53	0
54	MG	1a	1659	1/1	0.86	0.23	64,64,64,64	0
54	MG	1A	3142	1/1	0.86	0.14	58,58,58,58	0
54	MG	2A	3059	1/1	0.86	0.17	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3377	1/1	0.86	0.13	58,58,58,58	0
54	MG	2o	101	1/1	0.86	0.16	69,69,69,69	0
54	MG	2A	3622	1/1	0.86	0.14	66,66,66,66	0
54	MG	1B	203	1/1	0.86	0.26	69,69,69,69	0
54	MG	2A	3624	1/1	0.86	0.17	76,76,76,76	0
54	MG	1A	3331	1/1	0.86	0.10	30,30,30,30	0
54	MG	2A	3660	1/1	0.86	0.09	31,31,31,31	0
54	MG	1B	206	1/1	0.86	0.19	64,64,64,64	0
54	MG	1A	3754	1/1	0.87	0.20	48,48,48,48	0
54	MG	1A	3973	1/1	0.87	0.12	44,44,44,44	0
54	MG	2A	3470	1/1	0.87	0.14	84,84,84,84	0
54	MG	1a	1674	1/1	0.87	0.20	76,76,76,76	0
54	MG	1A	3144	1/1	0.87	0.14	69,69,69,69	0
54	MG	1A	3584	1/1	0.87	0.19	53,53,53,53	0
54	MG	1A	3763	1/1	0.87	0.19	65,65,65,65	0
54	MG	1D	314	1/1	0.87	0.11	60,60,60,60	0
54	MG	1A	3124	1/1	0.87	0.14	39,39,39,39	0
54	MG	1A	3873	1/1	0.87	0.10	47,47,47,47	0
54	MG	2A	3502	1/1	0.87	0.14	69,69,69,69	0
54	MG	1A	3548	1/1	0.87	0.10	38,38,38,38	0
54	MG	2A	3298	1/1	0.87	0.16	64,64,64,64	0
54	MG	1A	3875	1/1	0.87	0.13	69,69,69,69	0
54	MG	1A	3989	1/1	0.87	0.14	53,53,53,53	0
54	MG	1A	3694	1/1	0.87	0.09	71,71,71,71	0
54	MG	2A	3520	1/1	0.87	0.14	62,62,62,62	0
54	MG	1a	1713	1/1	0.87	0.10	94,94,94,94	0
54	MG	2A	3057	1/1	0.87	0.20	58,58,58,58	0
54	MG	1A	3428	1/1	0.87	0.18	47,47,47,47	0
54	MG	1a	1822	1/1	0.87	0.13	71,71,71,71	0
54	MG	2a	3004	1/1	0.87	0.21	73,73,73,73	0
54	MG	1a	1722	1/1	0.87	0.17	61,61,61,61	0
54	MG	2A	3546	1/1	0.87	0.09	74,74,74,74	0
54	MG	2A	3342	1/1	0.87	0.13	40,40,40,40	0
54	MG	2a	3027	1/1	0.87	0.31	74,74,74,74	0
54	MG	2A	3083	1/1	0.87	0.15	48,48,48,48	0
54	MG	1A	3884	1/1	0.87	0.14	65,65,65,65	0
54	MG	1A	3308	1/1	0.87	0.36	49,49,49,49	0
54	MG	1a	1731	1/1	0.87	0.17	59,59,59,59	0
54	MG	1a	1734	1/1	0.87	0.28	69,69,69,69	0
54	MG	1A	3650	1/1	0.87	0.11	53,53,53,53	0
54	MG	1A	4012	1/1	0.87	0.21	69,69,69,69	0
54	MG	2a	3043	1/1	0.87	0.28	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2a	3045	1/1	0.87	0.22	84,84,84,84	0
54	MG	2A	3576	1/1	0.87	0.10	66,66,66,66	0
54	MG	2A	3100	1/1	0.87	0.28	63,63,63,63	0
54	MG	1A	4015	1/1	0.87	0.25	48,48,48,48	0
54	MG	1A	3468	1/1	0.87	0.14	60,60,60,60	0
54	MG	2A	3593	1/1	0.87	0.10	72,72,72,72	0
54	MG	2A	3137	1/1	0.87	0.15	51,51,51,51	0
54	MG	1a	1853	1/1	0.87	0.12	66,66,66,66	0
54	MG	1A	3792	1/1	0.87	0.13	35,35,35,35	0
54	MG	2A	3381	1/1	0.87	0.14	47,47,47,47	0
54	MG	10	107	1/1	0.87	0.14	73,73,73,73	0
54	MG	1A	3716	1/1	0.87	0.18	29,29,29,29	0
54	MG	2a	3075	1/1	0.87	0.17	70,70,70,70	0
54	MG	1A	4030	1/1	0.87	0.18	75,75,75,75	0
54	MG	1A	3606	1/1	0.87	0.18	50,50,50,50	0
54	MG	15	108	1/1	0.87	0.31	42,42,42,42	0
54	MG	2A	3189	1/1	0.87	0.25	66,66,66,66	0
54	MG	1A	3665	1/1	0.87	0.07	22,22,22,22	0
54	MG	2a	3110	1/1	0.87	0.23	77,77,77,77	0
54	MG	2a	3112	1/1	0.87	0.15	55,55,55,55	0
54	MG	1A	3561	1/1	0.87	0.12	54,54,54,54	0
54	MG	1A	3925	1/1	0.87	0.13	54,54,54,54	0
54	MG	2A	3414	1/1	0.87	0.15	91,91,91,91	0
54	MG	2a	3143	1/1	0.87	0.12	55,55,55,55	0
54	MG	2A	3198	1/1	0.87	0.29	77,77,77,77	0
54	MG	2A	3654	1/1	0.87	0.10	85,85,85,85	0
54	MG	2A	3417	1/1	0.87	0.19	68,68,68,68	0
54	MG	1a	1616	1/1	0.87	0.15	73,73,73,73	0
54	MG	2A	3663	1/1	0.87	0.16	85,85,85,85	0
54	MG	1A	3354	1/1	0.87	0.16	60,60,60,60	0
54	MG	1A	4045	1/1	0.87	0.16	64,64,64,64	0
54	MG	1A	3935	1/1	0.87	0.14	53,53,53,53	0
54	MG	2a	3179	1/1	0.87	0.18	69,69,69,69	0
54	MG	2A	3213	1/1	0.87	0.26	64,64,64,64	0
54	MG	2A	3434	1/1	0.87	0.11	63,63,63,63	0
54	MG	2a	3191	1/1	0.87	0.12	88,88,88,88	0
54	MG	2A	3438	1/1	0.87	0.12	54,54,54,54	0
54	MG	1A	3567	1/1	0.87	0.16	64,64,64,64	0
54	MG	1b	301	1/1	0.87	0.15	80,80,80,80	0
54	MG	1A	3834	1/1	0.87	0.15	59,59,59,59	0
54	MG	1A	3950	1/1	0.87	0.17	51,51,51,51	0
54	MG	2A	3701	1/1	0.87	0.15	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2p	101	1/1	0.87	0.44	67,67,67,67	0
54	MG	2t	201	1/1	0.87	0.15	54,54,54,54	0
54	MG	1B	202	1/1	0.87	0.14	74,74,74,74	0
54	MG	2A	3449	1/1	0.87	0.21	58,58,58,58	0
54	MG	1A	3952	1/1	0.87	0.07	68,68,68,68	0
54	MG	1A	3746	1/1	0.87	0.21	57,57,57,57	0
54	MG	1A	3164	1/1	0.87	0.18	51,51,51,51	0
54	MG	1A	3676	1/1	0.87	0.11	44,44,44,44	0
54	MG	1A	3916	1/1	0.88	0.11	39,39,39,39	0
54	MG	1A	4023	1/1	0.88	0.09	28,28,28,28	0
54	MG	1a	1804	1/1	0.88	0.10	71,71,71,71	0
54	MG	1A	3918	1/1	0.88	0.16	51,51,51,51	0
54	MG	1A	3484	1/1	0.88	0.10	30,30,30,30	0
54	MG	1A	3092	1/1	0.88	0.12	62,62,62,62	0
54	MG	2B	210	1/1	0.88	0.20	82,82,82,82	0
54	MG	1A	3538	1/1	0.88	0.17	63,63,63,63	0
54	MG	2A	3494	1/1	0.88	0.10	53,53,53,53	0
54	MG	1A	3600	1/1	0.88	0.16	44,44,44,44	0
54	MG	1a	1814	1/1	0.88	0.12	64,64,64,64	0
54	MG	1A	3601	1/1	0.88	0.12	66,66,66,66	0
54	MG	2D	310	1/1	0.88	0.10	31,31,31,31	0
54	MG	1A	4038	1/1	0.88	0.18	60,60,60,60	0
54	MG	2F	303	1/1	0.88	0.17	59,59,59,59	0
54	MG	1A	3487	1/1	0.88	0.14	34,34,34,34	0
54	MG	1A	3839	1/1	0.88	0.12	39,39,39,39	0
54	MG	2A	3308	1/1	0.88	0.16	67,67,67,67	0
54	MG	1A	3208	1/1	0.88	0.26	73,73,73,73	0
54	MG	1A	3462	1/1	0.88	0.17	43,43,43,43	0
54	MG	2A	3319	1/1	0.88	0.12	53,53,53,53	0
54	MG	28	102	1/1	0.88	0.20	60,60,60,60	0
54	MG	1a	1737	1/1	0.88	0.32	79,79,79,79	0
54	MG	1A	3463	1/1	0.88	0.11	27,27,27,27	0
54	MG	1a	1601	1/1	0.88	0.26	78,78,78,78	0
54	MG	2a	3008	1/1	0.88	0.43	75,75,75,75	0
54	MG	1A	3685	1/1	0.88	0.10	70,70,70,70	0
54	MG	1A	3508	1/1	0.88	0.10	47,47,47,47	0
54	MG	2A	3552	1/1	0.88	0.11	80,80,80,80	0
54	MG	2A	3553	1/1	0.88	0.09	75,75,75,75	0
54	MG	2A	3344	1/1	0.88	0.11	40,40,40,40	0
54	MG	2a	3033	1/1	0.88	0.20	65,65,65,65	0
54	MG	1a	1628	1/1	0.88	0.23	77,77,77,77	0
54	MG	2A	3347	1/1	0.88	0.12	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3099	1/1	0.88	0.13	65,65,65,65	0
54	MG	1a	1846	1/1	0.88	0.12	80,80,80,80	0
54	MG	1a	1751	1/1	0.88	0.20	64,64,64,64	0
54	MG	2A	3113	1/1	0.88	0.27	76,76,76,76	0
54	MG	1A	3560	1/1	0.88	0.12	42,42,42,42	0
54	MG	2A	3121	1/1	0.88	0.24	72,72,72,72	0
54	MG	2A	3124	1/1	0.88	0.17	76,76,76,76	0
54	MG	1a	1631	1/1	0.88	0.23	74,74,74,74	0
54	MG	2A	3370	1/1	0.88	0.24	73,73,73,73	0
54	MG	2A	3375	1/1	0.88	0.11	40,40,40,40	0
54	MG	2A	3142	1/1	0.88	0.18	68,68,68,68	0
54	MG	2a	3055	1/1	0.88	0.26	74,74,74,74	0
54	MG	1A	3689	1/1	0.88	0.15	47,47,47,47	0
54	MG	1a	1756	1/1	0.88	0.18	66,66,66,66	0
54	MG	1A	3976	1/1	0.88	0.15	53,53,53,53	0
54	MG	2A	3605	1/1	0.88	0.12	68,68,68,68	0
54	MG	1A	3394	1/1	0.88	0.11	37,37,37,37	0
54	MG	1A	3469	1/1	0.88	0.10	57,57,57,57	0
54	MG	2A	3170	1/1	0.88	0.20	67,67,67,67	0
54	MG	2a	3076	1/1	0.88	0.09	72,72,72,72	0
54	MG	2A	3388	1/1	0.88	0.20	72,72,72,72	0
54	MG	2A	3176	1/1	0.88	0.16	65,65,65,65	0
54	MG	1A	3784	1/1	0.88	0.12	49,49,49,49	0
54	MG	1a	1644	1/1	0.88	0.29	61,61,61,61	0
54	MG	2A	3186	1/1	0.88	0.25	54,54,54,54	0
54	MG	2a	3107	1/1	0.88	0.13	75,75,75,75	0
54	MG	1a	1645	1/1	0.88	0.29	74,74,74,74	0
54	MG	1a	1770	1/1	0.88	0.14	68,68,68,68	0
54	MG	1a	1653	1/1	0.88	0.21	59,59,59,59	0
54	MG	2a	3125	1/1	0.88	0.16	82,82,82,82	0
54	MG	2A	3628	1/1	0.88	0.16	90,90,90,90	0
54	MG	2a	3137	1/1	0.88	0.14	68,68,68,68	0
54	MG	2A	3195	1/1	0.88	0.23	67,67,67,67	0
54	MG	1a	1772	1/1	0.88	0.29	71,71,71,71	0
54	MG	2A	3658	1/1	0.88	0.11	42,42,42,42	0
54	MG	1B	218	1/1	0.88	0.10	59,59,59,59	0
54	MG	2a	3151	1/1	0.88	0.22	68,68,68,68	0
54	MG	1A	3265	1/1	0.88	0.17	62,62,62,62	0
54	MG	2A	3205	1/1	0.88	0.14	63,63,63,63	0
54	MG	2a	3157	1/1	0.88	0.14	93,93,93,93	0
54	MG	1a	1656	1/1	0.88	0.19	50,50,50,50	0
54	MG	2A	3680	1/1	0.88	0.12	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3430	1/1	0.88	0.12	60,60,60,60	0
54	MG	1A	3409	1/1	0.88	0.21	59,59,59,59	0
54	MG	2a	3176	1/1	0.88	0.23	63,63,63,63	0
54	MG	1A	3580	1/1	0.88	0.10	24,24,24,24	0
54	MG	2A	3437	1/1	0.88	0.12	69,69,69,69	0
54	MG	2a	3182	1/1	0.88	0.12	66,66,66,66	0
54	MG	1A	3411	1/1	0.88	0.23	73,73,73,73	0
54	MG	1h	202	1/1	0.88	0.14	64,64,64,64	0
54	MG	2a	3193	1/1	0.88	0.26	76,76,76,76	0
54	MG	2A	3218	1/1	0.88	0.29	72,72,72,72	0
54	MG	1A	3799	1/1	0.88	0.20	70,70,70,70	0
54	MG	1A	3481	1/1	0.88	0.14	40,40,40,40	0
54	MG	1A	3270	1/1	0.88	0.12	65,65,65,65	0
54	MG	1n	102	1/1	0.88	0.14	67,67,67,67	0
54	MG	2A	3720	1/1	0.88	0.13	57,57,57,57	0
54	MG	2A	3723	1/1	0.88	0.22	67,67,67,67	0
54	MG	2r	101	1/1	0.88	0.13	68,68,68,68	0
54	MG	1A	3904	1/1	0.88	0.10	69,69,69,69	0
56	MPD	1A	4058	8/8	0.88	0.20	51,55,64,66	0
54	MG	1A	3813	1/1	0.88	0.19	38,38,38,38	0
54	MG	2A	3730	1/1	0.88	0.24	74,74,74,74	0
54	MG	2A	3735	1/1	0.88	0.09	77,77,77,77	0
54	MG	1A	3820	1/1	0.88	0.15	53,53,53,53	0
54	MG	1A	4014	1/1	0.88	0.09	67,67,67,67	0
54	MG	1A	3913	1/1	0.88	0.10	29,29,29,29	0
58	ZN	24	501	1/1	0.88	0.20	157,157,157,157	0
54	MG	1B	228	1/1	0.89	0.09	68,68,68,68	0
54	MG	1A	3562	1/1	0.89	0.19	71,71,71,71	0
54	MG	1D	311	1/1	0.89	0.19	49,49,49,49	0
54	MG	1A	3889	1/1	0.89	0.11	45,45,45,45	0
54	MG	2A	3731	1/1	0.89	0.18	72,72,72,72	0
54	MG	2A	3732	1/1	0.89	0.09	74,74,74,74	0
54	MG	1a	1779	1/1	0.89	0.11	55,55,55,55	0
54	MG	2A	3221	1/1	0.89	0.12	65,65,65,65	0
54	MG	2A	3446	1/1	0.89	0.18	64,64,64,64	0
54	MG	2A	3448	1/1	0.89	0.14	56,56,56,56	0
54	MG	1A	3692	1/1	0.89	0.11	65,65,65,65	0
54	MG	1A	3693	1/1	0.89	0.17	69,69,69,69	0
54	MG	1A	3563	1/1	0.89	0.11	51,51,51,51	0
54	MG	1y	204	1/1	0.89	0.11	86,86,86,86	0
54	MG	2A	3455	1/1	0.89	0.13	42,42,42,42	0
54	MG	2A	3003	1/1	0.89	0.09	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3242	1/1	0.89	0.16	66,66,66,66	0
54	MG	2A	3010	1/1	0.89	0.16	73,73,73,73	0
54	MG	1a	1784	1/1	0.89	0.14	66,66,66,66	0
54	MG	2A	3471	1/1	0.89	0.10	55,55,55,55	0
54	MG	2A	3252	1/1	0.89	0.15	65,65,65,65	0
54	MG	2D	304	1/1	0.89	0.38	52,52,52,52	0
54	MG	2A	3016	1/1	0.89	0.28	74,74,74,74	0
54	MG	2D	309	1/1	0.89	0.27	42,42,42,42	0
54	MG	2A	3480	1/1	0.89	0.20	61,61,61,61	0
54	MG	2E	301	1/1	0.89	0.15	73,73,73,73	0
54	MG	2A	3482	1/1	0.89	0.09	64,64,64,64	0
54	MG	1A	3250	1/1	0.89	0.12	64,64,64,64	0
54	MG	2A	3488	1/1	0.89	0.09	73,73,73,73	0
54	MG	1a	1789	1/1	0.89	0.15	66,66,66,66	0
54	MG	1E	307	1/1	0.89	0.12	34,34,34,34	0
54	MG	1A	3907	1/1	0.89	0.09	53,53,53,53	0
54	MG	2R	203	1/1	0.89	0.22	60,60,60,60	0
54	MG	2W	203	1/1	0.89	0.15	64,64,64,64	0
54	MG	1A	3801	1/1	0.89	0.10	49,49,49,49	0
54	MG	1a	1677	1/1	0.89	0.14	63,63,63,63	0
54	MG	1F	315	1/1	0.89	0.13	47,47,47,47	0
54	MG	1a	1687	1/1	0.89	0.14	59,59,59,59	0
54	MG	2A	3286	1/1	0.89	0.17	52,52,52,52	0
54	MG	2A	3508	1/1	0.89	0.13	67,67,67,67	0
54	MG	1A	3369	1/1	0.89	0.17	65,65,65,65	0
54	MG	2a	3009	1/1	0.89	0.17	70,70,70,70	0
54	MG	2A	3294	1/1	0.89	0.09	43,43,43,43	0
54	MG	1A	3074	1/1	0.89	0.20	53,53,53,53	0
54	MG	2a	3021	1/1	0.89	0.20	71,71,71,71	0
54	MG	2a	3023	1/1	0.89	0.15	62,62,62,62	0
54	MG	2a	3025	1/1	0.89	0.23	70,70,70,70	0
54	MG	1N	203	1/1	0.89	0.12	63,63,63,63	0
54	MG	1N	205	1/1	0.89	0.15	60,60,60,60	0
54	MG	1A	3578	1/1	0.89	0.15	72,72,72,72	0
54	MG	1a	1809	1/1	0.89	0.10	72,72,72,72	0
54	MG	2A	3528	1/1	0.89	0.11	42,42,42,42	0
54	MG	2A	3535	1/1	0.89	0.09	67,67,67,67	0
54	MG	2A	3304	1/1	0.89	0.12	77,77,77,77	0
54	MG	1A	3299	1/1	0.89	0.21	67,67,67,67	0
54	MG	2A	3543	1/1	0.89	0.18	56,56,56,56	0
54	MG	1a	1706	1/1	0.89	0.19	60,60,60,60	0
54	MG	2A	3067	1/1	0.89	0.21	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1a	1709	1/1	0.89	0.15	56,56,56,56	0
54	MG	2A	3321	1/1	0.89	0.12	48,48,48,48	0
54	MG	1a	1711	1/1	0.89	0.14	74,74,74,74	0
54	MG	2A	3330	1/1	0.89	0.10	35,35,35,35	0
54	MG	2A	3560	1/1	0.89	0.11	44,44,44,44	0
54	MG	1A	3278	1/1	0.89	0.43	56,56,56,56	0
54	MG	1A	4028	1/1	0.89	0.12	51,51,51,51	0
54	MG	10	102	1/1	0.89	0.25	56,56,56,56	0
54	MG	1a	1720	1/1	0.89	0.19	70,70,70,70	0
54	MG	1A	3485	1/1	0.89	0.10	46,46,46,46	0
54	MG	1A	3829	1/1	0.89	0.17	45,45,45,45	0
54	MG	2a	3069	1/1	0.89	0.25	68,68,68,68	0
54	MG	2A	3346	1/1	0.89	0.14	42,42,42,42	0
54	MG	2a	3073	1/1	0.89	0.15	75,75,75,75	0
54	MG	1A	3421	1/1	0.89	0.12	29,29,29,29	0
54	MG	11	104	1/1	0.89	0.12	55,55,55,55	0
54	MG	1A	3424	1/1	0.89	0.12	69,69,69,69	0
54	MG	1A	3946	1/1	0.89	0.09	31,31,31,31	0
54	MG	1A	3181	1/1	0.89	0.17	58,58,58,58	0
54	MG	2a	3084	1/1	0.89	0.10	41,41,41,41	0
54	MG	2A	3118	1/1	0.89	0.29	45,45,45,45	0
54	MG	1A	3664	1/1	0.89	0.12	64,64,64,64	0
54	MG	2a	3096	1/1	0.89	0.13	65,65,65,65	0
54	MG	1A	3465	1/1	0.89	0.17	73,73,73,73	0
54	MG	2a	3102	1/1	0.89	0.28	66,66,66,66	0
54	MG	2a	3103	1/1	0.89	0.18	70,70,70,70	0
54	MG	2A	3125	1/1	0.89	0.24	66,66,66,66	0
54	MG	2a	3109	1/1	0.89	0.18	78,78,78,78	0
54	MG	2A	3132	1/1	0.89	0.10	54,54,54,54	0
54	MG	1A	3595	1/1	0.89	0.15	60,60,60,60	0
54	MG	2a	3113	1/1	0.89	0.14	69,69,69,69	0
54	MG	2A	3376	1/1	0.89	0.11	37,37,37,37	0
54	MG	2A	3613	1/1	0.89	0.13	61,61,61,61	0
54	MG	2a	3126	1/1	0.89	0.15	75,75,75,75	0
54	MG	1A	4049	1/1	0.89	0.12	62,62,62,62	0
54	MG	2A	3378	1/1	0.89	0.14	74,74,74,74	0
54	MG	1a	1605	1/1	0.89	0.20	67,67,67,67	0
54	MG	2A	3152	1/1	0.89	0.13	52,52,52,52	0
54	MG	2A	3621	1/1	0.89	0.22	64,64,64,64	0
54	MG	1A	3427	1/1	0.89	0.14	59,59,59,59	0
54	MG	1a	1858	1/1	0.89	0.11	61,61,61,61	0
54	MG	1A	3269	1/1	0.89	0.13	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2a	3155	1/1	0.89	0.17	54,54,54,54	0
54	MG	2A	3625	1/1	0.89	0.12	74,74,74,74	0
54	MG	1A	3603	1/1	0.89	0.10	45,45,45,45	0
54	MG	2A	3642	1/1	0.89	0.12	80,80,80,80	0
54	MG	2a	3161	1/1	0.89	0.18	64,64,64,64	0
54	MG	1A	3509	1/1	0.89	0.10	32,32,32,32	0
54	MG	2A	3656	1/1	0.89	0.16	33,33,33,33	0
54	MG	2A	3174	1/1	0.89	0.14	70,70,70,70	0
54	MG	1A	3325	1/1	0.89	0.08	39,39,39,39	0
54	MG	2A	3178	1/1	0.89	0.10	61,61,61,61	0
54	MG	2a	3180	1/1	0.89	0.10	76,76,76,76	0
54	MG	1A	3767	1/1	0.89	0.15	67,67,67,67	0
54	MG	2A	3670	1/1	0.89	0.10	71,71,71,71	0
54	MG	2a	3185	1/1	0.89	0.15	77,77,77,77	0
54	MG	2A	3672	1/1	0.89	0.10	48,48,48,48	0
54	MG	2a	3189	1/1	0.89	0.13	60,60,60,60	0
54	MG	1A	3679	1/1	0.89	0.11	70,70,70,70	0
54	MG	2a	3192	1/1	0.89	0.15	82,82,82,82	0
54	MG	1A	3610	1/1	0.89	0.37	41,41,41,41	0
54	MG	2A	3411	1/1	0.89	0.24	49,49,49,49	0
54	MG	2A	3412	1/1	0.89	0.11	50,50,50,50	0
54	MG	2A	3188	1/1	0.89	0.17	54,54,54,54	0
54	MG	1A	3476	1/1	0.89	0.12	51,51,51,51	0
54	MG	1A	3985	1/1	0.89	0.08	54,54,54,54	0
54	MG	1A	3616	1/1	0.89	0.22	38,38,38,38	0
54	MG	1a	1767	1/1	0.89	0.16	79,79,79,79	0
54	MG	1A	3783	1/1	0.89	0.14	43,43,43,43	0
54	MG	1a	1652	1/1	0.89	0.24	60,60,60,60	0
54	MG	2A	3700	1/1	0.89	0.14	61,61,61,61	0
54	MG	1d	303	1/1	0.89	0.24	74,74,74,74	0
54	MG	2A	3702	1/1	0.89	0.10	60,60,60,60	0
54	MG	2A	3705	1/1	0.89	0.13	51,51,51,51	0
54	MG	2A	3203	1/1	0.89	0.18	56,56,56,56	0
54	MG	1A	3622	1/1	0.89	0.20	69,69,69,69	0
54	MG	2A	3715	1/1	0.89	0.13	67,67,67,67	0
54	MG	1f	201	1/1	0.89	0.23	71,71,71,71	0
54	MG	2A	3462	1/1	0.90	0.11	56,56,56,56	0
54	MG	2A	3464	1/1	0.90	0.11	70,70,70,70	0
54	MG	1P	203	1/1	0.90	0.15	39,39,39,39	0
54	MG	1A	3353	1/1	0.90	0.12	47,47,47,47	0
54	MG	2A	3220	1/1	0.90	0.10	61,61,61,61	0
54	MG	1a	1877	1/1	0.90	0.16	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3479	1/1	0.90	0.12	42,42,42,42	0
54	MG	1A	3991	1/1	0.90	0.08	50,50,50,50	0
54	MG	1A	3853	1/1	0.90	0.12	50,50,50,50	0
54	MG	1A	3994	1/1	0.90	0.15	49,49,49,49	0
54	MG	1A	3995	1/1	0.90	0.21	46,46,46,46	0
54	MG	1g	201	1/1	0.90	0.23	67,67,67,67	0
54	MG	1a	1742	1/1	0.90	0.14	80,80,80,80	0
54	MG	2A	3245	1/1	0.90	0.21	62,62,62,62	0
54	MG	2A	3495	1/1	0.90	0.26	70,70,70,70	0
54	MG	1A	3575	1/1	0.90	0.14	47,47,47,47	0
54	MG	1A	3997	1/1	0.90	0.21	43,43,43,43	0
54	MG	1A	3010	1/1	0.90	0.14	58,58,58,58	0
54	MG	2N	201	1/1	0.90	0.09	77,77,77,77	0
54	MG	1A	4002	1/1	0.90	0.13	56,56,56,56	0
54	MG	13	103	1/1	0.90	0.10	69,69,69,69	0
54	MG	1A	4003	1/1	0.90	0.15	62,62,62,62	0
54	MG	2A	3269	1/1	0.90	0.30	66,66,66,66	0
54	MG	15	104	1/1	0.90	0.22	31,31,31,31	0
54	MG	25	101	1/1	0.90	0.22	70,70,70,70	0
54	MG	1y	203	1/1	0.90	0.24	80,80,80,80	0
54	MG	2A	3519	1/1	0.90	0.10	72,72,72,72	0
54	MG	1A	3262	1/1	0.90	0.18	51,51,51,51	0
54	MG	2A	3001	1/1	0.90	0.24	70,70,70,70	0
54	MG	2A	3002	1/1	0.90	0.15	50,50,50,50	0
54	MG	1A	3748	1/1	0.90	0.30	67,67,67,67	0
54	MG	1A	3579	1/1	0.90	0.10	62,62,62,62	0
54	MG	17	106	1/1	0.90	0.21	59,59,59,59	0
54	MG	1A	3649	1/1	0.90	0.20	40,40,40,40	0
54	MG	2a	3022	1/1	0.90	0.17	77,77,77,77	0
54	MG	1A	3196	1/1	0.90	0.32	67,67,67,67	0
54	MG	1A	3755	1/1	0.90	0.12	62,62,62,62	0
54	MG	2A	3545	1/1	0.90	0.18	77,77,77,77	0
54	MG	1A	3518	1/1	0.90	0.11	60,60,60,60	0
54	MG	1A	3757	1/1	0.90	0.14	46,46,46,46	0
54	MG	2A	3032	1/1	0.90	0.14	58,58,58,58	0
54	MG	2a	3034	1/1	0.90	0.18	73,73,73,73	0
54	MG	1A	3656	1/1	0.90	0.13	55,55,55,55	0
54	MG	1a	1618	1/1	0.90	0.11	65,65,65,65	0
54	MG	2A	3311	1/1	0.90	0.16	56,56,56,56	0
54	MG	1a	1620	1/1	0.90	0.11	64,64,64,64	0
54	MG	1A	3467	1/1	0.90	0.09	49,49,49,49	0
54	MG	2A	3564	1/1	0.90	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
54	MG	1a	1776	1/1	0.90	0.21	71,71,71,71	0
54	MG	1A	3414	1/1	0.90	0.25	59,59,59,59	0
54	MG	1A	3765	1/1	0.90	0.15	47,47,47,47	0
54	MG	2A	3329	1/1	0.90	0.11	51,51,51,51	0
54	MG	1A	3586	1/1	0.90	0.25	58,58,58,58	0
54	MG	2A	3332	1/1	0.90	0.18	67,67,67,67	0
54	MG	1a	1634	1/1	0.90	0.26	75,75,75,75	0
54	MG	1A	3300	1/1	0.90	0.20	68,68,68,68	0
54	MG	1A	3163	1/1	0.90	0.11	44,44,44,44	0
54	MG	1A	3133	1/1	0.90	0.40	51,51,51,51	0
54	MG	2a	3060	1/1	0.90	0.10	67,67,67,67	0
54	MG	1a	1640	1/1	0.90	0.14	83,83,83,83	0
54	MG	2a	3063	1/1	0.90	0.10	68,68,68,68	0
54	MG	1A	4043	1/1	0.90	0.10	62,62,62,62	0
54	MG	2A	3602	1/1	0.90	0.10	48,48,48,48	0
54	MG	2a	3071	1/1	0.90	0.28	69,69,69,69	0
54	MG	2A	3081	1/1	0.90	0.16	48,48,48,48	0
54	MG	1A	3908	1/1	0.90	0.23	40,40,40,40	0
54	MG	1A	3594	1/1	0.90	0.18	75,75,75,75	0
54	MG	1a	1650	1/1	0.90	0.21	69,69,69,69	0
54	MG	1A	3310	1/1	0.90	0.18	64,64,64,64	0
54	MG	1A	3598	1/1	0.90	0.13	68,68,68,68	0
54	MG	2A	3092	1/1	0.90	0.19	65,65,65,65	0
54	MG	1A	3678	1/1	0.90	0.19	42,42,42,42	0
54	MG	2a	3085	1/1	0.90	0.21	68,68,68,68	0
54	MG	2A	3094	1/1	0.90	0.09	55,55,55,55	0
54	MG	1A	3139	1/1	0.90	0.29	67,67,67,67	0
54	MG	2a	3095	1/1	0.90	0.09	58,58,58,58	0
54	MG	1A	3071	1/1	0.90	0.23	49,49,49,49	0
54	MG	1A	3429	1/1	0.90	0.09	29,29,29,29	0
54	MG	2A	3106	1/1	0.90	0.12	54,54,54,54	0
54	MG	2A	3107	1/1	0.90	0.18	58,58,58,58	0
54	MG	2a	3105	1/1	0.90	0.14	72,72,72,72	0
54	MG	1A	3378	1/1	0.90	0.11	46,46,46,46	0
54	MG	1a	1660	1/1	0.90	0.13	71,71,71,71	0
54	MG	1A	3187	1/1	0.90	0.12	59,59,59,59	0
54	MG	2A	3630	1/1	0.90	0.12	61,61,61,61	0
54	MG	2A	3640	1/1	0.90	0.14	74,74,74,74	0
54	MG	2a	3117	1/1	0.90	0.14	71,71,71,71	0
54	MG	1a	1665	1/1	0.90	0.27	77,77,77,77	0
54	MG	2A	3649	1/1	0.90	0.09	76,76,76,76	0
54	MG	2A	3652	1/1	0.90	0.10	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1a	1667	1/1	0.90	0.17	64,64,64,64	0
54	MG	1A	3014	1/1	0.90	0.31	65,65,65,65	0
54	MG	1A	3804	1/1	0.90	0.09	57,57,57,57	0
54	MG	1A	3386	1/1	0.90	0.15	67,67,67,67	0
54	MG	2a	3144	1/1	0.90	0.21	47,47,47,47	0
54	MG	2A	3134	1/1	0.90	0.17	70,70,70,70	0
54	MG	2A	3392	1/1	0.90	0.32	62,62,62,62	0
54	MG	1A	3558	1/1	0.90	0.16	64,64,64,64	0
54	MG	2a	3153	1/1	0.90	0.09	78,78,78,78	0
54	MG	1A	3283	1/1	0.90	0.11	49,49,49,49	0
54	MG	2A	3674	1/1	0.90	0.09	72,72,72,72	0
54	MG	2A	3146	1/1	0.90	0.17	56,56,56,56	0
54	MG	1A	3451	1/1	0.90	0.12	57,57,57,57	0
54	MG	1a	1680	1/1	0.90	0.37	75,75,75,75	0
54	MG	1A	3960	1/1	0.90	0.08	65,65,65,65	0
54	MG	1A	3501	1/1	0.90	0.08	67,67,67,67	0
54	MG	1A	3504	1/1	0.90	0.13	61,61,61,61	0
54	MG	1A	3965	1/1	0.90	0.12	59,59,59,59	0
54	MG	1A	3831	1/1	0.90	0.08	26,26,26,26	0
54	MG	2a	3177	1/1	0.90	0.23	72,72,72,72	0
54	MG	1a	1835	1/1	0.90	0.08	64,64,64,64	0
54	MG	2A	3694	1/1	0.90	0.13	69,69,69,69	0
54	MG	1A	3968	1/1	0.90	0.25	51,51,51,51	0
54	MG	2A	3696	1/1	0.90	0.13	63,63,63,63	0
54	MG	1A	3969	1/1	0.90	0.16	60,60,60,60	0
54	MG	2A	3180	1/1	0.90	0.21	69,69,69,69	0
54	MG	1a	1698	1/1	0.90	0.13	60,60,60,60	0
54	MG	1a	1847	1/1	0.90	0.21	73,73,73,73	0
54	MG	1A	3832	1/1	0.90	0.11	52,52,52,52	0
54	MG	1a	1702	1/1	0.90	0.16	56,56,56,56	0
54	MG	1a	1703	1/1	0.90	0.09	39,39,39,39	0
54	MG	1a	1705	1/1	0.90	0.11	78,78,78,78	0
54	MG	2d	301	1/1	0.90	0.18	67,67,67,67	0
54	MG	2e	201	1/1	0.90	0.16	65,65,65,65	0
54	MG	2A	3716	1/1	0.90	0.12	40,40,40,40	0
54	MG	2A	3192	1/1	0.90	0.25	65,65,65,65	0
54	MG	1A	3630	1/1	0.90	0.11	27,27,27,27	0
54	MG	1A	3709	1/1	0.90	0.15	66,66,66,66	0
54	MG	1A	3710	1/1	0.90	0.10	52,52,52,52	0
54	MG	1A	3390	1/1	0.90	0.12	28,28,28,28	0
54	MG	1A	3838	1/1	0.90	0.09	60,60,60,60	0
54	MG	1A	3638	1/1	0.90	0.23	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3204	1/1	0.90	0.16	68,68,68,68	0
54	MG	1A	3639	1/1	0.90	0.11	46,46,46,46	0
54	MG	1A	3845	1/1	0.90	0.30	60,60,60,60	0
54	MG	1A	3848	1/1	0.90	0.17	53,53,53,53	0
54	MG	1a	1727	1/1	0.90	0.20	46,46,46,46	0
54	MG	1O	201	1/1	0.90	0.12	59,59,59,59	0
54	MG	2A	3215	1/1	0.90	0.14	63,63,63,63	0
54	MG	1A	3459	1/1	0.91	0.10	52,52,52,52	0
54	MG	1a	1869	1/1	0.91	0.15	66,66,66,66	0
54	MG	1A	3766	1/1	0.91	0.07	31,31,31,31	0
54	MG	1A	3326	1/1	0.91	0.17	44,44,44,44	0
54	MG	1a	1872	1/1	0.91	0.14	65,65,65,65	0
54	MG	1a	1873	1/1	0.91	0.21	61,61,61,61	0
54	MG	2A	3206	1/1	0.91	0.30	55,55,55,55	0
54	MG	2B	206	1/1	0.91	0.18	69,69,69,69	0
54	MG	1A	3244	1/1	0.91	0.37	45,45,45,45	0
54	MG	1a	1875	1/1	0.91	0.12	87,87,87,87	0
54	MG	1A	3772	1/1	0.91	0.09	34,34,34,34	0
54	MG	2A	3211	1/1	0.91	0.23	64,64,64,64	0
54	MG	2A	3465	1/1	0.91	0.10	60,60,60,60	0
54	MG	1A	3061	1/1	0.91	0.13	55,55,55,55	0
54	MG	1a	1733	1/1	0.91	0.20	62,62,62,62	0
54	MG	2A	3472	1/1	0.91	0.17	62,62,62,62	0
54	MG	1A	3392	1/1	0.91	0.10	37,37,37,37	0
54	MG	11	105	1/1	0.91	0.10	44,44,44,44	0
54	MG	1A	4005	1/1	0.91	0.25	38,38,38,38	0
54	MG	1A	3260	1/1	0.91	0.13	62,62,62,62	0
54	MG	2A	3225	1/1	0.91	0.22	49,49,49,49	0
54	MG	2A	3483	1/1	0.91	0.08	61,61,61,61	0
54	MG	1A	3541	1/1	0.91	0.19	63,63,63,63	0
54	MG	2A	3487	1/1	0.91	0.12	52,52,52,52	0
54	MG	1A	3398	1/1	0.91	0.11	34,34,34,34	0
54	MG	1A	3893	1/1	0.91	0.13	60,60,60,60	0
54	MG	1A	4016	1/1	0.91	0.10	63,63,63,63	0
54	MG	1A	3895	1/1	0.91	0.21	39,39,39,39	0
54	MG	2Q	202	1/1	0.91	0.11	66,66,66,66	0
54	MG	1A	4020	1/1	0.91	0.15	61,61,61,61	0
54	MG	2T	201	1/1	0.91	0.25	68,68,68,68	0
54	MG	2A	3498	1/1	0.91	0.10	73,73,73,73	0
54	MG	2Y	201	1/1	0.91	0.18	60,60,60,60	0
54	MG	20	102	1/1	0.91	0.08	71,71,71,71	0
54	MG	2A	3244	1/1	0.91	0.09	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	4022	1/1	0.91	0.14	54,54,54,54	0
54	MG	1A	3896	1/1	0.91	0.13	49,49,49,49	0
54	MG	1y	201	1/1	0.91	0.09	76,76,76,76	0
54	MG	1a	1602	1/1	0.91	0.16	78,78,78,78	0
54	MG	1A	3343	1/1	0.91	0.09	43,43,43,43	0
54	MG	1A	3346	1/1	0.91	0.10	40,40,40,40	0
54	MG	2A	3513	1/1	0.91	0.12	56,56,56,56	0
54	MG	1a	1760	1/1	0.91	0.24	68,68,68,68	0
54	MG	2A	3268	1/1	0.91	0.22	58,58,58,58	0
54	MG	1a	1614	1/1	0.91	0.19	68,68,68,68	0
54	MG	1a	1615	1/1	0.91	0.11	57,57,57,57	0
54	MG	1A	3551	1/1	0.91	0.17	46,46,46,46	0
54	MG	2A	3522	1/1	0.91	0.18	64,64,64,64	0
54	MG	1A	3793	1/1	0.91	0.12	64,64,64,64	0
54	MG	2A	3017	1/1	0.91	0.12	61,61,61,61	0
54	MG	2A	3526	1/1	0.91	0.10	58,58,58,58	0
54	MG	2a	3030	1/1	0.91	0.15	73,73,73,73	0
54	MG	2A	3019	1/1	0.91	0.29	51,51,51,51	0
54	MG	1A	3795	1/1	0.91	0.14	70,70,70,70	0
54	MG	2A	3278	1/1	0.91	0.21	60,60,60,60	0
54	MG	1a	1621	1/1	0.91	0.14	58,58,58,58	0
54	MG	2a	3036	1/1	0.91	0.23	58,58,58,58	0
54	MG	2A	3287	1/1	0.91	0.18	65,65,65,65	0
54	MG	1A	3199	1/1	0.91	0.14	48,48,48,48	0
54	MG	1A	4036	1/1	0.91	0.09	65,65,65,65	0
54	MG	2A	3547	1/1	0.91	0.09	38,38,38,38	0
54	MG	1A	3288	1/1	0.91	0.14	46,46,46,46	0
54	MG	2a	3042	1/1	0.91	0.29	74,74,74,74	0
54	MG	1A	3625	1/1	0.91	0.10	30,30,30,30	0
54	MG	2A	3035	1/1	0.91	0.26	68,68,68,68	0
54	MG	1A	3093	1/1	0.91	0.13	64,64,64,64	0
54	MG	1A	3700	1/1	0.91	0.10	49,49,49,49	0
54	MG	1A	3359	1/1	0.91	0.12	41,41,41,41	0
54	MG	2A	3045	1/1	0.91	0.15	67,67,67,67	0
54	MG	1A	3423	1/1	0.91	0.09	32,32,32,32	0
54	MG	1A	3264	1/1	0.91	0.27	30,30,30,30	0
54	MG	1A	3938	1/1	0.91	0.08	59,59,59,59	0
54	MG	1a	1642	1/1	0.91	0.25	68,68,68,68	0
54	MG	1A	3637	1/1	0.91	0.08	46,46,46,46	0
54	MG	2a	3061	1/1	0.91	0.14	68,68,68,68	0
54	MG	2A	3327	1/1	0.91	0.10	42,42,42,42	0
54	MG	1A	4052	1/1	0.91	0.15	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1a	1785	1/1	0.91	0.12	79,79,79,79	0
54	MG	1A	3941	1/1	0.91	0.09	50,50,50,50	0
54	MG	2A	3589	1/1	0.91	0.09	66,66,66,66	0
54	MG	2A	3064	1/1	0.91	0.08	55,55,55,55	0
54	MG	1a	1788	1/1	0.91	0.11	73,73,73,73	0
54	MG	2A	3071	1/1	0.91	0.14	50,50,50,50	0
54	MG	1A	3943	1/1	0.91	0.12	65,65,65,65	0
54	MG	1a	1790	1/1	0.91	0.27	74,74,74,74	0
54	MG	1A	3822	1/1	0.91	0.11	31,31,31,31	0
54	MG	2a	3078	1/1	0.91	0.25	70,70,70,70	0
54	MG	1A	3425	1/1	0.91	0.12	32,32,32,32	0
54	MG	2a	3083	1/1	0.91	0.13	82,82,82,82	0
54	MG	1A	3949	1/1	0.91	0.09	60,60,60,60	0
54	MG	1A	3828	1/1	0.91	0.09	18,18,18,18	0
54	MG	2a	3086	1/1	0.91	0.15	62,62,62,62	0
54	MG	2a	3090	1/1	0.91	0.13	58,58,58,58	0
54	MG	1A	3715	1/1	0.91	0.14	28,28,28,28	0
54	MG	2A	3351	1/1	0.91	0.29	61,61,61,61	0
54	MG	1B	214	1/1	0.91	0.08	49,49,49,49	0
54	MG	1A	3956	1/1	0.91	0.12	67,67,67,67	0
54	MG	1a	1662	1/1	0.91	0.23	67,67,67,67	0
54	MG	2a	3098	1/1	0.91	0.11	85,85,85,85	0
54	MG	2a	3099	1/1	0.91	0.12	74,74,74,74	0
54	MG	2A	3616	1/1	0.91	0.09	58,58,58,58	0
54	MG	1A	3119	1/1	0.91	0.30	54,54,54,54	0
54	MG	1A	3718	1/1	0.91	0.18	53,53,53,53	0
54	MG	2A	3620	1/1	0.91	0.14	58,58,58,58	0
54	MG	1B	221	1/1	0.91	0.20	66,66,66,66	0
54	MG	2A	3367	1/1	0.91	0.09	66,66,66,66	0
54	MG	1a	1668	1/1	0.91	0.18	60,60,60,60	0
54	MG	1A	3961	1/1	0.91	0.12	69,69,69,69	0
54	MG	1A	3366	1/1	0.91	0.09	54,54,54,54	0
54	MG	2A	3111	1/1	0.91	0.14	51,51,51,51	0
54	MG	2A	3629	1/1	0.91	0.12	73,73,73,73	0
54	MG	1A	3963	1/1	0.91	0.10	66,66,66,66	0
54	MG	2a	3127	1/1	0.91	0.23	74,74,74,74	0
54	MG	2a	3131	1/1	0.91	0.10	53,53,53,53	0
54	MG	1A	3574	1/1	0.91	0.12	65,65,65,65	0
54	MG	1A	3643	1/1	0.91	0.23	38,38,38,38	0
54	MG	2a	3139	1/1	0.91	0.10	73,73,73,73	0
54	MG	2A	3647	1/1	0.91	0.10	53,53,53,53	0
54	MG	1A	3266	1/1	0.91	0.36	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1a	1679	1/1	0.91	0.28	72,72,72,72	0
54	MG	1A	3368	1/1	0.91	0.11	24,24,24,24	0
54	MG	2a	3148	1/1	0.91	0.12	67,67,67,67	0
54	MG	2A	3126	1/1	0.91	0.19	67,67,67,67	0
54	MG	1a	1823	1/1	0.91	0.10	65,65,65,65	0
54	MG	1D	316	1/1	0.91	0.15	53,53,53,53	0
54	MG	1A	3011	1/1	0.91	0.16	66,66,66,66	0
54	MG	2A	3138	1/1	0.91	0.33	62,62,62,62	0
54	MG	2A	3666	1/1	0.91	0.08	62,62,62,62	0
54	MG	1A	3309	1/1	0.91	0.34	41,41,41,41	0
54	MG	2a	3158	1/1	0.91	0.09	68,68,68,68	0
54	MG	2A	3402	1/1	0.91	0.09	45,45,45,45	0
54	MG	2A	3403	1/1	0.91	0.11	39,39,39,39	0
54	MG	1A	3214	1/1	0.91	0.13	58,58,58,58	0
54	MG	2A	3676	1/1	0.91	0.08	55,55,55,55	0
54	MG	2A	3147	1/1	0.91	0.33	79,79,79,79	0
54	MG	1A	3653	1/1	0.91	0.09	54,54,54,54	0
54	MG	1A	3317	1/1	0.91	0.32	54,54,54,54	0
54	MG	1a	1834	1/1	0.91	0.10	51,51,51,51	0
54	MG	2A	3158	1/1	0.91	0.20	44,44,44,44	0
54	MG	1a	1695	1/1	0.91	0.23	65,65,65,65	0
54	MG	2A	3686	1/1	0.91	0.13	67,67,67,67	0
54	MG	1A	3851	1/1	0.91	0.10	54,54,54,54	0
54	MG	1a	1697	1/1	0.91	0.29	68,68,68,68	0
54	MG	1F	314	1/1	0.91	0.31	43,43,43,43	0
54	MG	1A	3319	1/1	0.91	0.14	60,60,60,60	0
54	MG	2A	3422	1/1	0.91	0.15	61,61,61,61	0
54	MG	1a	1700	1/1	0.91	0.21	64,64,64,64	0
54	MG	1A	3515	1/1	0.91	0.12	28,28,28,28	0
54	MG	1A	3172	1/1	0.91	0.14	67,67,67,67	0
54	MG	2A	3432	1/1	0.91	0.23	78,78,78,78	0
54	MG	1A	3863	1/1	0.91	0.10	53,53,53,53	0
54	MG	1A	3864	1/1	0.91	0.09	51,51,51,51	0
54	MG	2A	3436	1/1	0.91	0.07	49,49,49,49	0
54	MG	2A	3709	1/1	0.91	0.20	74,74,74,74	0
54	MG	2A	3711	1/1	0.91	0.08	74,74,74,74	0
54	MG	1A	3867	1/1	0.91	0.18	45,45,45,45	0
54	MG	1a	1710	1/1	0.91	0.13	67,67,67,67	0
54	MG	1A	3193	1/1	0.91	0.11	64,64,64,64	0
54	MG	2A	3722	1/1	0.91	0.15	48,48,48,48	0
54	MG	1A	3383	1/1	0.91	0.11	54,54,54,54	0
54	MG	2A	3191	1/1	0.91	0.26	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3727	1/1	0.91	0.18	62,62,62,62	0
54	MG	1A	3458	1/1	0.91	0.12	55,55,55,55	0
54	MG	1T	201	1/1	0.91	0.12	52,52,52,52	0
54	MG	1a	1717	1/1	0.91	0.12	70,70,70,70	0
54	MG	2A	3447	1/1	0.91	0.10	44,44,44,44	0
54	MG	2A	3038	1/1	0.92	0.16	67,67,67,67	0
54	MG	1A	3255	1/1	0.92	0.17	47,47,47,47	0
54	MG	1A	3635	1/1	0.92	0.11	31,31,31,31	0
54	MG	1A	3566	1/1	0.92	0.08	61,61,61,61	0
54	MG	1A	3510	1/1	0.92	0.10	73,73,73,73	0
54	MG	1a	1792	1/1	0.92	0.12	66,66,66,66	0
54	MG	2A	3281	1/1	0.92	0.11	24,24,24,24	0
54	MG	2A	3285	1/1	0.92	0.12	54,54,54,54	0
54	MG	1A	3460	1/1	0.92	0.11	63,63,63,63	0
54	MG	2E	305	1/1	0.92	0.09	57,57,57,57	0
54	MG	2E	307	1/1	0.92	0.19	67,67,67,67	0
54	MG	1A	3512	1/1	0.92	0.11	60,60,60,60	0
54	MG	1A	3150	1/1	0.92	0.48	45,45,45,45	0
54	MG	1A	3713	1/1	0.92	0.11	54,54,54,54	0
54	MG	1F	316	1/1	0.92	0.12	57,57,57,57	0
54	MG	1a	1678	1/1	0.92	0.08	65,65,65,65	0
54	MG	2O	201	1/1	0.92	0.14	65,65,65,65	0
54	MG	1A	3210	1/1	0.92	0.10	55,55,55,55	0
54	MG	1A	3905	1/1	0.92	0.10	75,75,75,75	0
54	MG	1a	1682	1/1	0.92	0.20	59,59,59,59	0
54	MG	2A	3302	1/1	0.92	0.13	55,55,55,55	0
54	MG	2T	203	1/1	0.92	0.09	63,63,63,63	0
54	MG	2V	203	1/1	0.92	0.13	69,69,69,69	0
54	MG	2W	202	1/1	0.92	0.13	52,52,52,52	0
54	MG	1a	1807	1/1	0.92	0.19	60,60,60,60	0
54	MG	2A	3307	1/1	0.92	0.11	45,45,45,45	0
54	MG	1a	1683	1/1	0.92	0.18	78,78,78,78	0
54	MG	1A	3811	1/1	0.92	0.32	47,47,47,47	0
54	MG	2A	3533	1/1	0.92	0.13	57,57,57,57	0
54	MG	2A	3085	1/1	0.92	0.21	75,75,75,75	0
54	MG	1a	1686	1/1	0.92	0.13	66,66,66,66	0
54	MG	1A	3464	1/1	0.92	0.09	46,46,46,46	0
54	MG	2A	3320	1/1	0.92	0.14	69,69,69,69	0
54	MG	1A	3330	1/1	0.92	0.10	65,65,65,65	0
54	MG	1A	4006	1/1	0.92	0.12	18,18,18,18	0
54	MG	1a	1817	1/1	0.92	0.15	76,76,76,76	0
54	MG	2a	3010	1/1	0.92	0.14	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3548	1/1	0.92	0.12	72,72,72,72	0
54	MG	1A	4007	1/1	0.92	0.12	42,42,42,42	0
54	MG	2a	3020	1/1	0.92	0.18	63,63,63,63	0
54	MG	1A	3817	1/1	0.92	0.10	41,41,41,41	0
54	MG	1R	202	1/1	0.92	0.19	50,50,50,50	0
54	MG	1A	3098	1/1	0.92	0.10	59,59,59,59	0
54	MG	1A	3102	1/1	0.92	0.10	36,36,36,36	0
54	MG	1V	206	1/1	0.92	0.14	59,59,59,59	0
54	MG	1W	201	1/1	0.92	0.14	50,50,50,50	0
54	MG	1A	3725	1/1	0.92	0.07	36,36,36,36	0
54	MG	2A	3110	1/1	0.92	0.23	56,56,56,56	0
54	MG	1A	3728	1/1	0.92	0.12	39,39,39,39	0
54	MG	1A	3648	1/1	0.92	0.13	57,57,57,57	0
54	MG	1A	3063	1/1	0.92	0.12	42,42,42,42	0
54	MG	1A	3932	1/1	0.92	0.14	61,61,61,61	0
54	MG	2A	3352	1/1	0.92	0.18	65,65,65,65	0
54	MG	1a	1708	1/1	0.92	0.14	72,72,72,72	0
54	MG	2A	3582	1/1	0.92	0.10	60,60,60,60	0
54	MG	1A	3532	1/1	0.92	0.18	55,55,55,55	0
54	MG	1A	3936	1/1	0.92	0.12	47,47,47,47	0
54	MG	2A	3590	1/1	0.92	0.09	41,41,41,41	0
54	MG	2A	3591	1/1	0.92	0.12	49,49,49,49	0
54	MG	1a	1844	1/1	0.92	0.09	65,65,65,65	0
54	MG	2a	3048	1/1	0.92	0.14	74,74,74,74	0
54	MG	13	102	1/1	0.92	0.12	46,46,46,46	0
54	MG	2A	3597	1/1	0.92	0.10	41,41,41,41	0
54	MG	2A	3365	1/1	0.92	0.14	65,65,65,65	0
54	MG	1A	3740	1/1	0.92	0.10	31,31,31,31	0
54	MG	1a	1849	1/1	0.92	0.34	72,72,72,72	0
54	MG	1A	3741	1/1	0.92	0.08	51,51,51,51	0
54	MG	1a	1851	1/1	0.92	0.18	72,72,72,72	0
54	MG	2a	3057	1/1	0.92	0.08	88,88,88,88	0
54	MG	2A	3372	1/1	0.92	0.17	71,71,71,71	0
54	MG	2a	3059	1/1	0.92	0.23	75,75,75,75	0
54	MG	1A	3342	1/1	0.92	0.09	48,48,48,48	0
54	MG	1A	3121	1/1	0.92	0.13	49,49,49,49	0
54	MG	1a	1856	1/1	0.92	0.12	63,63,63,63	0
54	MG	2A	3151	1/1	0.92	0.20	67,67,67,67	0
54	MG	1a	1719	1/1	0.92	0.10	75,75,75,75	0
54	MG	2a	3065	1/1	0.92	0.17	64,64,64,64	0
54	MG	15	106	1/1	0.92	0.10	50,50,50,50	0
54	MG	1A	3945	1/1	0.92	0.07	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3344	1/1	0.92	0.09	32,32,32,32	0
54	MG	1A	3303	1/1	0.92	0.15	42,42,42,42	0
54	MG	1A	3236	1/1	0.92	0.24	64,64,64,64	0
54	MG	2A	3166	1/1	0.92	0.10	61,61,61,61	0
54	MG	2A	3167	1/1	0.92	0.14	53,53,53,53	0
54	MG	1A	3237	1/1	0.92	0.28	58,58,58,58	0
54	MG	2A	3397	1/1	0.92	0.11	57,57,57,57	0
54	MG	2A	3172	1/1	0.92	0.15	65,65,65,65	0
54	MG	2A	3401	1/1	0.92	0.10	50,50,50,50	0
54	MG	1a	1732	1/1	0.92	0.08	56,56,56,56	0
54	MG	2A	3175	1/1	0.92	0.26	75,75,75,75	0
54	MG	2A	3636	1/1	0.92	0.07	58,58,58,58	0
54	MG	2A	3637	1/1	0.92	0.07	64,64,64,64	0
54	MG	2A	3404	1/1	0.92	0.16	70,70,70,70	0
54	MG	1A	3951	1/1	0.92	0.10	68,68,68,68	0
54	MG	2A	3643	1/1	0.92	0.08	56,56,56,56	0
54	MG	2A	3177	1/1	0.92	0.10	71,71,71,71	0
54	MG	1A	3546	1/1	0.92	0.10	35,35,35,35	0
54	MG	1A	3955	1/1	0.92	0.09	31,31,31,31	0
54	MG	2A	3653	1/1	0.92	0.11	57,57,57,57	0
54	MG	1A	3039	1/1	0.92	0.14	57,57,57,57	0
54	MG	1a	1612	1/1	0.92	0.18	84,84,84,84	0
54	MG	1A	4048	1/1	0.92	0.14	54,54,54,54	0
54	MG	1A	3958	1/1	0.92	0.17	54,54,54,54	0
54	MG	1A	3273	1/1	0.92	0.10	39,39,39,39	0
54	MG	1a	1744	1/1	0.92	0.18	63,63,63,63	0
54	MG	2a	3111	1/1	0.92	0.15	66,66,66,66	0
54	MG	1A	3604	1/1	0.92	0.08	43,43,43,43	0
54	MG	2A	3669	1/1	0.92	0.12	60,60,60,60	0
54	MG	2a	3115	1/1	0.92	0.08	69,69,69,69	0
54	MG	1A	3444	1/1	0.92	0.10	50,50,50,50	0
54	MG	1a	1750	1/1	0.92	0.08	60,60,60,60	0
54	MG	2A	3194	1/1	0.92	0.09	47,47,47,47	0
54	MG	1A	3448	1/1	0.92	0.12	49,49,49,49	0
54	MG	1a	1624	1/1	0.92	0.12	59,59,59,59	0
54	MG	1A	3449	1/1	0.92	0.10	63,63,63,63	0
54	MG	2A	3678	1/1	0.92	0.07	62,62,62,62	0
54	MG	2a	3136	1/1	0.92	0.11	75,75,75,75	0
54	MG	2A	3679	1/1	0.92	0.08	48,48,48,48	0
54	MG	2a	3138	1/1	0.92	0.15	70,70,70,70	0
54	MG	1f	202	1/1	0.92	0.12	49,49,49,49	0
54	MG	1A	3557	1/1	0.92	0.13	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3314	1/1	0.92	0.20	39,39,39,39	0
54	MG	1A	3771	1/1	0.92	0.11	54,54,54,54	0
54	MG	2A	3439	1/1	0.92	0.18	52,52,52,52	0
54	MG	2a	3146	1/1	0.92	0.14	70,70,70,70	0
54	MG	1B	207	1/1	0.92	0.30	61,61,61,61	0
54	MG	2A	3687	1/1	0.92	0.11	62,62,62,62	0
54	MG	1A	3868	1/1	0.92	0.08	65,65,65,65	0
54	MG	1l	201	1/1	0.92	0.16	65,65,65,65	0
54	MG	1A	3619	1/1	0.92	0.10	44,44,44,44	0
54	MG	1B	215	1/1	0.92	0.18	56,56,56,56	0
54	MG	2A	3445	1/1	0.92	0.11	66,66,66,66	0
54	MG	2A	3212	1/1	0.92	0.14	67,67,67,67	0
54	MG	1B	216	1/1	0.92	0.19	69,69,69,69	0
54	MG	1o	3100	1/1	0.92	0.10	50,50,50,50	0
54	MG	1A	3775	1/1	0.92	0.09	34,34,34,34	0
54	MG	1A	3620	1/1	0.92	0.25	45,45,45,45	0
54	MG	2a	3172	1/1	0.92	0.14	78,78,78,78	0
54	MG	1a	1768	1/1	0.92	0.19	74,74,74,74	0
54	MG	2A	3452	1/1	0.92	0.12	38,38,38,38	0
54	MG	1a	1769	1/1	0.92	0.15	67,67,67,67	0
54	MG	1A	3559	1/1	0.92	0.09	52,52,52,52	0
54	MG	2A	3456	1/1	0.92	0.13	75,75,75,75	0
54	MG	1A	3399	1/1	0.92	0.08	40,40,40,40	0
54	MG	2A	3718	1/1	0.92	0.12	51,51,51,51	0
54	MG	1a	1649	1/1	0.92	0.23	63,63,63,63	0
54	MG	2A	3721	1/1	0.92	0.10	68,68,68,68	0
54	MG	1A	3980	1/1	0.92	0.12	57,57,57,57	0
54	MG	2A	3232	1/1	0.92	0.09	59,59,59,59	0
54	MG	1A	3981	1/1	0.92	0.10	60,60,60,60	0
54	MG	2A	3725	1/1	0.92	0.09	75,75,75,75	0
54	MG	1A	3982	1/1	0.92	0.13	51,51,51,51	0
54	MG	2A	3728	1/1	0.92	0.09	87,87,87,87	0
54	MG	2A	3466	1/1	0.92	0.10	73,73,73,73	0
54	MG	2A	3468	1/1	0.92	0.12	69,69,69,69	0
54	MG	1B	229	1/1	0.92	0.08	62,62,62,62	0
54	MG	2A	3243	1/1	0.92	0.12	44,44,44,44	0
54	MG	1A	3403	1/1	0.92	0.09	23,23,23,23	0
54	MG	1A	3880	1/1	0.92	0.09	57,57,57,57	0
54	MG	1D	312	1/1	0.92	0.30	44,44,44,44	0
54	MG	1D	313	1/1	0.92	0.12	66,66,66,66	0
54	MG	1a	1782	1/1	0.92	0.12	70,70,70,70	0
54	MG	1A	3245	1/1	0.92	0.22	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3033	1/1	0.92	0.17	53,53,53,53	0
54	MG	2A	3485	1/1	0.92	0.08	42,42,42,42	0
54	MG	1A	3145	1/1	0.92	0.17	56,56,56,56	0
54	MG	1a	1663	1/1	0.92	0.09	69,69,69,69	0
54	MG	1A	3788	1/1	0.92	0.11	66,66,66,66	0
54	MG	2A	3037	1/1	0.92	0.20	52,52,52,52	0
54	MG	2B	211	1/1	0.92	0.12	63,63,63,63	0
58	ZN	14	102	1/1	0.92	0.13	144,144,144,144	0
54	MG	2A	3492	1/1	0.92	0.12	54,54,54,54	0
54	MG	1a	1672	1/1	0.93	0.11	48,48,48,48	0
54	MG	1A	3088	1/1	0.93	0.29	40,40,40,40	0
54	MG	2A	3490	1/1	0.93	0.10	65,65,65,65	0
54	MG	1A	3974	1/1	0.93	0.12	64,64,64,64	0
54	MG	2A	3280	1/1	0.93	0.07	53,53,53,53	0
54	MG	1A	3205	1/1	0.93	0.24	43,43,43,43	0
54	MG	1A	3207	1/1	0.93	0.27	46,46,46,46	0
54	MG	2A	3497	1/1	0.93	0.12	45,45,45,45	0
54	MG	2B	216	1/1	0.93	0.16	69,69,69,69	0
54	MG	1A	3494	1/1	0.93	0.07	67,67,67,67	0
54	MG	2D	303	1/1	0.93	0.33	45,45,45,45	0
54	MG	1A	3495	1/1	0.93	0.09	31,31,31,31	0
54	MG	2A	3289	1/1	0.93	0.19	53,53,53,53	0
54	MG	2A	3074	1/1	0.93	0.12	58,58,58,58	0
54	MG	2A	3079	1/1	0.93	0.13	61,61,61,61	0
54	MG	2A	3504	1/1	0.93	0.10	63,63,63,63	0
54	MG	1E	304	1/1	0.93	0.09	52,52,52,52	0
54	MG	1a	1681	1/1	0.93	0.16	59,59,59,59	0
54	MG	1A	3854	1/1	0.93	0.12	48,48,48,48	0
54	MG	2A	3510	1/1	0.93	0.08	38,38,38,38	0
54	MG	2A	3511	1/1	0.93	0.15	66,66,66,66	0
54	MG	1A	3856	1/1	0.93	0.07	47,47,47,47	0
54	MG	1A	3747	1/1	0.93	0.08	65,65,65,65	0
54	MG	1A	3496	1/1	0.93	0.07	28,28,28,28	0
54	MG	2A	3518	1/1	0.93	0.07	61,61,61,61	0
54	MG	1A	3173	1/1	0.93	0.23	46,46,46,46	0
54	MG	1a	1688	1/1	0.93	0.29	77,77,77,77	0
54	MG	1A	3570	1/1	0.93	0.10	57,57,57,57	0
54	MG	2A	3309	1/1	0.93	0.10	55,55,55,55	0
54	MG	2A	3523	1/1	0.93	0.14	51,51,51,51	0
54	MG	2A	3310	1/1	0.93	0.11	67,67,67,67	0
54	MG	1A	3866	1/1	0.93	0.09	46,46,46,46	0
54	MG	2A	3096	1/1	0.93	0.11	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3315	1/1	0.93	0.11	30,30,30,30	0
54	MG	2A	3530	1/1	0.93	0.10	44,44,44,44	0
54	MG	1A	3572	1/1	0.93	0.09	25,25,25,25	0
54	MG	1A	3178	1/1	0.93	0.18	52,52,52,52	0
54	MG	1G	204	1/1	0.93	0.14	60,60,60,60	0
54	MG	2A	3539	1/1	0.93	0.06	56,56,56,56	0
54	MG	2a	3001	1/1	0.93	0.09	49,49,49,49	0
54	MG	1A	3990	1/1	0.93	0.16	61,61,61,61	0
54	MG	2A	3542	1/1	0.93	0.16	69,69,69,69	0
54	MG	1A	3371	1/1	0.93	0.08	34,34,34,34	0
54	MG	1a	1831	1/1	0.93	0.14	66,66,66,66	0
54	MG	1A	3438	1/1	0.93	0.13	61,61,61,61	0
54	MG	1A	3758	1/1	0.93	0.10	52,52,52,52	0
54	MG	2a	3014	1/1	0.93	0.16	63,63,63,63	0
54	MG	2A	3112	1/1	0.93	0.15	58,58,58,58	0
54	MG	2A	3551	1/1	0.93	0.11	53,53,53,53	0
54	MG	1A	3651	1/1	0.93	0.11	43,43,43,43	0
54	MG	1Q	202	1/1	0.93	0.07	36,36,36,36	0
54	MG	2A	3341	1/1	0.93	0.15	53,53,53,53	0
54	MG	2A	3556	1/1	0.93	0.10	65,65,65,65	0
54	MG	1Q	203	1/1	0.93	0.12	56,56,56,56	0
54	MG	1a	1838	1/1	0.93	0.13	74,74,74,74	0
54	MG	2A	3123	1/1	0.93	0.23	42,42,42,42	0
54	MG	2a	3028	1/1	0.93	0.29	67,67,67,67	0
54	MG	1a	1842	1/1	0.93	0.09	67,67,67,67	0
54	MG	1A	3577	1/1	0.93	0.12	46,46,46,46	0
54	MG	2a	3032	1/1	0.93	0.08	92,92,92,92	0
54	MG	1A	3507	1/1	0.93	0.10	46,46,46,46	0
54	MG	2A	3349	1/1	0.93	0.09	34,34,34,34	0
54	MG	2A	3569	1/1	0.93	0.11	71,71,71,71	0
54	MG	1A	3440	1/1	0.93	0.11	72,72,72,72	0
54	MG	1a	1848	1/1	0.93	0.15	66,66,66,66	0
54	MG	1A	4001	1/1	0.93	0.14	81,81,81,81	0
54	MG	1V	201	1/1	0.93	0.24	38,38,38,38	0
54	MG	1A	3267	1/1	0.93	0.29	55,55,55,55	0
54	MG	2A	3580	1/1	0.93	0.09	54,54,54,54	0
54	MG	2A	3360	1/1	0.93	0.17	50,50,50,50	0
54	MG	1A	3101	1/1	0.93	0.20	43,43,43,43	0
54	MG	2A	3362	1/1	0.93	0.12	62,62,62,62	0
54	MG	2a	3046	1/1	0.93	0.12	61,61,61,61	0
54	MG	1A	3147	1/1	0.93	0.16	45,45,45,45	0
54	MG	1A	3770	1/1	0.93	0.15	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3150	1/1	0.93	0.13	68,68,68,68	0
54	MG	1A	3186	1/1	0.93	0.10	60,60,60,60	0
54	MG	1A	3890	1/1	0.93	0.08	50,50,50,50	0
54	MG	1A	3328	1/1	0.93	0.13	65,65,65,65	0
54	MG	2A	3599	1/1	0.93	0.06	56,56,56,56	0
54	MG	2A	3154	1/1	0.93	0.16	59,59,59,59	0
54	MG	2A	3371	1/1	0.93	0.08	74,74,74,74	0
54	MG	11	101	1/1	0.93	0.13	45,45,45,45	0
54	MG	1a	1724	1/1	0.93	0.13	67,67,67,67	0
54	MG	1A	4009	1/1	0.93	0.16	64,64,64,64	0
54	MG	1A	4011	1/1	0.93	0.11	53,53,53,53	0
54	MG	2A	3163	1/1	0.93	0.10	63,63,63,63	0
54	MG	1a	1729	1/1	0.93	0.11	69,69,69,69	0
54	MG	2A	3612	1/1	0.93	0.14	57,57,57,57	0
54	MG	1A	3329	1/1	0.93	0.13	31,31,31,31	0
54	MG	1A	3517	1/1	0.93	0.08	44,44,44,44	0
54	MG	2a	3070	1/1	0.93	0.14	54,54,54,54	0
54	MG	1A	3675	1/1	0.93	0.17	55,55,55,55	0
54	MG	1A	3232	1/1	0.93	0.13	41,41,41,41	0
54	MG	1A	3387	1/1	0.93	0.13	41,41,41,41	0
54	MG	2A	3387	1/1	0.93	0.17	72,72,72,72	0
54	MG	1A	3070	1/1	0.93	0.08	44,44,44,44	0
54	MG	1A	3112	1/1	0.93	0.32	42,42,42,42	0
54	MG	1A	3681	1/1	0.93	0.12	56,56,56,56	0
54	MG	2A	3393	1/1	0.93	0.07	34,34,34,34	0
54	MG	2A	3394	1/1	0.93	0.19	64,64,64,64	0
54	MG	2A	3396	1/1	0.93	0.09	37,37,37,37	0
54	MG	1A	3682	1/1	0.93	0.12	56,56,56,56	0
54	MG	2A	3399	1/1	0.93	0.11	39,39,39,39	0
54	MG	1A	3791	1/1	0.93	0.17	65,65,65,65	0
54	MG	2a	3088	1/1	0.93	0.23	49,49,49,49	0
54	MG	2A	3631	1/1	0.93	0.10	71,71,71,71	0
54	MG	2A	3632	1/1	0.93	0.11	86,86,86,86	0
54	MG	2A	3633	1/1	0.93	0.14	61,61,61,61	0
54	MG	2a	3094	1/1	0.93	0.09	62,62,62,62	0
54	MG	2A	3635	1/1	0.93	0.09	59,59,59,59	0
54	MG	1A	3599	1/1	0.93	0.07	47,47,47,47	0
54	MG	1A	3335	1/1	0.93	0.08	32,32,32,32	0
54	MG	2A	3187	1/1	0.93	0.14	58,58,58,58	0
54	MG	1a	1745	1/1	0.93	0.08	57,57,57,57	0
54	MG	1A	4031	1/1	0.93	0.07	66,66,66,66	0
54	MG	2A	3645	1/1	0.93	0.07	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1a	1603	1/1	0.93	0.13	72,72,72,72	0
54	MG	2A	3407	1/1	0.93	0.20	70,70,70,70	0
54	MG	2A	3408	1/1	0.93	0.11	56,56,56,56	0
54	MG	1A	3914	1/1	0.93	0.07	38,38,38,38	0
54	MG	1A	3794	1/1	0.93	0.10	39,39,39,39	0
54	MG	1A	4035	1/1	0.93	0.11	62,62,62,62	0
54	MG	1A	3158	1/1	0.93	0.16	64,64,64,64	0
54	MG	1A	3243	1/1	0.93	0.11	46,46,46,46	0
54	MG	2A	3415	1/1	0.93	0.10	47,47,47,47	0
54	MG	1A	3798	1/1	0.93	0.13	65,65,65,65	0
54	MG	2a	3120	1/1	0.93	0.07	55,55,55,55	0
54	MG	2a	3122	1/1	0.93	0.11	78,78,78,78	0
54	MG	2a	3123	1/1	0.93	0.07	64,64,64,64	0
54	MG	1A	3161	1/1	0.93	0.10	43,43,43,43	0
54	MG	2A	3200	1/1	0.93	0.13	42,42,42,42	0
54	MG	1A	4042	1/1	0.93	0.11	67,67,67,67	0
54	MG	1A	3195	1/1	0.93	0.10	52,52,52,52	0
54	MG	1A	3934	1/1	0.93	0.08	63,63,63,63	0
54	MG	1A	3466	1/1	0.93	0.09	57,57,57,57	0
54	MG	1A	3608	1/1	0.93	0.12	56,56,56,56	0
54	MG	1A	3805	1/1	0.93	0.09	44,44,44,44	0
54	MG	1y	202	1/1	0.93	0.09	71,71,71,71	0
54	MG	2a	3141	1/1	0.93	0.09	64,64,64,64	0
54	MG	2A	3209	1/1	0.93	0.10	58,58,58,58	0
54	MG	1A	3806	1/1	0.93	0.26	42,42,42,42	0
54	MG	1A	3808	1/1	0.93	0.10	62,62,62,62	0
54	MG	1A	3810	1/1	0.93	0.10	64,64,64,64	0
54	MG	1A	3539	1/1	0.93	0.09	64,64,64,64	0
54	MG	2a	3147	1/1	0.93	0.12	64,64,64,64	0
54	MG	1A	4054	1/1	0.93	0.13	64,64,64,64	0
54	MG	1a	1639	1/1	0.93	0.14	68,68,68,68	0
54	MG	1A	3540	1/1	0.93	0.10	57,57,57,57	0
54	MG	1A	3701	1/1	0.93	0.30	41,41,41,41	0
54	MG	2A	3692	1/1	0.93	0.07	44,44,44,44	0
54	MG	1A	3615	1/1	0.93	0.19	38,38,38,38	0
54	MG	2A	3018	1/1	0.93	0.40	54,54,54,54	0
54	MG	1A	3289	1/1	0.93	0.18	58,58,58,58	0
54	MG	2A	3228	1/1	0.93	0.17	71,71,71,71	0
54	MG	1A	3408	1/1	0.93	0.19	57,57,57,57	0
54	MG	1A	3347	1/1	0.93	0.10	55,55,55,55	0
54	MG	1B	209	1/1	0.93	0.09	62,62,62,62	0
54	MG	1A	3953	1/1	0.93	0.07	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3290	1/1	0.93	0.13	56,56,56,56	0
54	MG	2A	3237	1/1	0.93	0.14	48,48,48,48	0
54	MG	2A	3241	1/1	0.93	0.19	54,54,54,54	0
54	MG	1A	3826	1/1	0.93	0.18	35,35,35,35	0
54	MG	2A	3710	1/1	0.93	0.09	63,63,63,63	0
54	MG	1A	3064	1/1	0.93	0.27	43,43,43,43	0
54	MG	2A	3712	1/1	0.93	0.12	61,61,61,61	0
54	MG	2A	3458	1/1	0.93	0.17	64,64,64,64	0
54	MG	2a	3183	1/1	0.93	0.11	70,70,70,70	0
54	MG	1A	3355	1/1	0.93	0.07	38,38,38,38	0
54	MG	1A	3251	1/1	0.93	0.28	76,76,76,76	0
54	MG	1A	3254	1/1	0.93	0.09	76,76,76,76	0
54	MG	2A	3463	1/1	0.93	0.11	56,56,56,56	0
54	MG	1A	3360	1/1	0.93	0.07	26,26,26,26	0
54	MG	1A	3720	1/1	0.93	0.25	43,43,43,43	0
54	MG	1A	3632	1/1	0.93	0.11	50,50,50,50	0
54	MG	2A	3467	1/1	0.93	0.11	34,34,34,34	0
54	MG	2A	3255	1/1	0.93	0.15	51,51,51,51	0
54	MG	2A	3259	1/1	0.93	0.10	49,49,49,49	0
54	MG	2A	3260	1/1	0.93	0.10	31,31,31,31	0
54	MG	2A	3044	1/1	0.93	0.20	65,65,65,65	0
54	MG	2A	3473	1/1	0.93	0.20	66,66,66,66	0
54	MG	2A	3264	1/1	0.93	0.24	73,73,73,73	0
54	MG	2A	3734	1/1	0.93	0.11	51,51,51,51	0
54	MG	1A	3724	1/1	0.93	0.12	54,54,54,54	0
54	MG	1A	3634	1/1	0.93	0.09	35,35,35,35	0
54	MG	1D	303	1/1	0.93	0.10	41,41,41,41	0
54	MG	2A	3738	1/1	0.93	0.12	81,81,81,81	0
54	MG	2A	3740	1/1	0.93	0.14	69,69,69,69	0
54	MG	1A	3197	1/1	0.93	0.10	56,56,56,56	0
54	MG	1A	3120	1/1	0.93	0.20	52,52,52,52	0
54	MG	2A	3055	1/1	0.93	0.12	43,43,43,43	0
54	MG	2B	203	1/1	0.93	0.22	70,70,70,70	0
54	MG	2A	3274	1/1	0.93	0.07	43,43,43,43	0
54	MG	1A	3970	1/1	0.93	0.10	70,70,70,70	0
54	MG	1A	3253	1/1	0.94	0.09	46,46,46,46	0
54	MG	1H	201	1/1	0.94	0.16	66,66,66,66	0
54	MG	1H	203	1/1	0.94	0.11	66,66,66,66	0
54	MG	1A	3589	1/1	0.94	0.17	69,69,69,69	0
54	MG	1A	3492	1/1	0.94	0.08	24,24,24,24	0
54	MG	1A	3047	1/1	0.94	0.32	48,48,48,48	0
54	MG	2A	3197	1/1	0.94	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
54	MG	1A	3402	1/1	0.94	0.12	29,29,29,29	0
54	MG	1A	3836	1/1	0.94	0.07	53,53,53,53	0
54	MG	1A	3048	1/1	0.94	0.24	47,47,47,47	0
54	MG	1A	3327	1/1	0.94	0.10	56,56,56,56	0
54	MG	1a	1714	1/1	0.94	0.14	73,73,73,73	0
54	MG	1A	3406	1/1	0.94	0.08	28,28,28,28	0
54	MG	1A	3711	1/1	0.94	0.07	39,39,39,39	0
54	MG	1d	301	1/1	0.94	0.26	75,75,75,75	0
54	MG	1R	204	1/1	0.94	0.11	52,52,52,52	0
54	MG	1A	3712	1/1	0.94	0.10	66,66,66,66	0
54	MG	1A	3846	1/1	0.94	0.09	55,55,55,55	0
54	MG	2A	3739	1/1	0.94	0.15	60,60,60,60	0
54	MG	2A	3459	1/1	0.94	0.09	73,73,73,73	0
54	MG	1T	205	1/1	0.94	0.10	62,62,62,62	0
54	MG	1U	201	1/1	0.94	0.15	41,41,41,41	0
54	MG	1A	3503	1/1	0.94	0.10	43,43,43,43	0
54	MG	1a	1728	1/1	0.94	0.11	56,56,56,56	0
54	MG	1V	204	1/1	0.94	0.14	54,54,54,54	0
54	MG	1V	205	1/1	0.94	0.12	63,63,63,63	0
54	MG	1A	3258	1/1	0.94	0.18	38,38,38,38	0
54	MG	1A	3602	1/1	0.94	0.09	53,53,53,53	0
54	MG	1m	201	1/1	0.94	0.07	79,79,79,79	0
54	MG	2A	3469	1/1	0.94	0.08	64,64,64,64	0
54	MG	2A	3226	1/1	0.94	0.24	57,57,57,57	0
54	MG	1A	3259	1/1	0.94	0.15	45,45,45,45	0
54	MG	1A	3506	1/1	0.94	0.10	53,53,53,53	0
54	MG	1n	103	1/1	0.94	0.20	73,73,73,73	0
54	MG	1A	3123	1/1	0.94	0.05	35,35,35,35	0
54	MG	2A	3476	1/1	0.94	0.10	61,61,61,61	0
54	MG	1A	3857	1/1	0.94	0.07	62,62,62,62	0
54	MG	2A	3478	1/1	0.94	0.14	34,34,34,34	0
54	MG	2D	306	1/1	0.94	0.15	47,47,47,47	0
54	MG	1A	3075	1/1	0.94	0.21	45,45,45,45	0
54	MG	1A	3607	1/1	0.94	0.08	49,49,49,49	0
54	MG	1A	3190	1/1	0.94	0.28	72,72,72,72	0
54	MG	2D	311	1/1	0.94	0.10	65,65,65,65	0
54	MG	2D	312	1/1	0.94	0.14	56,56,56,56	0
54	MG	1A	3420	1/1	0.94	0.10	29,29,29,29	0
54	MG	2E	302	1/1	0.94	0.23	52,52,52,52	0
54	MG	1A	3731	1/1	0.94	0.08	36,36,36,36	0
54	MG	1A	3076	1/1	0.94	0.19	44,44,44,44	0
54	MG	13	104	1/1	0.94	0.10	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3008	1/1	0.94	0.10	53,53,53,53	0
54	MG	2A	3247	1/1	0.94	0.07	60,60,60,60	0
54	MG	2A	3009	1/1	0.94	0.15	56,56,56,56	0
54	MG	1a	1748	1/1	0.94	0.14	67,67,67,67	0
54	MG	1A	3613	1/1	0.94	0.22	40,40,40,40	0
54	MG	1A	3869	1/1	0.94	0.09	39,39,39,39	0
54	MG	2A	3254	1/1	0.94	0.18	46,46,46,46	0
54	MG	2A	3496	1/1	0.94	0.10	72,72,72,72	0
54	MG	2R	202	1/1	0.94	0.12	46,46,46,46	0
54	MG	1A	3422	1/1	0.94	0.11	62,62,62,62	0
54	MG	2A	3256	1/1	0.94	0.10	57,57,57,57	0
54	MG	1A	3871	1/1	0.94	0.09	46,46,46,46	0
54	MG	2A	3500	1/1	0.94	0.10	61,61,61,61	0
54	MG	1a	1753	1/1	0.94	0.14	59,59,59,59	0
54	MG	2A	3022	1/1	0.94	0.18	51,51,51,51	0
54	MG	2A	3262	1/1	0.94	0.34	52,52,52,52	0
54	MG	1A	3513	1/1	0.94	0.07	23,23,23,23	0
54	MG	2A	3505	1/1	0.94	0.11	64,64,64,64	0
54	MG	1A	3617	1/1	0.94	0.12	48,48,48,48	0
54	MG	2A	3026	1/1	0.94	0.09	58,58,58,58	0
54	MG	27	101	1/1	0.94	0.28	45,45,45,45	0
54	MG	17	103	1/1	0.94	0.29	41,41,41,41	0
54	MG	1a	1757	1/1	0.94	0.19	56,56,56,56	0
54	MG	1a	1758	1/1	0.94	0.18	66,66,66,66	0
54	MG	2A	3512	1/1	0.94	0.21	45,45,45,45	0
54	MG	1A	3745	1/1	0.94	0.10	42,42,42,42	0
54	MG	2a	3005	1/1	0.94	0.09	54,54,54,54	0
54	MG	1A	3618	1/1	0.94	0.16	36,36,36,36	0
54	MG	18	102	1/1	0.94	0.12	45,45,45,45	0
54	MG	1a	1762	1/1	0.94	0.06	57,57,57,57	0
54	MG	2a	3012	1/1	0.94	0.14	68,68,68,68	0
54	MG	18	103	1/1	0.94	0.21	42,42,42,42	0
54	MG	1A	3876	1/1	0.94	0.07	29,29,29,29	0
54	MG	2a	3018	1/1	0.94	0.09	57,57,57,57	0
54	MG	2A	3279	1/1	0.94	0.07	32,32,32,32	0
54	MG	2A	3039	1/1	0.94	0.16	57,57,57,57	0
54	MG	2A	3041	1/1	0.94	0.06	34,34,34,34	0
54	MG	2A	3283	1/1	0.94	0.10	33,33,33,33	0
54	MG	2A	3284	1/1	0.94	0.09	44,44,44,44	0
54	MG	1A	4019	1/1	0.94	0.15	39,39,39,39	0
54	MG	1A	3337	1/1	0.94	0.10	18,18,18,18	0
54	MG	2A	3529	1/1	0.94	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
54	MG	1A	3194	1/1	0.94	0.09	54,54,54,54	0
54	MG	2A	3531	1/1	0.94	0.11	32,32,32,32	0
54	MG	2A	3532	1/1	0.94	0.07	54,54,54,54	0
54	MG	1a	1604	1/1	0.94	0.24	76,76,76,76	0
54	MG	1A	3079	1/1	0.94	0.31	45,45,45,45	0
54	MG	2A	3536	1/1	0.94	0.07	65,65,65,65	0
54	MG	2A	3291	1/1	0.94	0.09	50,50,50,50	0
54	MG	2A	3293	1/1	0.94	0.06	39,39,39,39	0
54	MG	2A	3047	1/1	0.94	0.08	59,59,59,59	0
54	MG	2A	3048	1/1	0.94	0.13	55,55,55,55	0
54	MG	2A	3050	1/1	0.94	0.09	42,42,42,42	0
54	MG	2A	3544	1/1	0.94	0.14	60,60,60,60	0
54	MG	1a	1607	1/1	0.94	0.09	67,67,67,67	0
54	MG	1a	1608	1/1	0.94	0.09	67,67,67,67	0
54	MG	1A	3883	1/1	0.94	0.08	28,28,28,28	0
54	MG	1a	1773	1/1	0.94	0.12	74,74,74,74	0
54	MG	2A	3550	1/1	0.94	0.12	55,55,55,55	0
54	MG	1A	4025	1/1	0.94	0.10	55,55,55,55	0
54	MG	2A	3305	1/1	0.94	0.12	69,69,69,69	0
54	MG	2A	3306	1/1	0.94	0.21	60,60,60,60	0
54	MG	1A	3052	1/1	0.94	0.09	44,44,44,44	0
54	MG	1A	3054	1/1	0.94	0.16	58,58,58,58	0
54	MG	2a	3053	1/1	0.94	0.17	64,64,64,64	0
54	MG	1A	3058	1/1	0.94	0.10	45,45,45,45	0
54	MG	2A	3062	1/1	0.94	0.12	61,61,61,61	0
54	MG	2A	3559	1/1	0.94	0.10	62,62,62,62	0
54	MG	2A	3063	1/1	0.94	0.09	48,48,48,48	0
54	MG	1a	1617	1/1	0.94	0.12	67,67,67,67	0
54	MG	2A	3314	1/1	0.94	0.07	49,49,49,49	0
54	MG	2A	3065	1/1	0.94	0.11	51,51,51,51	0
54	MG	1A	3059	1/1	0.94	0.08	37,37,37,37	0
54	MG	2A	3568	1/1	0.94	0.09	51,51,51,51	0
54	MG	2A	3318	1/1	0.94	0.09	40,40,40,40	0
54	MG	1A	3523	1/1	0.94	0.07	24,24,24,24	0
54	MG	1A	3631	1/1	0.94	0.10	59,59,59,59	0
54	MG	2a	3067	1/1	0.94	0.19	66,66,66,66	0
54	MG	2a	3068	1/1	0.94	0.15	72,72,72,72	0
54	MG	2A	3575	1/1	0.94	0.07	55,55,55,55	0
54	MG	1a	1623	1/1	0.94	0.20	58,58,58,58	0
54	MG	2A	3322	1/1	0.94	0.09	55,55,55,55	0
54	MG	2A	3578	1/1	0.94	0.06	50,50,50,50	0
54	MG	2A	3326	1/1	0.94	0.18	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3075	1/1	0.94	0.12	58,58,58,58	0
54	MG	2A	3076	1/1	0.94	0.10	54,54,54,54	0
54	MG	1A	3430	1/1	0.94	0.09	29,29,29,29	0
54	MG	2A	3080	1/1	0.94	0.17	68,68,68,68	0
54	MG	1A	3432	1/1	0.94	0.07	18,18,18,18	0
54	MG	1A	3433	1/1	0.94	0.08	40,40,40,40	0
54	MG	2A	3336	1/1	0.94	0.08	49,49,49,49	0
54	MG	2A	3337	1/1	0.94	0.21	67,67,67,67	0
54	MG	2A	3596	1/1	0.94	0.08	49,49,49,49	0
54	MG	1A	3351	1/1	0.94	0.09	52,52,52,52	0
54	MG	2A	3340	1/1	0.94	0.18	79,79,79,79	0
54	MG	1A	3095	1/1	0.94	0.11	51,51,51,51	0
54	MG	2a	3091	1/1	0.94	0.25	69,69,69,69	0
54	MG	2A	3087	1/1	0.94	0.11	49,49,49,49	0
54	MG	1A	3277	1/1	0.94	0.33	36,36,36,36	0
54	MG	1A	3148	1/1	0.94	0.10	51,51,51,51	0
54	MG	1A	3096	1/1	0.94	0.24	49,49,49,49	0
54	MG	1A	3035	1/1	0.94	0.12	53,53,53,53	0
54	MG	1A	3443	1/1	0.94	0.17	62,62,62,62	0
54	MG	1A	3544	1/1	0.94	0.06	24,24,24,24	0
54	MG	1A	3911	1/1	0.94	0.06	39,39,39,39	0
54	MG	2a	3100	1/1	0.94	0.12	60,60,60,60	0
54	MG	2A	3097	1/1	0.94	0.19	54,54,54,54	0
54	MG	1A	3777	1/1	0.94	0.07	38,38,38,38	0
54	MG	1A	3030	1/1	0.94	0.05	35,35,35,35	0
54	MG	1A	3022	1/1	0.94	0.08	45,45,45,45	0
54	MG	2a	3108	1/1	0.94	0.16	71,71,71,71	0
54	MG	1A	3549	1/1	0.94	0.12	51,51,51,51	0
54	MG	1A	3103	1/1	0.94	0.10	45,45,45,45	0
54	MG	2A	3108	1/1	0.94	0.06	57,57,57,57	0
54	MG	1A	3365	1/1	0.94	0.07	24,24,24,24	0
54	MG	1a	1806	1/1	0.94	0.10	74,74,74,74	0
54	MG	2a	3114	1/1	0.94	0.10	79,79,79,79	0
54	MG	1A	3221	1/1	0.94	0.23	41,41,41,41	0
54	MG	1B	204	1/1	0.94	0.08	52,52,52,52	0
54	MG	1A	3787	1/1	0.94	0.11	50,50,50,50	0
54	MG	2A	3115	1/1	0.94	0.15	56,56,56,56	0
54	MG	2A	3627	1/1	0.94	0.08	71,71,71,71	0
54	MG	1A	3230	1/1	0.94	0.34	47,47,47,47	0
54	MG	1A	3294	1/1	0.94	0.16	57,57,57,57	0
54	MG	1A	3105	1/1	0.94	0.10	70,70,70,70	0
54	MG	1A	3937	1/1	0.94	0.12	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1a	1815	1/1	0.94	0.15	67,67,67,67	0
54	MG	1a	1816	1/1	0.94	0.16	65,65,65,65	0
54	MG	1A	3657	1/1	0.94	0.20	56,56,56,56	0
54	MG	2A	3127	1/1	0.94	0.11	65,65,65,65	0
54	MG	1A	3170	1/1	0.94	0.20	54,54,54,54	0
54	MG	1A	3109	1/1	0.94	0.20	38,38,38,38	0
54	MG	2A	3136	1/1	0.94	0.15	62,62,62,62	0
54	MG	1A	3372	1/1	0.94	0.08	34,34,34,34	0
54	MG	2A	3644	1/1	0.94	0.09	62,62,62,62	0
54	MG	1A	3944	1/1	0.94	0.07	64,64,64,64	0
54	MG	2A	3386	1/1	0.94	0.10	40,40,40,40	0
54	MG	2A	3648	1/1	0.94	0.08	65,65,65,65	0
54	MG	1A	3066	1/1	0.94	0.19	39,39,39,39	0
54	MG	1A	3669	1/1	0.94	0.13	65,65,65,65	0
54	MG	2A	3389	1/1	0.94	0.11	40,40,40,40	0
54	MG	2A	3390	1/1	0.94	0.08	37,37,37,37	0
54	MG	2A	3655	1/1	0.94	0.09	49,49,49,49	0
54	MG	1a	1670	1/1	0.94	0.10	69,69,69,69	0
54	MG	1B	222	1/1	0.94	0.09	58,58,58,58	0
54	MG	2A	3149	1/1	0.94	0.09	40,40,40,40	0
54	MG	1A	3238	1/1	0.94	0.31	42,42,42,42	0
54	MG	2A	3661	1/1	0.94	0.08	80,80,80,80	0
54	MG	1a	1673	1/1	0.94	0.17	63,63,63,63	0
54	MG	2A	3664	1/1	0.94	0.07	62,62,62,62	0
54	MG	1A	3800	1/1	0.94	0.07	82,82,82,82	0
54	MG	2a	3165	1/1	0.94	0.12	79,79,79,79	0
54	MG	2a	3166	1/1	0.94	0.15	68,68,68,68	0
54	MG	2a	3169	1/1	0.94	0.09	73,73,73,73	0
54	MG	1A	3564	1/1	0.94	0.08	44,44,44,44	0
54	MG	1A	3672	1/1	0.94	0.08	50,50,50,50	0
54	MG	2A	3155	1/1	0.94	0.12	67,67,67,67	0
54	MG	1A	3377	1/1	0.94	0.07	32,32,32,32	0
54	MG	2A	3159	1/1	0.94	0.15	71,71,71,71	0
54	MG	2a	3178	1/1	0.94	0.11	58,58,58,58	0
54	MG	1A	3113	1/1	0.94	0.10	45,45,45,45	0
54	MG	1A	3179	1/1	0.94	0.16	40,40,40,40	0
54	MG	1A	3118	1/1	0.94	0.11	41,41,41,41	0
54	MG	1A	3809	1/1	0.94	0.11	61,61,61,61	0
54	MG	1A	3381	1/1	0.94	0.10	41,41,41,41	0
54	MG	1A	3312	1/1	0.94	0.08	47,47,47,47	0
54	MG	2A	3168	1/1	0.94	0.08	51,51,51,51	0
54	MG	2a	3187	1/1	0.94	0.19	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2a	3188	1/1	0.94	0.20	65,65,65,65	0
54	MG	1A	3475	1/1	0.94	0.12	51,51,51,51	0
54	MG	2A	3171	1/1	0.94	0.08	51,51,51,51	0
54	MG	2A	3413	1/1	0.94	0.26	59,59,59,59	0
54	MG	1A	3384	1/1	0.94	0.14	53,53,53,53	0
54	MG	2A	3173	1/1	0.94	0.11	62,62,62,62	0
54	MG	1A	3815	1/1	0.94	0.11	42,42,42,42	0
54	MG	1A	3313	1/1	0.94	0.17	52,52,52,52	0
54	MG	2A	3418	1/1	0.94	0.06	31,31,31,31	0
54	MG	2f	201	1/1	0.94	0.10	56,56,56,56	0
54	MG	1A	3249	1/1	0.94	0.18	56,56,56,56	0
54	MG	1A	3316	1/1	0.94	0.22	53,53,53,53	0
54	MG	1A	3045	1/1	0.94	0.24	56,56,56,56	0
54	MG	2A	3425	1/1	0.94	0.13	70,70,70,70	0
54	MG	2A	3179	1/1	0.94	0.11	52,52,52,52	0
54	MG	2A	3428	1/1	0.94	0.14	62,62,62,62	0
54	MG	1a	1693	1/1	0.94	0.22	68,68,68,68	0
55	CPF	1A	4056	24/24	0.94	0.13	34,46,55,61	0
55	CPF	2A	3741	24/24	0.94	0.12	39,44,56,58	0
54	MG	1A	3391	1/1	0.94	0.07	30,30,30,30	0
54	MG	2A	3184	1/1	0.94	0.17	66,66,66,66	0
54	MG	1A	3825	1/1	0.94	0.34	45,45,45,45	0
54	MG	1A	3318	1/1	0.94	0.08	30,30,30,30	0
54	MG	1A	3827	1/1	0.94	0.12	59,59,59,59	0
54	MG	1F	317	1/1	0.94	0.11	43,43,43,43	0
54	MG	1A	3183	1/1	0.94	0.18	34,34,34,34	0
54	MG	1A	3395	1/1	0.94	0.08	37,37,37,37	0
54	MG	2A	3717	1/1	0.94	0.11	64,64,64,64	0
54	MG	1A	3921	1/1	0.95	0.24	44,44,44,44	0
54	MG	2V	201	1/1	0.95	0.13	60,60,60,60	0
54	MG	1A	3612	1/1	0.95	0.10	62,62,62,62	0
54	MG	1A	4039	1/1	0.95	0.17	63,63,63,63	0
54	MG	1A	3128	1/1	0.95	0.06	44,44,44,44	0
54	MG	2A	3571	1/1	0.95	0.09	53,53,53,53	0
54	MG	20	101	1/1	0.95	0.13	65,65,65,65	0
54	MG	2A	3183	1/1	0.95	0.10	61,61,61,61	0
54	MG	2A	3382	1/1	0.95	0.07	53,53,53,53	0
54	MG	1A	4041	1/1	0.95	0.31	45,45,45,45	0
54	MG	23	101	1/1	0.95	0.17	59,59,59,59	0
54	MG	1A	3180	1/1	0.95	0.07	57,57,57,57	0
54	MG	1A	3279	1/1	0.95	0.07	51,51,51,51	0
54	MG	28	101	1/1	0.95	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
54	MG	1A	3707	1/1	0.95	0.17	50,50,50,50	0
54	MG	1A	3393	1/1	0.95	0.07	44,44,44,44	0
54	MG	1A	4046	1/1	0.95	0.13	69,69,69,69	0
54	MG	1A	3339	1/1	0.95	0.12	37,37,37,37	0
54	MG	2A	3588	1/1	0.95	0.06	38,38,38,38	0
54	MG	1A	3056	1/1	0.95	0.18	36,36,36,36	0
54	MG	2a	3006	1/1	0.95	0.25	58,58,58,58	0
54	MG	2a	3007	1/1	0.95	0.09	71,71,71,71	0
54	MG	2A	3006	1/1	0.95	0.15	54,54,54,54	0
54	MG	1A	3816	1/1	0.95	0.09	53,53,53,53	0
54	MG	1A	4050	1/1	0.95	0.15	76,76,76,76	0
54	MG	1A	3396	1/1	0.95	0.07	24,24,24,24	0
54	MG	2A	3395	1/1	0.95	0.06	61,61,61,61	0
54	MG	2a	3015	1/1	0.95	0.12	53,53,53,53	0
54	MG	1A	3818	1/1	0.95	0.07	48,48,48,48	0
54	MG	1A	3942	1/1	0.95	0.06	48,48,48,48	0
54	MG	1A	3621	1/1	0.95	0.11	34,34,34,34	0
54	MG	2A	3199	1/1	0.95	0.06	53,53,53,53	0
54	MG	1A	4055	1/1	0.95	0.10	57,57,57,57	0
54	MG	2A	3603	1/1	0.95	0.07	36,36,36,36	0
54	MG	1A	3072	1/1	0.95	0.27	32,32,32,32	0
54	MG	1a	1619	1/1	0.95	0.06	47,47,47,47	0
54	MG	1B	201	1/1	0.95	0.14	54,54,54,54	0
54	MG	2A	3607	1/1	0.95	0.10	54,54,54,54	0
54	MG	1A	3002	1/1	0.95	0.11	53,53,53,53	0
54	MG	2A	3025	1/1	0.95	0.10	52,52,52,52	0
54	MG	1A	3547	1/1	0.95	0.08	41,41,41,41	0
54	MG	2A	3027	1/1	0.95	0.14	39,39,39,39	0
54	MG	1A	3401	1/1	0.95	0.11	26,26,26,26	0
54	MG	1a	1626	1/1	0.95	0.12	64,64,64,64	0
54	MG	1A	3140	1/1	0.95	0.18	41,41,41,41	0
54	MG	1a	1629	1/1	0.95	0.14	51,51,51,51	0
54	MG	1A	3629	1/1	0.95	0.15	60,60,60,60	0
54	MG	1A	3723	1/1	0.95	0.07	32,32,32,32	0
54	MG	1A	3032	1/1	0.95	0.21	51,51,51,51	0
54	MG	1A	3474	1/1	0.95	0.09	45,45,45,45	0
54	MG	1A	3954	1/1	0.95	0.05	31,31,31,31	0
54	MG	1A	3241	1/1	0.95	0.13	48,48,48,48	0
54	MG	2A	3224	1/1	0.95	0.12	56,56,56,56	0
54	MG	1A	3730	1/1	0.95	0.10	67,67,67,67	0
54	MG	1A	3957	1/1	0.95	0.10	55,55,55,55	0
54	MG	2a	3047	1/1	0.95	0.09	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3023	1/1	0.95	0.11	30,30,30,30	0
54	MG	1B	219	1/1	0.95	0.07	35,35,35,35	0
54	MG	1A	3477	1/1	0.95	0.14	52,52,52,52	0
54	MG	1A	3736	1/1	0.95	0.09	46,46,46,46	0
54	MG	1A	3291	1/1	0.95	0.15	36,36,36,36	0
54	MG	2A	3233	1/1	0.95	0.10	72,72,72,72	0
54	MG	2A	3634	1/1	0.95	0.07	62,62,62,62	0
54	MG	1a	1646	1/1	0.95	0.23	58,58,58,58	0
54	MG	1a	1647	1/1	0.95	0.15	51,51,51,51	0
54	MG	2A	3236	1/1	0.95	0.19	62,62,62,62	0
54	MG	1A	3077	1/1	0.95	0.21	35,35,35,35	0
54	MG	2A	3238	1/1	0.95	0.07	61,61,61,61	0
54	MG	1A	3410	1/1	0.95	0.10	32,32,32,32	0
54	MG	1B	227	1/1	0.95	0.06	61,61,61,61	0
54	MG	1A	3078	1/1	0.95	0.14	52,52,52,52	0
54	MG	1A	3843	1/1	0.95	0.07	43,43,43,43	0
54	MG	1A	3640	1/1	0.95	0.23	48,48,48,48	0
54	MG	2A	3058	1/1	0.95	0.08	56,56,56,56	0
54	MG	2a	3066	1/1	0.95	0.09	63,63,63,63	0
54	MG	1A	3412	1/1	0.95	0.07	25,25,25,25	0
54	MG	2A	3060	1/1	0.95	0.14	44,44,44,44	0
54	MG	2A	3251	1/1	0.95	0.19	63,63,63,63	0
54	MG	1A	3356	1/1	0.95	0.07	27,27,27,27	0
54	MG	1A	3246	1/1	0.95	0.30	48,48,48,48	0
54	MG	1a	1803	1/1	0.95	0.07	50,50,50,50	0
54	MG	1A	3972	1/1	0.95	0.06	33,33,33,33	0
54	MG	2A	3659	1/1	0.95	0.07	34,34,34,34	0
54	MG	1A	3644	1/1	0.95	0.13	49,49,49,49	0
54	MG	2A	3258	1/1	0.95	0.35	44,44,44,44	0
54	MG	2A	3066	1/1	0.95	0.13	61,61,61,61	0
54	MG	1A	3751	1/1	0.95	0.06	32,32,32,32	0
54	MG	1A	3418	1/1	0.95	0.07	42,42,42,42	0
54	MG	2A	3667	1/1	0.95	0.07	62,62,62,62	0
54	MG	1D	317	1/1	0.95	0.09	52,52,52,52	0
54	MG	2A	3073	1/1	0.95	0.26	49,49,49,49	0
54	MG	1A	3247	1/1	0.95	0.10	42,42,42,42	0
54	MG	2A	3673	1/1	0.95	0.07	41,41,41,41	0
54	MG	2a	3089	1/1	0.95	0.05	60,60,60,60	0
54	MG	1A	3491	1/1	0.95	0.12	28,28,28,28	0
54	MG	1A	3248	1/1	0.95	0.12	45,45,45,45	0
54	MG	2A	3077	1/1	0.95	0.12	61,61,61,61	0
54	MG	2A	3271	1/1	0.95	0.06	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3078	1/1	0.95	0.07	53,53,53,53	0
54	MG	1a	1812	1/1	0.95	0.08	63,63,63,63	0
54	MG	1A	3192	1/1	0.95	0.22	45,45,45,45	0
54	MG	1A	3862	1/1	0.95	0.06	45,45,45,45	0
54	MG	1A	3363	1/1	0.95	0.13	63,63,63,63	0
54	MG	1A	3759	1/1	0.95	0.06	48,48,48,48	0
54	MG	1F	313	1/1	0.95	0.28	48,48,48,48	0
54	MG	2a	3101	1/1	0.95	0.09	66,66,66,66	0
54	MG	1A	3025	1/1	0.95	0.20	41,41,41,41	0
54	MG	2A	3088	1/1	0.95	0.24	57,57,57,57	0
54	MG	1A	3761	1/1	0.95	0.08	51,51,51,51	0
54	MG	2A	3689	1/1	0.95	0.08	59,59,59,59	0
54	MG	2A	3690	1/1	0.95	0.07	56,56,56,56	0
54	MG	1A	3081	1/1	0.95	0.51	47,47,47,47	0
54	MG	1A	3500	1/1	0.95	0.06	24,24,24,24	0
54	MG	1F	318	1/1	0.95	0.08	66,66,66,66	0
54	MG	1F	319	1/1	0.95	0.07	53,53,53,53	0
54	MG	1A	3020	1/1	0.95	0.31	41,41,41,41	0
54	MG	1A	3115	1/1	0.95	0.20	35,35,35,35	0
54	MG	1G	203	1/1	0.95	0.11	64,64,64,64	0
54	MG	1A	3660	1/1	0.95	0.23	53,53,53,53	0
54	MG	2A	3292	1/1	0.95	0.07	59,59,59,59	0
54	MG	1A	3992	1/1	0.95	0.06	19,19,19,19	0
54	MG	1A	3160	1/1	0.95	0.13	56,56,56,56	0
54	MG	2A	3295	1/1	0.95	0.10	44,44,44,44	0
54	MG	2A	3101	1/1	0.95	0.12	78,78,78,78	0
54	MG	1A	3769	1/1	0.95	0.06	29,29,29,29	0
54	MG	1A	3084	1/1	0.95	0.07	39,39,39,39	0
54	MG	1A	3583	1/1	0.95	0.11	37,37,37,37	0
54	MG	2A	3714	1/1	0.95	0.12	65,65,65,65	0
54	MG	2a	3135	1/1	0.95	0.08	69,69,69,69	0
54	MG	1A	3666	1/1	0.95	0.08	48,48,48,48	0
54	MG	1P	205	1/1	0.95	0.08	74,74,74,74	0
54	MG	1A	3201	1/1	0.95	0.21	49,49,49,49	0
54	MG	1A	3087	1/1	0.95	0.17	39,39,39,39	0
54	MG	1a	1845	1/1	0.95	0.19	60,60,60,60	0
54	MG	1A	3204	1/1	0.95	0.19	50,50,50,50	0
54	MG	1A	3779	1/1	0.95	0.11	51,51,51,51	0
54	MG	2A	3117	1/1	0.95	0.09	44,44,44,44	0
54	MG	1Q	205	1/1	0.95	0.12	54,54,54,54	0
54	MG	2A	3120	1/1	0.95	0.18	53,53,53,53	0
54	MG	1A	3053	1/1	0.95	0.10	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3122	1/1	0.95	0.36	45,45,45,45	0
54	MG	1A	3887	1/1	0.95	0.06	68,68,68,68	0
54	MG	1a	1701	1/1	0.95	0.11	66,66,66,66	0
54	MG	1R	206	1/1	0.95	0.19	58,58,58,58	0
54	MG	1A	3166	1/1	0.95	0.09	41,41,41,41	0
54	MG	1a	1704	1/1	0.95	0.08	46,46,46,46	0
54	MG	2A	3128	1/1	0.95	0.24	62,62,62,62	0
54	MG	2A	3130	1/1	0.95	0.13	64,64,64,64	0
54	MG	2A	3516	1/1	0.95	0.12	67,67,67,67	0
54	MG	2A	3131	1/1	0.95	0.18	64,64,64,64	0
54	MG	1A	3321	1/1	0.95	0.14	55,55,55,55	0
54	MG	1A	3323	1/1	0.95	0.21	37,37,37,37	0
54	MG	1A	3324	1/1	0.95	0.08	33,33,33,33	0
54	MG	1U	203	1/1	0.95	0.34	40,40,40,40	0
54	MG	2a	3168	1/1	0.95	0.08	71,71,71,71	0
54	MG	1U	205	1/1	0.95	0.33	33,33,33,33	0
54	MG	2a	3170	1/1	0.95	0.11	68,68,68,68	0
54	MG	1U	206	1/1	0.95	0.23	43,43,43,43	0
54	MG	2A	3143	1/1	0.95	0.13	42,42,42,42	0
54	MG	2B	205	1/1	0.95	0.15	53,53,53,53	0
54	MG	2a	3175	1/1	0.95	0.10	75,75,75,75	0
54	MG	2A	3145	1/1	0.95	0.17	52,52,52,52	0
54	MG	1A	3067	1/1	0.95	0.08	53,53,53,53	0
54	MG	1V	203	1/1	0.95	0.14	44,44,44,44	0
54	MG	1A	3596	1/1	0.95	0.08	19,19,19,19	0
54	MG	1A	3894	1/1	0.95	0.12	38,38,38,38	0
54	MG	1A	3209	1/1	0.95	0.31	43,43,43,43	0
54	MG	2B	212	1/1	0.95	0.17	72,72,72,72	0
54	MG	1A	3171	1/1	0.95	0.20	36,36,36,36	0
54	MG	1W	203	1/1	0.95	0.17	35,35,35,35	0
54	MG	1A	3037	1/1	0.95	0.09	53,53,53,53	0
54	MG	1A	3903	1/1	0.95	0.06	42,42,42,42	0
54	MG	1A	3385	1/1	0.95	0.12	58,58,58,58	0
54	MG	2A	3156	1/1	0.95	0.20	46,46,46,46	0
54	MG	1A	3094	1/1	0.95	0.11	38,38,38,38	0
54	MG	2D	305	1/1	0.95	0.39	48,48,48,48	0
54	MG	1A	3521	1/1	0.95	0.06	64,64,64,64	0
54	MG	2D	307	1/1	0.95	0.25	51,51,51,51	0
54	MG	1A	3215	1/1	0.95	0.15	38,38,38,38	0
54	MG	2A	3355	1/1	0.95	0.09	53,53,53,53	0
54	MG	11	103	1/1	0.95	0.09	55,55,55,55	0
54	MG	2A	3359	1/1	0.95	0.09	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3388	1/1	0.95	0.07	31,31,31,31	0
54	MG	1A	3525	1/1	0.95	0.10	63,63,63,63	0
54	MG	2A	3164	1/1	0.95	0.12	55,55,55,55	0
54	MG	1A	4027	1/1	0.95	0.10	59,59,59,59	0
54	MG	1A	3527	1/1	0.95	0.10	60,60,60,60	0
54	MG	1A	4029	1/1	0.95	0.09	46,46,46,46	0
54	MG	2F	301	1/1	0.95	0.32	48,48,48,48	0
54	MG	1A	3453	1/1	0.95	0.11	55,55,55,55	0
54	MG	2A	3555	1/1	0.95	0.08	72,72,72,72	0
54	MG	1a	1739	1/1	0.95	0.12	66,66,66,66	0
54	MG	15	101	1/1	0.95	0.13	41,41,41,41	0
54	MG	1A	3696	1/1	0.95	0.08	56,56,56,56	0
54	MG	1A	3915	1/1	0.95	0.15	25,25,25,25	0
54	MG	1A	3126	1/1	0.95	0.13	40,40,40,40	0
54	MG	2A	3374	1/1	0.95	0.07	54,54,54,54	0
57	ARG	1B	230	12/12	0.95	0.10	37,56,63,63	0
54	MG	2A	3563	1/1	0.95	0.07	38,38,38,38	0
54	MG	1A	3917	1/1	0.95	0.12	29,29,29,29	0
54	MG	1A	3457	1/1	0.95	0.09	64,64,64,64	0
54	MG	2A	3617	1/1	0.96	0.08	68,68,68,68	0
54	MG	1A	3780	1/1	0.96	0.12	48,48,48,48	0
54	MG	2A	3240	1/1	0.96	0.32	43,43,43,43	0
54	MG	1A	3024	1/1	0.96	0.15	26,26,26,26	0
54	MG	2A	3068	1/1	0.96	0.25	41,41,41,41	0
54	MG	1A	3358	1/1	0.96	0.09	34,34,34,34	0
54	MG	1A	3498	1/1	0.96	0.12	58,58,58,58	0
54	MG	1A	3499	1/1	0.96	0.10	51,51,51,51	0
54	MG	2A	3246	1/1	0.96	0.10	60,60,60,60	0
54	MG	1P	202	1/1	0.96	0.18	38,38,38,38	0
54	MG	1A	3674	1/1	0.96	0.17	48,48,48,48	0
54	MG	1A	3786	1/1	0.96	0.08	51,51,51,51	0
54	MG	1A	4013	1/1	0.96	0.08	47,47,47,47	0
54	MG	1A	3111	1/1	0.96	0.17	39,39,39,39	0
54	MG	1A	3086	1/1	0.96	0.06	49,49,49,49	0
54	MG	1A	3502	1/1	0.96	0.07	41,41,41,41	0
54	MG	1A	3361	1/1	0.96	0.09	50,50,50,50	0
54	MG	1A	3015	1/1	0.96	0.06	35,35,35,35	0
54	MG	2A	3084	1/1	0.96	0.08	42,42,42,42	0
54	MG	1a	1824	1/1	0.96	0.08	55,55,55,55	0
54	MG	1R	203	1/1	0.96	0.09	56,56,56,56	0
54	MG	1A	3906	1/1	0.96	0.07	64,64,64,64	0
54	MG	1a	1685	1/1	0.96	0.15	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1R	205	1/1	0.96	0.15	45,45,45,45	0
54	MG	1A	3295	1/1	0.96	0.11	41,41,41,41	0
54	MG	1A	3242	1/1	0.96	0.33	43,43,43,43	0
54	MG	1a	1832	1/1	0.96	0.06	75,75,75,75	0
54	MG	1T	203	1/1	0.96	0.15	65,65,65,65	0
54	MG	2A	3651	1/1	0.96	0.07	57,57,57,57	0
54	MG	1A	3017	1/1	0.96	0.18	34,34,34,34	0
54	MG	2A	3095	1/1	0.96	0.12	51,51,51,51	0
54	MG	1A	3191	1/1	0.96	0.19	38,38,38,38	0
54	MG	1A	3797	1/1	0.96	0.07	77,77,77,77	0
54	MG	1A	3152	1/1	0.96	0.22	33,33,33,33	0
54	MG	1A	3431	1/1	0.96	0.08	31,31,31,31	0
54	MG	1A	3304	1/1	0.96	0.22	39,39,39,39	0
54	MG	1a	1843	1/1	0.96	0.07	58,58,58,58	0
54	MG	2A	3102	1/1	0.96	0.11	56,56,56,56	0
54	MG	2A	3104	1/1	0.96	0.09	72,72,72,72	0
54	MG	2A	3105	1/1	0.96	0.18	55,55,55,55	0
54	MG	1A	3154	1/1	0.96	0.32	38,38,38,38	0
54	MG	1A	3306	1/1	0.96	0.14	24,24,24,24	0
54	MG	1A	4032	1/1	0.96	0.07	59,59,59,59	0
54	MG	1A	3155	1/1	0.96	0.18	42,42,42,42	0
54	MG	1A	3920	1/1	0.96	0.07	53,53,53,53	0
54	MG	1A	3116	1/1	0.96	0.08	39,39,39,39	0
54	MG	1W	202	1/1	0.96	0.11	54,54,54,54	0
54	MG	1A	3922	1/1	0.96	0.07	52,52,52,52	0
54	MG	2A	3114	1/1	0.96	0.10	49,49,49,49	0
54	MG	1A	3117	1/1	0.96	0.11	41,41,41,41	0
54	MG	10	101	1/1	0.96	0.13	47,47,47,47	0
54	MG	1A	3439	1/1	0.96	0.10	56,56,56,56	0
54	MG	1A	3159	1/1	0.96	0.10	38,38,38,38	0
54	MG	2A	3119	1/1	0.96	0.07	38,38,38,38	0
54	MG	1A	3198	1/1	0.96	0.19	45,45,45,45	0
54	MG	2A	3484	1/1	0.96	0.07	58,58,58,58	0
54	MG	1A	3933	1/1	0.96	0.06	36,36,36,36	0
54	MG	1A	3038	1/1	0.96	0.16	49,49,49,49	0
54	MG	1A	3029	1/1	0.96	0.11	40,40,40,40	0
54	MG	1A	3446	1/1	0.96	0.07	58,58,58,58	0
54	MG	1A	3524	1/1	0.96	0.14	51,51,51,51	0
54	MG	13	101	1/1	0.96	0.15	36,36,36,36	0
54	MG	1A	3043	1/1	0.96	0.12	17,17,17,17	0
54	MG	1A	3526	1/1	0.96	0.11	27,27,27,27	0
54	MG	1A	3614	1/1	0.96	0.26	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1a	1723	1/1	0.96	0.06	60,60,60,60	0
54	MG	1A	3819	1/1	0.96	0.09	48,48,48,48	0
54	MG	2a	3080	1/1	0.96	0.06	75,75,75,75	0
54	MG	1A	3256	1/1	0.96	0.08	44,44,44,44	0
54	MG	15	102	1/1	0.96	0.18	39,39,39,39	0
54	MG	2A	3699	1/1	0.96	0.06	66,66,66,66	0
54	MG	1A	3528	1/1	0.96	0.07	52,52,52,52	0
54	MG	2a	3087	1/1	0.96	0.06	53,53,53,53	0
54	MG	1A	3530	1/1	0.96	0.28	31,31,31,31	0
54	MG	1A	3060	1/1	0.96	0.07	62,62,62,62	0
54	MG	2A	3704	1/1	0.96	0.11	60,60,60,60	0
54	MG	1A	3824	1/1	0.96	0.08	41,41,41,41	0
54	MG	2A	3144	1/1	0.96	0.14	54,54,54,54	0
54	MG	1A	3008	1/1	0.96	0.05	45,45,45,45	0
54	MG	2A	3708	1/1	0.96	0.06	74,74,74,74	0
54	MG	1A	3206	1/1	0.96	0.13	47,47,47,47	0
54	MG	2A	3324	1/1	0.96	0.09	35,35,35,35	0
54	MG	17	105	1/1	0.96	0.30	49,49,49,49	0
54	MG	1d	304	1/1	0.96	0.17	65,65,65,65	0
54	MG	2A	3713	1/1	0.96	0.06	69,69,69,69	0
54	MG	1A	3721	1/1	0.96	0.17	40,40,40,40	0
54	MG	1A	3535	1/1	0.96	0.07	56,56,56,56	0
54	MG	1A	3167	1/1	0.96	0.09	51,51,51,51	0
54	MG	2A	3331	1/1	0.96	0.08	37,37,37,37	0
54	MG	1A	3012	1/1	0.96	0.10	44,44,44,44	0
54	MG	2a	3106	1/1	0.96	0.06	66,66,66,66	0
54	MG	19	101	1/1	0.96	0.18	56,56,56,56	0
54	MG	2A	3334	1/1	0.96	0.09	37,37,37,37	0
54	MG	1g	203	1/1	0.96	0.09	66,66,66,66	0
54	MG	1A	3125	1/1	0.96	0.27	46,46,46,46	0
54	MG	1A	3100	1/1	0.96	0.34	38,38,38,38	0
54	MG	1A	3729	1/1	0.96	0.10	52,52,52,52	0
54	MG	2A	3726	1/1	0.96	0.06	61,61,61,61	0
54	MG	1k	201	1/1	0.96	0.10	46,46,46,46	0
54	MG	1B	208	1/1	0.96	0.06	45,45,45,45	0
54	MG	2a	3116	1/1	0.96	0.09	58,58,58,58	0
54	MG	1A	3211	1/1	0.96	0.21	36,36,36,36	0
54	MG	1A	3005	1/1	0.96	0.10	29,29,29,29	0
54	MG	1a	1606	1/1	0.96	0.19	55,55,55,55	0
54	MG	1B	211	1/1	0.96	0.06	61,61,61,61	0
54	MG	2A	3733	1/1	0.96	0.08	64,64,64,64	0
54	MG	2A	3165	1/1	0.96	0.17	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3348	1/1	0.96	0.05	38,38,38,38	0
54	MG	1A	3542	1/1	0.96	0.27	35,35,35,35	0
54	MG	2a	3128	1/1	0.96	0.09	71,71,71,71	0
54	MG	1a	1609	1/1	0.96	0.06	60,60,60,60	0
54	MG	1A	3268	1/1	0.96	0.07	35,35,35,35	0
54	MG	1A	3737	1/1	0.96	0.21	41,41,41,41	0
54	MG	1a	1613	1/1	0.96	0.11	31,31,31,31	0
54	MG	1A	3080	1/1	0.96	0.33	46,46,46,46	0
54	MG	1A	3633	1/1	0.96	0.08	34,34,34,34	0
54	MG	1A	3065	1/1	0.96	0.22	35,35,35,35	0
54	MG	1A	3136	1/1	0.96	0.06	41,41,41,41	0
54	MG	1A	3272	1/1	0.96	0.32	39,39,39,39	0
54	MG	2A	3005	1/1	0.96	0.10	59,59,59,59	0
54	MG	1A	3397	1/1	0.96	0.10	27,27,27,27	0
54	MG	2A	3007	1/1	0.96	0.06	42,42,42,42	0
54	MG	1A	3217	1/1	0.96	0.17	42,42,42,42	0
54	MG	1B	225	1/1	0.96	0.05	44,44,44,44	0
54	MG	1A	3852	1/1	0.96	0.12	43,43,43,43	0
54	MG	1A	3274	1/1	0.96	0.10	63,63,63,63	0
54	MG	1a	1625	1/1	0.96	0.12	55,55,55,55	0
54	MG	1A	3552	1/1	0.96	0.08	55,55,55,55	0
54	MG	1A	3750	1/1	0.96	0.10	46,46,46,46	0
54	MG	1A	3400	1/1	0.96	0.07	45,45,45,45	0
54	MG	1D	305	1/1	0.96	0.12	46,46,46,46	0
54	MG	1A	3752	1/1	0.96	0.09	39,39,39,39	0
54	MG	2D	301	1/1	0.96	0.20	48,48,48,48	0
54	MG	2a	3159	1/1	0.96	0.11	59,59,59,59	0
54	MG	2D	302	1/1	0.96	0.13	46,46,46,46	0
54	MG	1A	3275	1/1	0.96	0.08	33,33,33,33	0
54	MG	1A	3050	1/1	0.96	0.21	32,32,32,32	0
54	MG	1A	3222	1/1	0.96	0.29	42,42,42,42	0
54	MG	1a	1636	1/1	0.96	0.07	40,40,40,40	0
54	MG	2a	3167	1/1	0.96	0.06	51,51,51,51	0
54	MG	1A	3224	1/1	0.96	0.25	42,42,42,42	0
54	MG	2A	3030	1/1	0.96	0.14	33,33,33,33	0
54	MG	1A	3405	1/1	0.96	0.05	24,24,24,24	0
54	MG	2a	3171	1/1	0.96	0.07	61,61,61,61	0
54	MG	1A	3345	1/1	0.96	0.11	50,50,50,50	0
54	MG	1A	3407	1/1	0.96	0.07	26,26,26,26	0
54	MG	1A	3482	1/1	0.96	0.05	26,26,26,26	0
54	MG	1A	3280	1/1	0.96	0.26	52,52,52,52	0
54	MG	1a	1643	1/1	0.96	0.19	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3225	1/1	0.96	0.13	59,59,59,59	0
54	MG	1E	305	1/1	0.96	0.11	27,27,27,27	0
54	MG	1A	3226	1/1	0.96	0.20	34,34,34,34	0
54	MG	1a	1786	1/1	0.96	0.17	60,60,60,60	0
54	MG	1A	3352	1/1	0.96	0.09	29,29,29,29	0
54	MG	1A	3568	1/1	0.96	0.06	52,52,52,52	0
54	MG	1F	304	1/1	0.96	0.12	34,34,34,34	0
54	MG	1F	308	1/1	0.96	0.18	31,31,31,31	0
54	MG	1F	310	1/1	0.96	0.20	54,54,54,54	0
54	MG	2A	3585	1/1	0.96	0.07	61,61,61,61	0
54	MG	1A	3569	1/1	0.96	0.11	51,51,51,51	0
54	MG	1a	1793	1/1	0.96	0.06	74,74,74,74	0
54	MG	2a	3190	1/1	0.96	0.10	62,62,62,62	0
54	MG	2Q	203	1/1	0.96	0.10	61,61,61,61	0
54	MG	2A	3049	1/1	0.96	0.16	47,47,47,47	0
54	MG	2A	3217	1/1	0.96	0.08	51,51,51,51	0
54	MG	1A	3659	1/1	0.96	0.11	68,68,68,68	0
54	MG	2A	3594	1/1	0.96	0.10	58,58,58,58	0
54	MG	2A	3051	1/1	0.96	0.10	62,62,62,62	0
54	MG	1A	3106	1/1	0.96	0.19	34,34,34,34	0
54	MG	2W	201	1/1	0.96	0.27	49,49,49,49	0
54	MG	2A	3222	1/1	0.96	0.07	52,52,52,52	0
54	MG	2A	3223	1/1	0.96	0.27	40,40,40,40	0
54	MG	1A	3571	1/1	0.96	0.19	46,46,46,46	0
54	MG	1a	1797	1/1	0.96	0.10	56,56,56,56	0
54	MG	1a	1798	1/1	0.96	0.07	80,80,80,80	0
54	MG	1A	3663	1/1	0.96	0.07	29,29,29,29	0
54	MG	1A	3998	1/1	0.96	0.09	83,83,83,83	0
54	MG	1a	1661	1/1	0.96	0.12	72,72,72,72	0
54	MG	23	102	1/1	0.96	0.10	48,48,48,48	0
54	MG	1A	3999	1/1	0.96	0.09	62,62,62,62	0
54	MG	2A	3231	1/1	0.96	0.09	41,41,41,41	0
56	MPD	18	104	8/8	0.96	0.12	32,39,43,43	0
54	MG	1A	3413	1/1	0.96	0.06	42,42,42,42	0
54	MG	1A	3107	1/1	0.96	0.24	42,42,42,42	0
54	MG	1A	3285	1/1	0.96	0.10	64,64,64,64	0
54	MG	2A	3419	1/1	0.96	0.15	55,55,55,55	0
54	MG	1a	1666	1/1	0.96	0.10	63,63,63,63	0
54	MG	1A	3417	1/1	0.96	0.09	36,36,36,36	0
54	MG	1A	3184	1/1	0.96	0.18	46,46,46,46	0
54	MG	2A	3423	1/1	0.96	0.23	66,66,66,66	0
54	MG	2A	3139	1/1	0.97	0.15	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3140	1/1	0.97	0.17	54,54,54,54	0
54	MG	2a	3024	1/1	0.97	0.19	65,65,65,65	0
54	MG	2A	3296	1/1	0.97	0.10	39,39,39,39	0
54	MG	1N	201	1/1	0.97	0.11	46,46,46,46	0
54	MG	1N	202	1/1	0.97	0.10	42,42,42,42	0
54	MG	1A	3003	1/1	0.97	0.05	27,27,27,27	0
54	MG	2a	3029	1/1	0.97	0.08	40,40,40,40	0
54	MG	1A	3926	1/1	0.97	0.04	66,66,66,66	0
54	MG	1A	3928	1/1	0.97	0.07	56,56,56,56	0
54	MG	1P	201	1/1	0.97	0.25	38,38,38,38	0
54	MG	1A	3929	1/1	0.97	0.07	58,58,58,58	0
54	MG	1A	3293	1/1	0.97	0.17	49,49,49,49	0
54	MG	2A	3004	1/1	0.97	0.07	45,45,45,45	0
54	MG	1P	204	1/1	0.97	0.17	52,52,52,52	0
54	MG	1A	3588	1/1	0.97	0.10	45,45,45,45	0
54	MG	1A	3743	1/1	0.97	0.10	53,53,53,53	0
54	MG	1Q	201	1/1	0.97	0.12	36,36,36,36	0
54	MG	2A	3665	1/1	0.97	0.09	66,66,66,66	0
54	MG	1A	3185	1/1	0.97	0.12	50,50,50,50	0
54	MG	2A	3312	1/1	0.97	0.14	44,44,44,44	0
54	MG	1A	3590	1/1	0.97	0.10	50,50,50,50	0
54	MG	2a	3044	1/1	0.97	0.21	60,60,60,60	0
54	MG	2A	3011	1/1	0.97	0.07	41,41,41,41	0
54	MG	1a	1658	1/1	0.97	0.08	72,72,72,72	0
54	MG	2A	3014	1/1	0.97	0.08	49,49,49,49	0
54	MG	2A	3317	1/1	0.97	0.10	53,53,53,53	0
54	MG	2A	3015	1/1	0.97	0.19	39,39,39,39	0
54	MG	1A	3830	1/1	0.97	0.08	36,36,36,36	0
54	MG	1A	3348	1/1	0.97	0.07	56,56,56,56	0
54	MG	1A	3592	1/1	0.97	0.11	54,54,54,54	0
54	MG	2A	3491	1/1	0.97	0.07	42,42,42,42	0
54	MG	1A	3939	1/1	0.97	0.05	61,61,61,61	0
54	MG	2A	3323	1/1	0.97	0.10	36,36,36,36	0
54	MG	2A	3020	1/1	0.97	0.16	49,49,49,49	0
54	MG	2A	3021	1/1	0.97	0.07	43,43,43,43	0
54	MG	1A	3085	1/1	0.97	0.15	44,44,44,44	0
54	MG	1A	3296	1/1	0.97	0.11	33,33,33,33	0
54	MG	1A	3057	1/1	0.97	0.05	35,35,35,35	0
54	MG	1A	3298	1/1	0.97	0.21	60,60,60,60	0
54	MG	1T	202	1/1	0.97	0.08	65,65,65,65	0
54	MG	1A	3127	1/1	0.97	0.29	40,40,40,40	0
54	MG	1A	3533	1/1	0.97	0.05	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3029	1/1	0.97	0.07	45,45,45,45	0
54	MG	1A	3046	1/1	0.97	0.18	42,42,42,42	0
54	MG	1A	3301	1/1	0.97	0.26	44,44,44,44	0
54	MG	2A	3506	1/1	0.97	0.08	62,62,62,62	0
54	MG	2A	3338	1/1	0.97	0.10	41,41,41,41	0
54	MG	1U	202	1/1	0.97	0.13	33,33,33,33	0
54	MG	1A	3948	1/1	0.97	0.11	62,62,62,62	0
54	MG	2A	3181	1/1	0.97	0.12	58,58,58,58	0
54	MG	1U	204	1/1	0.97	0.25	40,40,40,40	0
54	MG	1A	3841	1/1	0.97	0.12	49,49,49,49	0
54	MG	1A	3257	1/1	0.97	0.22	39,39,39,39	0
54	MG	2A	3514	1/1	0.97	0.11	62,62,62,62	0
54	MG	1U	207	1/1	0.97	0.24	40,40,40,40	0
54	MG	1A	3844	1/1	0.97	0.08	47,47,47,47	0
54	MG	1A	3218	1/1	0.97	0.06	43,43,43,43	0
54	MG	2A	3040	1/1	0.97	0.11	44,44,44,44	0
54	MG	2a	3082	1/1	0.97	0.06	80,80,80,80	0
54	MG	1A	3219	1/1	0.97	0.10	37,37,37,37	0
54	MG	1A	3220	1/1	0.97	0.06	41,41,41,41	0
54	MG	1A	3019	1/1	0.97	0.21	33,33,33,33	0
54	MG	1A	3132	1/1	0.97	0.07	51,51,51,51	0
54	MG	1A	3419	1/1	0.97	0.05	29,29,29,29	0
54	MG	1A	3609	1/1	0.97	0.06	40,40,40,40	0
54	MG	1A	3680	1/1	0.97	0.11	57,57,57,57	0
54	MG	1A	3855	1/1	0.97	0.12	50,50,50,50	0
54	MG	2A	3719	1/1	0.97	0.09	66,66,66,66	0
54	MG	1A	3263	1/1	0.97	0.20	38,38,38,38	0
54	MG	10	103	1/1	0.97	0.13	52,52,52,52	0
54	MG	10	104	1/1	0.97	0.09	50,50,50,50	0
54	MG	1A	3311	1/1	0.97	0.17	55,55,55,55	0
54	MG	2A	3201	1/1	0.97	0.20	56,56,56,56	0
54	MG	1a	1692	1/1	0.97	0.11	66,66,66,66	0
54	MG	1a	1819	1/1	0.97	0.07	61,61,61,61	0
54	MG	1A	3223	1/1	0.97	0.16	41,41,41,41	0
54	MG	2A	3537	1/1	0.97	0.06	63,63,63,63	0
54	MG	1A	3016	1/1	0.97	0.26	38,38,38,38	0
54	MG	1A	3488	1/1	0.97	0.09	33,33,33,33	0
54	MG	11	102	1/1	0.97	0.07	59,59,59,59	0
54	MG	2a	3104	1/1	0.97	0.09	81,81,81,81	0
54	MG	2A	3541	1/1	0.97	0.07	64,64,64,64	0
54	MG	1A	3134	1/1	0.97	0.10	38,38,38,38	0
54	MG	2A	3373	1/1	0.97	0.06	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3490	1/1	0.97	0.06	63,63,63,63	0
54	MG	1A	3776	1/1	0.97	0.05	45,45,45,45	0
54	MG	1A	3315	1/1	0.97	0.09	55,55,55,55	0
54	MG	1A	3971	1/1	0.97	0.12	45,45,45,45	0
54	MG	1A	3049	1/1	0.97	0.22	40,40,40,40	0
54	MG	2A	3214	1/1	0.97	0.07	49,49,49,49	0
54	MG	1a	1830	1/1	0.97	0.11	64,64,64,64	0
54	MG	1A	3493	1/1	0.97	0.07	40,40,40,40	0
54	MG	1A	3695	1/1	0.97	0.12	48,48,48,48	0
54	MG	1A	3228	1/1	0.97	0.28	44,44,44,44	0
54	MG	2A	3219	1/1	0.97	0.07	51,51,51,51	0
54	MG	2A	3069	1/1	0.97	0.10	55,55,55,55	0
54	MG	1A	3697	1/1	0.97	0.05	61,61,61,61	0
54	MG	1a	1707	1/1	0.97	0.08	45,45,45,45	0
54	MG	15	103	1/1	0.97	0.30	43,43,43,43	0
54	MG	1A	3698	1/1	0.97	0.19	50,50,50,50	0
54	MG	1A	3556	1/1	0.97	0.09	64,64,64,64	0
54	MG	1a	1839	1/1	0.97	0.09	55,55,55,55	0
54	MG	1a	1840	1/1	0.97	0.05	64,64,64,64	0
54	MG	2a	3132	1/1	0.97	0.08	52,52,52,52	0
54	MG	1A	3229	1/1	0.97	0.23	40,40,40,40	0
54	MG	2A	3566	1/1	0.97	0.10	59,59,59,59	0
54	MG	1A	3137	1/1	0.97	0.05	35,35,35,35	0
54	MG	1A	3168	1/1	0.97	0.09	33,33,33,33	0
54	MG	1A	3233	1/1	0.97	0.27	38,38,38,38	0
54	MG	2B	218	1/1	0.97	0.07	55,55,55,55	0
54	MG	2a	3140	1/1	0.97	0.07	72,72,72,72	0
54	MG	2A	3082	1/1	0.97	0.50	49,49,49,49	0
54	MG	2A	3398	1/1	0.97	0.17	66,66,66,66	0
54	MG	17	104	1/1	0.97	0.11	38,38,38,38	0
54	MG	1A	3322	1/1	0.97	0.08	44,44,44,44	0
54	MG	1A	3705	1/1	0.97	0.12	43,43,43,43	0
54	MG	1A	3706	1/1	0.97	0.09	53,53,53,53	0
54	MG	1A	3885	1/1	0.97	0.06	44,44,44,44	0
54	MG	1D	301	1/1	0.97	0.29	44,44,44,44	0
54	MG	2A	3239	1/1	0.97	0.48	46,46,46,46	0
54	MG	2a	3150	1/1	0.97	0.06	78,78,78,78	0
54	MG	1A	3062	1/1	0.97	0.12	44,44,44,44	0
54	MG	2a	3152	1/1	0.97	0.10	57,57,57,57	0
54	MG	1a	1854	1/1	0.97	0.06	62,62,62,62	0
54	MG	1A	3031	1/1	0.97	0.08	22,22,22,22	0
54	MG	1A	3051	1/1	0.97	0.33	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3382	1/1	0.97	0.06	50,50,50,50	0
54	MG	2E	303	1/1	0.97	0.09	47,47,47,47	0
54	MG	1A	3276	1/1	0.97	0.10	37,37,37,37	0
54	MG	1A	3097	1/1	0.97	0.19	36,36,36,36	0
54	MG	2E	306	1/1	0.97	0.10	32,32,32,32	0
54	MG	1A	3714	1/1	0.97	0.04	39,39,39,39	0
54	MG	2a	3163	1/1	0.97	0.05	71,71,71,71	0
54	MG	2A	3248	1/1	0.97	0.11	57,57,57,57	0
54	MG	2F	302	1/1	0.97	0.06	44,44,44,44	0
54	MG	1A	3239	1/1	0.97	0.19	37,37,37,37	0
54	MG	2F	304	1/1	0.97	0.17	46,46,46,46	0
54	MG	1A	3240	1/1	0.97	0.17	64,64,64,64	0
54	MG	1A	3802	1/1	0.97	0.10	29,29,29,29	0
54	MG	1A	3717	1/1	0.97	0.07	48,48,48,48	0
54	MG	1E	302	1/1	0.97	0.09	41,41,41,41	0
54	MG	1A	3176	1/1	0.97	0.28	46,46,46,46	0
54	MG	1A	3203	1/1	0.97	0.17	40,40,40,40	0
54	MG	2Q	201	1/1	0.97	0.06	64,64,64,64	0
54	MG	1A	3177	1/1	0.97	0.24	53,53,53,53	0
54	MG	1A	3807	1/1	0.97	0.04	57,57,57,57	0
54	MG	2A	3424	1/1	0.97	0.07	39,39,39,39	0
54	MG	1A	3333	1/1	0.97	0.14	52,52,52,52	0
54	MG	1A	3334	1/1	0.97	0.05	28,28,28,28	0
54	MG	2T	202	1/1	0.97	0.19	68,68,68,68	0
54	MG	2A	3427	1/1	0.97	0.11	37,37,37,37	0
54	MG	2A	3609	1/1	0.97	0.14	62,62,62,62	0
54	MG	1F	303	1/1	0.97	0.16	34,34,34,34	0
54	MG	1A	3021	1/1	0.97	0.09	41,41,41,41	0
54	MG	2A	3263	1/1	0.97	0.07	52,52,52,52	0
54	MG	2A	3431	1/1	0.97	0.05	52,52,52,52	0
54	MG	1a	1747	1/1	0.97	0.10	54,54,54,54	0
54	MG	2A	3265	1/1	0.97	0.06	32,32,32,32	0
54	MG	1F	306	1/1	0.97	0.17	38,38,38,38	0
54	MG	2A	3267	1/1	0.97	0.08	52,52,52,52	0
54	MG	1F	307	1/1	0.97	0.06	37,37,37,37	0
54	MG	1a	1622	1/1	0.97	0.04	48,48,48,48	0
54	MG	1A	3336	1/1	0.97	0.05	33,33,33,33	0
54	MG	1A	3099	1/1	0.97	0.21	36,36,36,36	0
54	MG	1A	3726	1/1	0.97	0.07	52,52,52,52	0
54	MG	1e	201	1/1	0.97	0.08	59,59,59,59	0
54	MG	1e	202	1/1	0.97	0.07	68,68,68,68	0
54	MG	1A	4010	1/1	0.97	0.04	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3626	1/1	0.97	0.04	60,60,60,60	0
54	MG	2k	201	1/1	0.97	0.09	57,57,57,57	0
54	MG	1a	1627	1/1	0.97	0.06	52,52,52,52	0
54	MG	1A	3814	1/1	0.97	0.07	44,44,44,44	0
54	MG	1A	3041	1/1	0.97	0.05	23,23,23,23	0
54	MG	1A	3287	1/1	0.97	0.10	18,18,18,18	0
54	MG	1A	3341	1/1	0.97	0.10	34,34,34,34	0
54	MG	1A	3582	1/1	0.97	0.09	28,28,28,28	0
54	MG	1a	1633	1/1	0.97	0.09	47,47,47,47	0
54	MG	1A	3734	1/1	0.97	0.07	39,39,39,39	0
54	MG	1A	3026	1/1	0.97	0.18	32,32,32,32	0
54	MG	2a	3013	1/1	0.97	0.19	54,54,54,54	0
54	MG	1A	4018	1/1	0.97	0.07	50,50,50,50	0
54	MG	1A	3151	1/1	0.97	0.07	41,41,41,41	0
54	MG	2A	3133	1/1	0.97	0.06	51,51,51,51	0
54	MG	2a	3017	1/1	0.97	0.06	58,58,58,58	0
54	MG	1A	3083	1/1	0.97	0.08	46,46,46,46	0
54	MG	1A	3923	1/1	0.97	0.07	57,57,57,57	0
54	MG	1H	202	1/1	0.97	0.09	59,59,59,59	0
58	ZN	2Y	202	1/1	0.97	0.05	97,97,97,97	0
54	MG	1A	3652	1/1	0.97	0.05	39,39,39,39	0
58	ZN	2n	102	1/1	0.97	0.06	102,102,102,102	0
54	MG	1D	304	1/1	0.98	0.06	46,46,46,46	0
54	MG	1A	3252	1/1	0.98	0.17	31,31,31,31	0
54	MG	1D	306	1/1	0.98	0.08	17,17,17,17	0
54	MG	2a	3081	1/1	0.98	0.06	74,74,74,74	0
54	MG	1D	307	1/1	0.98	0.04	40,40,40,40	0
54	MG	1D	308	1/1	0.98	0.10	33,33,33,33	0
54	MG	1A	3661	1/1	0.98	0.06	31,31,31,31	0
54	MG	1D	310	1/1	0.98	0.22	29,29,29,29	0
54	MG	1A	3013	1/1	0.98	0.04	26,26,26,26	0
54	MG	1a	1862	1/1	0.98	0.05	65,65,65,65	0
54	MG	1A	3455	1/1	0.98	0.06	31,31,31,31	0
54	MG	1a	1864	1/1	0.98	0.06	62,62,62,62	0
54	MG	2A	3169	1/1	0.98	0.05	45,45,45,45	0
54	MG	1A	3861	1/1	0.98	0.05	34,34,34,34	0
54	MG	1A	3042	1/1	0.98	0.19	29,29,29,29	0
54	MG	2A	3638	1/1	0.98	0.08	40,40,40,40	0
54	MG	1A	3114	1/1	0.98	0.12	33,33,33,33	0
54	MG	2A	3641	1/1	0.98	0.07	63,63,63,63	0
54	MG	1A	3727	1/1	0.98	0.04	71,71,71,71	0
54	MG	1A	3033	1/1	0.98	0.06	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3292	1/1	0.98	0.06	51,51,51,51	0
54	MG	1E	301	1/1	0.98	0.18	45,45,45,45	0
54	MG	2A	3646	1/1	0.98	0.11	59,59,59,59	0
54	MG	1A	4021	1/1	0.98	0.07	30,30,30,30	0
54	MG	1A	3668	1/1	0.98	0.04	47,47,47,47	0
54	MG	2A	3070	1/1	0.98	0.07	28,28,28,28	0
54	MG	2A	3650	1/1	0.98	0.09	57,57,57,57	0
54	MG	2A	3288	1/1	0.98	0.07	35,35,35,35	0
54	MG	1A	3135	1/1	0.98	0.14	26,26,26,26	0
54	MG	1A	3732	1/1	0.98	0.05	57,57,57,57	0
54	MG	1A	3162	1/1	0.98	0.23	42,42,42,42	0
54	MG	1A	3373	1/1	0.98	0.11	36,36,36,36	0
54	MG	1E	308	1/1	0.98	0.07	62,62,62,62	0
54	MG	1A	3514	1/1	0.98	0.07	27,27,27,27	0
54	MG	1d	302	1/1	0.98	0.16	65,65,65,65	0
54	MG	2R	201	1/1	0.98	0.19	49,49,49,49	0
54	MG	1F	301	1/1	0.98	0.13	39,39,39,39	0
54	MG	1A	3415	1/1	0.98	0.04	31,31,31,31	0
54	MG	1A	3055	1/1	0.98	0.09	51,51,51,51	0
54	MG	2A	3662	1/1	0.98	0.04	57,57,57,57	0
54	MG	1F	305	1/1	0.98	0.06	38,38,38,38	0
54	MG	1A	3375	1/1	0.98	0.09	48,48,48,48	0
54	MG	2V	202	1/1	0.98	0.12	44,44,44,44	0
54	MG	1A	3877	1/1	0.98	0.05	46,46,46,46	0
54	MG	2A	3534	1/1	0.98	0.04	69,69,69,69	0
54	MG	17	101	1/1	0.98	0.10	38,38,38,38	0
54	MG	2A	3668	1/1	0.98	0.04	44,44,44,44	0
54	MG	2X	101	1/1	0.98	0.07	58,58,58,58	0
54	MG	2a	3129	1/1	0.98	0.05	65,65,65,65	0
54	MG	2a	3130	1/1	0.98	0.06	70,70,70,70	0
54	MG	2A	3303	1/1	0.98	0.06	27,27,27,27	0
54	MG	17	102	1/1	0.98	0.12	43,43,43,43	0
54	MG	2a	3133	1/1	0.98	0.05	76,76,76,76	0
54	MG	2A	3671	1/1	0.98	0.07	64,64,64,64	0
54	MG	1A	3068	1/1	0.98	0.05	31,31,31,31	0
54	MG	1F	309	1/1	0.98	0.15	34,34,34,34	0
54	MG	1A	3227	1/1	0.98	0.11	29,29,29,29	0
54	MG	1F	311	1/1	0.98	0.06	37,37,37,37	0
54	MG	17	107	1/1	0.98	0.06	52,52,52,52	0
54	MG	1A	3881	1/1	0.98	0.05	42,42,42,42	0
54	MG	1A	3742	1/1	0.98	0.04	23,23,23,23	0
54	MG	1A	3165	1/1	0.98	0.06	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3744	1/1	0.98	0.09	53,53,53,53	0
54	MG	1A	3138	1/1	0.98	0.17	39,39,39,39	0
54	MG	1A	3623	1/1	0.98	0.06	47,47,47,47	0
54	MG	2A	3549	1/1	0.98	0.04	25,25,25,25	0
54	MG	1A	3044	1/1	0.98	0.05	31,31,31,31	0
54	MG	1A	3966	1/1	0.98	0.09	49,49,49,49	0
54	MG	1A	3573	1/1	0.98	0.06	48,48,48,48	0
54	MG	1A	3231	1/1	0.98	0.20	39,39,39,39	0
54	MG	2A	3435	1/1	0.98	0.05	59,59,59,59	0
54	MG	1A	3009	1/1	0.98	0.05	35,35,35,35	0
54	MG	2a	3011	1/1	0.98	0.08	49,49,49,49	0
54	MG	1A	3169	1/1	0.98	0.15	31,31,31,31	0
54	MG	2A	3103	1/1	0.98	0.06	30,30,30,30	0
54	MG	1A	3687	1/1	0.98	0.14	31,31,31,31	0
54	MG	1A	3234	1/1	0.98	0.12	31,31,31,31	0
54	MG	2A	3325	1/1	0.98	0.10	34,34,34,34	0
54	MG	2A	3697	1/1	0.98	0.05	68,68,68,68	0
54	MG	1a	1610	1/1	0.98	0.33	56,56,56,56	0
54	MG	2A	3562	1/1	0.98	0.05	62,62,62,62	0
54	MG	2a	3162	1/1	0.98	0.07	79,79,79,79	0
54	MG	1A	3141	1/1	0.98	0.15	37,37,37,37	0
54	MG	1A	3690	1/1	0.98	0.05	51,51,51,51	0
54	MG	1A	3307	1/1	0.98	0.21	40,40,40,40	0
54	MG	2A	3703	1/1	0.98	0.07	55,55,55,55	0
54	MG	1A	3897	1/1	0.98	0.03	32,32,32,32	0
54	MG	1N	204	1/1	0.98	0.04	55,55,55,55	0
54	MG	1A	3977	1/1	0.98	0.06	27,27,27,27	0
54	MG	1A	3001	1/1	0.98	0.04	40,40,40,40	0
54	MG	1A	3143	1/1	0.98	0.05	40,40,40,40	0
54	MG	2A	3335	1/1	0.98	0.06	37,37,37,37	0
54	MG	2A	3572	1/1	0.98	0.08	41,41,41,41	0
54	MG	2A	3573	1/1	0.98	0.05	58,58,58,58	0
54	MG	1A	3028	1/1	0.98	0.28	33,33,33,33	0
54	MG	1A	3349	1/1	0.98	0.07	28,28,28,28	0
54	MG	2A	3454	1/1	0.98	0.04	47,47,47,47	0
54	MG	2A	3013	1/1	0.98	0.07	26,26,26,26	0
54	MG	1A	3350	1/1	0.98	0.04	37,37,37,37	0
54	MG	1A	3762	1/1	0.98	0.14	38,38,38,38	0
54	MG	1A	3174	1/1	0.98	0.12	36,36,36,36	0
54	MG	1a	1721	1/1	0.98	0.12	63,63,63,63	0
54	MG	2A	3583	1/1	0.98	0.06	71,71,71,71	0
54	MG	2a	3184	1/1	0.98	0.06	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3175	1/1	0.98	0.17	36,36,36,36	0
54	MG	1A	3436	1/1	0.98	0.04	34,34,34,34	0
54	MG	2A	3586	1/1	0.98	0.08	73,73,73,73	0
54	MG	1A	3122	1/1	0.98	0.05	67,67,67,67	0
54	MG	1a	1725	1/1	0.98	0.05	62,62,62,62	0
54	MG	1A	3146	1/1	0.98	0.31	39,39,39,39	0
54	MG	1A	3007	1/1	0.98	0.09	43,43,43,43	0
54	MG	1R	201	1/1	0.98	0.08	42,42,42,42	0
54	MG	1A	3091	1/1	0.98	0.05	24,24,24,24	0
54	MG	1A	3149	1/1	0.98	0.17	50,50,50,50	0
54	MG	1A	3442	1/1	0.98	0.05	18,18,18,18	0
54	MG	1B	212	1/1	0.98	0.08	47,47,47,47	0
54	MG	1A	3004	1/1	0.98	0.06	41,41,41,41	0
54	MG	1A	3919	1/1	0.98	0.04	19,19,19,19	0
54	MG	2A	3358	1/1	0.98	0.07	42,42,42,42	0
54	MG	1A	3708	1/1	0.98	0.04	37,37,37,37	0
54	MG	1a	1736	1/1	0.98	0.06	67,67,67,67	0
54	MG	1A	3545	1/1	0.98	0.07	44,44,44,44	0
54	MG	1a	1738	1/1	0.98	0.05	56,56,56,56	0
54	MG	1A	3842	1/1	0.98	0.04	33,33,33,33	0
54	MG	1A	3108	1/1	0.98	0.07	42,42,42,42	0
54	MG	2A	3481	1/1	0.98	0.07	57,57,57,57	0
54	MG	1A	3597	1/1	0.98	0.07	52,52,52,52	0
54	MG	1A	3445	1/1	0.98	0.05	43,43,43,43	0
54	MG	1A	3018	1/1	0.98	0.15	28,28,28,28	0
54	MG	1A	3040	1/1	0.98	0.09	35,35,35,35	0
54	MG	1A	3129	1/1	0.98	0.15	35,35,35,35	0
54	MG	1A	3850	1/1	0.98	0.08	44,44,44,44	0
54	MG	1A	3655	1/1	0.98	0.06	39,39,39,39	0
54	MG	2A	3257	1/1	0.98	0.08	21,21,21,21	0
54	MG	1A	3156	1/1	0.98	0.14	39,39,39,39	0
54	MG	1V	202	1/1	0.98	0.15	35,35,35,35	0
54	MG	1A	3286	1/1	0.98	0.07	22,22,22,22	0
58	ZN	1Y	501	1/1	0.98	0.04	58,58,58,58	0
54	MG	1a	1651	1/1	0.98	0.07	46,46,46,46	0
58	ZN	15	109	1/1	0.98	0.04	61,61,61,61	0
54	MG	1A	3658	1/1	0.98	0.05	54,54,54,54	0
54	MG	1A	3553	1/1	0.98	0.17	59,59,59,59	0
58	ZN	26	501	1/1	0.98	0.03	67,67,67,67	0
58	ZN	29	501	1/1	0.98	0.04	76,76,76,76	0
54	MG	2A	3157	1/1	0.98	0.18	54,54,54,54	0
59	SF4	1d	306	8/8	0.98	0.05	60,71,79,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	SF4	2d	302	8/8	0.98	0.05	71,83,87,87	0
54	MG	2A	3135	1/1	0.99	0.09	43,43,43,43	0
54	MG	2A	3527	1/1	0.99	0.07	54,54,54,54	0
54	MG	2A	3691	1/1	0.99	0.03	51,51,51,51	0
54	MG	1A	3302	1/1	0.99	0.07	47,47,47,47	0
54	MG	1B	223	1/1	0.99	0.06	58,58,58,58	0
54	MG	2A	3581	1/1	0.99	0.04	34,34,34,34	0
54	MG	1A	3901	1/1	0.99	0.04	43,43,43,43	0
54	MG	1A	3902	1/1	0.99	0.06	28,28,28,28	0
54	MG	2A	3639	1/1	0.99	0.06	42,42,42,42	0
54	MG	1A	3110	1/1	0.99	0.13	35,35,35,35	0
54	MG	2A	3282	1/1	0.99	0.06	53,53,53,53	0
54	MG	2A	3141	1/1	0.99	0.07	61,61,61,61	0
54	MG	2a	3118	1/1	0.99	0.04	56,56,56,56	0
54	MG	2A	3587	1/1	0.99	0.04	46,46,46,46	0
54	MG	1A	3789	1/1	0.99	0.03	29,29,29,29	0
54	MG	2a	3121	1/1	0.99	0.10	67,67,67,67	0
54	MG	1A	3104	1/1	0.99	0.14	37,37,37,37	0
54	MG	1A	3089	1/1	0.99	0.04	42,42,42,42	0
54	MG	2a	3124	1/1	0.99	0.03	80,80,80,80	0
54	MG	1A	3090	1/1	0.99	0.16	26,26,26,26	0
54	MG	2A	3592	1/1	0.99	0.04	42,42,42,42	0
54	MG	1D	302	1/1	0.99	0.05	55,55,55,55	0
54	MG	1A	3069	1/1	0.99	0.07	35,35,35,35	0
54	MG	1A	3153	1/1	0.99	0.15	38,38,38,38	0
54	MG	1A	3847	1/1	0.99	0.03	26,26,26,26	0
54	MG	1A	3470	1/1	0.99	0.04	48,48,48,48	0
54	MG	1A	3912	1/1	0.99	0.03	49,49,49,49	0
54	MG	1A	3006	1/1	0.99	0.04	25,25,25,25	0
54	MG	1A	3472	1/1	0.99	0.03	57,57,57,57	0
54	MG	2A	3601	1/1	0.99	0.04	46,46,46,46	0
54	MG	1A	3473	1/1	0.99	0.06	39,39,39,39	0
54	MG	1A	3773	1/1	0.99	0.05	43,43,43,43	0
54	MG	1A	3774	1/1	0.99	0.05	43,43,43,43	0
54	MG	1A	3200	1/1	0.99	0.23	39,39,39,39	0
54	MG	1a	1841	1/1	0.99	0.03	63,63,63,63	0
54	MG	1A	3684	1/1	0.99	0.04	61,61,61,61	0
54	MG	1a	1716	1/1	0.99	0.06	46,46,46,46	0
54	MG	1A	3529	1/1	0.99	0.03	25,25,25,25	0
54	MG	1a	1718	1/1	0.99	0.09	40,40,40,40	0
54	MG	2A	3353	1/1	0.99	0.05	42,42,42,42	0
54	MG	1A	3130	1/1	0.99	0.32	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3858	1/1	0.99	0.11	39,39,39,39	0
54	MG	1A	3626	1/1	0.99	0.08	29,29,29,29	0
54	MG	1A	3212	1/1	0.99	0.11	33,33,33,33	0
54	MG	1A	3733	1/1	0.99	0.05	42,42,42,42	0
54	MG	1A	3073	1/1	0.99	0.06	42,42,42,42	0
54	MG	1a	1852	1/1	0.99	0.08	40,40,40,40	0
54	MG	1B	213	1/1	0.99	0.04	39,39,39,39	0
54	MG	1A	3927	1/1	0.99	0.07	56,56,56,56	0
54	MG	1A	3461	1/1	0.99	0.03	52,52,52,52	0
54	MG	1A	3691	1/1	0.99	0.03	36,36,36,36	0
54	MG	1A	3865	1/1	0.99	0.06	55,55,55,55	0
54	MG	1a	1648	1/1	0.99	0.13	51,51,51,51	0
54	MG	2A	3129	1/1	0.99	0.04	33,33,33,33	0
58	ZN	19	103	1/1	0.99	0.03	50,50,50,50	0
58	ZN	1n	104	1/1	0.99	0.03	77,77,77,77	0
54	MG	2A	3369	1/1	0.99	0.04	51,51,51,51	0
54	MG	1A	3479	1/1	0.99	0.06	42,42,42,42	0
58	ZN	25	102	1/1	0.99	0.03	71,71,71,71	0
54	MG	1A	3447	1/1	0.99	0.04	32,32,32,32	0
54	MG	2A	3685	1/1	0.99	0.04	47,47,47,47	0
54	MG	1F	302	1/1	0.99	0.05	34,34,34,34	0
54	MG	1A	3898	1/1	0.99	0.04	42,42,42,42	0
54	MG	1A	3899	1/1	0.99	0.07	41,41,41,41	0
54	MG	2A	3357	1/1	1.00	0.05	34,34,34,34	0
54	MG	1A	3978	1/1	1.00	0.04	33,33,33,33	0
54	MG	1A	3879	1/1	1.00	0.07	35,35,35,35	0
54	MG	1A	3931	1/1	1.00	0.04	47,47,47,47	0
54	MG	2A	3475	1/1	1.00	0.08	37,37,37,37	0
58	ZN	16	501	1/1	1.00	0.05	48,48,48,48	0
54	MG	1A	3338	1/1	1.00	0.05	34,34,34,34	0
54	MG	1A	3454	1/1	1.00	0.05	28,28,28,28	0

6.5 Other polymers (i)

There are no such residues in this entry.