wwPDB X-ray Structure Validation Summary Report (i)

Sep 15, 2026 – 09:36 PM EDT

PDB ID	:	7RQD / pdb_00007rqd
Title	:	Crystal structure of the Thermus thermophilus 70S ribosome in complex with protein Y, A-site deacylated tRNA analog CACCA, P-site MTI-tripeptidyl-tRNA analog ACCA-ITM, and chloramphenicol at 2.50A resolution
Authors	:	Syroegin, E.A.; Flemmich, L.; Klepacki, D.; Vazquez-Laslop, N.; Micura, R.; Polikanov, Y.S.
Deposited on	:	2021-08-06
Resolution	:	2.50 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 ⓘ) were used in the production of this report:

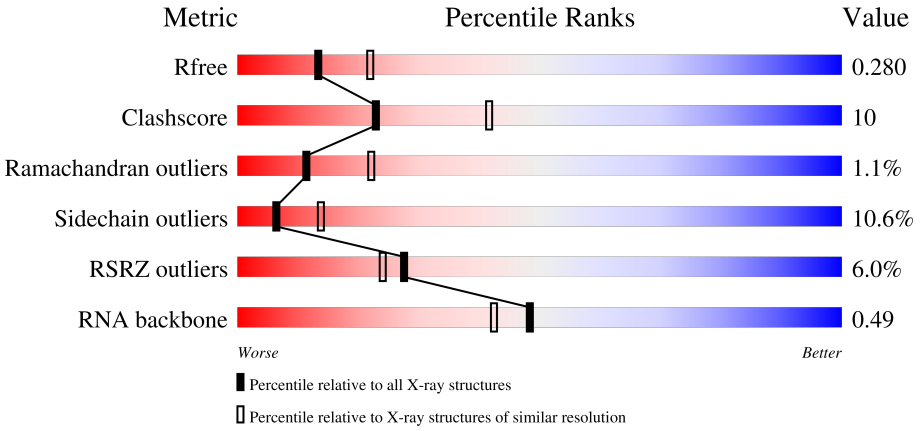
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)
RNA backbone	3983	1003 (2.78-2.22)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1A	2915	4% 61% 31% 7% •
1	2A	2915	5% 55% 35% 8% •
2	1B	121	% 67% 27% 5% •
2	2B	121	% 60% 37% ••

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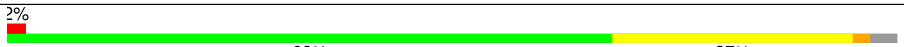
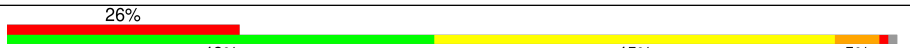
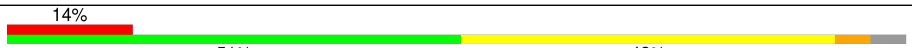
Mol	Chain	Length	Quality of chain
3	1D	276	
3	2D	276	
4	1E	206	
4	2E	206	
5	1F	210	
5	2F	210	
6	1G	182	
6	2G	182	
7	1H	180	
7	2H	180	
8	1I	148	
8	2I	148	
9	1N	140	
9	2N	140	
10	1O	122	
10	2O	122	
11	1P	150	
11	2P	150	
12	1Q	141	
12	2Q	141	
13	1R	118	
13	2R	118	
14	1S	112	
14	2S	112	
15	1T	146	

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Mol	Chain	Length	Quality of chain
15	2T	146	2% 62% 26% 10%
16	1U	118	81% 18%
16	2U	118	3% 64% 32%
17	1V	101	79% 20%
17	2V	101	4% 59% 37%
18	1W	113	% 79% 19%
18	2W	113	2% 73% 24%
19	1X	96	% 57% 38%
19	2X	96	8% 69% 28%
20	1Y	110	2% 64% 31%
20	2Y	110	7% 57% 34% 6%
21	1Z	206	2% 70% 24%
21	2Z	206	6% 67% 26% 5%
22	10	85	7% 74% 22%
22	20	85	7% 65% 32%
23	11	98	68% 30%
23	21	98	% 56% 39%
24	12	72	3% 65% 28%
24	22	72	60% 35%
25	13	60	63% 32%
25	23	60	5% 77% 22%
26	14	71	15% 52% 39% 6%
26	24	71	35% 35% 45% 15%
27	15	60	2% 77% 20%
27	25	60	75% 20%

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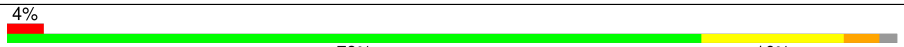
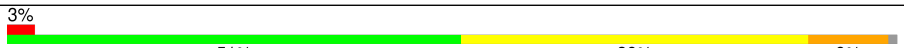
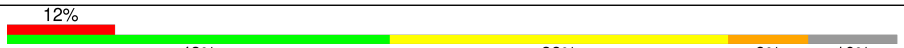
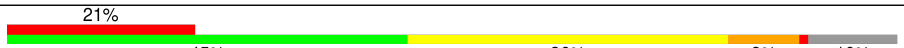
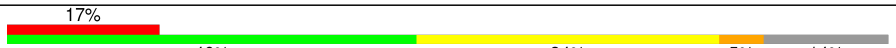
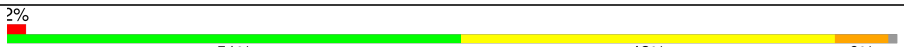
Mol	Chain	Length	Quality of chain
28	16	54	
28	26	54	
29	17	49	
29	27	49	
30	18	65	
30	28	65	
31	19	37	
31	29	37	
32	1a	1521	
32	2a	1521	
33	1b	256	
33	2b	256	
34	1c	239	
34	2c	239	
35	1d	209	
35	2d	209	
36	1e	162	
36	2e	162	
37	1f	101	
37	2f	101	
38	1g	156	
38	2g	156	
39	1h	138	
39	2h	138	
40	1i	128	

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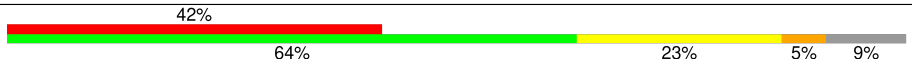
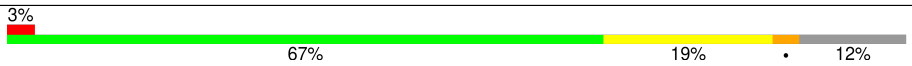
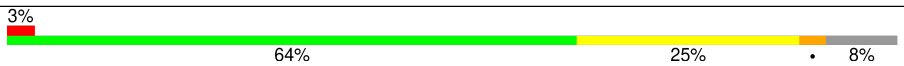
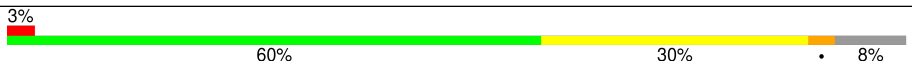
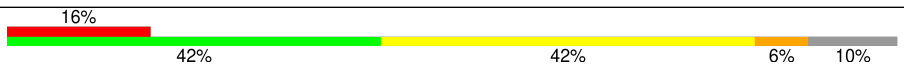
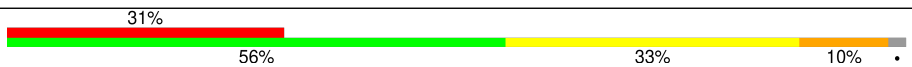
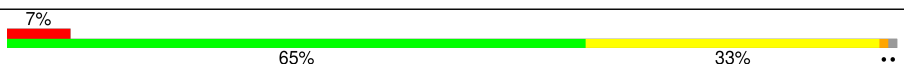
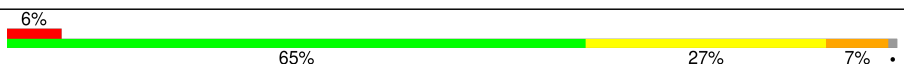
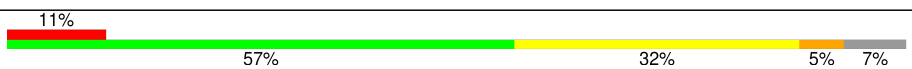
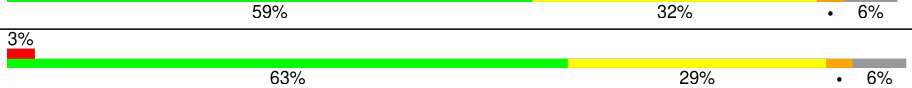
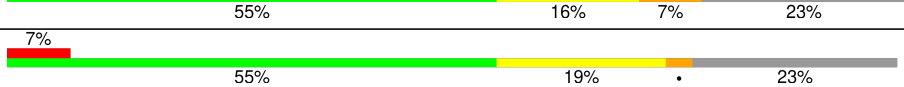
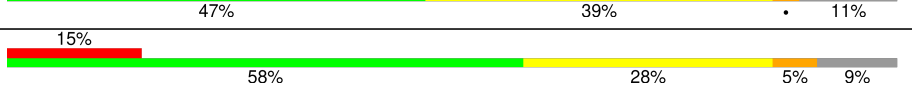
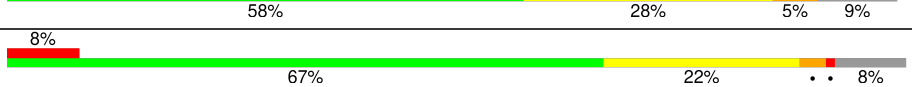
Mol	Chain	Length	Quality of chain
40	2i	128	
41	1j	105	
41	2j	105	
42	1k	129	
42	2k	129	
43	1l	132	
43	2l	132	
44	1m	126	
44	2m	126	
45	1n	61	
45	2n	61	
46	1o	89	
46	2o	89	
47	1p	88	
47	2p	88	
48	1q	105	
48	2q	105	
49	1r	88	
49	2r	88	
50	1s	93	
50	2s	93	
51	1t	106	
51	2t	106	
52	1u	27	
52	2u	27	

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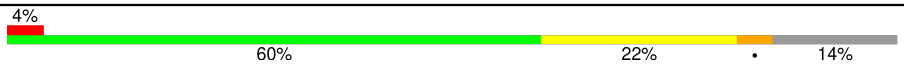
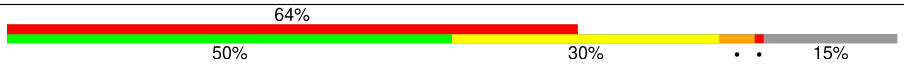
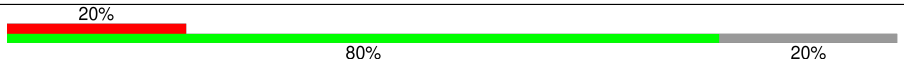
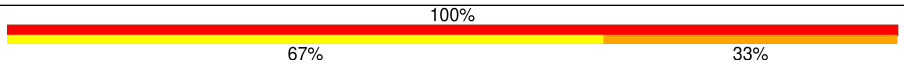
Mol	Chain	Length	Quality of chain
53	1y	113	
53	2y	113	
54	1w	5	
54	2w	5	
55	1x	4	
55	2x	4	
56	1v	3	
56	2v	3	

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
62	SF4	1d	306	-	-	X	-

2 Entry composition (i)

There are 63 unique types of molecules in this entry. The entry contains 297633 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
1	1A	2872	Total	C	N	O	P	0	0	0
			61869	27540	11574	19884	2871			
1	2A	2867	Total	C	N	O	P	0	0	0
			61758	27491	11552	19850	2865			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	1B	120	Total	C	N	O	P	0	0	0
			2572	1145	476	832	119			
2	2B	120	Total	C	N	O	P	0	0	0
			2573	1146	476	832	119			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	1D	275	Total	C	N	O	S	0	0	0
			2131	1346	422	360	3			
3	2D	275	Total	C	N	O	S	0	0	0
			2136	1349	423	361	3			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	1G	181	Total	C	N	O	S	0	0	0
			1426	916	253	253	4			
6	2G	181	Total	C	N	O	S	0	0	0
			1424	912	259	249	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	1H	174	Total	C	N	O	S	0	0	0
			1330	845	248	236	1			
7	2H	173	Total	C	N	O	S	0	0	0
			1324	842	247	234	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	1I	147	Total	C	N	O	S	0	0	0
			1094	699	191	203	1			
8	2I	146	Total	C	N	O	S	0	0	0
			1076	687	186	202	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	1N	140	Total	C	N	O	S	0	0	0
			1121	722	208	187	4			
9	2N	140	Total	C	N	O	S	0	0	0
			1117	719	207	187	4			

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	1S	110	Total	C	N	O	0	0	0
			877	553	175	149			
14	2S	110	Total	C	N	O	0	0	0
			870	549	173	148			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	1V	101	Total	C	N	O	S	0	0	0
			775	498	141	135	1			
17	2V	101	Total	C	N	O	S	0	0	0
			771	495	140	135	1			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	1Y	107	Total	C	N	O	S	0	0	0
			810	520	153	131	6			
20	2Y	107	Total	C	N	O	S	0	0	0
			810	519	153	132	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	1Z	203	Total	C	N	O	S	0	0	0
			1587	1011	282	292	2			
21	2Z	201	Total	C	N	O	S	0	0	0
			1557	995	274	286	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	10	83	Total	C	N	O	S	0	0	0
			653	404	139	109	1			
22	20	83	Total	C	N	O	S	0	0	0
			650	401	139	109	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	11	97	Total	C	N	O	S	0	0	0
			754	475	148	130	1			
23	21	97	Total	C	N	O	S	0	0	0
			759	478	149	131	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	12	70	Total	C	N	O	S	0	0	0
			588	365	118	103	2			
24	22	70	Total	C	N	O	S	0	0	0
			592	368	119	103	2			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	14	69	Total	C	N	O	S	0	0	0
			546	346	96	99	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	24	69	Total	C	N	O	S	0	0	0
			536	342	98	91	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	15	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			
27	25	59	Total	C	N	O	S	0	0	0
			455	285	89	76	5			

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	1a	1500	Total	C	N	O	P	0	0	0
			32246	14358	5975	10413	1500			
32	2a	1504	Total	C	N	O	P	0	0	0
			32331	14396	5990	10441	1504			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	1b	231	Total	C	N	O	S	0	0	0
			1842	1175	330	332	5			
33	2b	231	Total	C	N	O	S	0	0	0
			1825	1167	326	327	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	1c	206	Total	C	N	O	S	0	0	0
			1558	979	305	273	1			
34	2c	206	Total	C	N	O	S	0	0	0
			1542	968	300	273	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	1d	208	Total	C	N	O	S	0	0	0
			1665	1043	329	286	7			
35	2d	208	Total	C	N	O	S	0	0	0
			1668	1047	330	284	7			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	1f	100	Total	C	N	O	S	0	0	0
			814	516	144	151	3			
37	2f	100	Total	C	N	O	S	0	0	0
			816	516	146	151	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	1g	155	Total	C	N	O	S	0	0	0
			1235	769	244	216	6			
38	2g	155	Total	C	N	O	S	0	0	0
			1229	766	241	216	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	1h	137	Total	C	N	O	S	0	0	0
			1098	694	210	192	2			
39	2h	137	Total	C	N	O	S	0	0	0
			1088	689	206	191	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
40	1i	127	Total	C	N	O	0	0	0
			986	625	193	168			
40	2i	126	Total	C	N	O	0	0	0
			966	613	186	167			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
41	1j	97	Total	C	N	O	0	0	0
			719	446	142	131			
41	2j	96	Total	C	N	O	0	0	0
			710	442	137	131			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	1k	114	Total	C	N	O	S	0	0	0
			834	520	156	155	3			

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	1m	116	Total	C	N	O	S	0	0	0
			914	564	189	159	2			
44	2m	114	Total	C	N	O	S	0	0	0
			895	550	186	157	2			

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	1s	83	Total	C	N	O	S	0	0	0
			648	415	120	111	2			
50	2s	83	Total	C	N	O	S	0	0	0
			645	410	118	115	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	1t	96	Total	C	N	O	S	0	0	0
			732	449	157	124	2			
51	2t	98	Total	C	N	O	S	0	0	0
			733	451	154	126	2			

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

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

- Molecule 53 is a protein called Ribosome-associated inhibitor A.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	1w	4	Total	C	N	O	P	0	0	1
			63	28	11	21	3			
54	2w	4	Total	C	N	O	P	0	0	1
			63	28	11	21	3			

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

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

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

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	1A	1021	Total	Mg	0	0
			1021	1021		
57	1B	31	Total	Mg	0	0
			31	31		
57	1D	18	Total	Mg	0	0
			18	18		
57	1E	9	Total	Mg	0	0
			9	9		
57	1F	18	Total	Mg	0	0
			18	18		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	1G	4	Total Mg 4 4	0	0
57	1H	2	Total Mg 2 2	0	0
57	1N	5	Total Mg 5 5	0	0
57	1O	1	Total Mg 1 1	0	0
57	1P	4	Total Mg 4 4	0	0
57	1Q	4	Total Mg 4 4	0	0
57	1R	3	Total Mg 3 3	0	0
57	1T	6	Total Mg 6 6	0	0
57	1U	7	Total Mg 7 7	0	0
57	1V	6	Total Mg 6 6	0	0
57	1W	5	Total Mg 5 5	0	0
57	1X	1	Total Mg 1 1	0	0
57	1Y	1	Total Mg 1 1	0	0
57	1Z	1	Total Mg 1 1	0	0
57	10	8	Total Mg 8 8	0	0
57	11	5	Total Mg 5 5	0	0
57	13	3	Total Mg 3 3	0	0
57	15	10	Total Mg 10 10	0	0
57	17	5	Total Mg 5 5	0	0
57	18	2	Total Mg 2 2	0	0
57	19	2	Total Mg 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	1a	270	Total Mg 270 270	0	0
57	1b	1	Total Mg 1 1	0	0
57	1d	5	Total Mg 5 5	0	0
57	1e	1	Total Mg 1 1	0	0
57	1f	2	Total Mg 2 2	0	0
57	1g	3	Total Mg 3 3	0	0
57	1h	2	Total Mg 2 2	0	0
57	1i	2	Total Mg 2 2	0	0
57	1l	2	Total Mg 2 2	0	0
57	1m	2	Total Mg 2 2	0	0
57	1n	3	Total Mg 3 3	0	0
57	1o	2	Total Mg 2 2	0	0
57	1t	2	Total Mg 2 2	0	0
57	1y	3	Total Mg 3 3	0	0
57	2A	726	Total Mg 726 726	0	0
57	2B	17	Total Mg 17 17	0	0
57	2D	9	Total Mg 9 9	0	0
57	2E	8	Total Mg 8 8	0	0
57	2F	4	Total Mg 4 4	0	0
57	2G	3	Total Mg 3 3	0	0
57	2I	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	2N	1	Total Mg 1 1	0	0
57	2O	2	Total Mg 2 2	0	0
57	2P	2	Total Mg 2 2	0	0
57	2Q	3	Total Mg 3 3	0	0
57	2R	2	Total Mg 2 2	0	0
57	2T	4	Total Mg 4 4	0	0
57	2U	1	Total Mg 1 1	0	0
57	2V	3	Total Mg 3 3	0	0
57	2W	2	Total Mg 2 2	0	0
57	2Y	1	Total Mg 1 1	0	0
57	20	2	Total Mg 2 2	0	0
57	21	3	Total Mg 3 3	0	0
57	23	1	Total Mg 1 1	0	0
57	25	4	Total Mg 4 4	0	0
57	27	3	Total Mg 3 3	0	0
57	28	3	Total Mg 3 3	0	0
57	29	1	Total Mg 1 1	0	0
57	2a	189	Total Mg 189 189	0	0
57	2e	1	Total Mg 1 1	0	0
57	2f	1	Total Mg 1 1	0	0
57	2j	1	Total Mg 1 1	0	0

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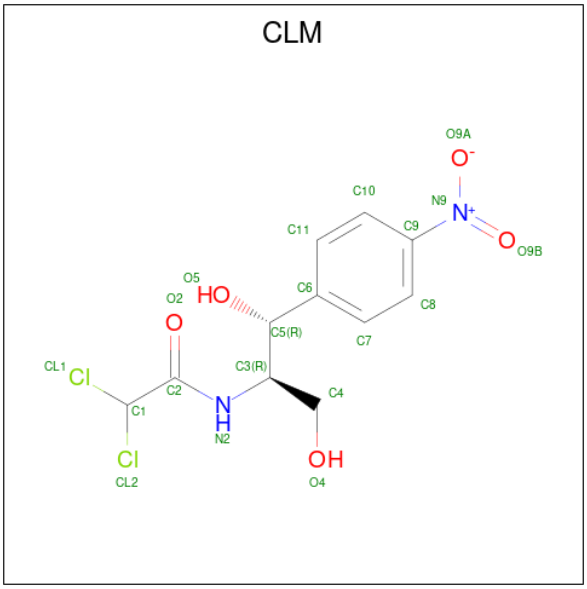
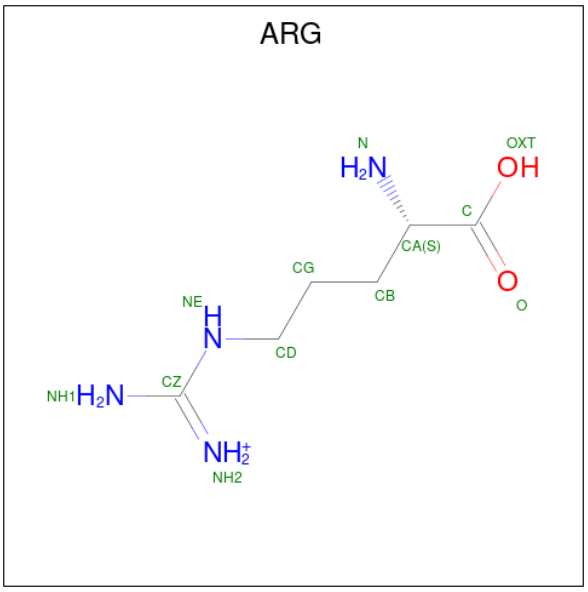
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	2l	2	Total Mg 2 2	0	0
57	2n	1	Total Mg 1 1	0	0
57	2p	1	Total Mg 1 1	0	0
57	2t	1	Total Mg 1 1	0	0
57	2x	1	Total Mg 1 1	0	0

- Molecule 58 is CHLORAMPHENICOL (CCD ID: CLM) (formula: $C_{11}H_{12}Cl_2N_2O_5$).



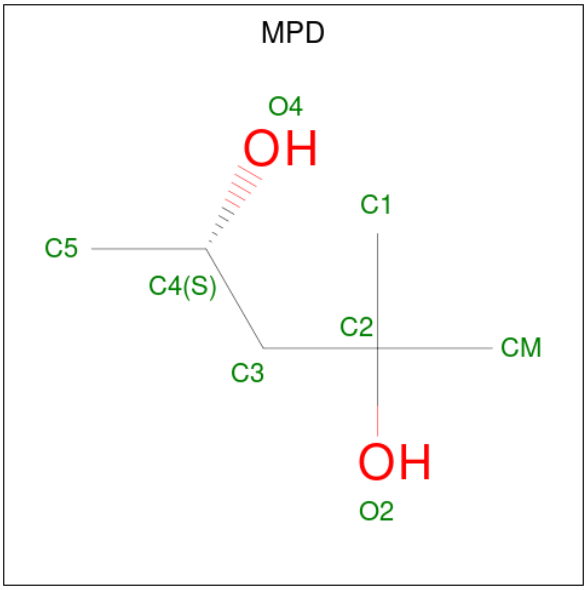
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	1A	1	Total C Cl N O 20 11 2 2 5	0	0
58	2A	1	Total C Cl N O 20 11 2 2 5	0	0

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



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

- Molecule 60 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	1A	1	Total C O 8 6 2	0	0
60	1T	1	Total C O 8 6 2	0	0

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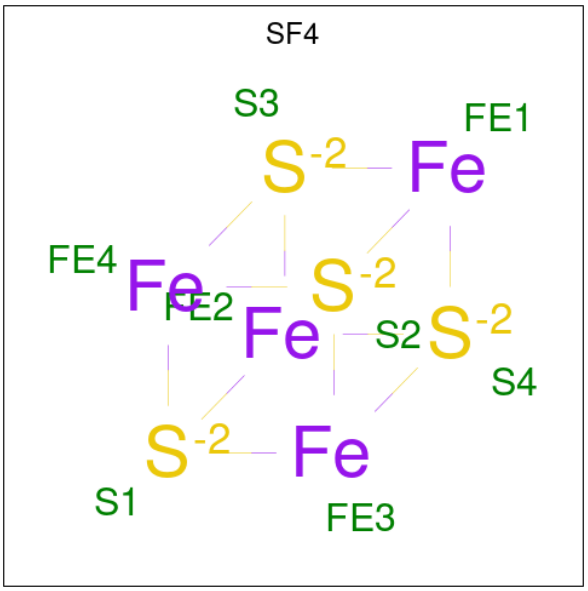
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	18	1	Total C O 8 6 2	0	0
60	1a	1	Total C O 8 6 2	0	0
60	2A	1	Total C O 8 6 2	0	0
60	2B	1	Total C O 8 6 2	0	0

- Molecule 61 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1Y	1	Total Zn 1 1	0	0
61	14	1	Total Zn 1 1	0	0
61	15	1	Total Zn 1 1	0	0
61	16	1	Total Zn 1 1	0	0
61	19	1	Total Zn 1 1	0	0
61	1n	1	Total Zn 1 1	0	0
61	2Y	1	Total Zn 1 1	0	0
61	24	1	Total Zn 1 1	0	0
61	25	1	Total Zn 1 1	0	0
61	26	1	Total Zn 1 1	0	0
61	29	1	Total Zn 1 1	0	0
61	2n	1	Total Zn 1 1	0	0

- Molecule 62 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
62	1d	1	Total Fe S 8 4 4	0	0
62	2d	1	Total Fe S 8 4 4	0	0

- Molecule 63 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
63	1A	3946	Total O 3946 3946	0	0
63	1B	90	Total O 90 90	0	0
63	1D	121	Total O 121 121	0	0
63	1E	80	Total O 80 80	0	0
63	1F	59	Total O 59 59	0	0
63	1G	19	Total O 19 19	0	0
63	1H	13	Total O 13 13	0	0
63	1I	5	Total O 5 5	0	0
63	1N	50	Total O 50 50	0	0
63	1O	33	Total O 33 33	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
63	1P	65	Total O 65 65	0	0
63	1Q	35	Total O 35 35	0	0
63	1R	32	Total O 32 32	0	0
63	1S	15	Total O 15 15	0	0
63	1T	28	Total O 28 28	0	0
63	1U	46	Total O 46 46	0	0
63	1V	41	Total O 41 41	0	0
63	1W	30	Total O 30 30	0	0
63	1X	28	Total O 28 28	0	0
63	1Y	21	Total O 21 21	0	0
63	1Z	13	Total O 13 13	0	0
63	10	25	Total O 25 25	0	0
63	11	26	Total O 26 26	0	0
63	12	15	Total O 15 15	0	0
63	13	24	Total O 24 24	0	0
63	14	2	Total O 2 2	0	0
63	15	24	Total O 24 24	0	0
63	16	18	Total O 18 18	0	0
63	17	17	Total O 17 17	0	0
63	18	26	Total O 26 26	0	0
63	19	7	Total O 7 7	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
63	1a	412	Total O 412 412	0	0
63	1b	1	Total O 1 1	0	0
63	1c	1	Total O 1 1	0	0
63	1d	7	Total O 7 7	0	0
63	1e	2	Total O 2 2	0	0
63	1f	3	Total O 3 3	0	0
63	1h	1	Total O 1 1	0	0
63	1j	1	Total O 1 1	0	0
63	1l	5	Total O 5 5	0	0
63	1o	2	Total O 2 2	0	0
63	1p	3	Total O 3 3	0	0
63	1t	1	Total O 1 1	0	0
63	1y	5	Total O 5 5	0	0
63	1w	5	Total O 5 5	0	0
63	1x	5	Total O 5 5	0	0
63	2A	2126	Total O 2126 2126	0	0
63	2B	46	Total O 46 46	0	0
63	2D	54	Total O 54 54	0	0
63	2E	26	Total O 26 26	0	0
63	2F	24	Total O 24 24	0	0
63	2G	7	Total O 7 7	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
63	2H	3	Total O 3 3	0	0
63	2I	6	Total O 6 6	0	0
63	2N	3	Total O 3 3	0	0
63	2O	22	Total O 22 22	0	0
63	2P	28	Total O 28 28	0	0
63	2Q	19	Total O 19 19	0	0
63	2R	17	Total O 17 17	0	0
63	2S	4	Total O 4 4	0	0
63	2T	11	Total O 11 11	0	0
63	2U	13	Total O 13 13	0	0
63	2V	7	Total O 7 7	0	0
63	2W	19	Total O 19 19	0	0
63	2X	9	Total O 9 9	0	0
63	2Y	4	Total O 4 4	0	0
63	2Z	10	Total O 10 10	0	0
63	20	12	Total O 12 12	0	0
63	21	20	Total O 20 20	0	0
63	22	2	Total O 2 2	0	0
63	23	3	Total O 3 3	0	0
63	24	1	Total O 1 1	0	0
63	25	10	Total O 10 10	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
63	26	5	Total O 5 5	0	0
63	27	8	Total O 8 8	0	0
63	28	13	Total O 13 13	0	0
63	29	1	Total O 1 1	0	0
63	2a	294	Total O 294 294	0	0
63	2d	2	Total O 2 2	0	0
63	2e	2	Total O 2 2	0	0
63	2f	2	Total O 2 2	0	0
63	2j	2	Total O 2 2	0	0
63	2l	2	Total O 2 2	0	0
63	2n	1	Total O 1 1	0	0
63	2o	3	Total O 3 3	0	0
63	2p	1	Total O 1 1	0	0
63	2r	3	Total O 3 3	0	0
63	2t	2	Total O 2 2	0	0
63	2y	2	Total O 2 2	0	0
63	2w	2	Total O 2 2	0	0
63	2x	2	Total O 2 2	0	0

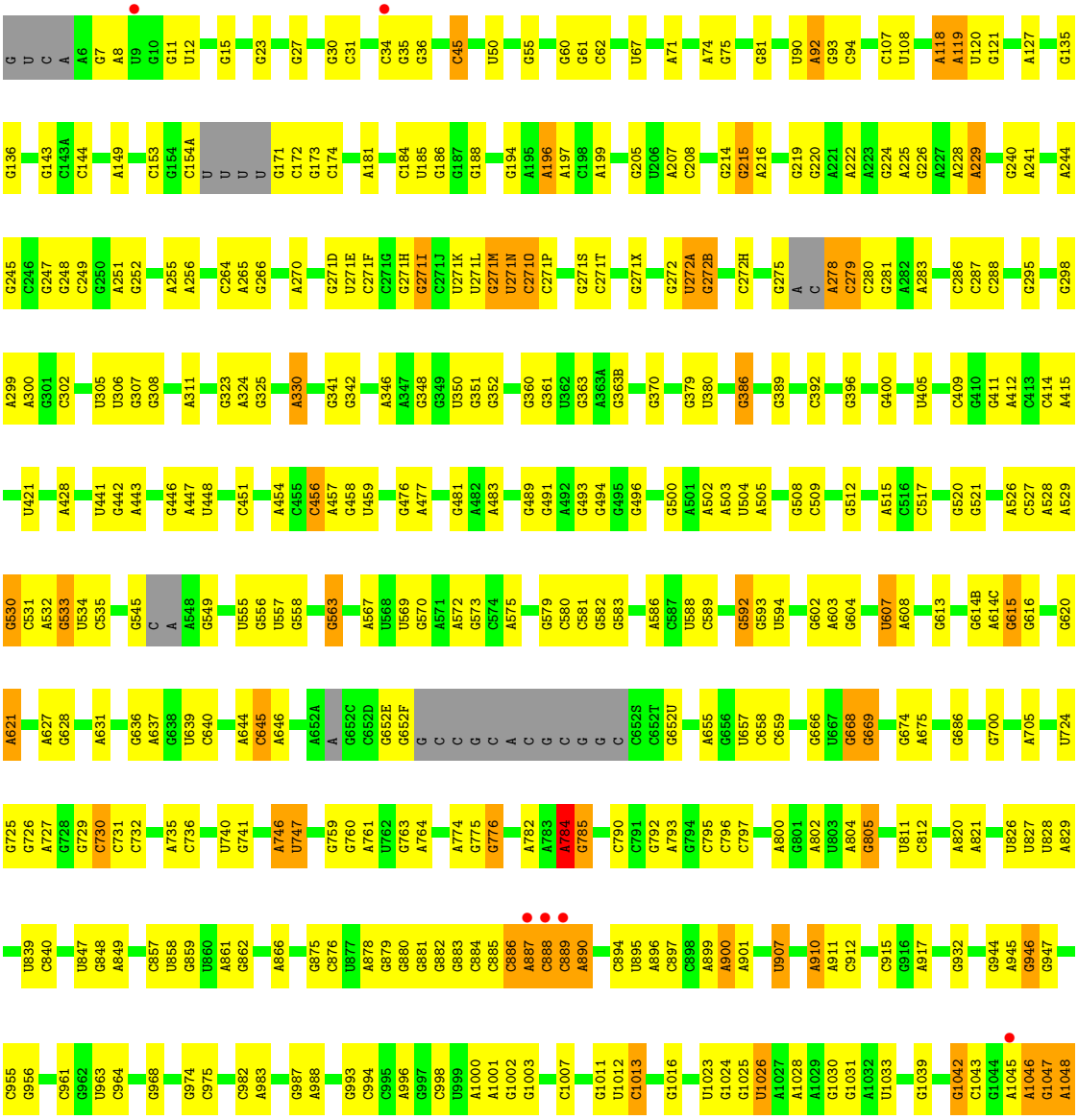
3 Residue-property plots (i)

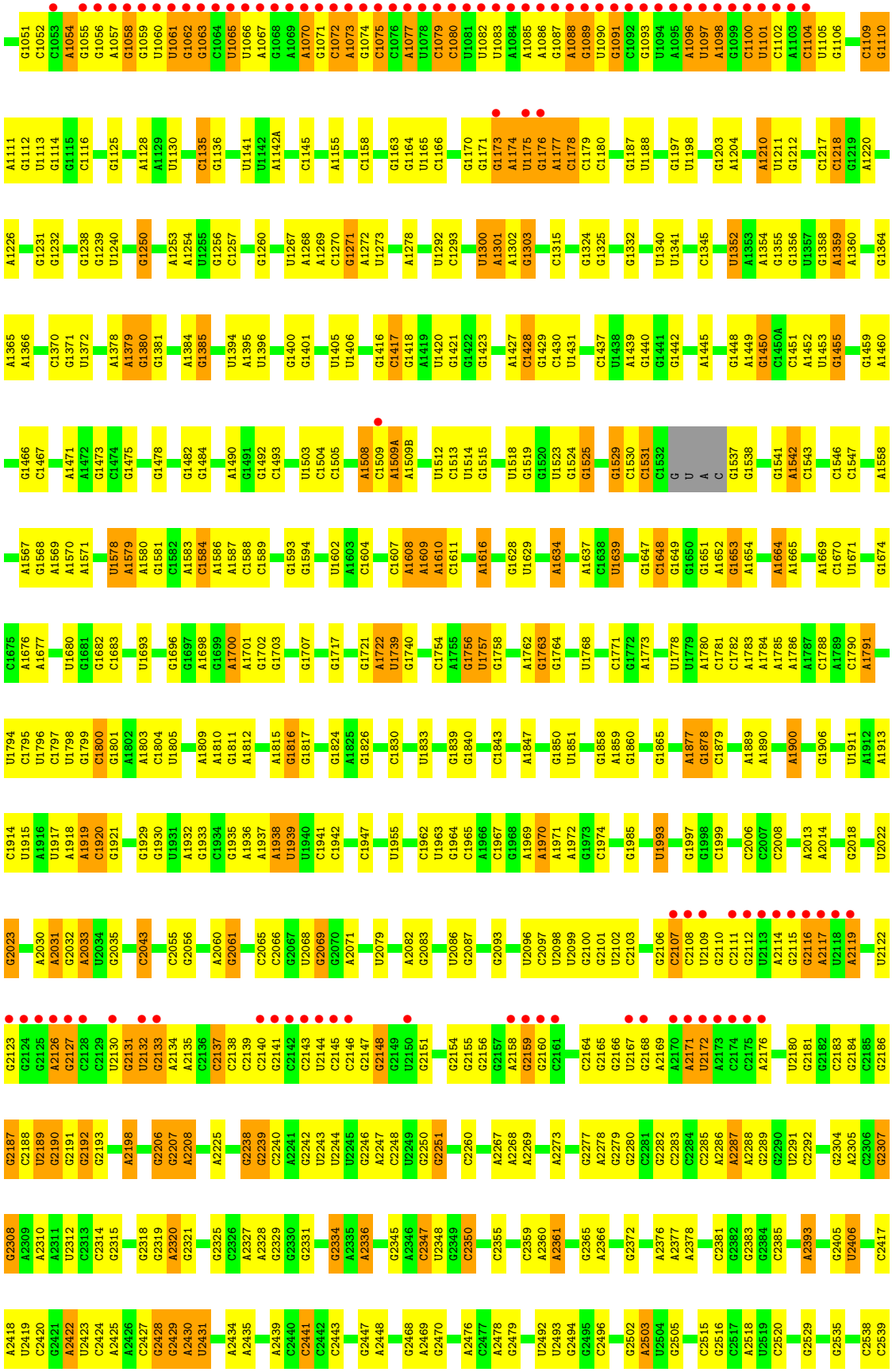
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

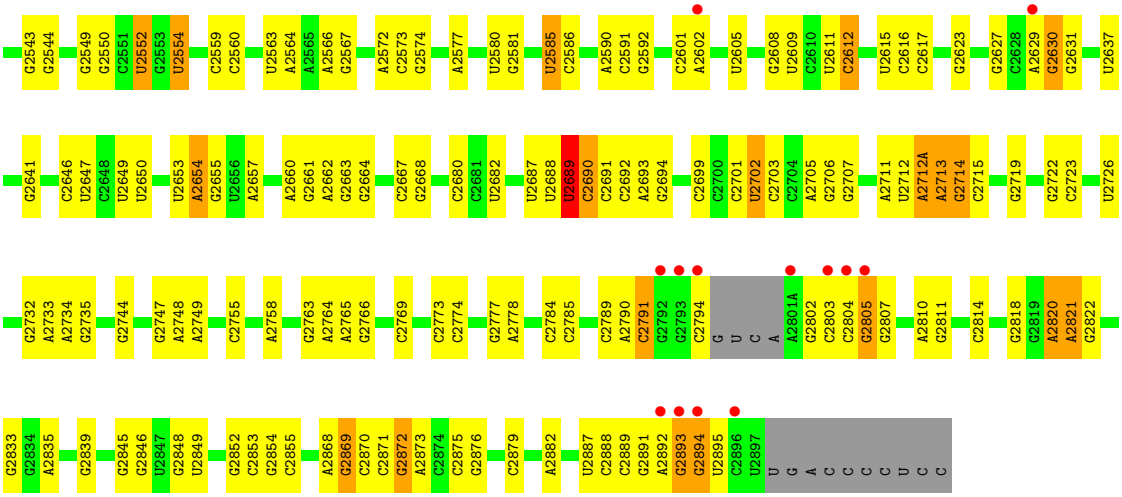
- Molecule 1: 23S Ribosomal RNA

Chain 1A:





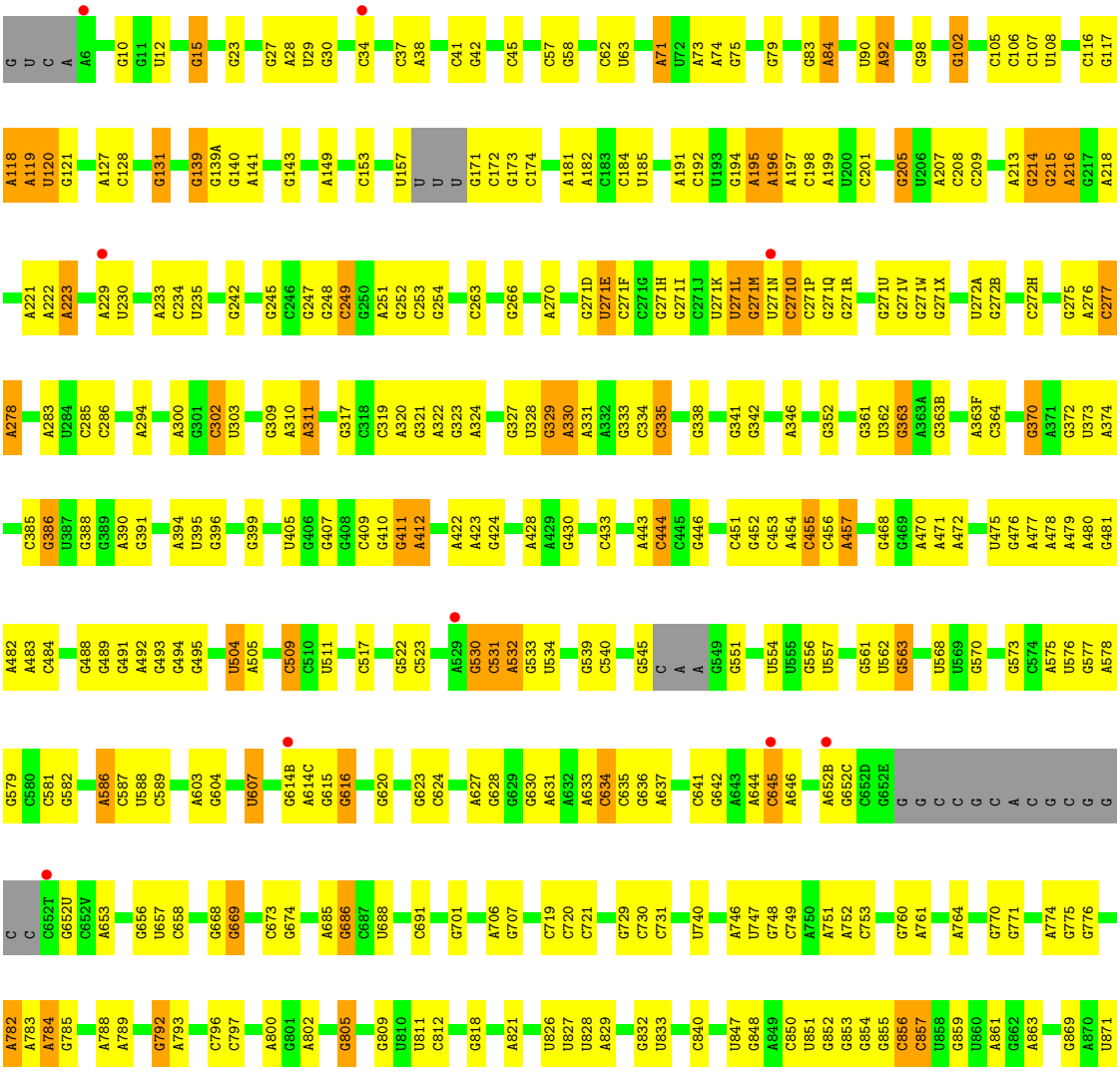


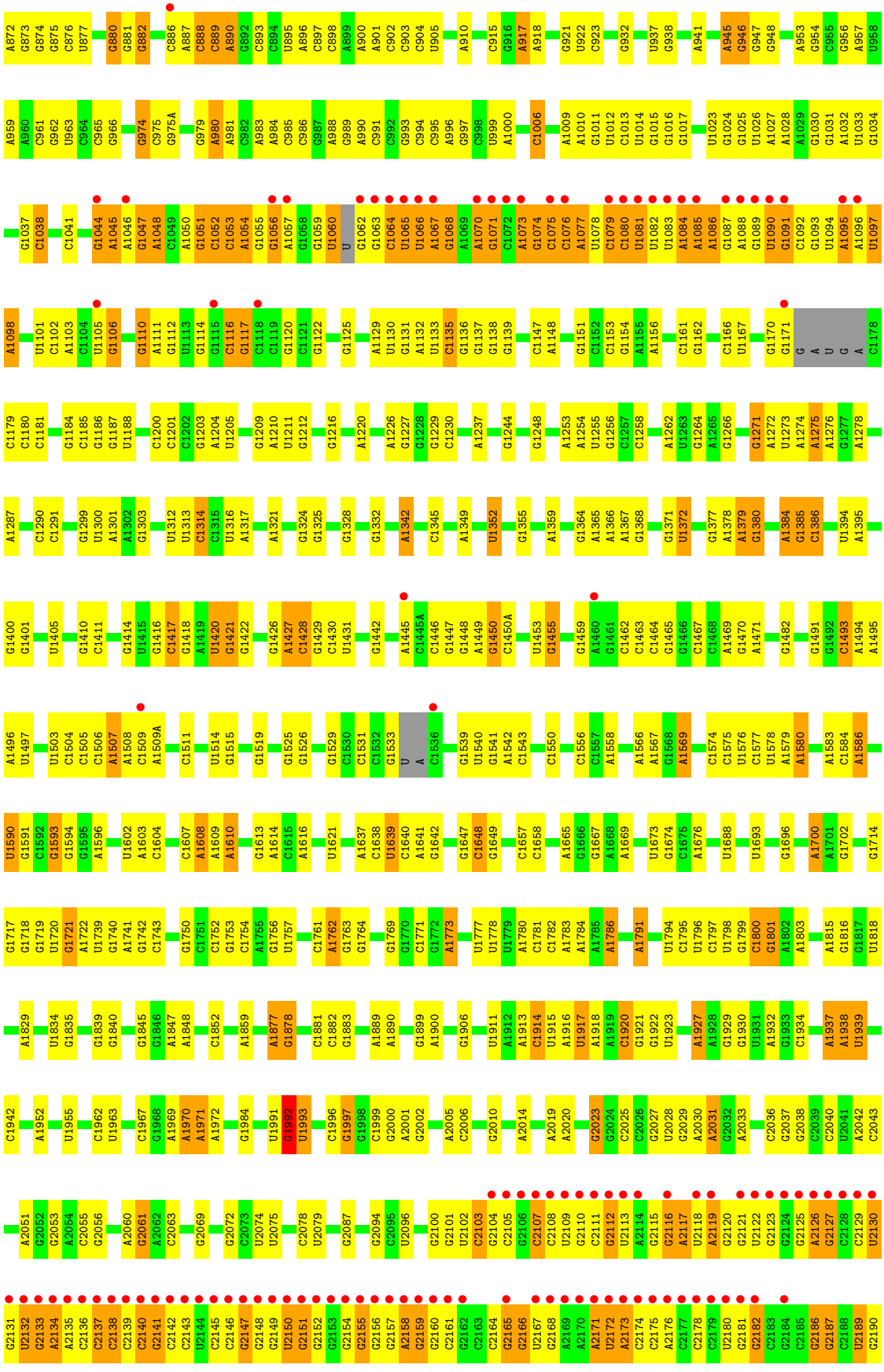


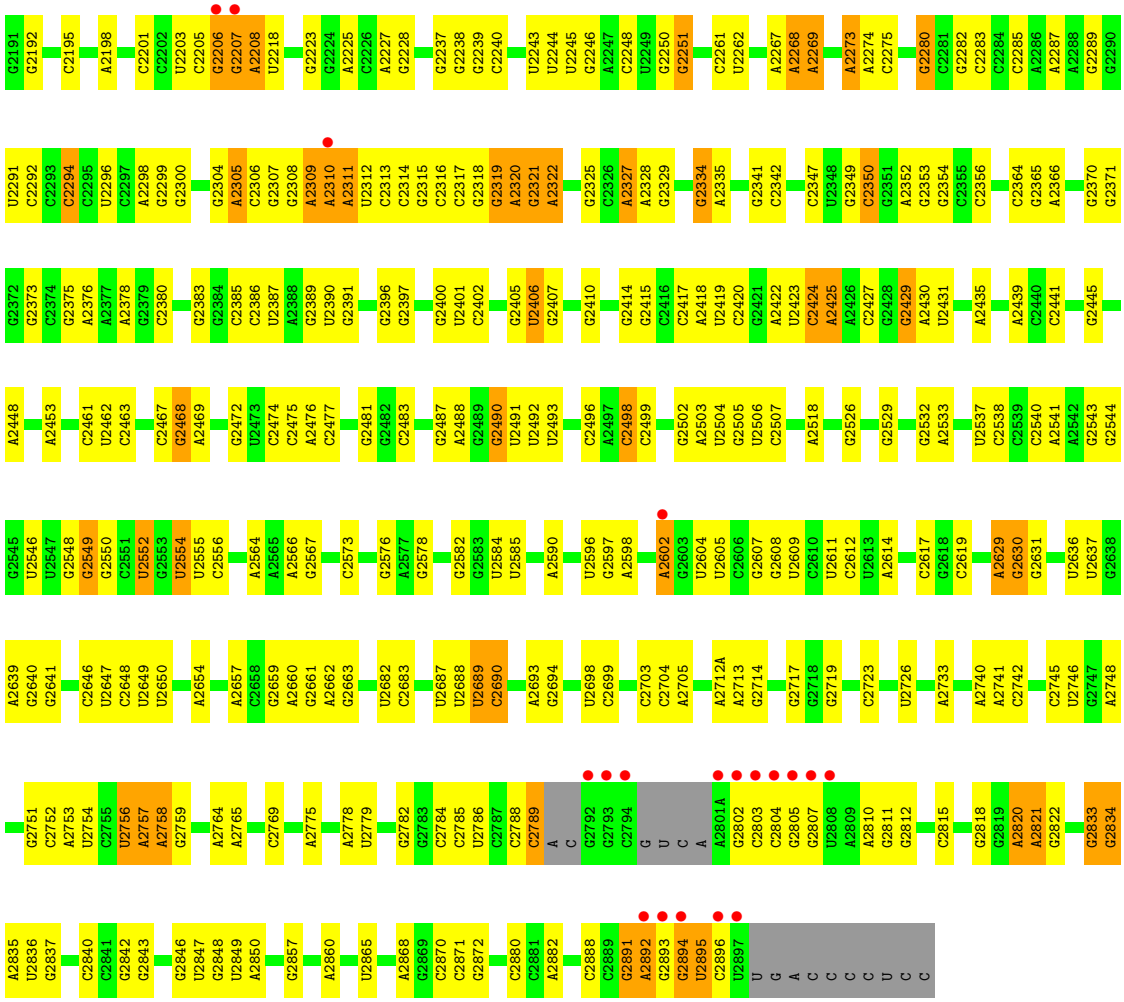
• Molecule 1: 23S Ribosomal RNA

Chain 2A:



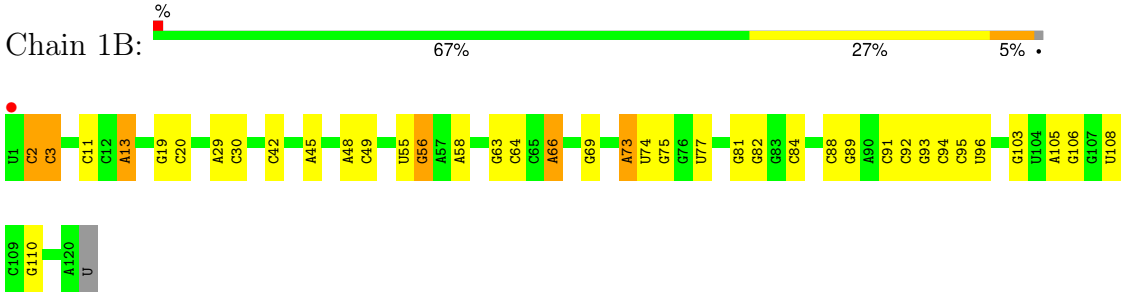






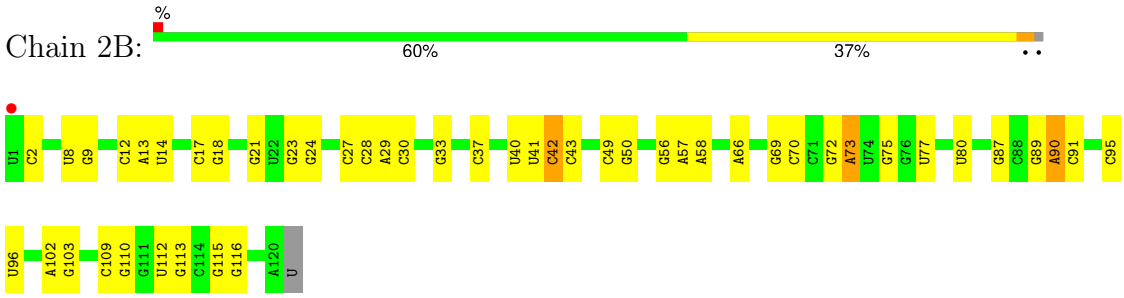
• Molecule 2: 5S Ribosomal RNA

Chain 1B:



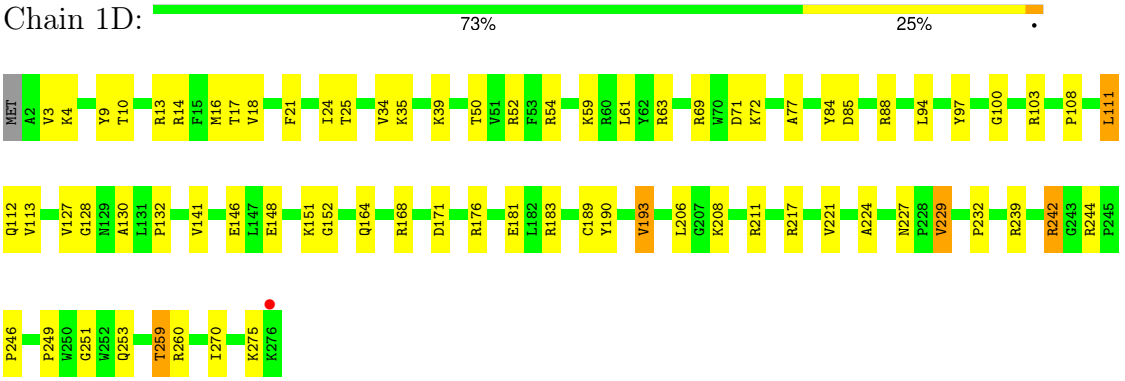
• Molecule 2: 5S Ribosomal RNA

Chain 2B:



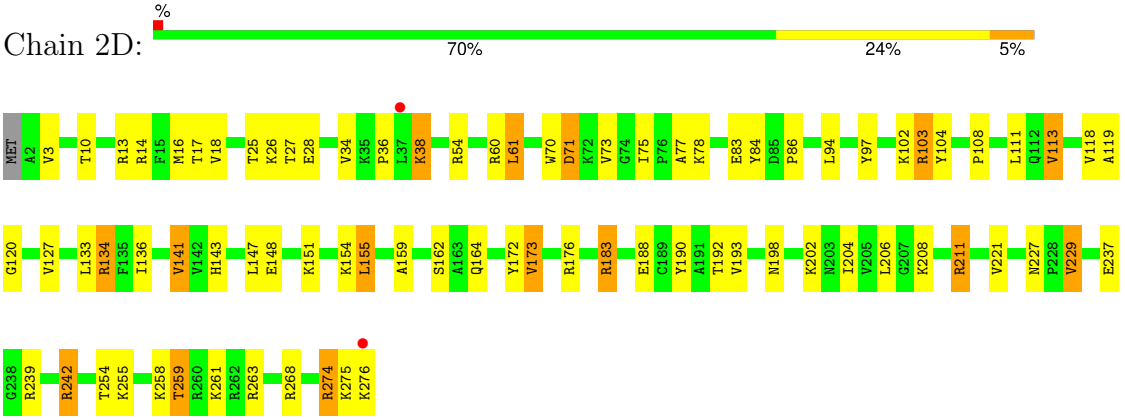
• Molecule 3: 50S ribosomal protein L2

Chain 1D:



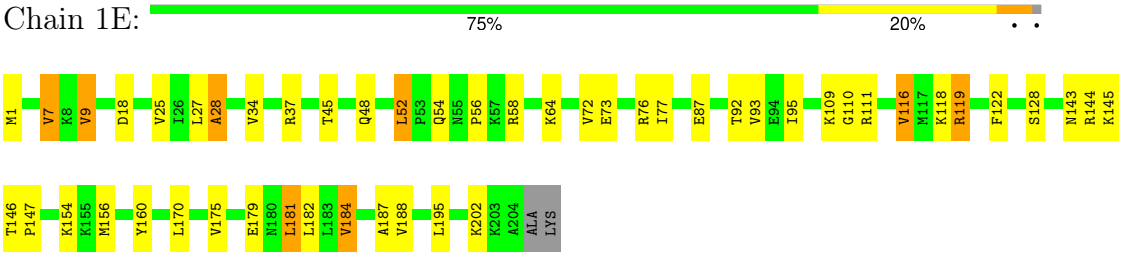
• Molecule 3: 50S ribosomal protein L2

Chain 2D:



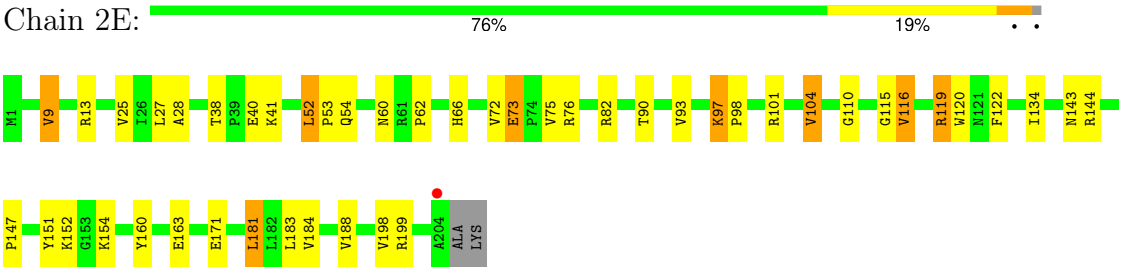
• Molecule 4: 50S ribosomal protein L3

Chain 1E:



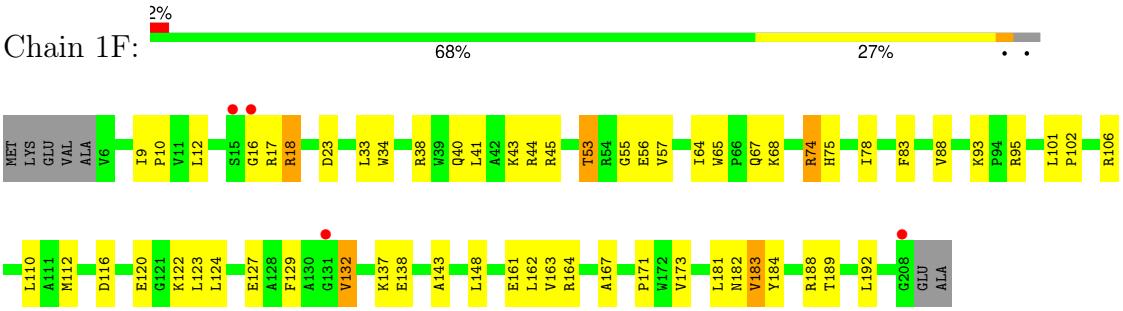
• Molecule 4: 50S ribosomal protein L3

Chain 2E:



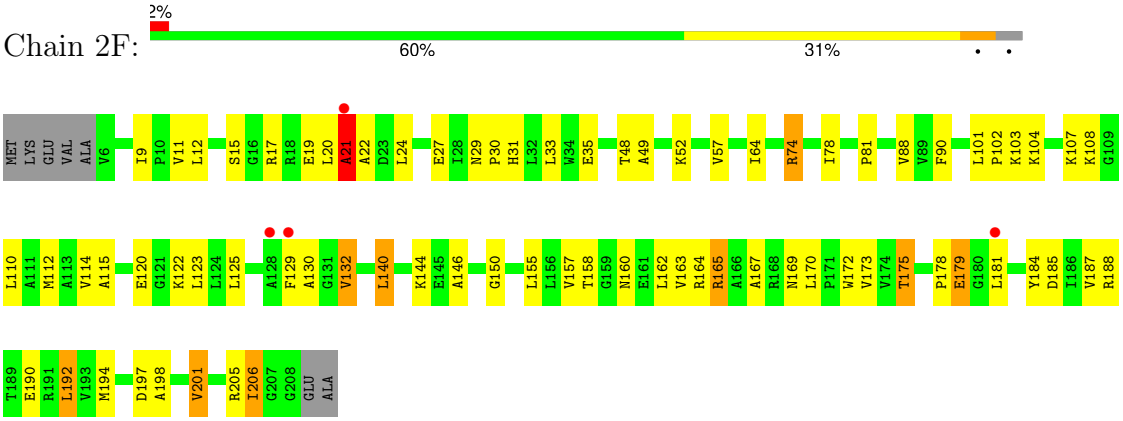
• Molecule 5: 50S ribosomal protein L4

Chain 1F:



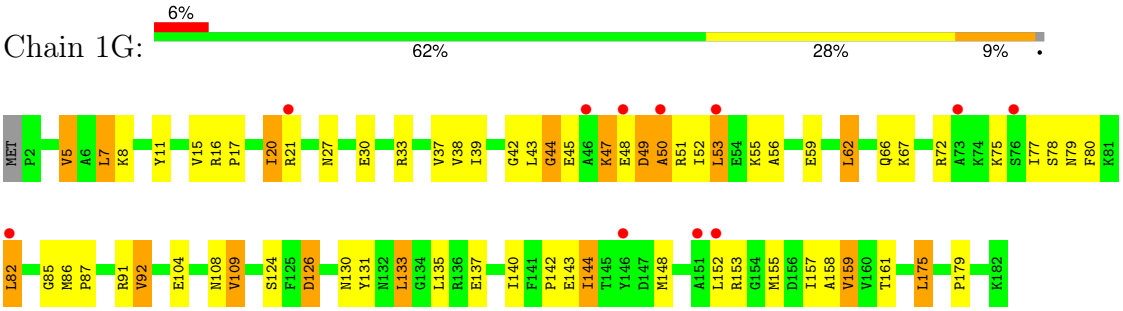
• Molecule 5: 50S ribosomal protein L4

Chain 2F:



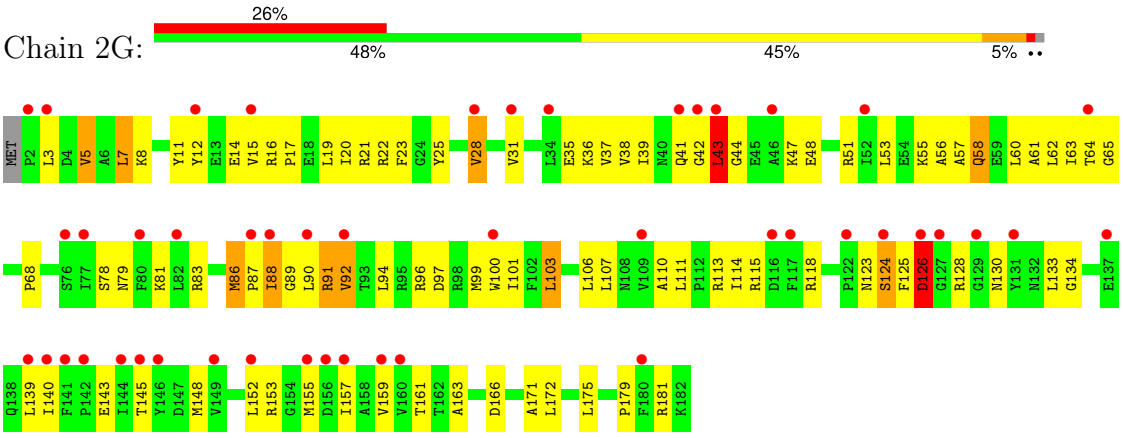
• Molecule 6: 50S ribosomal protein L5

Chain 1G:



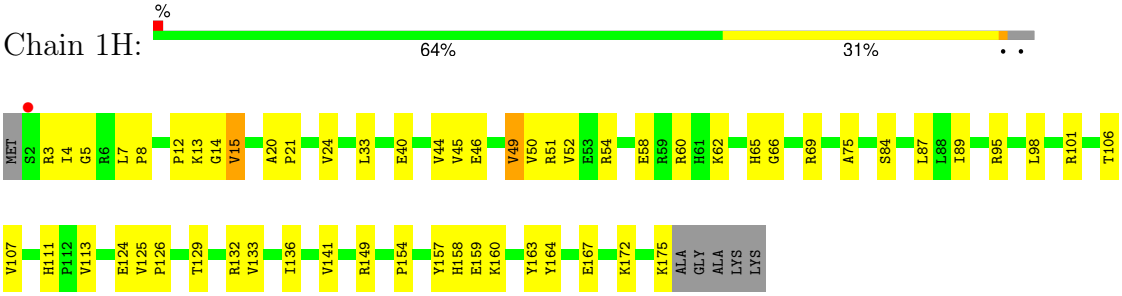
• Molecule 6: 50S ribosomal protein L5

Chain 2G:



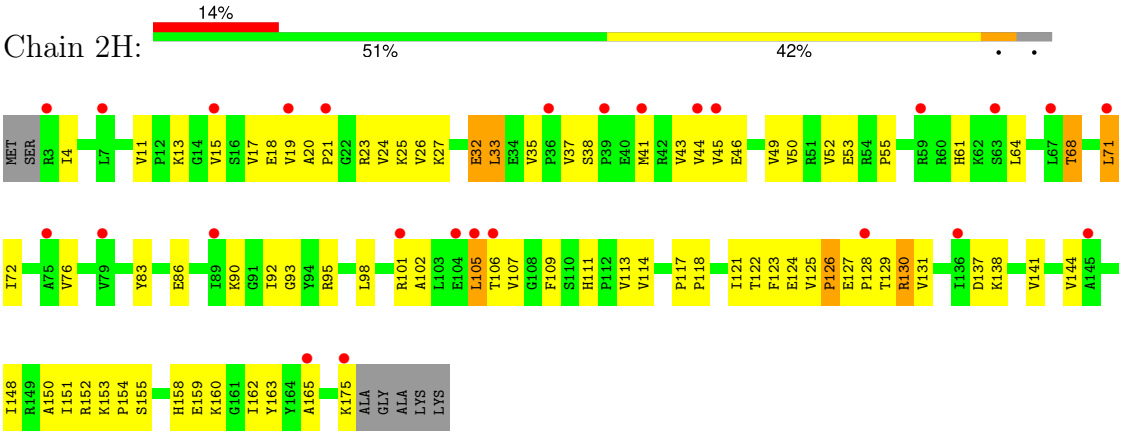
• Molecule 7: 50S ribosomal protein L6

Chain 1H:



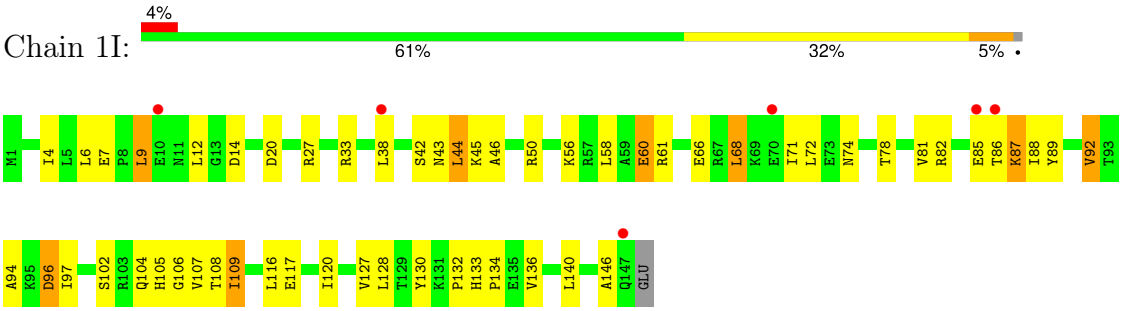
• Molecule 7: 50S ribosomal protein L6

Chain 2H:



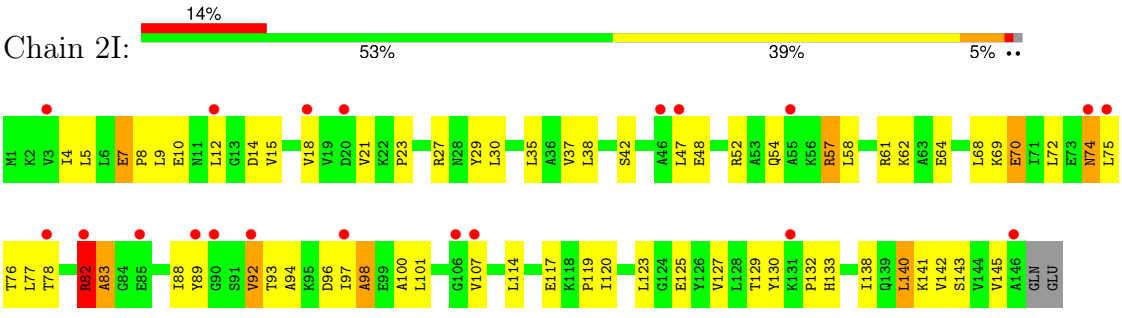
• Molecule 8: 50S ribosomal protein L9

Chain 1I:



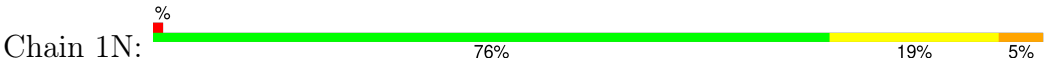
• Molecule 8: 50S ribosomal protein L9

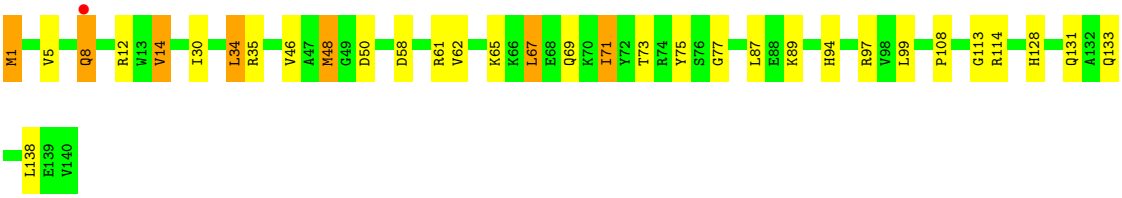
Chain 2I:



• Molecule 9: 50S ribosomal protein L13

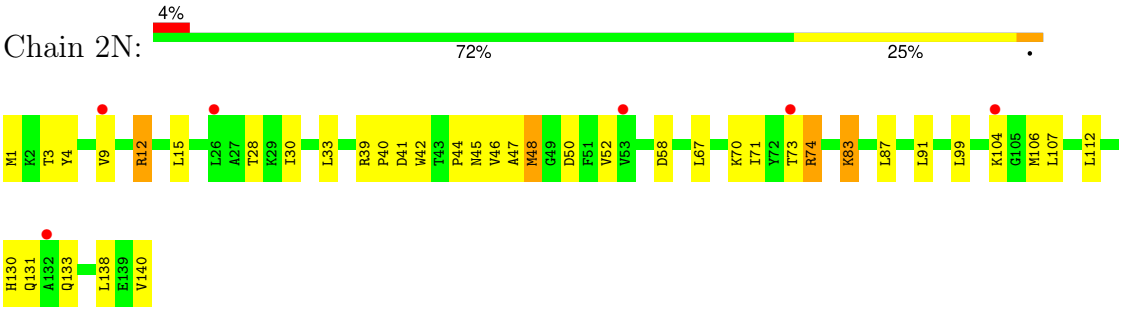
Chain 1N:





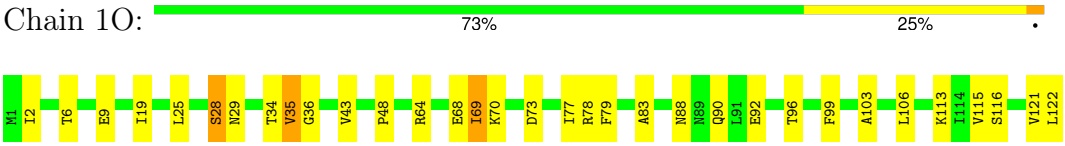
• Molecule 9: 50S ribosomal protein L13

Chain 2N:



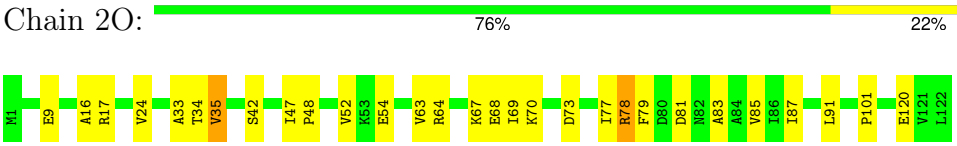
• Molecule 10: 50S ribosomal protein L14

Chain 1O:



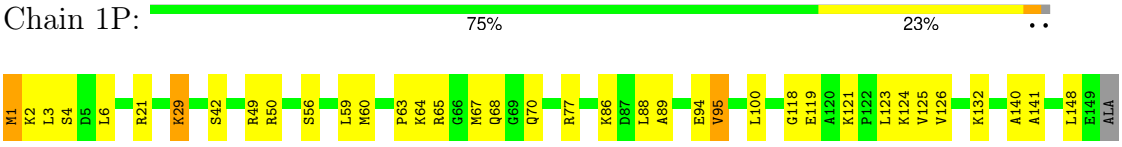
• Molecule 10: 50S ribosomal protein L14

Chain 2O:



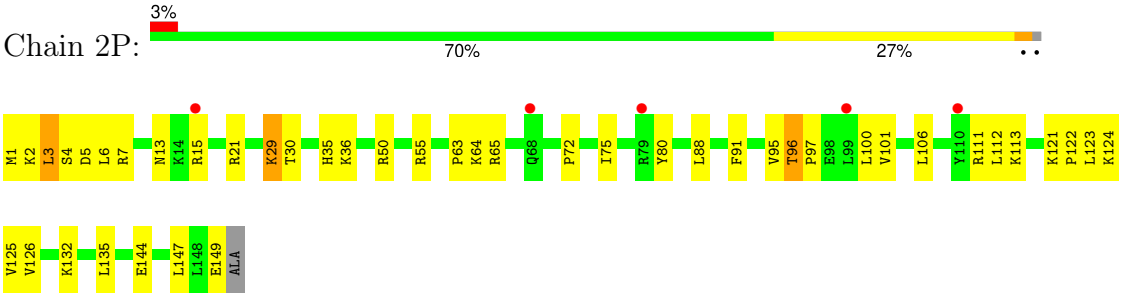
• Molecule 11: 50S ribosomal protein L15

Chain 1P:



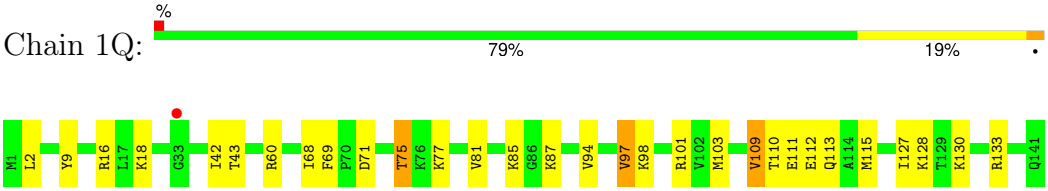
• Molecule 11: 50S ribosomal protein L15

Chain 2P:



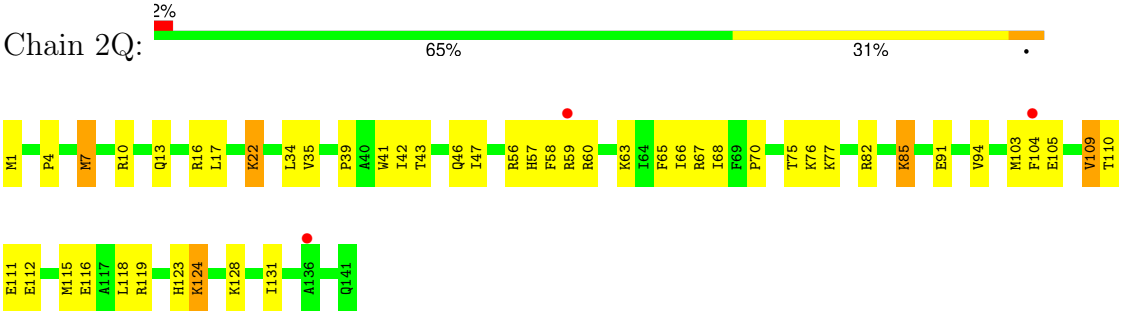
• Molecule 12: 50S ribosomal protein L16

Chain 1Q:



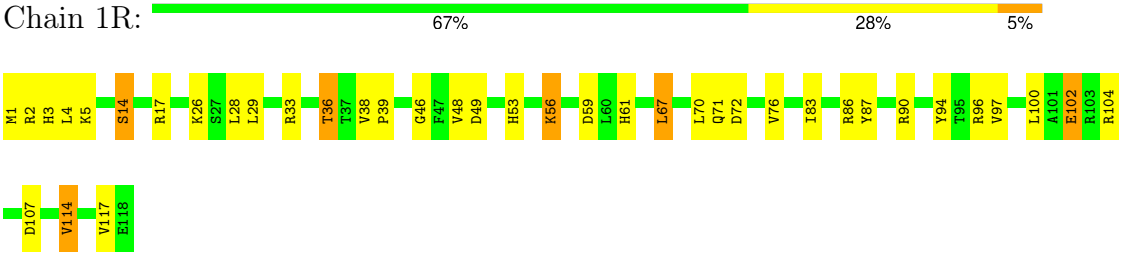
• Molecule 12: 50S ribosomal protein L16

Chain 2Q:



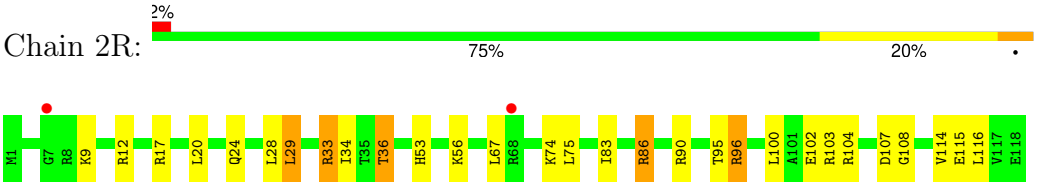
• Molecule 13: 50S ribosomal protein L17

Chain 1R:



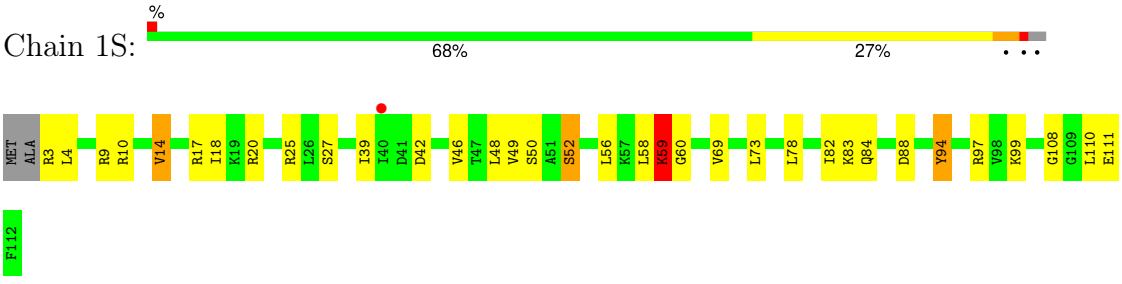
• Molecule 13: 50S ribosomal protein L17

Chain 2R:



• Molecule 14: 50S ribosomal protein L18

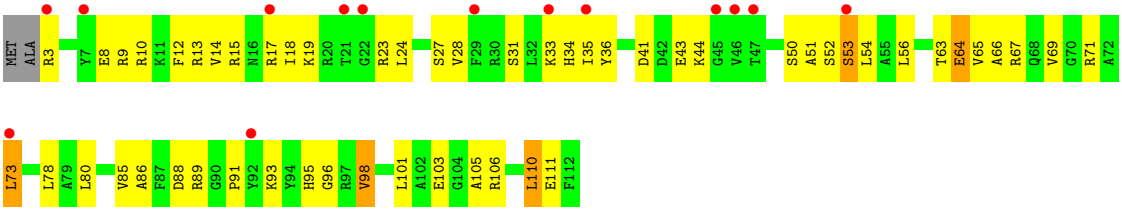
Chain 1S:



• Molecule 14: 50S ribosomal protein L18

Chain 2S:

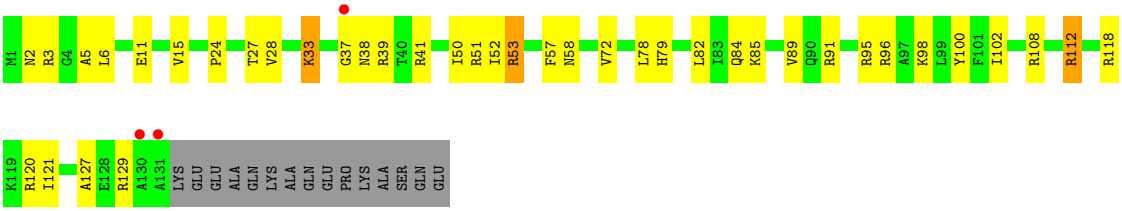




• Molecule 15: 50S ribosomal protein L19

Chain 1T:

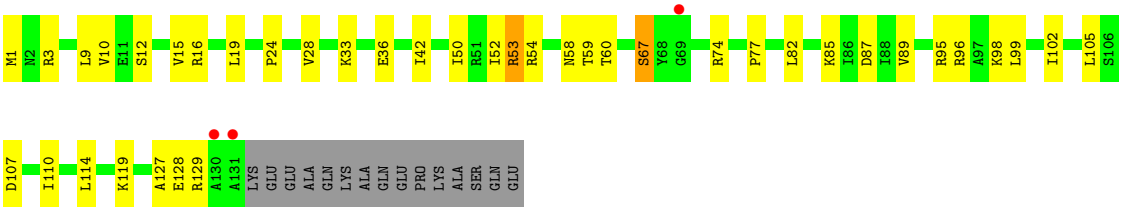




• Molecule 15: 50S ribosomal protein L19

Chain 2T:

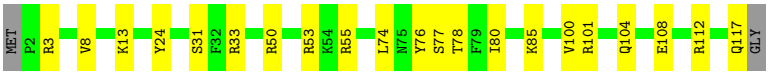




• Molecule 16: 50S ribosomal protein L20

Chain 1U:

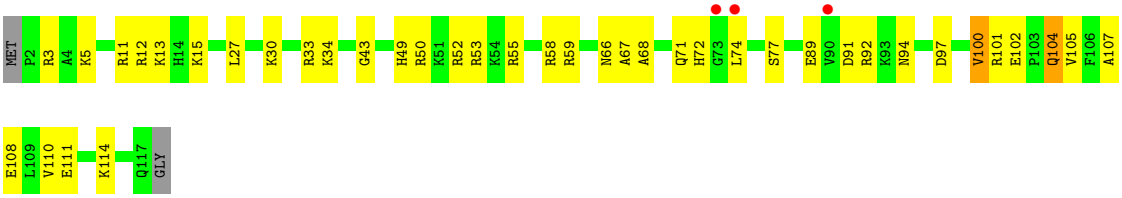




• Molecule 16: 50S ribosomal protein L20

Chain 2U:





• Molecule 17: 50S ribosomal protein L21

Chain 1V:



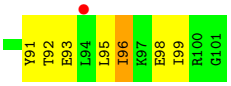


• Molecule 17: 50S ribosomal protein L21

Chain 2V:







• Molecule 18: 50S ribosomal protein L22

Chain 1W:

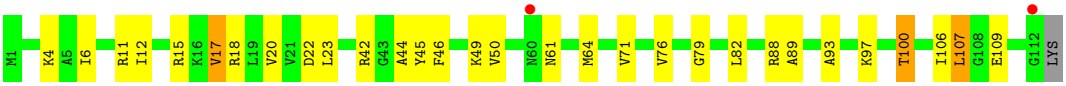




• Molecule 18: 50S ribosomal protein L22

Chain 2W:





• Molecule 19: 50S ribosomal protein L23

Chain 1X:



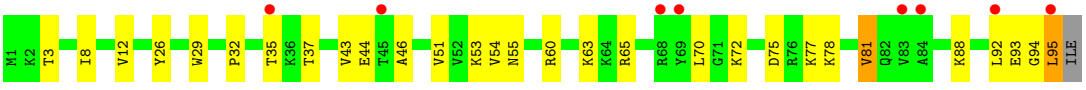




• Molecule 19: 50S ribosomal protein L23

Chain 2X:

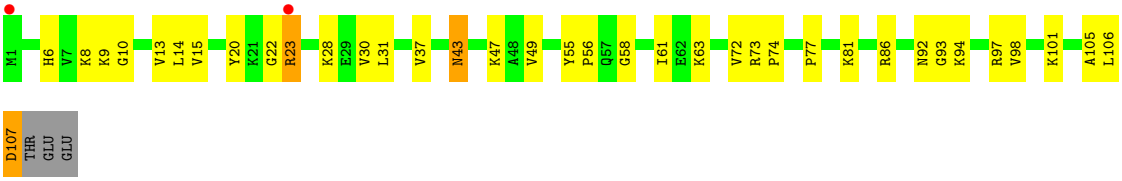




• Molecule 20: 50S ribosomal protein L24

Chain 1Y:

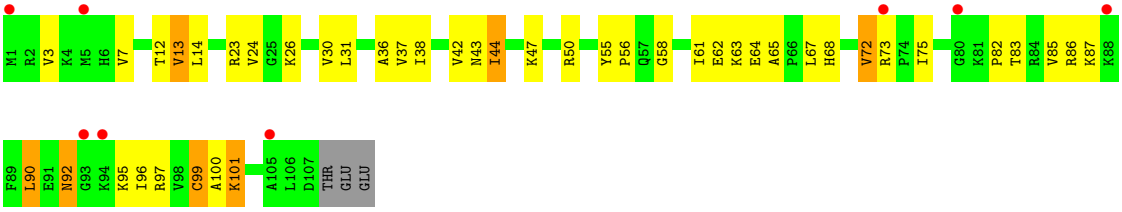




• Molecule 20: 50S ribosomal protein L24

Chain 2Y:

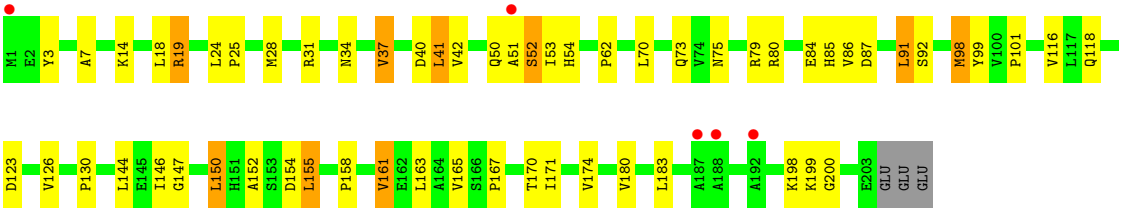




• Molecule 21: 50S ribosomal protein L25

Chain 1Z:

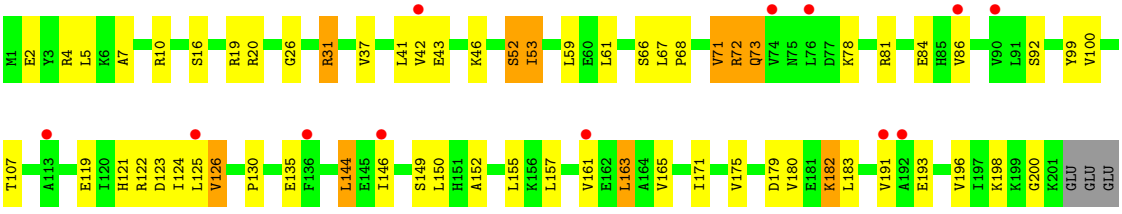




• Molecule 21: 50S ribosomal protein L25

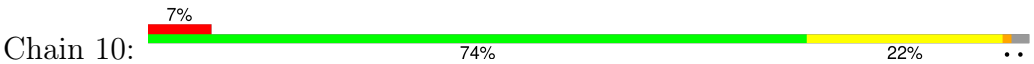
Chain 2Z:

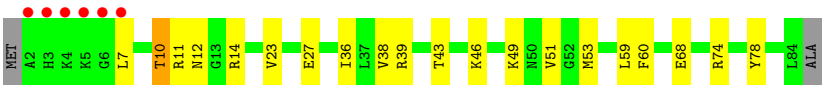




• Molecule 22: 50S ribosomal protein L27

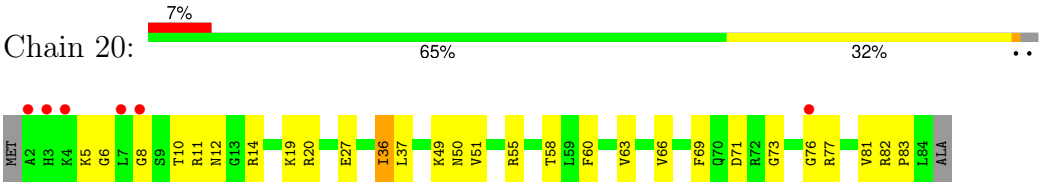
Chain 10:





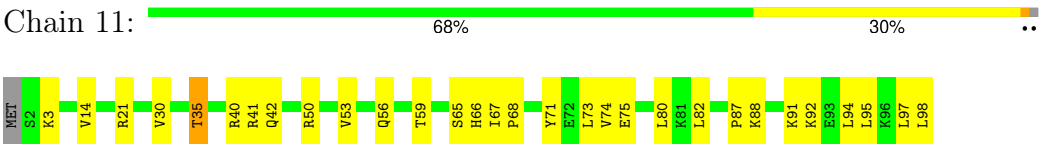
• Molecule 22: 50S ribosomal protein L27

Chain 20:



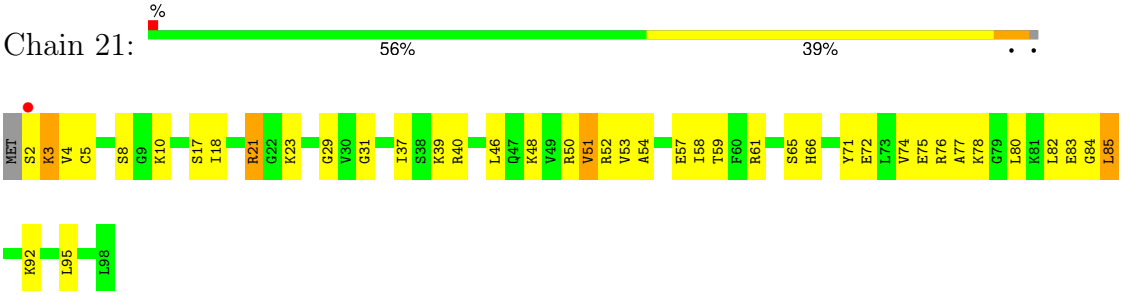
• Molecule 23: 50S ribosomal protein L28

Chain 11:



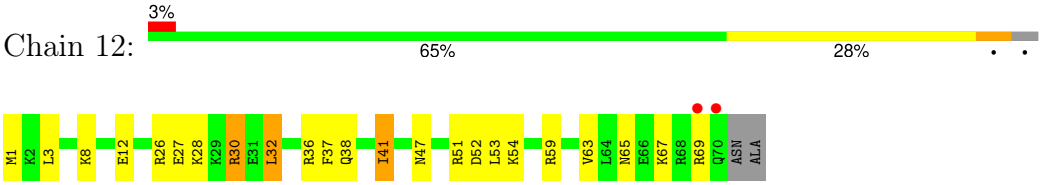
• Molecule 23: 50S ribosomal protein L28

Chain 21:



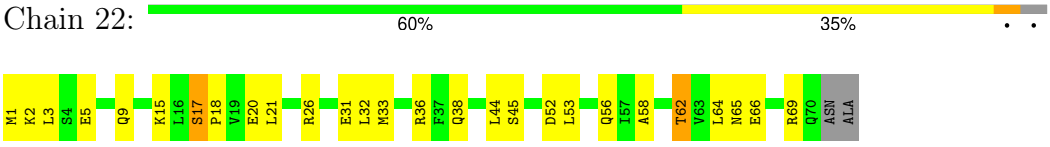
• Molecule 24: 50S ribosomal protein L29

Chain 12:



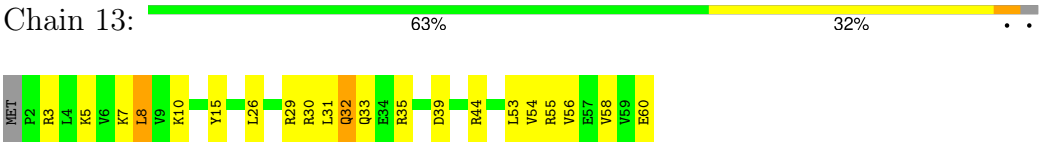
• Molecule 24: 50S ribosomal protein L29

Chain 22:



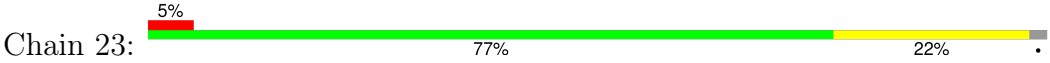
• Molecule 25: 50S ribosomal protein L30

Chain 13:



• Molecule 25: 50S ribosomal protein L30

Chain 23:

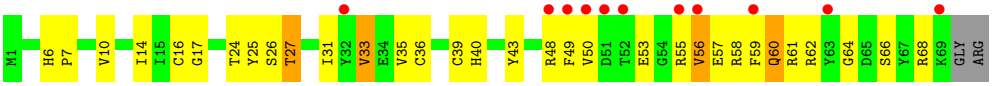




• Molecule 26: 50S ribosomal protein L31

Chain 14:

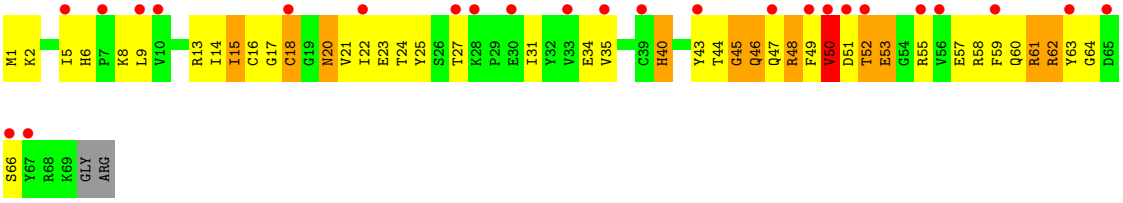




• Molecule 26: 50S ribosomal protein L31

Chain 24:

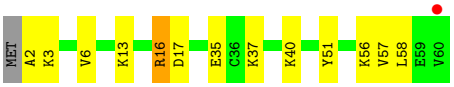




• Molecule 27: 50S ribosomal protein L32

Chain 15:

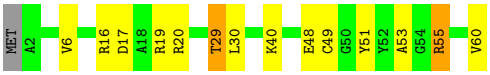




• Molecule 27: 50S ribosomal protein L32

Chain 25:

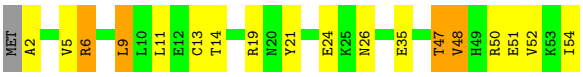




• Molecule 28: 50S ribosomal protein L33

Chain 16:





• Molecule 28: 50S ribosomal protein L33

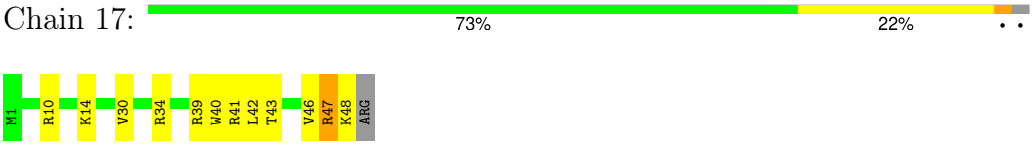
Chain 26:





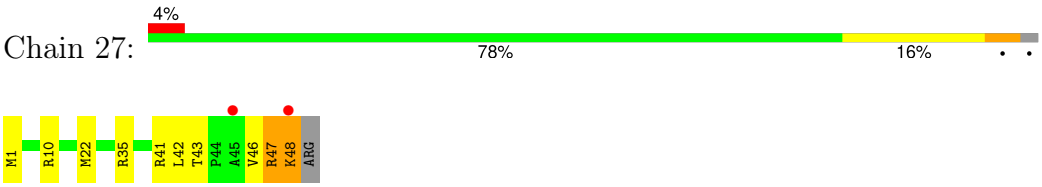
• Molecule 29: 50S ribosomal protein L34

Chain 17:



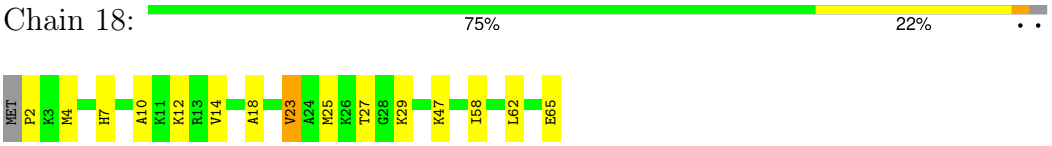
• Molecule 29: 50S ribosomal protein L34

Chain 27:



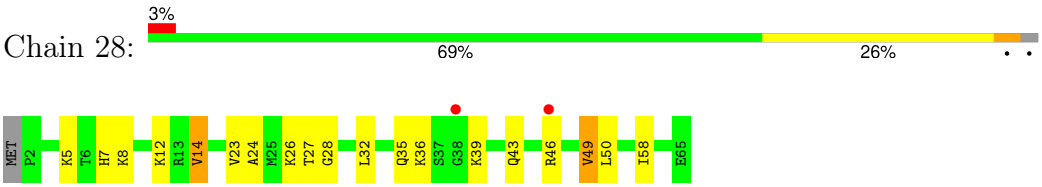
• Molecule 30: 50S ribosomal protein L35

Chain 18:



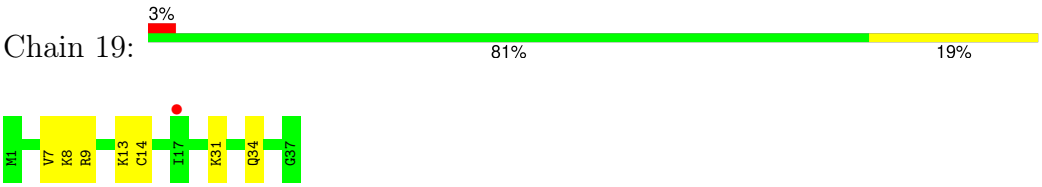
• Molecule 30: 50S ribosomal protein L35

Chain 28:



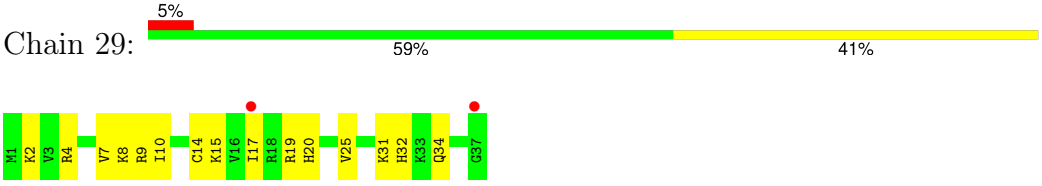
• Molecule 31: 50S ribosomal protein L36

Chain 19:



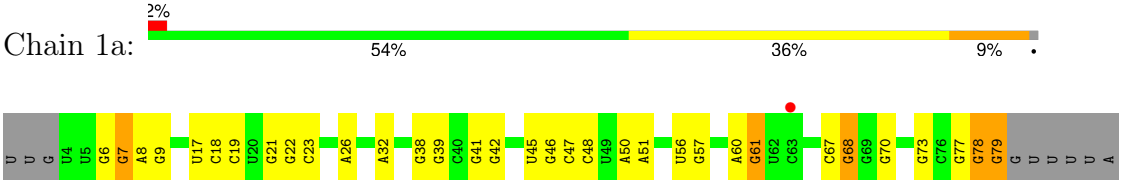
• Molecule 31: 50S ribosomal protein L36

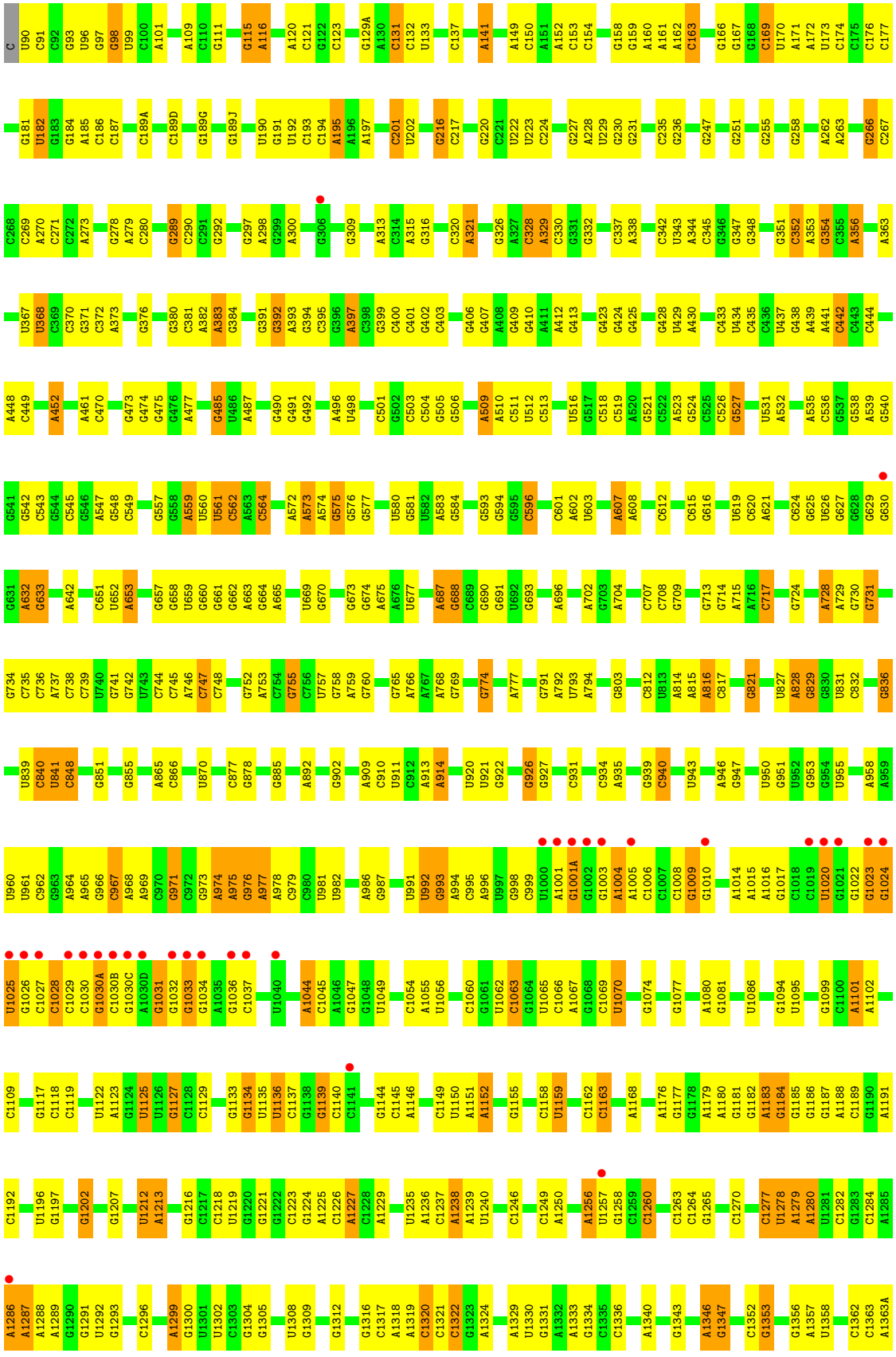
Chain 29:

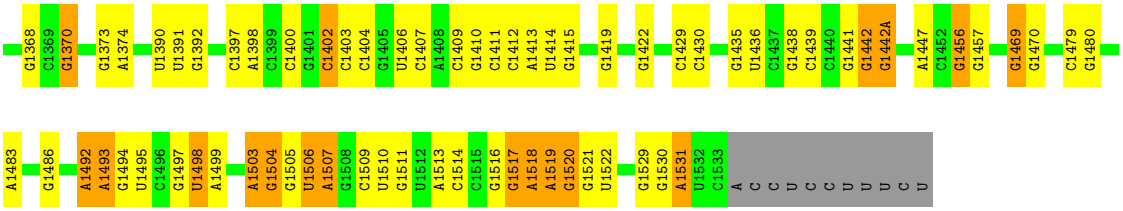


• Molecule 32: 16S Ribosomal RNA

Chain 1a:



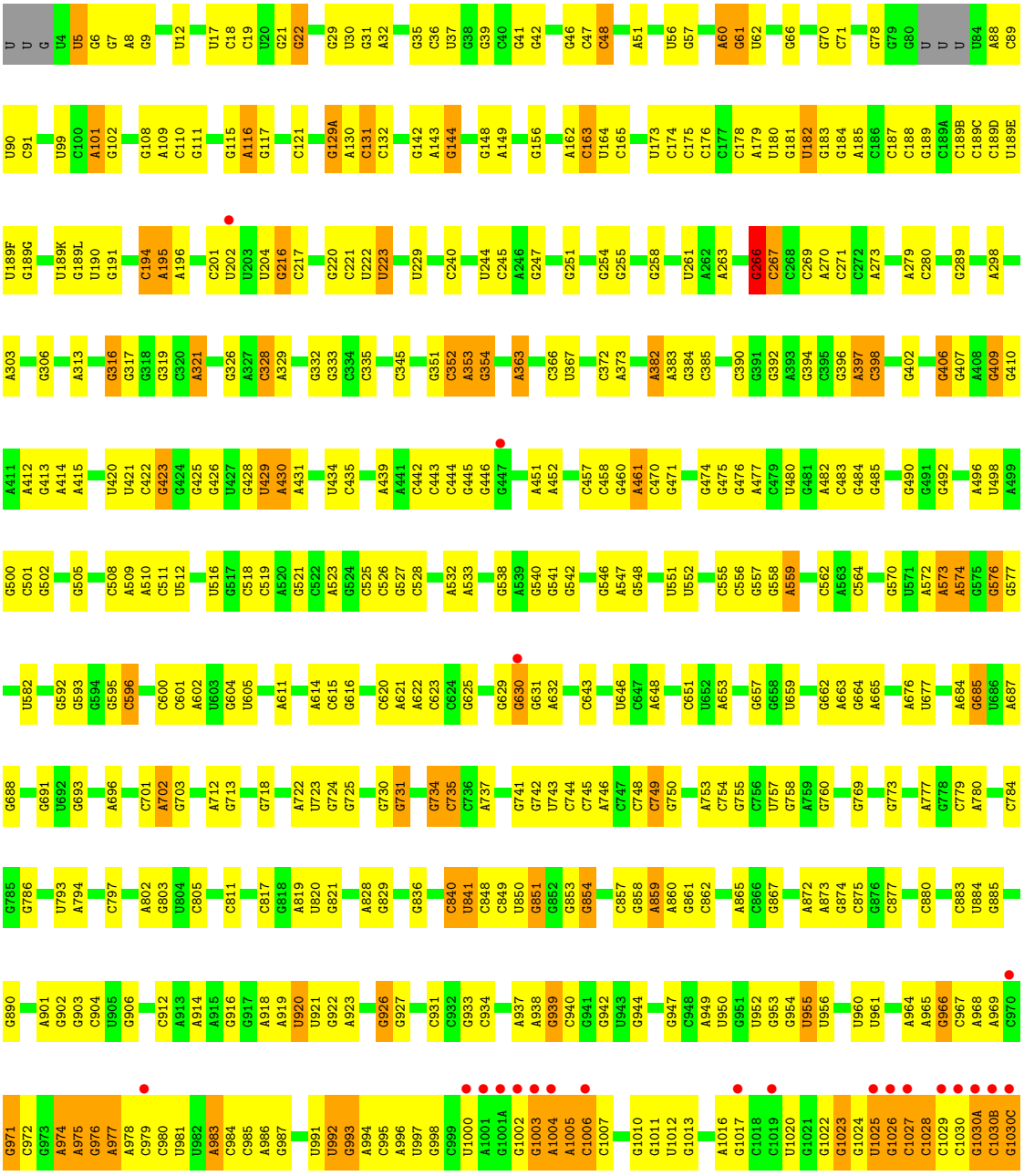


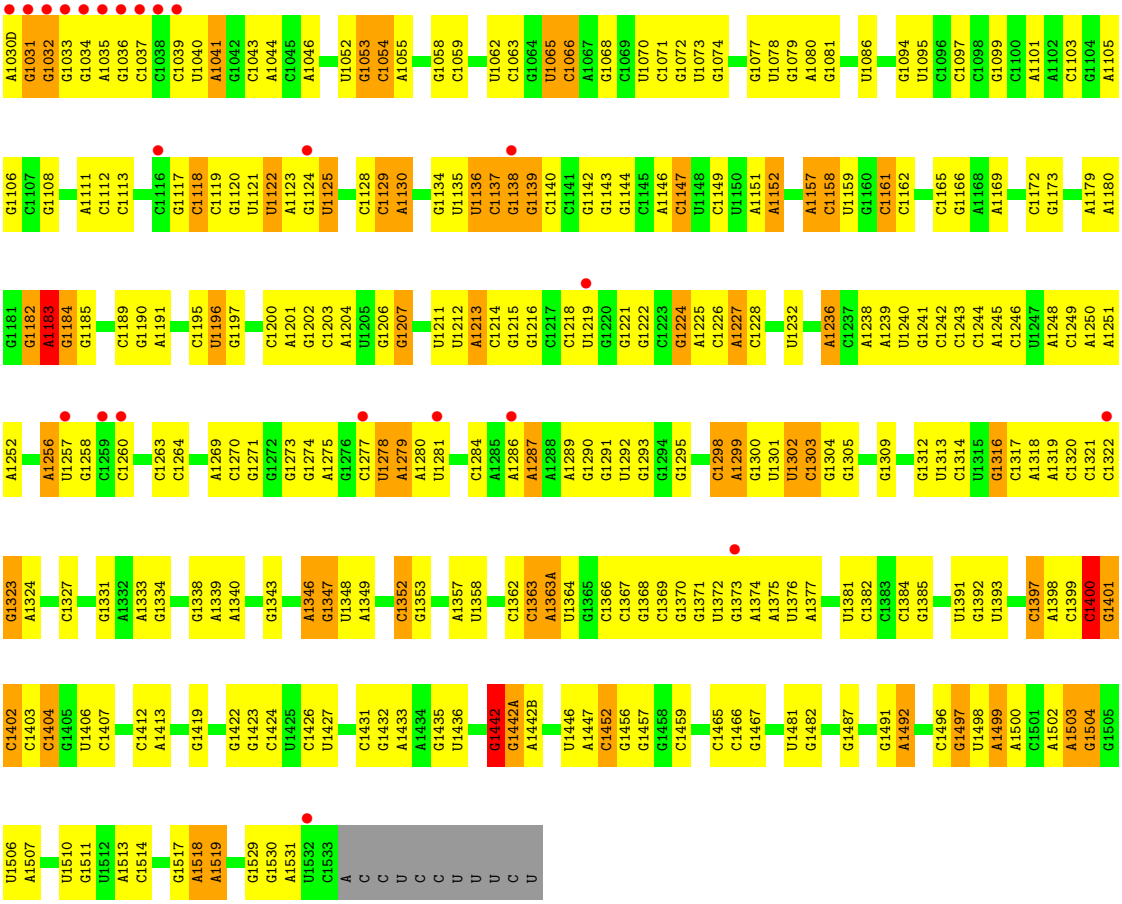


• Molecule 32: 16S Ribosomal RNA

Chain 2a:



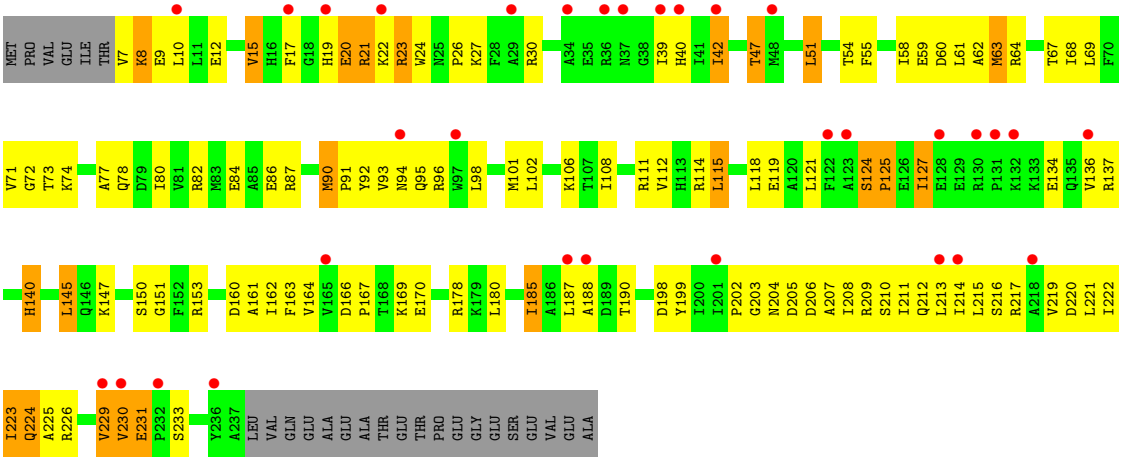




• Molecule 33: 30S ribosomal protein S2

Chain 1b:

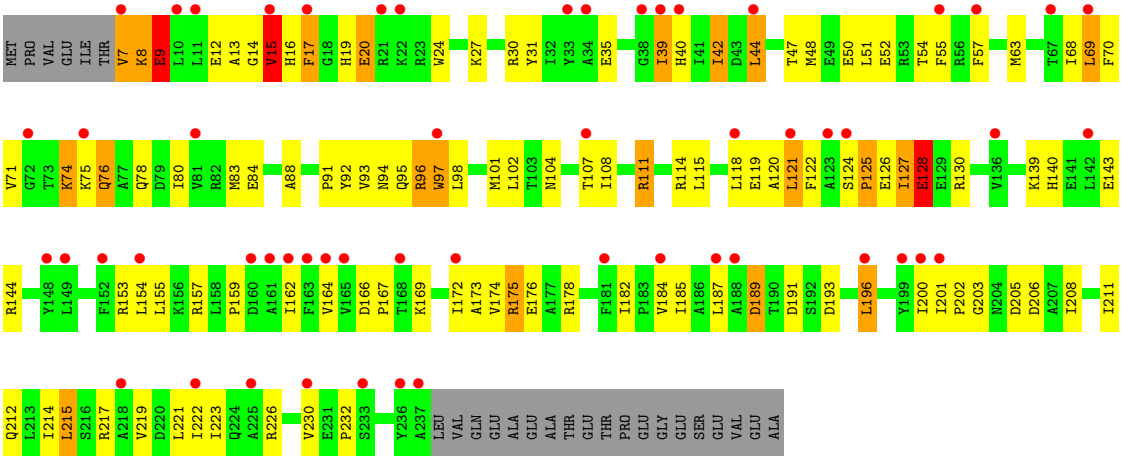




• Molecule 33: 30S ribosomal protein S2

Chain 2b:

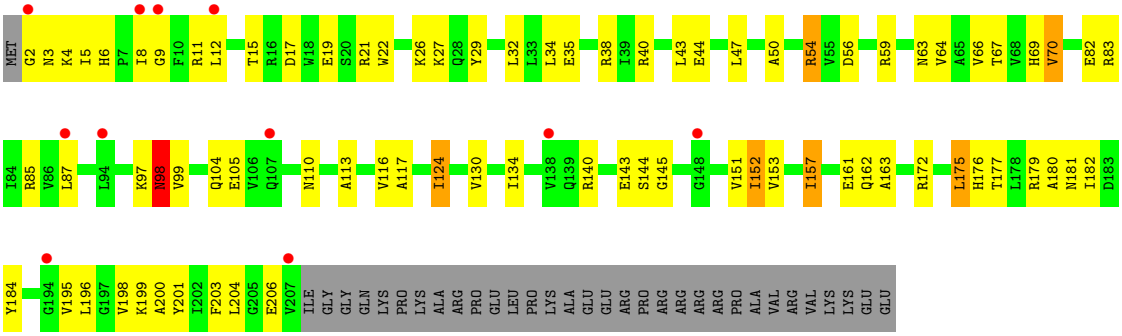




• Molecule 34: 30S ribosomal protein S3

Chain 1c:

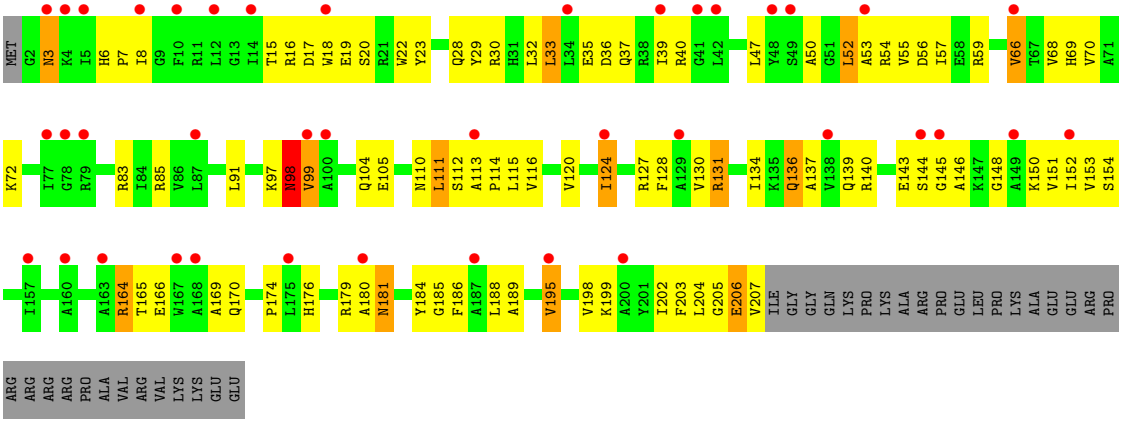




• Molecule 34: 30S ribosomal protein S3

Chain 2c:

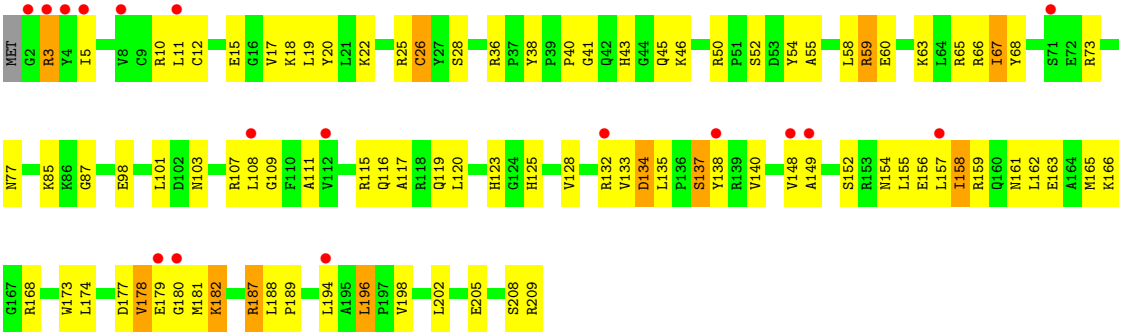




• Molecule 35: 30S ribosomal protein S4

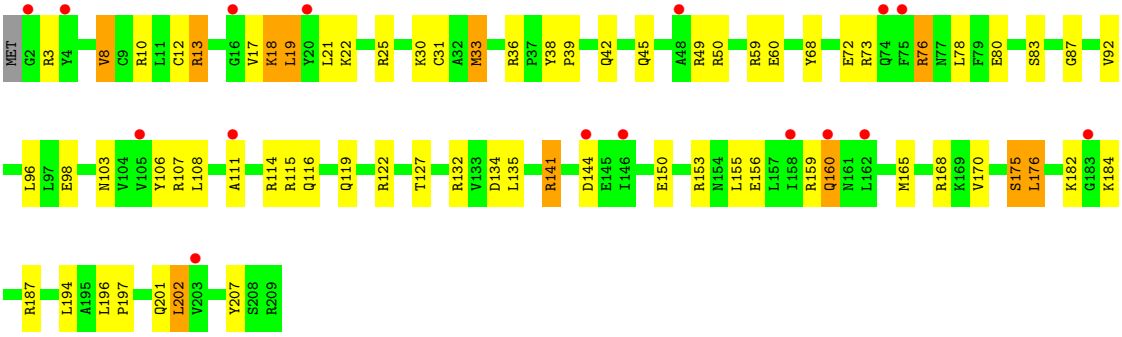
Chain 1d:





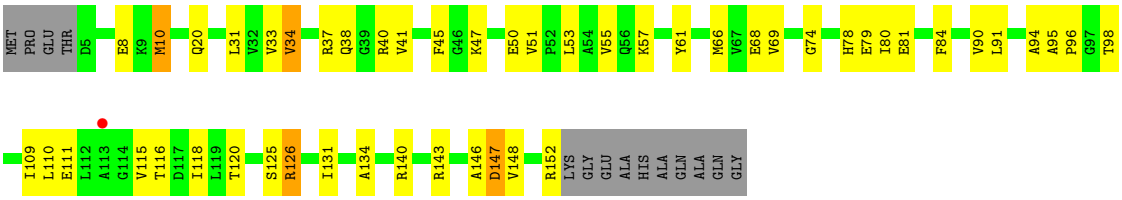
• Molecule 35: 30S ribosomal protein S4





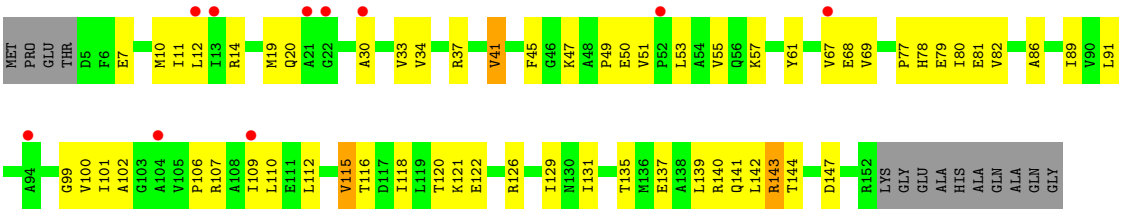
• Molecule 36: 30S ribosomal protein S5





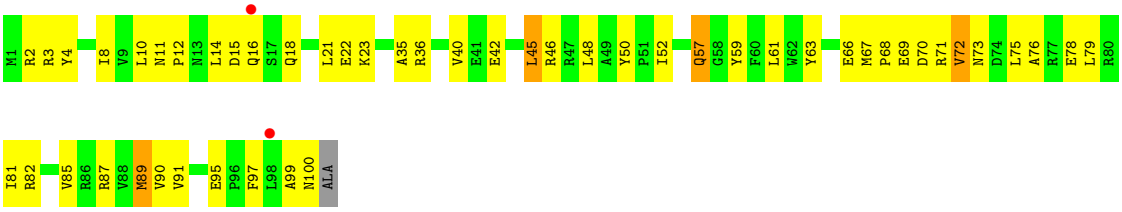
• Molecule 36: 30S ribosomal protein S5





• Molecule 37: 30S ribosomal protein S6

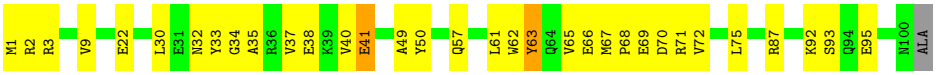




• Molecule 37: 30S ribosomal protein S6

Chain 2f:

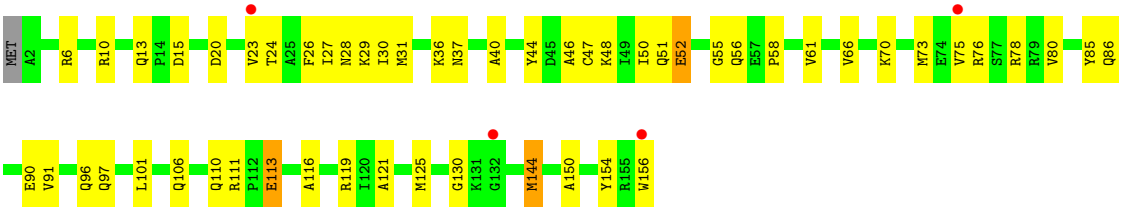




• Molecule 38: 30S ribosomal protein S7

Chain 1g:

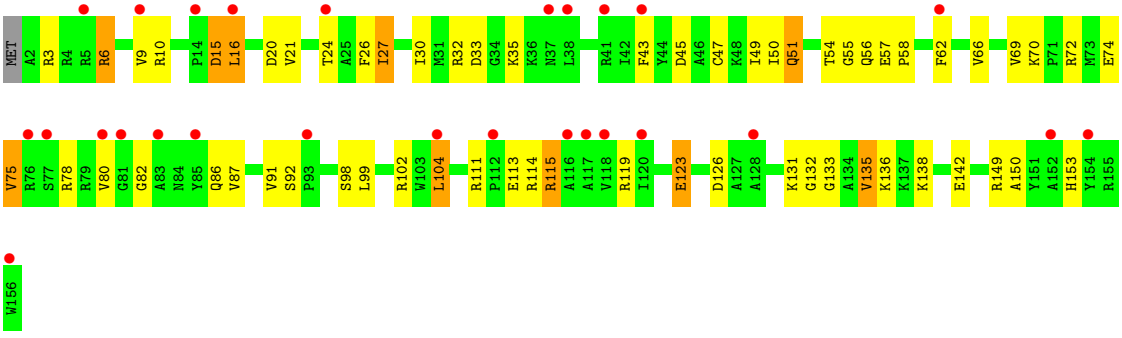




• Molecule 38: 30S ribosomal protein S7

Chain 2g:

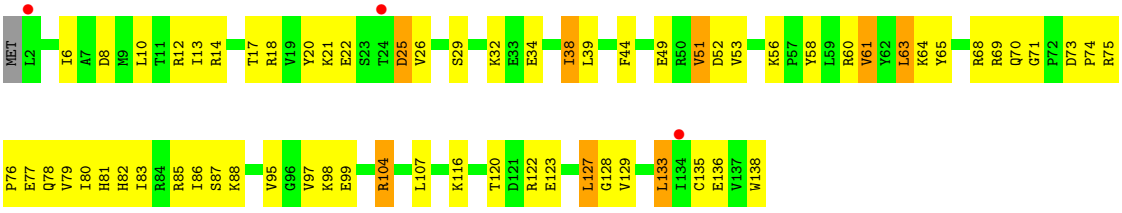




• Molecule 39: 30S ribosomal protein S8

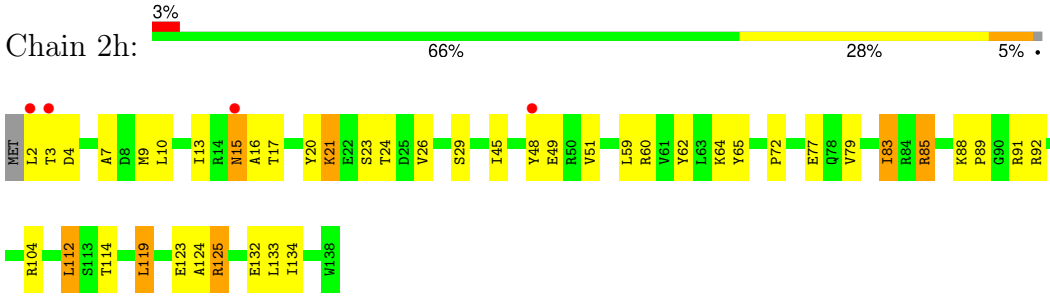
Chain 1h:





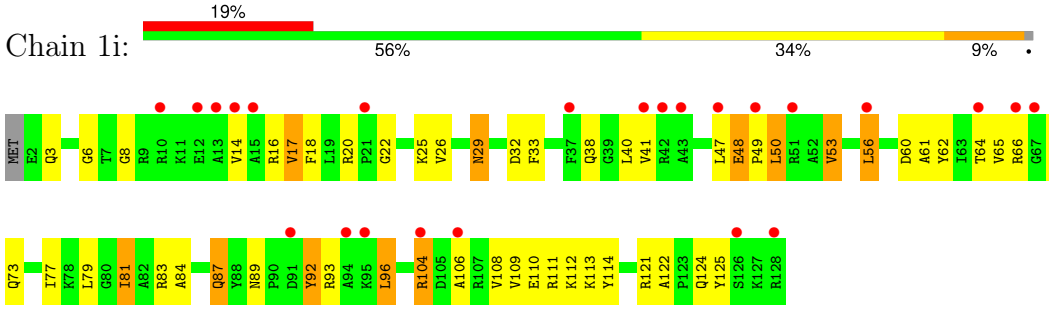
• Molecule 39: 30S ribosomal protein S8

Chain 2h:



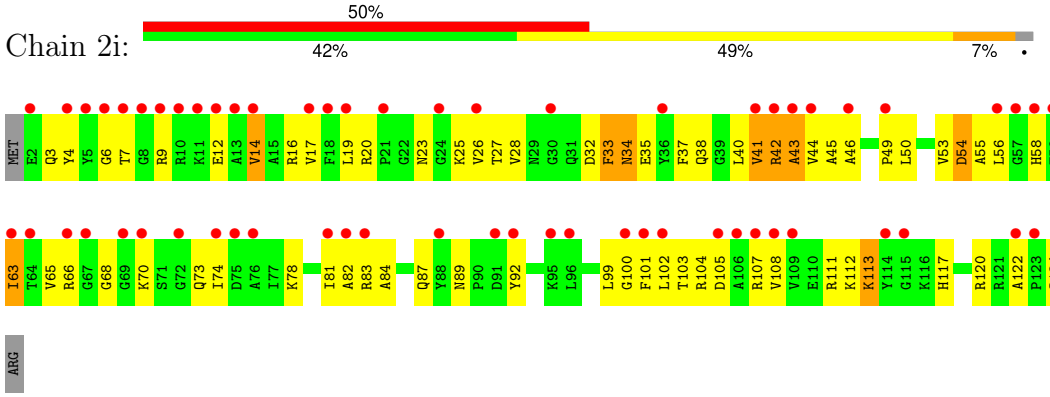
• Molecule 40: 30S ribosomal protein S9

Chain 1i:



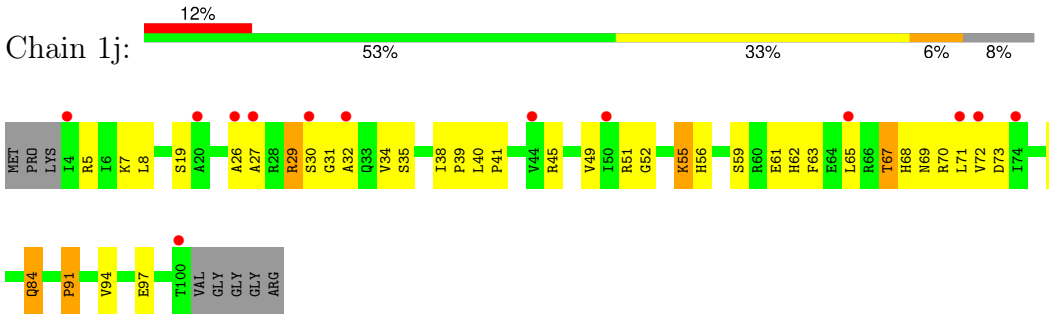
• Molecule 40: 30S ribosomal protein S9

Chain 2i:



• Molecule 41: 30S ribosomal protein S10

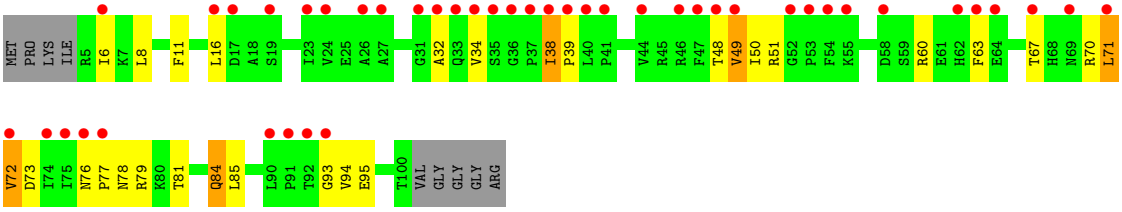
Chain 1j:



• Molecule 41: 30S ribosomal protein S10

Chain 2j:

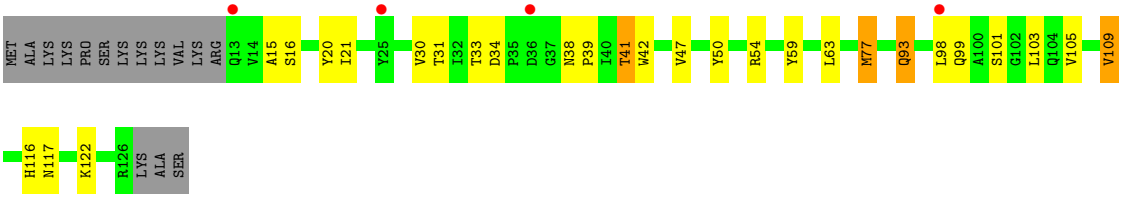




• Molecule 42: 30S ribosomal protein S11

Chain 1k:

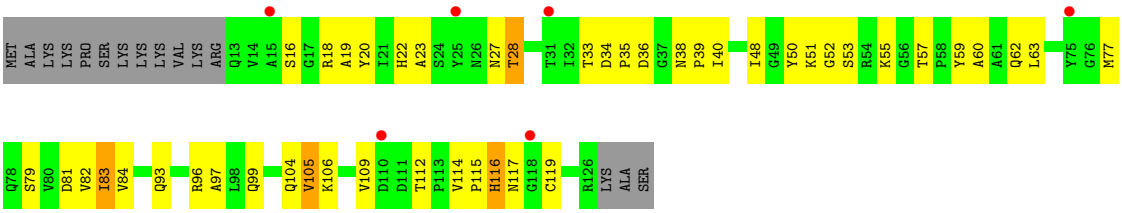




• Molecule 42: 30S ribosomal protein S11

Chain 2k:

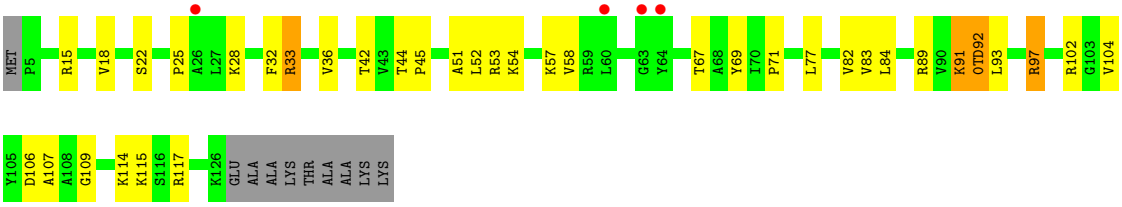




• Molecule 43: 30S ribosomal protein S12

Chain 1l:

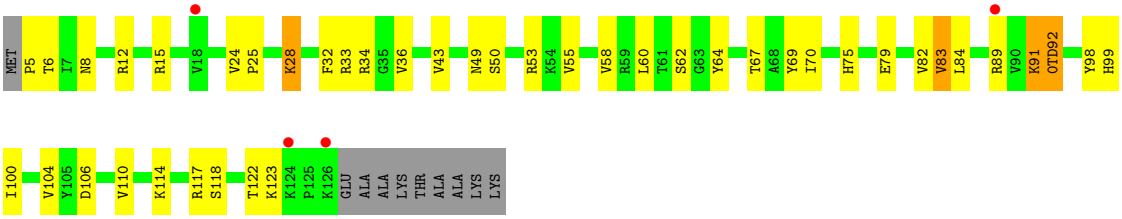




• Molecule 43: 30S ribosomal protein S12

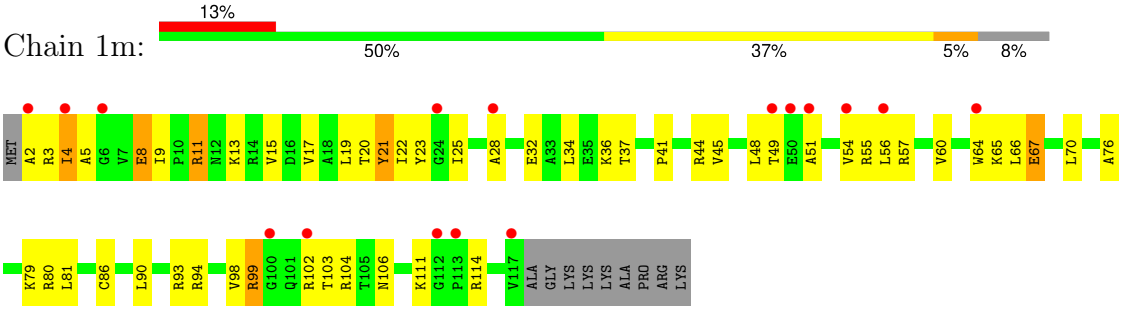
Chain 2l:





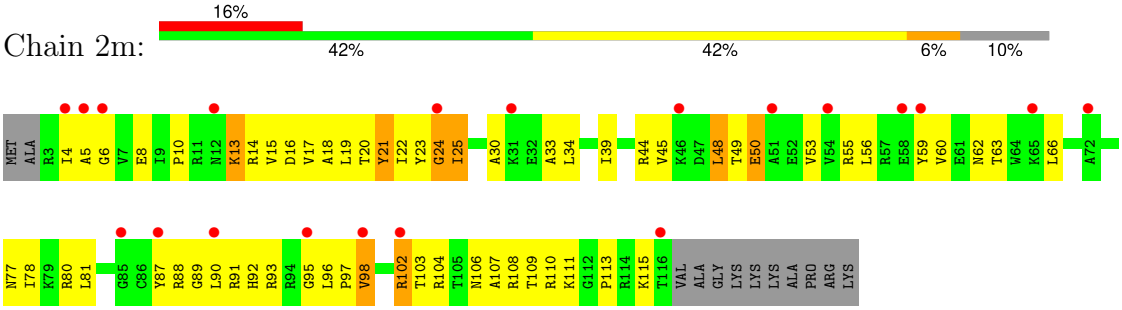
• Molecule 44: 30S ribosomal protein S13

Chain 1m:



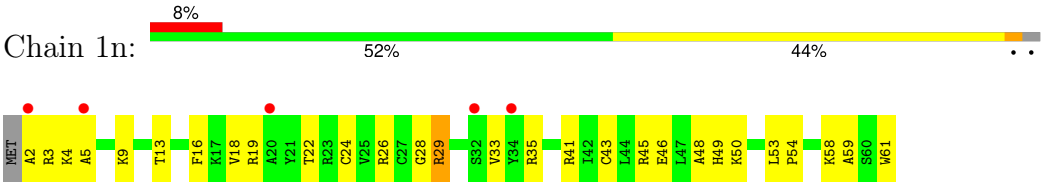
• Molecule 44: 30S ribosomal protein S13

Chain 2m:



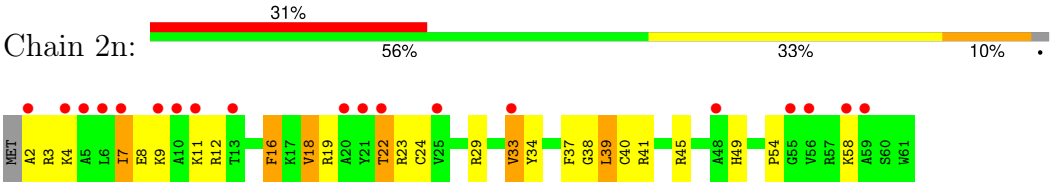
• Molecule 45: 30S ribosomal protein S14 type Z

Chain 1n:



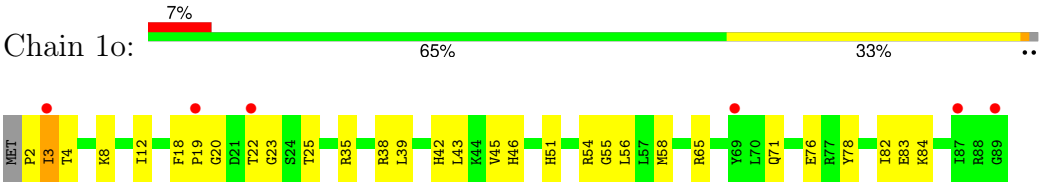
• Molecule 45: 30S ribosomal protein S14 type Z

Chain 2n:



• Molecule 46: 30S ribosomal protein S15

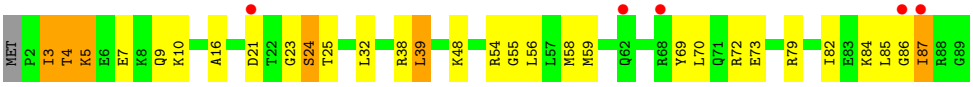
Chain 1o:



• Molecule 46: 30S ribosomal protein S15

Chain 2o:

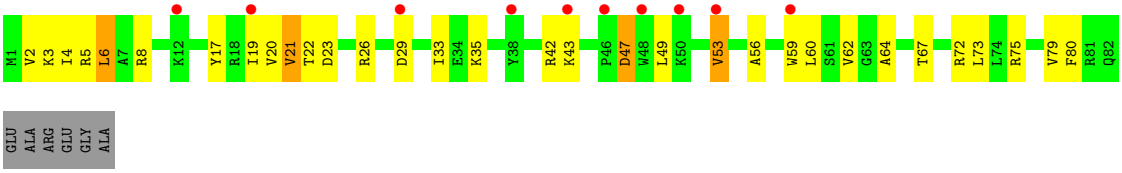




• Molecule 47: 30S ribosomal protein S16

Chain 1p:

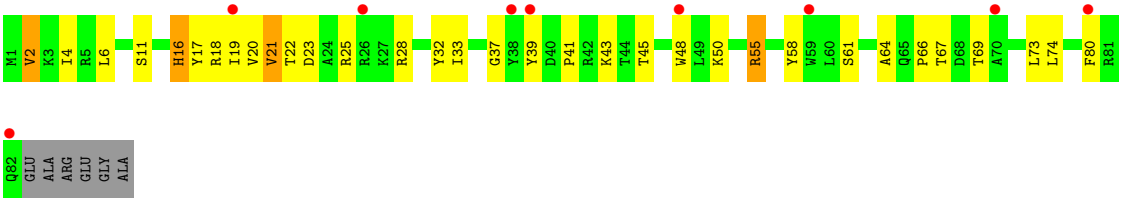




• Molecule 47: 30S ribosomal protein S16

Chain 2p:

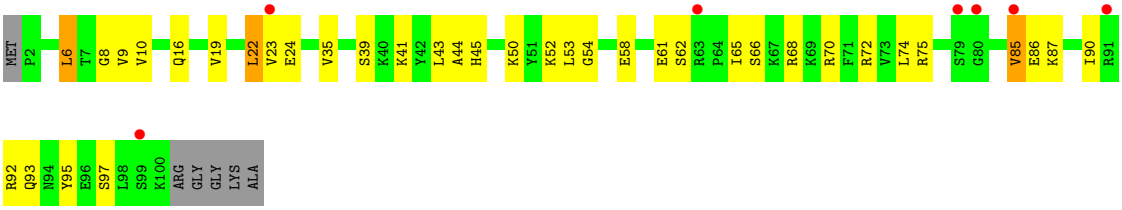




• Molecule 48: 30S ribosomal protein S17

Chain 1q:

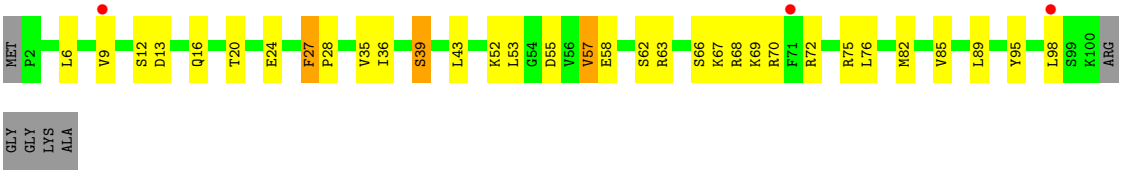




• Molecule 48: 30S ribosomal protein S17

Chain 2q:

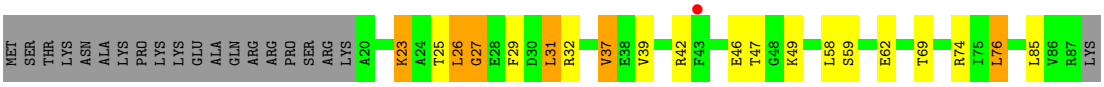




• Molecule 49: 30S ribosomal protein S18

Chain 1r:

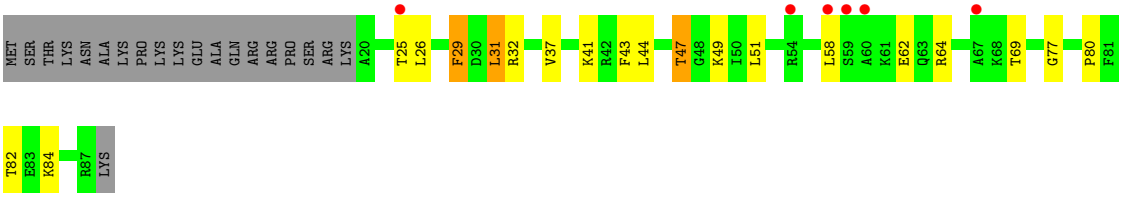




• Molecule 49: 30S ribosomal protein S18

Chain 2r:

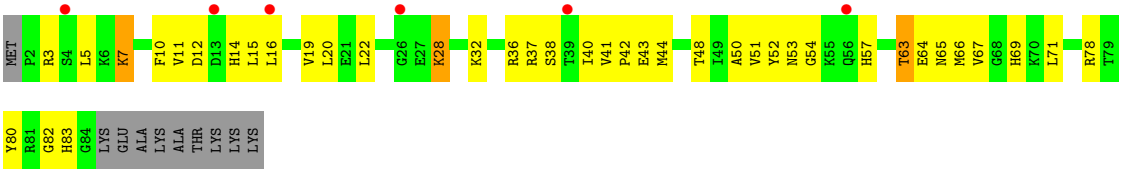




• Molecule 50: 30S ribosomal protein S19

Chain 1s:

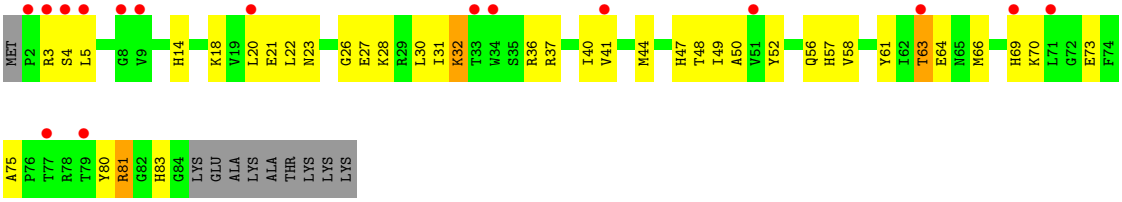




• Molecule 50: 30S ribosomal protein S19

Chain 2s:

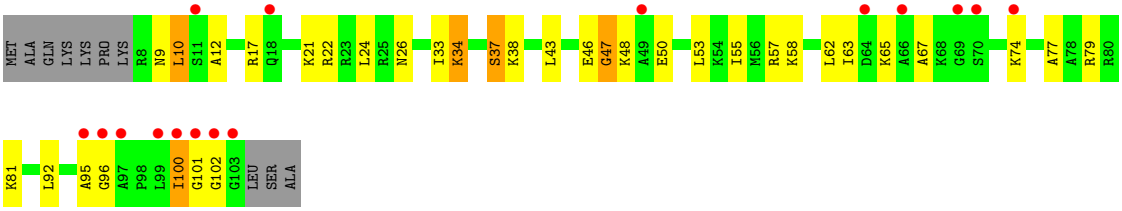




• Molecule 51: 30S ribosomal protein S20

Chain 1t:

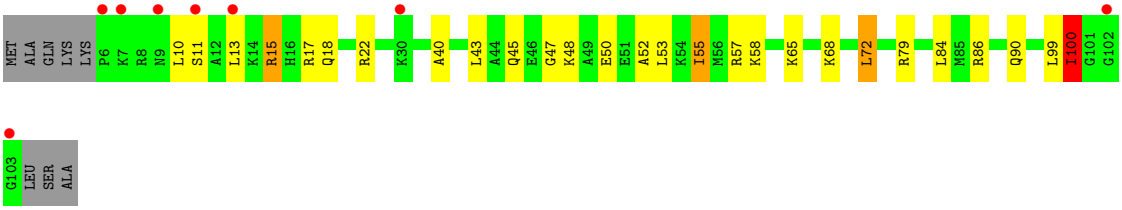




• Molecule 51: 30S ribosomal protein S20

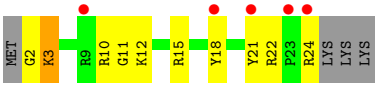
Chain 2t:





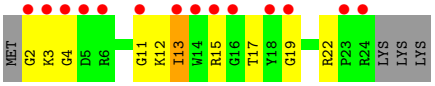
• Molecule 52: 30S ribosomal protein Thx





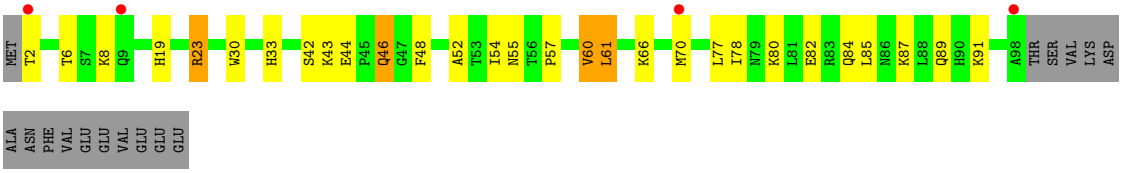
• Molecule 52: 30S ribosomal protein Thx





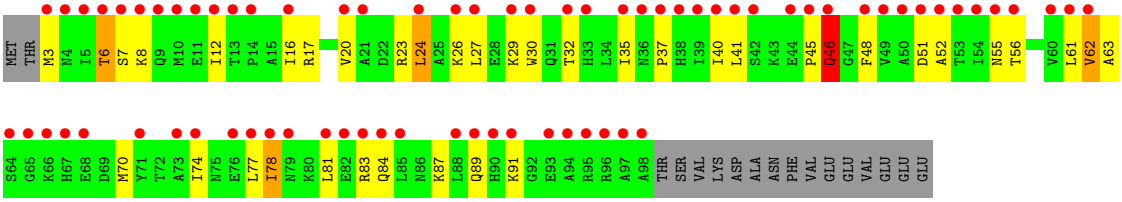
• Molecule 53: Ribosome-associated inhibitor A



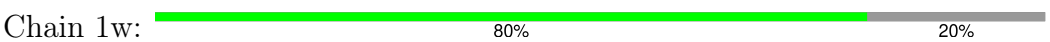


• Molecule 53: Ribosome-associated inhibitor A





• Molecule 54: A-site Deacylated tRNA Analog





• Molecule 54: A-site Deacylated tRNA Analog

Chain 2w:





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

Chain 1x:





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

Chain 2x:





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

Chain 1v:





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

Chain 2v:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	209.71Å 449.95Å 621.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	224.98 – 2.50 224.98 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.5 (224.98-2.50) 98.5 (224.98-2.50)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.16 (at 2.52Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.229 , 0.280 0.230 , 0.280	Depositor DCC
R_{free} test set	98581 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å^2)	46.2	Xtriage
Anisotropy	0.157	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 65.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.35$, $< L^2 > = 0.18$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	297633	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.63% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: G7M, 5MU, 2MU, MG, MA6, 0TD, 2MG, 8AN, 5MC, 4OC, SF4, MPD, UR3, OMC, ZN, M2G, OMG, PSU, CLM, 2MA

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	0.29	0/69030	0.49	4/107750 (0.0%)
1	2A	0.23	0/68902	0.43	1/107548 (0.0%)
2	1B	0.25	0/2876	0.44	0/4486
2	2B	0.19	0/2878	0.37	0/4490
3	1D	0.28	0/2181	0.52	0/2940
3	2D	0.24	0/2186	0.51	0/2944
4	1E	0.26	0/1592	0.51	0/2149
4	2E	0.22	0/1592	0.45	0/2149
5	1F	0.27	0/1619	0.50	0/2193
5	2F	0.23	0/1615	0.51	2/2188 (0.1%)
6	1G	0.21	0/1451	0.45	0/1961
6	2G	0.21	0/1449	0.46	0/1957
7	1H	0.23	0/1356	0.45	0/1834
7	2H	0.21	0/1350	0.45	0/1826
8	1I	0.20	0/1109	0.45	0/1512
8	2I	1.30	3/1091 (0.3%)	0.82	3/1490 (0.2%)
9	1N	0.26	0/1148	0.49	0/1547
9	2N	0.22	0/1144	0.42	0/1543
10	1O	0.26	0/943	0.48	0/1269
10	2O	0.23	0/943	0.42	0/1269
11	1P	0.28	0/1152	0.53	0/1533
11	2P	0.21	0/1152	0.49	0/1533
12	1Q	0.26	0/1143	0.50	0/1527
12	2Q	0.24	0/1143	0.49	0/1527
13	1R	0.28	0/982	0.51	0/1312
13	2R	0.24	0/982	0.48	0/1312
14	1S	0.23	0/887	0.49	0/1180
14	2S	0.21	0/880	0.44	0/1172
15	1T	0.26	0/1105	0.52	0/1477
15	2T	0.22	0/1097	0.42	0/1468
16	1U	0.29	0/977	0.51	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
16	2U	0.21	0/977	0.43	0/1301
17	1V	0.28	0/786	0.52	0/1053
17	2V	0.20	0/782	0.45	0/1049
18	1W	0.29	0/897	0.48	0/1205
18	2W	0.23	0/897	0.43	0/1205
19	1X	0.27	0/764	0.52	0/1025
19	2X	0.22	0/764	0.46	0/1025
20	1Y	0.25	0/823	0.51	0/1099
20	2Y	0.21	0/823	0.45	0/1100
21	1Z	0.23	0/1620	0.44	0/2200
21	2Z	0.20	0/1590	0.47	0/2162
22	10	0.27	0/662	0.53	0/881
22	20	0.23	0/659	0.55	0/877
23	11	0.24	0/761	0.43	0/1013
23	21	0.22	0/766	0.43	0/1018
24	12	0.23	0/590	0.48	0/781
24	22	0.20	0/594	0.40	0/785
25	13	0.26	0/474	0.50	0/635
25	23	0.22	0/469	0.50	0/630
26	14	0.25	0/559	0.57	0/754
26	24	0.32	0/549	0.70	0/741
27	15	0.34	0/473	0.57	0/639
27	25	0.21	0/469	0.48	0/635
28	16	0.24	0/460	0.46	0/613
28	26	0.21	0/456	0.46	0/608
29	17	0.31	0/426	0.56	0/561
29	27	0.24	0/426	0.49	0/561
30	18	0.28	0/525	0.55	0/691
30	28	0.22	0/525	0.40	0/691
31	19	0.27	0/310	0.50	0/407
31	29	0.24	0/310	0.46	0/407
32	1a	0.34	6/35795 (0.0%)	0.39	0/55864
32	2a	0.20	0/35890	0.39	4/56012 (0.0%)
33	1b	0.22	0/1876	0.47	0/2533
33	2b	0.23	0/1860	0.54	1/2518 (0.0%)
34	1c	0.19	0/1582	0.45	0/2137
34	2c	0.20	0/1566	0.45	0/2119
35	1d	0.21	0/1695	0.48	0/2274
35	2d	0.21	0/1698	0.45	0/2277
36	1e	0.21	0/1149	0.46	0/1548
36	2e	0.20	0/1149	0.43	0/1548
37	1f	0.19	0/827	0.43	0/1120
37	2f	0.20	0/829	0.44	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
38	1g	0.19	0/1254	0.39	0/1683
38	2g	0.19	0/1248	0.39	0/1676
39	1h	0.19	0/1118	0.45	0/1506
39	2h	0.20	0/1108	0.44	0/1494
40	1i	0.21	0/1005	0.47	0/1351
40	2i	0.23	0/985	0.54	0/1329
41	1j	0.19	0/732	0.40	0/993
41	2j	0.23	0/723	0.45	0/984
42	1k	0.20	0/849	0.42	0/1150
42	2k	0.18	0/848	0.42	0/1149
43	1l	0.21	0/937	0.45	0/1260
43	2l	0.20	0/937	0.43	0/1260
44	1m	0.21	0/924	0.46	0/1242
44	2m	0.23	0/905	0.47	0/1217
45	1n	0.21	0/501	0.47	0/664
45	2n	0.22	0/501	0.48	0/664
46	1o	0.21	0/739	0.40	0/985
46	2o	0.18	0/739	0.38	0/985
47	1p	0.21	0/697	0.50	0/939
47	2p	0.20	0/693	0.48	0/935
48	1q	0.20	0/836	0.40	0/1117
48	2q	0.20	0/836	0.45	0/1117
49	1r	0.20	0/560	0.46	0/746
49	2r	0.19	0/560	0.42	0/746
50	1s	0.19	0/663	0.42	0/895
50	2s	0.20	0/660	0.45	0/893
51	1t	0.21	0/734	0.47	0/969
51	2t	0.20	0/736	0.42	0/976
52	1u	0.19	0/203	0.45	0/266
52	2u	0.18	0/203	0.48	0/266
53	1y	0.20	0/776	0.42	0/1048
53	2y	0.22	0/761	0.39	0/1030
54	1w	0.26	0/69	0.45	0/106
54	2w	0.21	0/69	0.34	0/106
55	1x	0.32	0/44	0.50	0/67
55	2x	0.41	0/44	0.48	0/67
56	1v	0.33	0/22	0.38	0/28
56	2v	0.26	0/22	0.62	0/28
All	All	0.27	9/310298 (0.0%)	0.45	15/463749 (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
26	24	0	1
33	1b	0	1
All	All	0	2

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	2I	82	ARG	CD-NE	39.05	2.00	1.46
32	1a	368	U	N3-C4	24.40	1.87	1.38
32	1a	368	U	C2-N3	23.32	1.84	1.37
32	1a	368	U	N1-C2	20.62	1.79	1.38
32	1a	368	U	C4-C5	19.52	1.82	1.43

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	2I	82	ARG	CD-NE-CZ	21.88	155.03	124.40
8	2I	82	ARG	CG-CD-NE	10.58	135.28	112.00
1	1A	1042	G	OP1-P-O3'	-9.20	80.39	108.00
1	1A	1042	G	OP2-P-O3'	-7.56	85.32	108.00
8	2I	82	ARG	NE-CZ-NH1	7.49	128.99	121.50

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
33	1b	231	GLU	Peptide
26	24	18	CYS	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	31202	761	0
1	2A	61758	0	31151	860	0
2	1B	2572	0	1305	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	2B	2573	0	1306	33	0
3	1D	2131	0	2207	54	0
3	2D	2136	0	2218	67	0
4	1E	1559	0	1618	35	0
4	2E	1559	0	1618	28	0
5	1F	1584	0	1625	42	0
5	2F	1580	0	1619	54	0
6	1G	1426	0	1445	44	0
6	2G	1424	0	1441	69	0
7	1H	1330	0	1407	40	0
7	2H	1324	0	1402	49	0
8	1I	1094	0	1127	26	0
8	2I	1076	0	1094	37	7
9	1N	1121	0	1195	18	0
9	2N	1117	0	1184	25	0
10	1O	933	0	996	23	0
10	2O	933	0	996	18	0
11	1P	1135	0	1212	37	0
11	2P	1135	0	1212	33	0
12	1Q	1122	0	1179	25	0
12	2Q	1122	0	1177	35	0
13	1R	968	0	1033	29	0
13	2R	968	0	1033	20	0
14	1S	877	0	938	23	0
14	2S	870	0	923	35	0
15	1T	1091	0	1151	28	0
15	2T	1083	0	1136	27	0
16	1U	959	0	1019	13	0
16	2U	959	0	1019	33	0
17	1V	775	0	841	19	0
17	2V	771	0	830	25	0
18	1W	886	0	940	10	0
18	2W	886	0	940	23	0
19	1X	750	0	814	28	0
19	2X	750	0	814	21	0
20	1Y	810	0	892	28	0
20	2Y	810	0	887	27	0
21	1Z	1587	0	1598	35	0
21	2Z	1557	0	1564	40	0
22	10	653	0	674	18	0
22	20	650	0	665	22	0
23	11	754	0	823	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	21	759	0	837	32	0
24	12	588	0	643	17	0
24	22	592	0	654	14	0
25	13	469	0	518	13	0
25	23	464	0	514	8	0
26	14	546	0	522	26	0
26	24	536	0	514	32	0
27	15	459	0	476	9	0
27	25	455	0	465	9	0
28	16	453	0	473	12	0
28	26	449	0	469	9	0
29	17	418	0	467	9	0
29	27	418	0	467	7	0
30	18	517	0	582	16	0
30	28	517	0	582	14	0
31	19	307	0	335	4	0
31	29	307	0	335	9	0
32	1a	32246	0	16294	478	7
32	2a	32331	0	16338	506	0
33	1b	1842	0	1862	81	0
33	2b	1825	0	1828	73	0
34	1c	1558	0	1557	54	0
34	2c	1542	0	1517	63	0
35	1d	1665	0	1687	68	0
35	2d	1668	0	1703	55	0
36	1e	1133	0	1191	29	0
36	2e	1133	0	1191	40	0
37	1f	814	0	808	33	0
37	2f	816	0	808	22	0
38	1g	1235	0	1249	33	0
38	2g	1229	0	1238	42	0
39	1h	1098	0	1143	49	0
39	2h	1088	0	1126	27	0
40	1i	986	0	990	44	0
40	2i	966	0	953	64	0
41	1j	719	0	672	29	0
41	2j	710	0	661	21	0
42	1k	834	0	838	18	0
42	2k	833	0	836	32	0
43	1l	932	0	981	24	0
43	2l	932	0	981	26	0
44	1m	914	0	954	38	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	2m	895	0	920	40	0
45	1n	492	0	529	29	0
45	2n	492	0	529	25	0
46	1o	728	0	760	18	0
46	2o	728	0	760	20	0
47	1p	681	0	697	17	0
47	2p	677	0	686	17	0
48	1q	823	0	891	21	0
48	2q	823	0	891	22	0
49	1r	555	0	618	18	0
49	2r	555	0	618	12	0
50	1s	648	0	658	29	0
50	2s	645	0	635	33	0
51	1t	732	0	809	21	0
51	2t	733	0	795	17	0
52	1u	199	0	208	9	0
52	2u	199	0	208	9	0
53	1y	764	0	785	16	0
53	2y	749	0	757	27	0
54	1w	63	0	34	0	0
54	2w	63	0	34	0	0
55	1x	63	0	33	1	0
55	2x	63	0	33	1	0
56	1v	23	0	29	3	0
56	2v	23	0	29	4	0
57	10	8	0	0	0	0
57	11	5	0	0	0	0
57	13	3	0	0	0	0
57	15	10	0	0	0	0
57	17	5	0	0	0	0
57	18	2	0	0	0	0
57	19	2	0	0	0	0
57	1A	1021	0	0	0	0
57	1B	31	0	0	0	0
57	1D	18	0	0	0	0
57	1E	9	0	0	0	0
57	1F	18	0	0	0	0
57	1G	4	0	0	0	0
57	1H	2	0	0	0	0
57	1N	5	0	0	0	0
57	1O	1	0	0	0	0
57	1P	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	1Q	4	0	0	0	0
57	1R	3	0	0	0	0
57	1T	6	0	0	0	0
57	1U	7	0	0	0	0
57	1V	6	0	0	0	0
57	1W	5	0	0	0	0
57	1X	1	0	0	0	0
57	1Y	1	0	0	0	0
57	1Z	1	0	0	0	0
57	1a	270	0	0	0	0
57	1b	1	0	0	0	0
57	1d	5	0	0	0	0
57	1e	1	0	0	0	0
57	1f	2	0	0	0	0
57	1g	3	0	0	0	0
57	1h	2	0	0	0	0
57	1i	2	0	0	0	0
57	1l	2	0	0	0	0
57	1m	2	0	0	0	0
57	1n	3	0	0	0	0
57	1o	2	0	0	0	0
57	1t	2	0	0	0	0
57	1y	3	0	0	0	0
57	20	2	0	0	0	0
57	21	3	0	0	0	0
57	23	1	0	0	0	0
57	25	4	0	0	0	0
57	27	3	0	0	0	0
57	28	3	0	0	0	0
57	29	1	0	0	0	0
57	2A	726	0	0	0	0
57	2B	17	0	0	0	0
57	2D	9	0	0	0	0
57	2E	8	0	0	0	0
57	2F	4	0	0	0	0
57	2G	3	0	0	0	0
57	2I	1	0	0	0	0
57	2N	1	0	0	0	0
57	2O	2	0	0	0	0
57	2P	2	0	0	0	0
57	2Q	3	0	0	0	0
57	2R	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	2T	4	0	0	0	0
57	2U	1	0	0	0	0
57	2V	3	0	0	0	0
57	2W	2	0	0	0	0
57	2Y	1	0	0	0	0
57	2a	189	0	0	0	0
57	2e	1	0	0	0	0
57	2f	1	0	0	0	0
57	2j	1	0	0	0	0
57	2l	2	0	0	0	0
57	2n	1	0	0	0	0
57	2p	1	0	0	0	0
57	2t	1	0	0	0	0
57	2x	1	0	0	0	0
58	1A	20	0	11	2	0
58	2A	20	0	11	1	0
59	1A	12	0	12	2	0
59	1B	12	0	12	1	0
60	18	8	0	14	0	0
60	1A	8	0	14	1	0
60	1T	8	0	14	1	0
60	1a	8	0	14	3	0
60	2A	8	0	14	0	0
60	2B	8	0	14	0	0
61	14	1	0	0	0	0
61	15	1	0	0	0	0
61	16	1	0	0	0	0
61	19	1	0	0	0	0
61	1Y	1	0	0	0	0
61	1n	1	0	0	0	0
61	24	1	0	0	0	0
61	25	1	0	0	0	0
61	26	1	0	0	0	0
61	29	1	0	0	0	0
61	2Y	1	0	0	0	0
61	2n	1	0	0	0	0
62	1d	8	0	0	2	0
62	2d	8	0	0	0	0
63	10	25	0	0	0	0
63	11	26	0	0	1	0
63	12	15	0	0	2	0
63	13	24	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
63	14	2	0	0	0	0
63	15	24	0	0	0	0
63	16	18	0	0	1	0
63	17	17	0	0	1	0
63	18	26	0	0	0	0
63	19	7	0	0	0	0
63	1A	3946	0	0	162	0
63	1B	90	0	0	6	0
63	1D	121	0	0	3	0
63	1E	80	0	0	5	0
63	1F	59	0	0	3	0
63	1G	19	0	0	0	0
63	1H	13	0	0	1	0
63	1I	5	0	0	0	0
63	1N	50	0	0	3	0
63	1O	33	0	0	1	0
63	1P	65	0	0	3	0
63	1Q	35	0	0	3	0
63	1R	32	0	0	2	0
63	1S	15	0	0	1	0
63	1T	28	0	0	0	0
63	1U	46	0	0	4	0
63	1V	41	0	0	3	0
63	1W	30	0	0	1	0
63	1X	28	0	0	0	0
63	1Y	21	0	0	3	0
63	1Z	13	0	0	0	0
63	1a	412	0	0	25	0
63	1b	1	0	0	0	0
63	1c	1	0	0	0	0
63	1d	7	0	0	2	0
63	1e	2	0	0	0	0
63	1f	3	0	0	0	0
63	1h	1	0	0	0	0
63	1j	1	0	0	0	0
63	1l	5	0	0	1	0
63	1o	2	0	0	0	0
63	1p	3	0	0	0	0
63	1t	1	0	0	0	0
63	1w	5	0	0	0	0
63	1x	5	0	0	0	0
63	1y	5	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
63	20	12	0	0	1	0
63	21	20	0	0	3	0
63	22	2	0	0	0	0
63	23	3	0	0	1	0
63	24	1	0	0	0	0
63	25	10	0	0	0	0
63	26	5	0	0	2	0
63	27	8	0	0	0	0
63	28	13	0	0	3	0
63	29	1	0	0	0	0
63	2A	2126	0	0	161	0
63	2B	46	0	0	6	0
63	2D	54	0	0	9	0
63	2E	26	0	0	1	0
63	2F	24	0	0	4	0
63	2G	7	0	0	0	0
63	2H	3	0	0	0	0
63	2I	6	0	0	1	0
63	2N	3	0	0	0	0
63	2O	22	0	0	2	0
63	2P	28	0	0	3	0
63	2Q	19	0	0	2	0
63	2R	17	0	0	2	0
63	2S	4	0	0	0	0
63	2T	11	0	0	0	0
63	2U	13	0	0	1	0
63	2V	7	0	0	1	0
63	2W	19	0	0	3	0
63	2X	9	0	0	0	0
63	2Y	4	0	0	0	0
63	2Z	10	0	0	2	0
63	2a	294	0	0	18	0
63	2d	2	0	0	0	0
63	2e	2	0	0	0	0
63	2f	2	0	0	0	0
63	2j	2	0	0	0	0
63	2l	2	0	0	0	0
63	2n	1	0	0	0	0
63	2o	3	0	0	0	0
63	2p	1	0	0	0	0
63	2r	3	0	0	0	0
63	2t	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
63	2w	2	0	0	0	0
63	2x	2	0	0	0	0
63	2y	2	0	0	0	0
All	All	297633	0	194805	4850	7

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 10.

The worst 5 of 4850 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:368:U:C4	32:1a:368:U:C5	1.82	1.66
32:1a:368:U:C6	32:1a:368:U:N1	1.76	1.50
32:1a:368:U:N1	32:1a:368:U:C2	1.79	1.48
32:1a:368:U:C2	32:1a:368:U:N3	1.84	1.46
32:1a:368:U:C4	32:1a:368:U:N3	1.87	1.41

The worst 5 of 7 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:368:U:N3	8:2I:82:ARG:NE[2_655]	1.69	0.51
32:1a:368:U:N1	8:2I:82:ARG:NE[2_655]	1.71	0.49
32:1a:368:U:C2	8:2I:82:ARG:NE[2_655]	1.72	0.48
32:1a:368:U:C6	8:2I:82:ARG:NE[2_655]	1.93	0.27
32:1a:368:U:C4	8:2I:82:ARG:NE[2_655]	1.94	0.26

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%)	258 (94%)	15 (6%)	0	100	100
3	2D	273/276 (99%)	255 (93%)	18 (7%)	0	100	100
4	1E	202/206 (98%)	193 (96%)	7 (4%)	2 (1%)	12	24
4	2E	202/206 (98%)	187 (93%)	14 (7%)	1 (0%)	24	43
5	1F	201/210 (96%)	193 (96%)	7 (4%)	1 (0%)	24	43
5	2F	201/210 (96%)	189 (94%)	9 (4%)	3 (2%)	8	16
6	1G	179/182 (98%)	157 (88%)	17 (10%)	5 (3%)	4	6
6	2G	179/182 (98%)	149 (83%)	24 (13%)	6 (3%)	3	4
7	1H	172/180 (96%)	160 (93%)	10 (6%)	2 (1%)	10	20
7	2H	171/180 (95%)	138 (81%)	31 (18%)	2 (1%)	10	20
8	1I	145/148 (98%)	126 (87%)	16 (11%)	3 (2%)	5	9
8	2I	144/148 (97%)	126 (88%)	13 (9%)	5 (4%)	3	4
9	1N	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
9	2N	138/140 (99%)	126 (91%)	12 (9%)	0	100	100
10	1O	120/122 (98%)	112 (93%)	7 (6%)	1 (1%)	16	31
10	2O	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
11	1P	147/150 (98%)	136 (92%)	10 (7%)	1 (1%)	18	34
11	2P	147/150 (98%)	137 (93%)	9 (6%)	1 (1%)	18	34
12	1Q	139/141 (99%)	131 (94%)	8 (6%)	0	100	100
12	2Q	139/141 (99%)	131 (94%)	8 (6%)	0	100	100
13	1R	116/118 (98%)	112 (97%)	3 (3%)	1 (1%)	14	27
13	2R	116/118 (98%)	110 (95%)	6 (5%)	0	100	100
14	1S	108/112 (96%)	100 (93%)	6 (6%)	2 (2%)	6	11
14	2S	108/112 (96%)	100 (93%)	7 (6%)	1 (1%)	14	27
15	1T	129/146 (88%)	119 (92%)	10 (8%)	0	100	100
15	2T	129/146 (88%)	121 (94%)	7 (5%)	1 (1%)	16	31
16	1U	114/118 (97%)	112 (98%)	2 (2%)	0	100	100
16	2U	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
17	1V	99/101 (98%)	93 (94%)	6 (6%)	0	100	100
17	2V	99/101 (98%)	90 (91%)	8 (8%)	1 (1%)	12	24
18	1W	110/113 (97%)	107 (97%)	3 (3%)	0	100	100
18	2W	110/113 (97%)	107 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
19	1X	93/96 (97%)	89 (96%)	2 (2%)	2 (2%)	5 9
19	2X	93/96 (97%)	91 (98%)	2 (2%)	0	100 100
20	1Y	105/110 (96%)	95 (90%)	10 (10%)	0	100 100
20	2Y	105/110 (96%)	96 (91%)	9 (9%)	0	100 100
21	1Z	201/206 (98%)	182 (90%)	18 (9%)	1 (0%)	24 43
21	2Z	199/206 (97%)	172 (86%)	26 (13%)	1 (0%)	24 43
22	10	81/85 (95%)	78 (96%)	3 (4%)	0	100 100
22	20	81/85 (95%)	73 (90%)	8 (10%)	0	100 100
23	11	95/98 (97%)	89 (94%)	6 (6%)	0	100 100
23	21	95/98 (97%)	89 (94%)	5 (5%)	1 (1%)	11 22
24	12	68/72 (94%)	68 (100%)	0	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%)	53 (93%)	4 (7%)	0	100 100
26	14	67/71 (94%)	47 (70%)	17 (25%)	3 (4%)	2 2
26	24	67/71 (94%)	44 (66%)	14 (21%)	9 (13%)	0 0
27	15	57/60 (95%)	55 (96%)	2 (4%)	0	100 100
27	25	57/60 (95%)	56 (98%)	1 (2%)	0	100 100
28	16	51/54 (94%)	49 (96%)	2 (4%)	0	100 100
28	26	51/54 (94%)	48 (94%)	3 (6%)	0	100 100
29	17	46/49 (94%)	45 (98%)	1 (2%)	0	100 100
29	27	46/49 (94%)	46 (100%)	0	0	100 100
30	18	62/65 (95%)	62 (100%)	0	0	100 100
30	28	62/65 (95%)	61 (98%)	1 (2%)	0	100 100
31	19	35/37 (95%)	35 (100%)	0	0	100 100
31	29	35/37 (95%)	33 (94%)	2 (6%)	0	100 100
33	1b	229/256 (90%)	189 (82%)	30 (13%)	10 (4%)	2 2
33	2b	229/256 (90%)	182 (80%)	37 (16%)	10 (4%)	2 2
34	1c	204/239 (85%)	180 (88%)	23 (11%)	1 (0%)	24 43
34	2c	204/239 (85%)	160 (78%)	37 (18%)	7 (3%)	3 4
35	1d	206/209 (99%)	185 (90%)	21 (10%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
35	2d	206/209 (99%)	184 (89%)	20 (10%)	2 (1%)	12 24
36	1e	146/162 (90%)	136 (93%)	8 (6%)	2 (1%)	9 17
36	2e	146/162 (90%)	134 (92%)	12 (8%)	0	100 100
37	1f	98/101 (97%)	94 (96%)	4 (4%)	0	100 100
37	2f	98/101 (97%)	90 (92%)	8 (8%)	0	100 100
38	1g	153/156 (98%)	143 (94%)	8 (5%)	2 (1%)	9 18
38	2g	153/156 (98%)	139 (91%)	12 (8%)	2 (1%)	9 18
39	1h	135/138 (98%)	126 (93%)	9 (7%)	0	100 100
39	2h	135/138 (98%)	124 (92%)	11 (8%)	0	100 100
40	1i	125/128 (98%)	111 (89%)	11 (9%)	3 (2%)	4 8
40	2i	124/128 (97%)	108 (87%)	12 (10%)	4 (3%)	3 4
41	1j	95/105 (90%)	80 (84%)	11 (12%)	4 (4%)	2 2
41	2j	94/105 (90%)	77 (82%)	15 (16%)	2 (2%)	5 9
42	1k	112/129 (87%)	102 (91%)	10 (9%)	0	100 100
42	2k	112/129 (87%)	101 (90%)	10 (9%)	1 (1%)	14 27
43	1l	119/132 (90%)	109 (92%)	9 (8%)	1 (1%)	16 31
43	2l	119/132 (90%)	108 (91%)	10 (8%)	1 (1%)	16 31
44	1m	114/126 (90%)	100 (88%)	11 (10%)	3 (3%)	4 7
44	2m	112/126 (89%)	95 (85%)	12 (11%)	5 (4%)	2 2
45	1n	58/61 (95%)	52 (90%)	6 (10%)	0	100 100
45	2n	58/61 (95%)	51 (88%)	6 (10%)	1 (2%)	7 13
46	1o	86/89 (97%)	79 (92%)	6 (7%)	1 (1%)	10 20
46	2o	86/89 (97%)	78 (91%)	7 (8%)	1 (1%)	10 20
47	1p	80/88 (91%)	74 (92%)	6 (8%)	0	100 100
47	2p	80/88 (91%)	69 (86%)	11 (14%)	0	100 100
48	1q	97/105 (92%)	88 (91%)	9 (9%)	0	100 100
48	2q	97/105 (92%)	90 (93%)	6 (6%)	1 (1%)	12 24
49	1r	66/88 (75%)	60 (91%)	5 (8%)	1 (2%)	8 16
49	2r	66/88 (75%)	60 (91%)	6 (9%)	0	100 100
50	1s	81/93 (87%)	69 (85%)	12 (15%)	0	100 100
50	2s	81/93 (87%)	68 (84%)	13 (16%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
51	1t	94/106 (89%)	83 (88%)	9 (10%)	2 (2%)	5 9
51	2t	96/106 (91%)	82 (85%)	12 (12%)	2 (2%)	5 9
52	1u	21/27 (78%)	20 (95%)	1 (5%)	0	100 100
52	2u	21/27 (78%)	16 (76%)	5 (24%)	0	100 100
53	1y	95/113 (84%)	93 (98%)	2 (2%)	0	100 100
53	2y	94/113 (83%)	87 (93%)	5 (5%)	2 (2%)	5 9
56	1v	1/3 (33%)	1 (100%)	0	0	100 100
56	2v	1/3 (33%)	1 (100%)	0	0	100 100
All	All	11643/12360 (94%)	10591 (91%)	925 (8%)	127 (1%)	11 22

5 of 127 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	1G	47	LYS
8	1I	86	THR
14	1S	59	LYS
19	1X	94	GLY
26	14	61	ARG

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%)	200 (94%)	14 (6%)	15 32
3	2D	215/218 (99%)	191 (89%)	24 (11%)	6 12
4	1E	164/166 (99%)	155 (94%)	9 (6%)	19 40
4	2E	164/166 (99%)	148 (90%)	16 (10%)	7 16
5	1F	160/166 (96%)	148 (92%)	12 (8%)	12 26
5	2F	159/166 (96%)	140 (88%)	19 (12%)	5 11
6	1G	144/156 (92%)	125 (87%)	19 (13%)	4 8
6	2G	142/156 (91%)	119 (84%)	23 (16%)	2 4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
7	1H	144/148 (97%)	135 (94%)	9 (6%)	16 34
7	2H	143/148 (97%)	124 (87%)	19 (13%)	4 8
8	1I	111/124 (90%)	88 (79%)	23 (21%)	1 2
8	2I	108/124 (87%)	87 (81%)	21 (19%)	1 2
9	1N	119/119 (100%)	106 (89%)	13 (11%)	6 13
9	2N	118/119 (99%)	104 (88%)	14 (12%)	5 11
10	1O	100/100 (100%)	94 (94%)	6 (6%)	17 36
10	2O	100/100 (100%)	95 (95%)	5 (5%)	22 44
11	1P	115/116 (99%)	112 (97%)	3 (3%)	40 68
11	2P	115/116 (99%)	105 (91%)	10 (9%)	9 21
12	1Q	111/111 (100%)	104 (94%)	7 (6%)	16 34
12	2Q	111/111 (100%)	103 (93%)	8 (7%)	13 28
13	1R	101/101 (100%)	93 (92%)	8 (8%)	11 24
13	2R	101/101 (100%)	90 (89%)	11 (11%)	6 13
14	1S	87/88 (99%)	79 (91%)	8 (9%)	8 19
14	2S	85/88 (97%)	69 (81%)	16 (19%)	1 3
15	1T	115/127 (91%)	108 (94%)	7 (6%)	17 35
15	2T	113/127 (89%)	106 (94%)	7 (6%)	16 34
16	1U	93/94 (99%)	87 (94%)	6 (6%)	15 32
16	2U	93/94 (99%)	87 (94%)	6 (6%)	15 32
17	1V	81/82 (99%)	77 (95%)	4 (5%)	22 45
17	2V	80/82 (98%)	65 (81%)	15 (19%)	1 3
18	1W	90/92 (98%)	81 (90%)	9 (10%)	7 15
18	2W	90/92 (98%)	85 (94%)	5 (6%)	19 39
19	1X	77/78 (99%)	71 (92%)	6 (8%)	11 24
19	2X	77/78 (99%)	75 (97%)	2 (3%)	40 68
20	1Y	86/91 (94%)	79 (92%)	7 (8%)	11 23
20	2Y	86/91 (94%)	72 (84%)	14 (16%)	2 4
21	1Z	169/179 (94%)	151 (89%)	18 (11%)	6 13
21	2Z	165/179 (92%)	142 (86%)	23 (14%)	3 7
22	10	65/67 (97%)	63 (97%)	2 (3%)	35 62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
22	20	64/67 (96%)	62 (97%)	2 (3%)	35 62
23	11	79/83 (95%)	75 (95%)	4 (5%)	21 43
23	21	81/83 (98%)	74 (91%)	7 (9%)	10 21
24	12	65/67 (97%)	60 (92%)	5 (8%)	12 25
24	22	66/67 (98%)	58 (88%)	8 (12%)	5 10
25	13	51/52 (98%)	45 (88%)	6 (12%)	5 11
25	23	50/52 (96%)	45 (90%)	5 (10%)	7 15
26	14	58/63 (92%)	51 (88%)	7 (12%)	5 10
26	24	54/63 (86%)	43 (80%)	11 (20%)	1 2
27	15	51/52 (98%)	47 (92%)	4 (8%)	11 24
27	25	50/52 (96%)	45 (90%)	5 (10%)	7 15
28	16	51/52 (98%)	44 (86%)	7 (14%)	3 7
28	26	50/52 (96%)	43 (86%)	7 (14%)	3 7
29	17	41/42 (98%)	37 (90%)	4 (10%)	7 16
29	27	41/42 (98%)	36 (88%)	5 (12%)	5 10
30	18	54/55 (98%)	50 (93%)	4 (7%)	13 27
30	28	54/55 (98%)	48 (89%)	6 (11%)	6 12
31	19	34/34 (100%)	33 (97%)	1 (3%)	37 65
31	29	34/34 (100%)	32 (94%)	2 (6%)	18 37
33	1b	191/220 (87%)	164 (86%)	27 (14%)	3 7
33	2b	187/220 (85%)	157 (84%)	30 (16%)	2 5
34	1c	144/188 (77%)	132 (92%)	12 (8%)	10 22
34	2c	140/188 (74%)	117 (84%)	23 (16%)	2 4
35	1d	171/181 (94%)	147 (86%)	24 (14%)	3 7
35	2d	172/181 (95%)	150 (87%)	22 (13%)	4 9
36	1e	114/123 (93%)	104 (91%)	10 (9%)	9 20
36	2e	114/123 (93%)	103 (90%)	11 (10%)	8 17
37	1f	85/90 (94%)	72 (85%)	13 (15%)	3 5
37	2f	85/90 (94%)	77 (91%)	8 (9%)	8 18
38	1g	120/127 (94%)	110 (92%)	10 (8%)	10 22
38	2g	119/127 (94%)	102 (86%)	17 (14%)	3 6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
39	1h	116/119 (98%)	102 (88%)	14 (12%)	5 10
39	2h	114/119 (96%)	99 (87%)	15 (13%)	4 8
40	1i	91/99 (92%)	78 (86%)	13 (14%)	3 6
40	2i	88/99 (89%)	77 (88%)	11 (12%)	4 9
41	1j	68/92 (74%)	60 (88%)	8 (12%)	5 11
41	2j	68/92 (74%)	59 (87%)	9 (13%)	4 8
42	1k	83/99 (84%)	75 (90%)	8 (10%)	8 17
42	2k	83/99 (84%)	73 (88%)	10 (12%)	5 10
43	1l	96/108 (89%)	87 (91%)	9 (9%)	8 18
43	2l	96/108 (89%)	84 (88%)	12 (12%)	4 9
44	1m	90/101 (89%)	82 (91%)	8 (9%)	9 20
44	2m	87/101 (86%)	72 (83%)	15 (17%)	2 4
45	1n	49/50 (98%)	43 (88%)	6 (12%)	5 10
45	2n	49/50 (98%)	42 (86%)	7 (14%)	3 6
46	1o	78/80 (98%)	71 (91%)	7 (9%)	9 19
46	2o	78/80 (98%)	71 (91%)	7 (9%)	9 19
47	1p	69/74 (93%)	56 (81%)	13 (19%)	1 3
47	2p	68/74 (92%)	58 (85%)	10 (15%)	3 6
48	1q	94/97 (97%)	84 (89%)	10 (11%)	6 14
48	2q	94/97 (97%)	90 (96%)	4 (4%)	26 51
49	1r	59/77 (77%)	50 (85%)	9 (15%)	3 5
49	2r	59/77 (77%)	53 (90%)	6 (10%)	7 15
50	1s	68/80 (85%)	61 (90%)	7 (10%)	7 14
50	2s	67/80 (84%)	61 (91%)	6 (9%)	9 19
51	1t	71/82 (87%)	64 (90%)	7 (10%)	7 16
51	2t	70/82 (85%)	65 (93%)	5 (7%)	13 29
52	1u	18/22 (82%)	17 (94%)	1 (6%)	19 39
52	2u	18/22 (82%)	17 (94%)	1 (6%)	19 39
53	1y	82/98 (84%)	75 (92%)	7 (8%)	10 22
53	2y	79/98 (81%)	69 (87%)	10 (13%)	4 9
56	1v	3/3 (100%)	2 (67%)	1 (33%)	0 0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
56	2v	3/3 (100%)	2 (67%)	1 (33%)	0 0
All	All	9537/10266 (93%)	8525 (89%)	1012 (11%)	6 14

5 of 1012 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	2D	75	ILE
39	2h	21	LYS
8	2I	125	GLU
38	2g	92	SER
44	2m	49	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 153 such sidechains are listed below:

Mol	Chain	Res	Type
35	2d	116	GLN
46	2o	9	GLN
35	2d	201	GLN
40	2i	58	HIS
53	2y	46	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2865/2915 (98%)	428 (14%)	28 (0%)
1	2A	2858/2915 (98%)	497 (17%)	35 (1%)
2	1B	119/121 (98%)	9 (7%)	0
2	2B	119/121 (98%)	16 (13%)	0
32	1a	1497/1521 (98%)	266 (17%)	0
32	2a	1501/1521 (98%)	290 (19%)	0
54	1w	2/5 (40%)	0	0
54	2w	2/5 (40%)	0	0
55	1x	1/4 (25%)	0	0
55	2x	1/4 (25%)	0	0
All	All	8965/9132 (98%)	1506 (16%)	63 (0%)

5 of 1506 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	15	G

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Mol	Chain	Res	Type
1	1A	34	C
1	1A	45	C
1	1A	50	U
1	1A	71	A

5 of 63 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2A	195	A
1	2A	2126	A
1	2A	752	A
1	2A	1992	G
1	2A	2406	U

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

50 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	5MU	1A	1915	1	19,22,23	1.41	5 (26%)	27,32,35	2.32	9 (33%)
43	0TD	2l	92	43	8,9,10	4.31	1 (12%)	6,11,13	7.37	3 (50%)
32	5MC	1a	967	32	19,22,23	1.55	3 (15%)	26,32,35	1.05	2 (7%)
55	8AN	1x	76	55,56,57	21,24,25	1.37	3 (14%)	26,35,38	2.39	11 (42%)
1	2MU	2A	2552	1,57	19,22,24	1.18	2 (10%)	25,31,36	1.83	6 (24%)
1	5MU	2A	1939	1,57	19,22,23	1.38	5 (26%)	27,32,35	2.08	6 (22%)
32	5MC	2a	967	32	19,22,23	1.69	3 (15%)	26,32,35	1.04	2 (7%)
32	MA6	2a	1518	32	23,26,27	0.40	0	33,38,41	2.01	9 (27%)
32	G7M	2a	527	32	23,26,27	1.49	3 (13%)	34,39,42	1.70	5 (14%)
32	4OC	2a	1402	32	20,23,24	0.78	0	25,32,35	1.03	1 (4%)
32	5MC	2a	1404	32	19,22,23	1.67	3 (15%)	26,32,35	1.17	3 (11%)
1	OMG	1A	2251	55,1	23,26,27	1.27	3 (13%)	32,38,41	2.05	6 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	2MA	1A	2503	1,57	22,25,26	1.44	5 (22%)	32,37,40	2.25	9 (28%)
1	OMG	2A	2251	12,55,1,57	23,26,27	1.20	3 (13%)	32,38,41	2.11	7 (21%)
1	PSU	1A	2605	1	18,21,22	1.50	4 (22%)	21,30,33	2.12	5 (23%)
32	PSU	1a	516	32,57	18,21,22	1.39	2 (11%)	21,30,33	1.90	5 (23%)
1	5MC	1A	1962	1,57	19,22,23	1.62	3 (15%)	26,32,35	1.10	1 (3%)
32	M2G	2a	966	32,57	24,27,28	1.36	4 (16%)	33,40,43	1.82	5 (15%)
55	8AN	2x	76	55,56,57	21,24,25	1.37	3 (14%)	26,35,38	2.21	10 (38%)
32	5MC	1a	1404	32	19,22,23	1.70	2 (10%)	26,32,35	1.19	4 (15%)
32	5MC	2a	1400	32	19,22,23	1.52	3 (15%)	26,32,35	1.24	3 (11%)
32	UR3	1a	1498	32	19,22,23	0.99	1 (5%)	26,32,35	1.76	2 (7%)
32	4OC	1a	1402	32	20,23,24	0.75	0	25,32,35	0.98	1 (4%)
32	M2G	1a	966	32	24,27,28	1.29	3 (12%)	33,40,43	1.88	6 (18%)
1	5MU	2A	1915	1	19,22,23	1.47	4 (21%)	27,32,35	2.12	8 (29%)
32	2MG	1a	1207	32	23,26,27	1.22	2 (8%)	33,38,41	2.24	8 (24%)
1	OMC	2A	1920	1	19,22,23	0.81	0	25,31,34	0.97	1 (4%)
1	PSU	2A	1911	1	18,21,22	1.43	3 (16%)	21,30,33	1.99	5 (23%)
1	2MU	1A	2552	1,57	19,22,24	1.31	3 (15%)	25,31,36	1.84	6 (24%)
32	MA6	2a	1519	32	23,26,27	0.45	0	33,38,41	2.13	10 (30%)
1	5MU	1A	1939	1	19,22,23	1.39	5 (26%)	27,32,35	2.01	7 (25%)
32	MA6	1a	1519	32	23,26,27	0.45	0	33,38,41	2.06	10 (30%)
32	5MC	1a	1407	32	19,22,23	1.69	2 (10%)	26,32,35	1.16	3 (11%)
32	5MC	1a	1400	32	19,22,23	1.62	3 (15%)	26,32,35	1.16	2 (7%)
1	5MC	2A	1942	1	19,22,23	1.68	3 (15%)	26,32,35	1.16	2 (7%)
32	MA6	1a	1518	32	23,26,27	0.40	0	33,38,41	1.93	9 (27%)
32	5MC	2a	1407	32	19,22,23	1.69	2 (10%)	26,32,35	1.19	3 (11%)
32	UR3	2a	1498	32	19,22,23	1.01	2 (10%)	26,32,35	1.70	4 (15%)
32	PSU	2a	516	32,57	18,21,22	1.41	3 (16%)	21,30,33	2.12	5 (23%)
1	PSU	1A	1917	1	18,21,22	1.35	2 (11%)	21,30,33	1.97	3 (14%)
32	G7M	1a	527	32,57	23,26,27	1.54	4 (17%)	34,39,42	1.64	4 (11%)
1	5MC	1A	1942	1,57	19,22,23	1.42	3 (15%)	26,32,35	1.08	2 (7%)
43	0TD	1l	92	43	8,9,10	4.68	2 (25%)	6,11,13	4.48	3 (50%)
1	2MA	2A	2503	1,57	22,25,26	1.43	3 (13%)	32,37,40	2.38	9 (28%)
1	OMC	1A	1920	1	19,22,23	0.87	0	25,31,34	1.22	2 (8%)
1	PSU	2A	2605	1	18,21,22	1.37	3 (16%)	21,30,33	1.96	4 (19%)
32	2MG	2a	1207	32	23,26,27	1.22	3 (13%)	33,38,41	2.09	8 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	5MC	2A	1962	1	19,22,23	1.77	3 (15%)	26,32,35	1.21	4 (15%)
1	PSU	1A	1911	1	18,21,22	1.38	2 (11%)	21,30,33	2.01	4 (19%)
1	PSU	2A	1917	1	18,21,22	1.34	3 (16%)	21,30,33	2.02	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	5MU	1A	1915	1	-	2/7/25/26	0/2/2/2
43	0TD	2l	92	43	-	3/7/12/14	-
32	5MC	1a	967	32	-	0/7/25/26	0/2/2/2
55	8AN	1x	76	55,56,57	-	1/7/25/26	0/3/3/3
1	2MU	2A	2552	1,57	-	0/9/27/28	0/2/2/2
1	5MU	2A	1939	1,57	-	0/7/25/26	0/2/2/2
32	5MC	2a	967	32	-	0/7/25/26	0/2/2/2
32	MA6	2a	1518	32	-	0/11/29/30	0/3/3/3
32	G7M	2a	527	32	-	3/7/25/26	0/3/3/3
32	4OC	2a	1402	32	-	0/9/29/30	0/2/2/2
32	5MC	2a	1404	32	-	0/7/25/26	0/2/2/2
1	OMG	1A	2251	55,1	-	0/9/27/28	0/3/3/3
1	2MA	1A	2503	1,57	-	2/7/25/26	0/3/3/3
1	OMG	2A	2251	12,55,1,57	-	0/9/27/28	0/3/3/3
1	PSU	1A	2605	1	-	0/7/25/26	0/2/2/2
32	PSU	1a	516	32,57	-	0/7/25/26	0/2/2/2
1	5MC	1A	1962	1,57	-	2/7/25/26	0/2/2/2
32	M2G	2a	966	32,57	-	0/11/29/30	0/3/3/3
55	8AN	2x	76	55,56,57	-	1/7/25/26	0/3/3/3
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
32	5MC	2a	1400	32	-	3/7/25/26	0/2/2/2
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
32	4OC	1a	1402	32	-	2/9/29/30	0/2/2/2
32	M2G	1a	966	32	-	0/11/29/30	0/3/3/3
1	5MU	2A	1915	1	-	2/7/25/26	0/2/2/2
32	2MG	1a	1207	32	-	0/9/27/28	0/3/3/3
1	OMC	2A	1920	1	-	1/9/27/28	0/2/2/2
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
1	2MU	1A	2552	1,57	-	0/9/27/28	0/2/2/2
32	MA6	2a	1519	32	-	1/11/29/30	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5MU	1A	1939	1	-	0/7/25/26	0/2/2/2
32	MA6	1a	1519	32	-	2/11/29/30	0/3/3/3
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
32	5MC	1a	1400	32	-	0/7/25/26	0/2/2/2
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
32	MA6	1a	1518	32	-	0/11/29/30	0/3/3/3
32	5MC	2a	1407	32	-	0/7/25/26	0/2/2/2
32	UR3	2a	1498	32	-	0/7/25/26	0/2/2/2
32	PSU	2a	516	32,57	-	0/7/25/26	0/2/2/2
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
32	G7M	1a	527	32,57	-	1/7/25/26	0/3/3/3
1	5MC	1A	1942	1,57	-	0/7/25/26	0/2/2/2
43	0TD	1l	92	43	-	4/7/12/14	-
1	2MA	2A	2503	1,57	-	1/7/25/26	0/3/3/3
1	OMC	1A	1920	1	-	2/9/27/28	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
32	2MG	2a	1207	32	-	2/9/27/28	0/3/3/3
1	5MC	2A	1962	1	-	0/7/25/26	0/2/2/2
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2

The worst 5 of 124 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	1l	92	0TD	CB-SB	-12.66	1.69	1.82
43	2l	92	0TD	CB-SB	-11.75	1.70	1.82
1	2A	1962	5MC	C5-C4	6.54	1.49	1.44
32	1a	1404	5MC	C5-C4	6.30	1.48	1.44
32	2a	1407	5MC	C5-C4	6.15	1.48	1.44

The worst 5 of 250 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	2l	92	0TD	CSB-SB-CB	17.52	133.86	102.36
43	1l	92	0TD	CSB-SB-CB	10.23	120.76	102.36
1	2A	2503	2MA	C5-C4-N3	-8.00	118.75	127.18
1	1A	2503	2MA	C5-C4-N3	-7.85	118.91	127.18
32	1a	1498	UR3	C4-N3-C2	-7.06	118.90	124.58

There are no chirality outliers.

5 of 35 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
43	1l	92	0TD	O-C-CA-CB
43	1l	92	0TD	CG-CB-SB-CSB
1	2A	1915	5MU	O4'-C1'-N1-C2

There are no ring outliers.

24 monomers are involved in 37 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
43	2l	92	0TD	4	0
32	1a	967	5MC	1	0
1	2A	2552	2MU	1	0
1	2A	1939	5MU	2	0
32	2a	1518	MA6	1	0
32	2a	1402	4OC	2	0
32	2a	1404	5MC	1	0
1	1A	2251	OMG	1	0
1	1A	2503	2MA	1	0
1	2A	2251	OMG	1	0
32	2a	1400	5MC	2	0
32	1a	1498	UR3	1	0
32	1a	1402	4OC	2	0
1	2A	1920	OMC	2	0
1	1A	2552	2MU	2	0
32	2a	1519	MA6	1	0
1	1A	1939	5MU	1	0
32	1a	1519	MA6	5	0
32	1a	1518	MA6	2	0
32	1a	527	G7M	1	0
43	1l	92	0TD	1	0
1	1A	1920	OMC	2	0
32	2a	1207	2MG	1	0
1	2A	1917	PSU	2	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2510 ligands modelled in this entry, 2498 are monoatomic - leaving 12 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
59	ARG	1A	4023	-	10,11,11	0.77	1 (10%)	9,13,13	0.99	1 (11%)
60	MPD	1A	4024	-	7,7,7	0.30	0	9,10,10	0.18	0
60	MPD	2A	3728	-	7,7,7	0.27	0	9,10,10	0.17	0
58	CLM	2A	3727	-	20,20,20	0.96	1 (5%)	23,27,27	0.90	1 (4%)
62	SF4	1d	306	35	0,12,12	-	-	-		
62	SF4	2d	501	35	0,12,12	-	-	-		
60	MPD	18	103	-	7,7,7	0.29	0	9,10,10	0.24	0
60	MPD	1a	3271	-	7,7,7	0.40	0	9,10,10	0.57	0
60	MPD	1T	207	-	7,7,7	0.29	0	9,10,10	0.19	0
58	CLM	1A	4022	-	20,20,20	1.06	2 (10%)	23,27,27	1.17	3 (13%)
60	MPD	2B	218	-	7,7,7	0.33	0	9,10,10	0.32	0
59	ARG	1B	232	57	10,11,11	0.78	1 (10%)	9,13,13	0.95	1 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	ARG	1A	4023	-	-	1/11/11/11	-
60	MPD	1A	4024	-	-	1/5/5/5	-
60	MPD	2A	3728	-	-	0/5/5/5	-
58	CLM	2A	3727	-	-	0/20/22/22	0/1/1/1
62	SF4	1d	306	35	-	-	0/6/5/5
62	SF4	2d	501	35	-	-	0/6/5/5
60	MPD	18	103	-	-	2/5/5/5	-
60	MPD	1a	3271	-	-	2/5/5/5	-
60	MPD	1T	207	-	-	2/5/5/5	-
58	CLM	1A	4022	-	-	4/20/22/22	0/1/1/1
60	MPD	2B	218	-	-	4/5/5/5	-
59	ARG	1B	232	57	-	3/11/11/11	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	1A	4022	CLM	C6-C5	-2.39	1.48	1.51
59	1B	232	ARG	OXT-C	-2.38	1.23	1.30
58	2A	3727	CLM	C6-C5	-2.25	1.48	1.51
59	1A	4023	ARG	OXT-C	-2.17	1.23	1.30
58	1A	4022	CLM	C9-N9	-2.05	1.40	1.45

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
59	1A	4023	ARG	OXT-C-O	-2.82	117.69	124.08
59	1B	232	ARG	OXT-C-O	-2.62	118.14	124.08
58	1A	4022	CLM	C10-C9-N9	2.57	121.58	119.34
58	1A	4022	CLM	C3-N2-C2	-2.31	119.22	123.25
58	1A	4022	CLM	O5-C5-C6	-2.20	106.42	111.20

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	1A	4022	CLM	C5-C3-N2-C2
59	1B	232	ARG	O-C-CA-N
60	2B	218	MPD	C2-C3-C4-C5
59	1A	4023	ARG	CA-CB-CG-CD
58	1A	4022	CLM	C5-C3-C4-O4

There are no ring outliers.

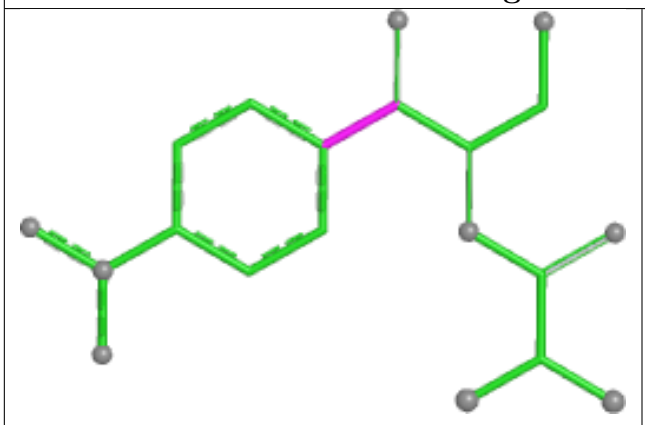
8 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
59	1A	4023	ARG	2	0
60	1A	4024	MPD	1	0
58	2A	3727	CLM	1	0
62	1d	306	SF4	2	0
60	1a	3271	MPD	3	0
60	1T	207	MPD	1	0
58	1A	4022	CLM	2	0
59	1B	232	ARG	1	0

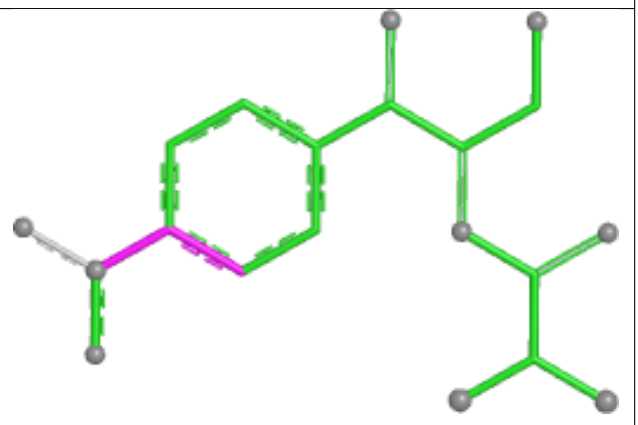
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

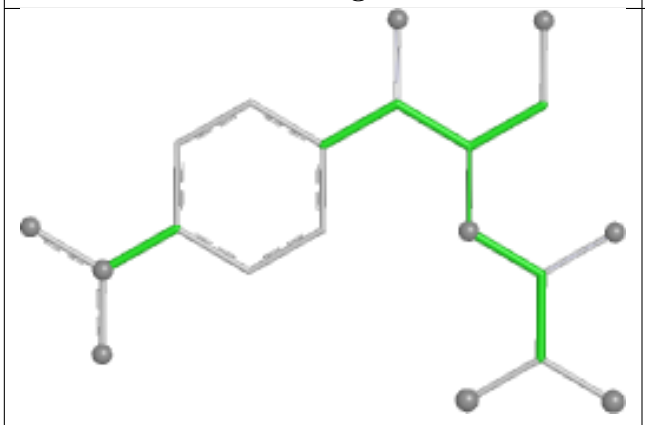
Ligand CLM 2A 3727



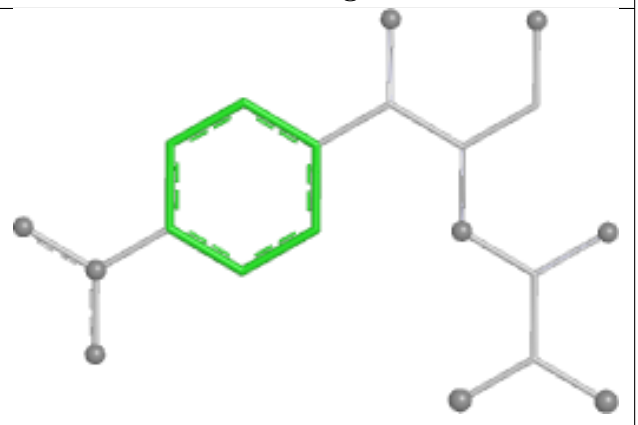
Bond lengths



Bond angles

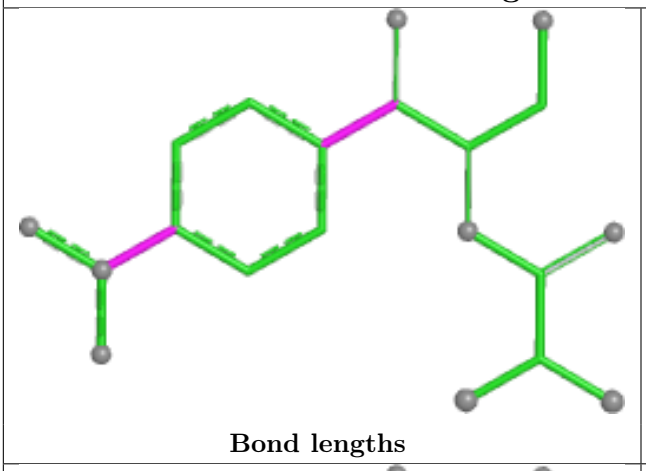


Torsions

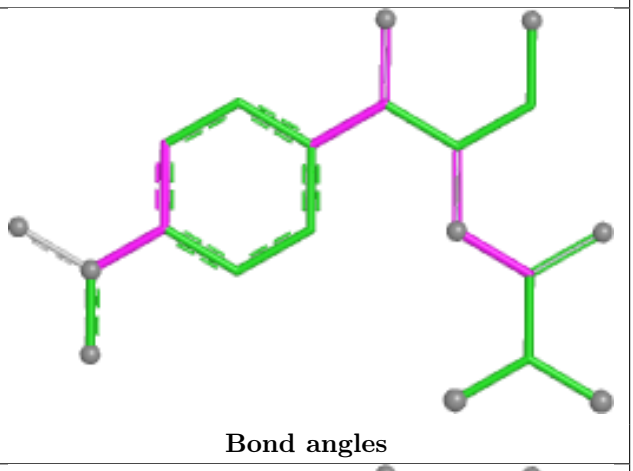


Rings

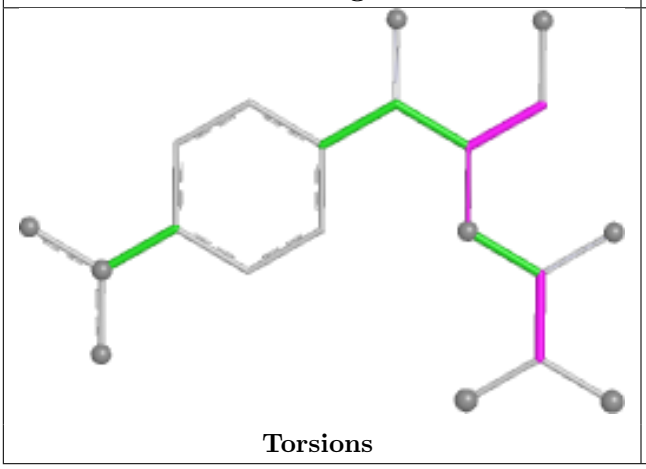
Ligand CLM 1A 4022



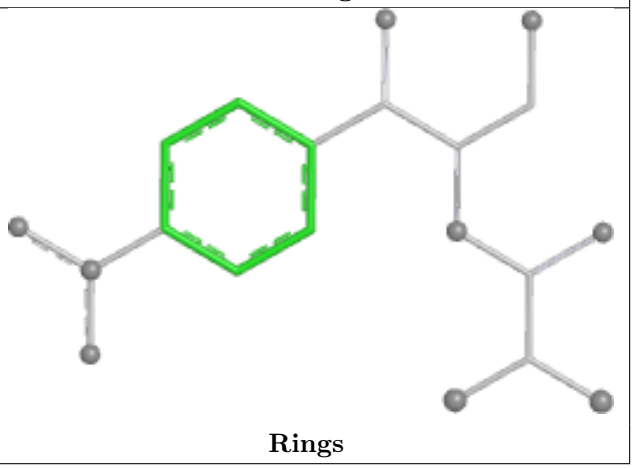
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	-0.46	116 (4%) 41 37	15, 32, 79, 90	0
1	2A	2856/2915 (97%)	-0.01	141 (4%) 35 31	27, 48, 81, 90	0
2	1B	120/121 (99%)	-0.29	1 (0%) 82 80	24, 43, 54, 68	0
2	2B	120/121 (99%)	0.50	1 (0%) 82 80	49, 64, 71, 75	0
3	1D	275/276 (99%)	-0.11	1 (0%) 88 86	18, 33, 44, 58	0
3	2D	275/276 (99%)	0.18	2 (0%) 84 81	27, 43, 54, 67	0
4	1E	204/206 (99%)	-0.05	0 100 100	16, 36, 52, 64	0
4	2E	204/206 (99%)	0.36	1 (0%) 87 85	25, 48, 62, 68	0
5	1F	203/210 (96%)	0.07	4 (1%) 65 61	14, 36, 58, 74	0
5	2F	203/210 (96%)	0.57	4 (1%) 65 61	28, 55, 65, 73	0
6	1G	181/182 (99%)	0.83	11 (6%) 27 23	40, 56, 66, 72	0
6	2G	181/182 (99%)	1.50	47 (25%) 1 1	58, 68, 74, 77	0
7	1H	174/180 (96%)	0.32	1 (0%) 85 83	30, 45, 55, 58	0
7	2H	173/180 (96%)	1.31	26 (15%) 5 4	58, 66, 72, 76	0
8	1I	147/148 (99%)	0.84	6 (4%) 41 37	37, 61, 70, 76	0
8	2I	146/148 (98%)	1.19	20 (13%) 6 5	46, 64, 72, 76	0
9	1N	140/140 (100%)	-0.09	1 (0%) 84 81	22, 32, 48, 65	0
9	2N	140/140 (100%)	0.58	6 (4%) 40 35	39, 52, 62, 70	0
10	1O	122/122 (100%)	-0.10	0 100 100	23, 35, 50, 57	0
10	2O	122/122 (100%)	0.35	0 100 100	38, 47, 59, 64	0
11	1P	149/150 (99%)	0.16	0 100 100	15, 40, 58, 63	0
11	2P	149/150 (99%)	0.60	5 (3%) 48 43	31, 55, 67, 72	0
12	1Q	141/141 (100%)	0.01	1 (0%) 84 81	22, 34, 45, 51	0
12	2Q	141/141 (100%)	0.77	3 (2%) 63 59	37, 52, 61, 68	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	1R	118/118 (100%)	-0.23	0 100 100	21, 30, 43, 50	0
13	2R	118/118 (100%)	0.30	2 (1%) 69 65	33, 44, 52, 58	0
14	1S	110/112 (98%)	0.30	1 (0%) 81 78	32, 43, 54, 58	0
14	2S	110/112 (98%)	1.11	14 (12%) 8 6	52, 59, 63, 68	0
15	1T	131/146 (89%)	0.13	3 (2%) 61 57	28, 38, 57, 70	0
15	2T	131/146 (89%)	0.48	3 (2%) 61 57	39, 50, 63, 68	0
16	1U	116/118 (98%)	-0.27	0 100 100	17, 26, 40, 51	0
16	2U	116/118 (98%)	0.52	3 (2%) 57 52	33, 48, 61, 68	0
17	1V	101/101 (100%)	-0.09	0 100 100	16, 35, 49, 54	0
17	2V	101/101 (100%)	0.75	4 (3%) 42 38	38, 57, 63, 67	0
18	1W	112/113 (99%)	-0.17	1 (0%) 81 78	18, 26, 45, 62	0
18	2W	112/113 (99%)	0.19	2 (1%) 67 64	32, 42, 57, 76	0
19	1X	95/96 (98%)	0.01	1 (1%) 78 75	22, 33, 52, 63	0
19	2X	95/96 (98%)	0.74	8 (8%) 17 15	38, 52, 64, 69	0
20	1Y	107/110 (97%)	0.21	2 (1%) 66 62	32, 42, 55, 63	0
20	2Y	107/110 (97%)	0.94	8 (7%) 20 18	45, 57, 66, 72	0
21	1Z	203/206 (98%)	0.55	5 (2%) 58 54	32, 49, 61, 71	0
21	2Z	201/206 (97%)	1.12	12 (5%) 27 24	50, 62, 69, 77	0
22	10	83/85 (97%)	0.21	6 (7%) 21 19	23, 32, 58, 68	0
22	20	83/85 (97%)	0.84	6 (7%) 21 19	40, 51, 62, 69	0
23	11	97/98 (98%)	0.18	0 100 100	24, 39, 59, 61	0
23	21	97/98 (98%)	0.47	1 (1%) 79 76	35, 48, 63, 68	0
24	12	70/72 (97%)	0.25	2 (2%) 53 49	30, 43, 51, 62	0
24	22	70/72 (97%)	0.72	0 100 100	46, 58, 62, 65	0
25	13	59/60 (98%)	-0.03	0 100 100	22, 31, 49, 56	0
25	23	59/60 (98%)	0.61	3 (5%) 33 29	41, 49, 63, 72	0
26	14	69/71 (97%)	1.20	11 (15%) 5 4	50, 68, 75, 79	0
26	24	69/71 (97%)	1.78	25 (36%) 1 1	67, 73, 79, 81	0
27	15	59/60 (98%)	-0.11	1 (1%) 69 65	17, 28, 44, 55	0
27	25	59/60 (98%)	0.05	0 100 100	27, 42, 55, 65	0
28	16	53/54 (98%)	-0.14	0 100 100	27, 36, 49, 51	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
28	26	53/54 (98%)	0.35	0 100 100	44, 51, 59, 63	0
29	17	48/49 (97%)	-0.23	0 100 100	16, 23, 48, 51	0
29	27	48/49 (97%)	0.14	2 (4%) 40 36	29, 36, 51, 62	0
30	18	64/65 (98%)	-0.15	0 100 100	22, 29, 36, 50	0
30	28	64/65 (98%)	0.46	2 (3%) 51 47	36, 45, 50, 59	0
31	19	37/37 (100%)	0.18	1 (2%) 56 51	26, 35, 50, 53	0
31	29	37/37 (100%)	0.87	2 (5%) 31 27	46, 54, 64, 66	0
32	1a	1488/1521 (97%)	0.35	33 (2%) 62 58	33, 60, 78, 90	0
32	2a	1492/1521 (98%)	0.53	45 (3%) 52 48	41, 65, 80, 90	0
33	1b	231/256 (90%)	1.25	32 (13%) 6 5	56, 66, 73, 79	0
33	2b	231/256 (90%)	1.46	55 (23%) 2 1	59, 69, 75, 80	0
34	1c	206/239 (86%)	0.97	11 (5%) 32 28	52, 63, 71, 74	0
34	2c	206/239 (86%)	1.46	40 (19%) 3 2	57, 69, 74, 80	0
35	1d	208/209 (99%)	1.01	17 (8%) 17 15	48, 61, 69, 73	0
35	2d	208/209 (99%)	1.03	16 (7%) 19 17	49, 61, 67, 70	0
36	1e	148/162 (91%)	0.64	1 (0%) 84 81	42, 57, 64, 69	0
36	2e	148/162 (91%)	1.00	10 (6%) 23 20	51, 61, 69, 74	0
37	1f	100/101 (99%)	0.71	2 (2%) 65 61	46, 58, 65, 67	0
37	2f	100/101 (99%)	0.65	0 100 100	48, 60, 65, 67	0
38	1g	155/156 (99%)	0.88	4 (2%) 57 52	52, 62, 67, 72	0
38	2g	155/156 (99%)	1.28	27 (17%) 4 3	59, 67, 71, 75	0
39	1h	137/138 (99%)	0.76	3 (2%) 62 58	47, 59, 64, 67	0
39	2h	137/138 (99%)	0.90	4 (2%) 53 49	54, 61, 66, 68	0
40	1i	127/128 (99%)	1.46	24 (18%) 3 2	56, 66, 72, 74	0
40	2i	126/128 (98%)	2.02	64 (50%) 0 0	61, 70, 75, 79	0
41	1j	97/105 (92%)	1.29	13 (13%) 7 5	55, 66, 73, 78	0
41	2j	96/105 (91%)	1.99	44 (45%) 0 0	61, 70, 75, 77	0
42	1k	114/129 (88%)	0.64	4 (3%) 47 42	40, 55, 64, 67	0
42	2k	114/129 (88%)	0.90	6 (5%) 32 28	49, 61, 68, 71	0
43	1l	121/132 (91%)	0.68	4 (3%) 49 45	45, 53, 60, 63	0
43	2l	121/132 (91%)	0.79	4 (3%) 49 45	44, 56, 63, 70	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
44	1m	116/126 (92%)	1.18	16 (13%) 6 5	54, 65, 70, 77	0
44	2m	114/126 (90%)	1.47	20 (17%) 4 3	61, 69, 73, 76	0
45	1n	60/61 (98%)	1.11	5 (8%) 17 15	54, 61, 66, 71	0
45	2n	60/61 (98%)	1.92	19 (31%) 1 1	60, 68, 73, 79	0
46	1o	88/89 (98%)	0.83	6 (6%) 23 20	38, 55, 66, 72	0
46	2o	88/89 (98%)	1.01	5 (5%) 29 26	51, 61, 67, 74	0
47	1p	82/88 (93%)	1.37	10 (12%) 8 7	50, 61, 67, 74	0
47	2p	82/88 (93%)	1.18	9 (10%) 10 8	54, 60, 66, 70	0
48	1q	99/105 (94%)	1.01	7 (7%) 22 19	45, 58, 64, 69	0
48	2q	99/105 (94%)	0.77	3 (3%) 52 48	47, 59, 66, 70	0
49	1r	68/88 (77%)	0.73	1 (1%) 72 68	48, 57, 66, 73	0
49	2r	68/88 (77%)	0.97	6 (8%) 15 14	52, 61, 69, 74	0
50	1s	83/93 (89%)	1.10	6 (7%) 21 19	56, 65, 70, 76	0
50	2s	83/93 (89%)	1.59	16 (19%) 3 2	59, 70, 74, 78	0
51	1t	96/106 (90%)	1.26	16 (16%) 4 3	53, 61, 68, 70	0
51	2t	98/106 (92%)	1.01	8 (8%) 17 15	50, 60, 66, 71	0
52	1u	23/27 (85%)	1.31	5 (21%) 2 2	59, 62, 66, 69	0
52	2u	23/27 (85%)	2.20	14 (60%) 0 0	62, 68, 70, 71	0
53	1y	97/113 (85%)	0.84	4 (4%) 41 37	47, 56, 67, 71	0
53	2y	96/113 (84%)	2.55	72 (75%) 0 0	66, 74, 80, 82	0
54	1w	4/5 (80%)	0.51	0 100 100	45, 49, 56, 71	0
54	2w	4/5 (80%)	0.76	1 (25%) 2 1	50, 58, 65, 72	0
55	1x	3/4 (75%)	2.18	2 (66%) 0 0	61, 61, 67, 73	0
55	2x	3/4 (75%)	1.38	1 (33%) 1 1	65, 65, 69, 77	0
56	1v	3/3 (100%)	3.05	2 (66%) 0 0	50, 50, 59, 61	0
56	2v	3/3 (100%)	3.58	3 (100%) 0 0	58, 58, 66, 67	0
All	All	20798/21492 (96%)	0.41	1249 (6%) 27 24	14, 54, 74, 90	0

The worst 5 of 1249 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
45	2n	2	ALA	8.2
1	1A	1087	G	7.2

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Mol	Chain	Res	Type	RSRZ
53	2y	98	ALA	6.6
45	1n	2	ALA	6.0
1	2A	2125	G	5.7

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	0.77	0.14	63,76,78,90	0
1	PSU	2A	1917	20/21	0.85	0.11	63,70,85,92	0
32	M2G	2a	966	25/26	0.85	0.17	57,64,74,84	0
55	8AN	1x	76	22/23	0.85	0.17	42,60,70,72	0
32	2MG	2a	1207	24/25	0.87	0.13	67,73,77,83	0
1	PSU	2A	1911	20/21	0.87	0.11	62,67,77,78	0
55	8AN	2x	76	22/23	0.87	0.15	49,64,72,84	0
32	5MC	1a	967	21/22	0.89	0.14	57,62,69,73	0
1	5MU	1A	1915	21/22	0.90	0.11	54,65,69,74	0
32	2MG	1a	1207	24/25	0.91	0.11	54,65,69,72	0
1	PSU	1A	1917	20/21	0.92	0.09	54,62,70,72	0
32	PSU	2a	516	20/21	0.92	0.09	63,68,75,76	0
1	PSU	1A	1911	20/21	0.93	0.09	49,57,64,68	0
43	0TD	2l	92	10/11	0.93	0.12	53,60,62,62	0
1	OMC	2A	1920	21/22	0.93	0.12	52,60,66,69	0
32	5MC	2a	967	21/22	0.93	0.13	60,65,71,72	0
32	5MC	1a	1407	21/22	0.94	0.10	40,50,54,58	0
32	4OC	2a	1402	22/23	0.94	0.11	53,59,65,67	0
32	MA6	2a	1518	24/25	0.94	0.12	52,58,61,64	0
32	G7M	2a	527	24/25	0.94	0.10	53,57,60,66	0
43	0TD	1l	92	10/11	0.94	0.12	45,52,57,58	0
32	PSU	1a	516	20/21	0.94	0.09	54,60,67,78	0
32	5MC	1a	1400	21/22	0.95	0.11	42,50,61,61	0
32	5MC	2a	1404	21/22	0.95	0.09	51,55,58,60	0
32	5MC	2a	1407	21/22	0.95	0.11	50,59,63,67	0
32	UR3	2a	1498	21/22	0.95	0.09	52,56,60,63	0
32	4OC	1a	1402	22/23	0.95	0.09	47,49,53,62	0
32	MA6	2a	1519	24/25	0.95	0.12	46,55,60,63	0
1	5MC	2A	1942	21/22	0.95	0.09	39,46,52,58	0
32	G7M	1a	527	24/25	0.95	0.09	44,51,55,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
32	5MC	2a	1400	21/22	0.95	0.13	51,68,74,76	0
32	M2G	1a	966	25/26	0.96	0.09	46,54,61,62	0
32	5MC	1a	1404	21/22	0.96	0.09	40,47,50,53	0
1	PSU	1A	2605	20/21	0.96	0.08	18,26,29,29	0
1	5MU	2A	1939	21/22	0.96	0.09	32,38,43,44	0
32	UR3	1a	1498	21/22	0.96	0.09	38,46,49,62	0
1	5MC	2A	1962	21/22	0.96	0.08	32,41,47,52	0
1	2MU	2A	2552	21/23	0.96	0.08	28,37,42,43	0
32	MA6	1a	1518	24/25	0.96	0.10	36,43,49,55	0
32	MA6	1a	1519	24/25	0.96	0.09	40,43,49,50	0
1	OMC	1A	1920	21/22	0.96	0.10	41,51,58,59	0
1	5MC	1A	1942	21/22	0.96	0.07	28,33,38,42	0
1	2MA	2A	2503	23/24	0.97	0.08	23,29,34,35	0
1	OMG	2A	2251	24/25	0.97	0.08	33,37,42,46	0
1	PSU	2A	2605	20/21	0.97	0.08	26,36,43,44	0
1	5MU	1A	1939	21/22	0.98	0.06	19,24,27,28	0
1	5MC	1A	1962	21/22	0.98	0.07	26,30,35,38	0
1	OMG	1A	2251	24/25	0.98	0.07	15,21,32,36	0
1	2MA	1A	2503	23/24	0.98	0.06	14,19,22,23	0
1	2MU	1A	2552	21/23	0.98	0.07	20,28,33,34	0

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3866	1/1	0.55	0.18	65,65,65,65	0
57	MG	2O	202	1/1	0.58	0.19	73,73,73,73	0
57	MG	1a	3182	1/1	0.62	0.20	77,77,77,77	0
57	MG	2A	3624	1/1	0.63	0.19	70,70,70,70	0
57	MG	1A	3977	1/1	0.64	0.20	34,34,34,34	0
57	MG	2A	3459	1/1	0.64	0.20	53,53,53,53	0
57	MG	1A	3504	1/1	0.65	0.17	50,50,50,50	0
57	MG	2A	3528	1/1	0.66	0.16	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3883	1/1	0.67	0.20	57,57,57,57	0
57	MG	1a	3174	1/1	0.68	0.15	75,75,75,75	0
57	MG	1A	3408	1/1	0.68	0.13	71,71,71,71	0
57	MG	1P	203	1/1	0.70	0.25	42,42,42,42	0
57	MG	2A	3559	1/1	0.70	0.19	62,62,62,62	0
57	MG	1A	3803	1/1	0.71	0.16	73,73,73,73	0
57	MG	1A	3437	1/1	0.71	0.24	64,64,64,64	0
57	MG	1a	3228	1/1	0.72	0.15	72,72,72,72	0
57	MG	1A	3852	1/1	0.72	0.14	52,52,52,52	0
57	MG	2A	3240	1/1	0.73	0.14	66,66,66,66	0
57	MG	2G	203	1/1	0.73	0.20	65,65,65,65	0
57	MG	1a	3203	1/1	0.73	0.17	59,59,59,59	0
57	MG	1A	3969	1/1	0.74	0.12	30,30,30,30	0
57	MG	2A	3121	1/1	0.74	0.20	73,73,73,73	0
57	MG	1A	3663	1/1	0.74	0.18	62,62,62,62	0
57	MG	2A	3235	1/1	0.75	0.28	62,62,62,62	0
57	MG	1a	3063	1/1	0.75	0.21	69,69,69,69	0
57	MG	1A	3984	1/1	0.75	0.24	38,38,38,38	0
57	MG	1A	3535	1/1	0.75	0.21	71,71,71,71	0
57	MG	2A	3159	1/1	0.76	0.17	63,63,63,63	0
57	MG	2A	3433	1/1	0.76	0.13	76,76,76,76	0
57	MG	1a	3102	1/1	0.77	0.17	61,61,61,61	0
57	MG	1A	3528	1/1	0.77	0.14	44,44,44,44	0
57	MG	2A	3627	1/1	0.77	0.19	58,58,58,58	0
57	MG	1A	3990	1/1	0.77	0.13	82,82,82,82	0
57	MG	2A	3539	1/1	0.77	0.16	56,56,56,56	0
57	MG	2a	3008	1/1	0.77	0.20	63,63,63,63	0
57	MG	2A	3377	1/1	0.78	0.18	70,70,70,70	0
57	MG	1A	3742	1/1	0.78	0.13	74,74,74,74	0
57	MG	1A	3783	1/1	0.78	0.22	59,59,59,59	0
57	MG	1a	3188	1/1	0.78	0.13	68,68,68,68	0
57	MG	1A	3996	1/1	0.78	0.19	83,83,83,83	0
57	MG	1A	3957	1/1	0.78	0.14	67,67,67,67	0
57	MG	2A	3572	1/1	0.78	0.15	42,42,42,42	0
57	MG	1A	3262	1/1	0.78	0.16	68,68,68,68	0
57	MG	1a	3092	1/1	0.78	0.21	68,68,68,68	0
57	MG	2A	3207	1/1	0.78	0.19	64,64,64,64	0
57	MG	1A	3283	1/1	0.78	0.10	66,66,66,66	0
57	MG	1a	3144	1/1	0.78	0.20	78,78,78,78	0
57	MG	1A	3514	1/1	0.79	0.12	53,53,53,53	0
57	MG	1D	315	1/1	0.79	0.16	68,68,68,68	0
57	MG	1A	3939	1/1	0.79	0.17	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3509	1/1	0.79	0.20	55,55,55,55	0
57	MG	1A	3361	1/1	0.79	0.10	27,27,27,27	0
57	MG	1a	3229	1/1	0.79	0.19	63,63,63,63	0
57	MG	1a	3239	1/1	0.79	0.21	74,74,74,74	0
57	MG	1A	3785	1/1	0.79	0.17	59,59,59,59	0
57	MG	1A	3413	1/1	0.79	0.14	62,62,62,62	0
57	MG	1A	3594	1/1	0.79	0.24	66,66,66,66	0
57	MG	2E	301	1/1	0.79	0.19	39,39,39,39	0
57	MG	1a	3150	1/1	0.79	0.15	59,59,59,59	0
57	MG	1A	3509	1/1	0.79	0.13	28,28,28,28	0
57	MG	2A	3341	1/1	0.79	0.13	42,42,42,42	0
59	ARG	1A	4023	12/12	0.79	0.18	43,60,64,64	0
57	MG	1A	3705	1/1	0.80	0.13	64,64,64,64	0
57	MG	1A	3940	1/1	0.80	0.11	74,74,74,74	0
57	MG	1A	3881	1/1	0.80	0.15	38,38,38,38	0
57	MG	2A	3486	1/1	0.80	0.16	54,54,54,54	0
57	MG	1a	3077	1/1	0.80	0.29	65,65,65,65	0
57	MG	1A	3753	1/1	0.80	0.15	45,45,45,45	0
57	MG	2A	3279	1/1	0.80	0.23	61,61,61,61	0
57	MG	2a	3133	1/1	0.80	0.20	72,72,72,72	0
57	MG	2a	3182	1/1	0.80	0.13	82,82,82,82	0
57	MG	1a	3262	1/1	0.80	0.16	61,61,61,61	0
57	MG	2A	3540	1/1	0.81	0.11	55,55,55,55	0
57	MG	2A	3299	1/1	0.81	0.12	33,33,33,33	0
57	MG	1a	3172	1/1	0.81	0.18	65,65,65,65	0
57	MG	2A	3591	1/1	0.81	0.11	38,38,38,38	0
57	MG	1A	3858	1/1	0.81	0.15	43,43,43,43	0
57	MG	2A	3404	1/1	0.81	0.12	52,52,52,52	0
57	MG	2A	3668	1/1	0.81	0.15	68,68,68,68	0
57	MG	1a	3097	1/1	0.81	0.58	81,81,81,81	0
57	MG	2A	3454	1/1	0.81	0.16	72,72,72,72	0
57	MG	1a	3187	1/1	0.81	0.24	68,68,68,68	0
57	MG	2U	201	1/1	0.81	0.32	72,72,72,72	0
57	MG	1A	3568	1/1	0.81	0.10	71,71,71,71	0
57	MG	2a	3124	1/1	0.81	0.15	64,64,64,64	0
57	MG	1A	3889	1/1	0.81	0.12	52,52,52,52	0
57	MG	1A	3924	1/1	0.81	0.17	57,57,57,57	0
57	MG	2a	3187	1/1	0.81	0.17	57,57,57,57	0
57	MG	1a	3155	1/1	0.81	0.18	73,73,73,73	0
57	MG	1A	3516	1/1	0.82	0.14	52,52,52,52	0
57	MG	2A	3324	1/1	0.82	0.15	58,58,58,58	0
57	MG	2A	3328	1/1	0.82	0.17	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3078	1/1	0.82	0.14	54,54,54,54	0
57	MG	2A	3609	1/1	0.82	0.17	51,51,51,51	0
57	MG	2A	3611	1/1	0.82	0.12	33,33,33,33	0
57	MG	1A	3913	1/1	0.82	0.11	27,27,27,27	0
57	MG	1A	3921	1/1	0.82	0.13	58,58,58,58	0
57	MG	2A	3413	1/1	0.82	0.16	55,55,55,55	0
57	MG	2B	207	1/1	0.82	0.16	59,59,59,59	0
57	MG	1A	3604	1/1	0.82	0.14	55,55,55,55	0
57	MG	2A	3439	1/1	0.82	0.15	53,53,53,53	0
57	MG	2A	3441	1/1	0.82	0.14	61,61,61,61	0
57	MG	2A	3191	1/1	0.82	0.25	65,65,65,65	0
57	MG	1A	3634	1/1	0.82	0.21	26,26,26,26	0
57	MG	2a	3034	1/1	0.82	0.27	70,70,70,70	0
57	MG	2A	3477	1/1	0.82	0.13	51,51,51,51	0
57	MG	1a	3199	1/1	0.82	0.12	69,69,69,69	0
57	MG	1B	218	1/1	0.82	0.17	64,64,64,64	0
57	MG	1A	3418	1/1	0.82	0.11	19,19,19,19	0
57	MG	2A	3297	1/1	0.82	0.13	51,51,51,51	0
60	MPD	1A	4024	8/8	0.82	0.24	46,51,56,64	0
57	MG	1A	3646	1/1	0.83	0.13	59,59,59,59	0
57	MG	1A	3550	1/1	0.83	0.15	58,58,58,58	0
57	MG	1A	3684	1/1	0.83	0.09	54,54,54,54	0
57	MG	1A	3519	1/1	0.83	0.14	51,51,51,51	0
57	MG	1D	312	1/1	0.83	0.29	46,46,46,46	0
57	MG	1A	3355	1/1	0.83	0.06	20,20,20,20	0
57	MG	2A	3311	1/1	0.83	0.11	53,53,53,53	0
57	MG	2A	3312	1/1	0.83	0.19	59,59,59,59	0
57	MG	1A	3598	1/1	0.83	0.12	40,40,40,40	0
57	MG	1A	3533	1/1	0.83	0.19	48,48,48,48	0
57	MG	1a	3073	1/1	0.83	0.15	53,53,53,53	0
57	MG	1A	3611	1/1	0.83	0.25	34,34,34,34	0
57	MG	1a	3236	1/1	0.83	0.16	46,46,46,46	0
57	MG	2A	3405	1/1	0.83	0.16	55,55,55,55	0
57	MG	1A	3620	1/1	0.83	0.12	34,34,34,34	0
57	MG	2A	3424	1/1	0.83	0.13	44,44,44,44	0
57	MG	1A	3848	1/1	0.83	0.17	61,61,61,61	0
57	MG	2A	3054	1/1	0.83	0.23	66,66,66,66	0
57	MG	2a	3024	1/1	0.83	0.11	58,58,58,58	0
57	MG	1A	3966	1/1	0.83	0.17	41,41,41,41	0
57	MG	2A	3446	1/1	0.83	0.16	46,46,46,46	0
57	MG	1A	3478	1/1	0.83	0.14	26,26,26,26	0
57	MG	2a	3135	1/1	0.83	0.22	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3167	1/1	0.83	0.18	46,46,46,46	0
57	MG	2A	3190	1/1	0.83	0.27	49,49,49,49	0
57	MG	1A	3644	1/1	0.83	0.15	40,40,40,40	0
57	MG	2A	3499	1/1	0.83	0.16	49,49,49,49	0
57	MG	1A	4012	1/1	0.84	0.15	40,40,40,40	0
57	MG	1A	3178	1/1	0.84	0.20	52,52,52,52	0
57	MG	1a	3105	1/1	0.84	0.30	64,64,64,64	0
57	MG	2A	3564	1/1	0.84	0.11	67,67,67,67	0
57	MG	1a	3126	1/1	0.84	0.17	65,65,65,65	0
57	MG	2A	3576	1/1	0.84	0.12	49,49,49,49	0
57	MG	1a	3255	1/1	0.84	0.12	61,61,61,61	0
57	MG	1B	219	1/1	0.84	0.10	46,46,46,46	0
57	MG	1A	3525	1/1	0.84	0.18	56,56,56,56	0
57	MG	2A	3621	1/1	0.84	0.13	28,28,28,28	0
57	MG	2A	3057	1/1	0.84	0.15	56,56,56,56	0
57	MG	1A	3863	1/1	0.84	0.12	51,51,51,51	0
57	MG	2A	3659	1/1	0.84	0.16	65,65,65,65	0
57	MG	2A	3126	1/1	0.84	0.18	57,57,57,57	0
57	MG	2A	3725	1/1	0.84	0.27	64,64,64,64	0
57	MG	1G	202	1/1	0.84	0.10	56,56,56,56	0
57	MG	1A	3492	1/1	0.84	0.14	34,34,34,34	0
57	MG	2A	3436	1/1	0.84	0.09	65,65,65,65	0
57	MG	2A	3168	1/1	0.84	0.15	58,58,58,58	0
57	MG	2T	202	1/1	0.84	0.16	61,61,61,61	0
57	MG	1a	3179	1/1	0.84	0.13	55,55,55,55	0
57	MG	10	106	1/1	0.84	0.13	50,50,50,50	0
57	MG	1A	3821	1/1	0.84	0.29	36,36,36,36	0
57	MG	2A	3208	1/1	0.84	0.17	56,56,56,56	0
57	MG	2a	3057	1/1	0.84	0.25	68,68,68,68	0
57	MG	1A	3986	1/1	0.84	0.10	28,28,28,28	0
57	MG	1A	3466	1/1	0.84	0.13	37,37,37,37	0
57	MG	2A	3487	1/1	0.84	0.15	48,48,48,48	0
57	MG	2a	3147	1/1	0.84	0.17	67,67,67,67	0
57	MG	1A	3950	1/1	0.84	0.13	61,61,61,61	0
57	MG	2a	3185	1/1	0.84	0.22	63,63,63,63	0
57	MG	1a	3210	1/1	0.84	0.16	59,59,59,59	0
57	MG	2A	3522	1/1	0.84	0.16	38,38,38,38	0
57	MG	2A	3298	1/1	0.84	0.15	71,71,71,71	0
57	MG	2A	3218	1/1	0.85	0.34	71,71,71,71	0
57	MG	1a	3065	1/1	0.85	0.27	61,61,61,61	0
57	MG	1A	3027	1/1	0.85	0.10	56,56,56,56	0
57	MG	2A	3256	1/1	0.85	0.18	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3543	1/1	0.85	0.11	33,33,33,33	0
57	MG	1a	3204	1/1	0.85	0.13	47,47,47,47	0
57	MG	1a	3076	1/1	0.85	0.14	56,56,56,56	0
57	MG	1A	3344	1/1	0.85	0.16	53,53,53,53	0
57	MG	1a	3082	1/1	0.85	0.11	56,56,56,56	0
57	MG	2A	3582	1/1	0.85	0.10	42,42,42,42	0
57	MG	1a	3233	1/1	0.85	0.19	61,61,61,61	0
57	MG	1A	3542	1/1	0.85	0.09	31,31,31,31	0
57	MG	1A	3267	1/1	0.85	0.30	58,58,58,58	0
57	MG	2A	3618	1/1	0.85	0.15	57,57,57,57	0
57	MG	1A	3531	1/1	0.85	0.16	43,43,43,43	0
57	MG	2A	3336	1/1	0.85	0.14	44,44,44,44	0
57	MG	1A	3696	1/1	0.85	0.23	40,40,40,40	0
57	MG	2A	3003	1/1	0.85	0.11	58,58,58,58	0
57	MG	1A	3697	1/1	0.85	0.15	59,59,59,59	0
57	MG	2A	3718	1/1	0.85	0.18	63,63,63,63	0
57	MG	2A	3719	1/1	0.85	0.15	47,47,47,47	0
57	MG	1N	204	1/1	0.85	0.10	50,50,50,50	0
57	MG	2B	206	1/1	0.85	0.13	54,54,54,54	0
57	MG	2A	3058	1/1	0.85	0.12	51,51,51,51	0
57	MG	2A	3080	1/1	0.85	0.12	78,78,78,78	0
57	MG	2G	202	1/1	0.85	0.15	70,70,70,70	0
57	MG	2A	3426	1/1	0.85	0.16	57,57,57,57	0
57	MG	1A	3700	1/1	0.85	0.25	40,40,40,40	0
57	MG	1A	3987	1/1	0.85	0.13	47,47,47,47	0
57	MG	2T	204	1/1	0.85	0.11	60,60,60,60	0
57	MG	2A	3136	1/1	0.85	0.18	61,61,61,61	0
57	MG	28	102	1/1	0.85	0.20	45,45,45,45	0
57	MG	2A	3148	1/1	0.85	0.20	57,57,57,57	0
57	MG	1a	3022	1/1	0.85	0.20	55,55,55,55	0
57	MG	1a	3033	1/1	0.85	0.29	60,60,60,60	0
57	MG	1a	3049	1/1	0.85	0.21	63,63,63,63	0
57	MG	2a	3106	1/1	0.85	0.25	52,52,52,52	0
57	MG	2A	3463	1/1	0.85	0.19	58,58,58,58	0
57	MG	2a	3132	1/1	0.85	0.12	58,58,58,58	0
57	MG	2A	3473	1/1	0.85	0.10	58,58,58,58	0
57	MG	2A	3189	1/1	0.85	0.23	59,59,59,59	0
57	MG	2A	3484	1/1	0.85	0.13	57,57,57,57	0
57	MG	2a	3180	1/1	0.85	0.17	63,63,63,63	0
57	MG	1a	3054	1/1	0.85	0.15	62,62,62,62	0
57	MG	1a	3058	1/1	0.85	0.16	61,61,61,61	0
57	MG	2A	3496	1/1	0.85	0.11	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2e	201	1/1	0.85	0.21	63,63,63,63	0
57	MG	1A	3631	1/1	0.85	0.10	30,30,30,30	0
57	MG	1a	3197	1/1	0.85	0.13	49,49,49,49	0
57	MG	2A	3400	1/1	0.86	0.10	41,41,41,41	0
57	MG	1B	203	1/1	0.86	0.13	56,56,56,56	0
57	MG	2A	3143	1/1	0.86	0.14	42,42,42,42	0
57	MG	2A	3407	1/1	0.86	0.18	56,56,56,56	0
57	MG	1a	3191	1/1	0.86	0.15	59,59,59,59	0
57	MG	1a	3069	1/1	0.86	0.29	54,54,54,54	0
57	MG	1A	3461	1/1	0.86	0.17	55,55,55,55	0
57	MG	2A	3649	1/1	0.86	0.12	53,53,53,53	0
57	MG	2A	3653	1/1	0.86	0.11	27,27,27,27	0
57	MG	1A	3194	1/1	0.86	0.28	54,54,54,54	0
57	MG	1A	3876	1/1	0.86	0.09	24,24,24,24	0
57	MG	2A	3695	1/1	0.86	0.18	53,53,53,53	0
57	MG	2A	3704	1/1	0.86	0.08	42,42,42,42	0
57	MG	2A	3714	1/1	0.86	0.13	61,61,61,61	0
57	MG	2A	3717	1/1	0.86	0.15	61,61,61,61	0
57	MG	1A	3878	1/1	0.86	0.08	25,25,25,25	0
57	MG	1a	3217	1/1	0.86	0.19	54,54,54,54	0
57	MG	2A	3442	1/1	0.86	0.15	60,60,60,60	0
57	MG	2A	3194	1/1	0.86	0.18	59,59,59,59	0
57	MG	1A	3669	1/1	0.86	0.19	45,45,45,45	0
57	MG	2B	212	1/1	0.86	0.12	53,53,53,53	0
57	MG	2A	3456	1/1	0.86	0.14	53,53,53,53	0
57	MG	1A	3975	1/1	0.86	0.10	56,56,56,56	0
57	MG	1A	3617	1/1	0.86	0.11	16,16,16,16	0
57	MG	2O	201	1/1	0.86	0.10	47,47,47,47	0
57	MG	2A	3472	1/1	0.86	0.17	59,59,59,59	0
57	MG	2Q	203	1/1	0.86	0.10	55,55,55,55	0
57	MG	1A	3470	1/1	0.86	0.11	41,41,41,41	0
57	MG	2A	3474	1/1	0.86	0.18	61,61,61,61	0
57	MG	1a	3019	1/1	0.86	0.20	53,53,53,53	0
57	MG	20	102	1/1	0.86	0.15	59,59,59,59	0
57	MG	1a	3252	1/1	0.86	0.12	46,46,46,46	0
57	MG	2A	3264	1/1	0.86	0.22	54,54,54,54	0
57	MG	2a	3023	1/1	0.86	0.21	59,59,59,59	0
57	MG	2A	3278	1/1	0.86	0.29	57,57,57,57	0
57	MG	2a	3031	1/1	0.86	0.24	71,71,71,71	0
57	MG	1a	3141	1/1	0.86	0.12	59,59,59,59	0
57	MG	2a	3037	1/1	0.86	0.11	67,67,67,67	0
57	MG	2a	3043	1/1	0.86	0.18	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3584	1/1	0.86	0.12	35,35,35,35	0
57	MG	2a	3069	1/1	0.86	0.16	62,62,62,62	0
57	MG	2a	3086	1/1	0.86	0.14	60,60,60,60	0
57	MG	2A	3507	1/1	0.86	0.16	59,59,59,59	0
57	MG	2a	3122	1/1	0.86	0.26	69,69,69,69	0
57	MG	1a	3029	1/1	0.86	0.14	53,53,53,53	0
57	MG	1A	3919	1/1	0.86	0.12	46,46,46,46	0
57	MG	1a	3045	1/1	0.86	0.17	60,60,60,60	0
57	MG	2A	3530	1/1	0.86	0.17	55,55,55,55	0
57	MG	2a	3137	1/1	0.86	0.13	45,45,45,45	0
57	MG	1A	3197	1/1	0.86	0.28	53,53,53,53	0
57	MG	2a	3167	1/1	0.86	0.14	73,73,73,73	0
57	MG	2A	3064	1/1	0.86	0.13	51,51,51,51	0
57	MG	1A	3446	1/1	0.86	0.11	58,58,58,58	0
57	MG	2A	3094	1/1	0.86	0.09	61,61,61,61	0
57	MG	1A	3710	1/1	0.86	0.20	21,21,21,21	0
57	MG	1A	4014	1/1	0.86	0.09	27,27,27,27	0
57	MG	2A	3397	1/1	0.86	0.12	50,50,50,50	0
57	MG	2A	3399	1/1	0.86	0.26	66,66,66,66	0
57	MG	1A	3655	1/1	0.87	0.09	40,40,40,40	0
57	MG	2A	3660	1/1	0.87	0.11	58,58,58,58	0
57	MG	1A	3893	1/1	0.87	0.14	47,47,47,47	0
57	MG	2A	3679	1/1	0.87	0.13	58,58,58,58	0
57	MG	2A	3690	1/1	0.87	0.11	50,50,50,50	0
57	MG	2A	3693	1/1	0.87	0.10	50,50,50,50	0
57	MG	2A	3187	1/1	0.87	0.14	52,52,52,52	0
57	MG	1A	3765	1/1	0.87	0.10	25,25,25,25	0
57	MG	2A	3708	1/1	0.87	0.11	62,62,62,62	0
57	MG	1A	3659	1/1	0.87	0.10	36,36,36,36	0
57	MG	2A	3716	1/1	0.87	0.12	45,45,45,45	0
57	MG	1A	3660	1/1	0.87	0.11	18,18,18,18	0
57	MG	1A	3794	1/1	0.87	0.27	39,39,39,39	0
57	MG	2A	3448	1/1	0.87	0.21	43,43,43,43	0
57	MG	2A	3723	1/1	0.87	0.18	58,58,58,58	0
57	MG	2A	3196	1/1	0.87	0.26	55,55,55,55	0
57	MG	1a	3227	1/1	0.87	0.13	62,62,62,62	0
57	MG	1B	227	1/1	0.87	0.10	58,58,58,58	0
57	MG	2B	208	1/1	0.87	0.29	57,57,57,57	0
57	MG	1B	229	1/1	0.87	0.10	46,46,46,46	0
57	MG	2D	306	1/1	0.87	0.25	41,41,41,41	0
57	MG	2A	3226	1/1	0.87	0.11	52,52,52,52	0
57	MG	1a	3232	1/1	0.87	0.11	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1a	3085	1/1	0.87	0.08	57,57,57,57	0
57	MG	1A	3359	1/1	0.87	0.10	43,43,43,43	0
57	MG	2A	3479	1/1	0.87	0.17	66,66,66,66	0
57	MG	1A	3665	1/1	0.87	0.11	47,47,47,47	0
57	MG	2A	3275	1/1	0.87	0.14	53,53,53,53	0
57	MG	1E	303	1/1	0.87	0.10	22,22,22,22	0
57	MG	1a	3104	1/1	0.87	0.35	61,61,61,61	0
57	MG	1a	3261	1/1	0.87	0.14	60,60,60,60	0
57	MG	1A	3944	1/1	0.87	0.10	21,21,21,21	0
57	MG	1n	103	1/1	0.87	0.13	60,60,60,60	0
57	MG	2A	3511	1/1	0.87	0.16	61,61,61,61	0
57	MG	1A	3831	1/1	0.87	0.10	25,25,25,25	0
57	MG	2A	3005	1/1	0.87	0.13	58,58,58,58	0
57	MG	2A	3033	1/1	0.87	0.20	58,58,58,58	0
57	MG	1A	3284	1/1	0.87	0.12	64,64,64,64	0
57	MG	1A	3571	1/1	0.87	0.14	49,49,49,49	0
57	MG	1a	3149	1/1	0.87	0.10	51,51,51,51	0
57	MG	2a	3058	1/1	0.87	0.27	63,63,63,63	0
57	MG	2A	3350	1/1	0.87	0.08	28,28,28,28	0
57	MG	2a	3079	1/1	0.87	0.14	60,60,60,60	0
57	MG	2a	3085	1/1	0.87	0.13	67,67,67,67	0
57	MG	2A	3359	1/1	0.87	0.09	37,37,37,37	0
57	MG	2A	3568	1/1	0.87	0.11	37,37,37,37	0
57	MG	2a	3107	1/1	0.87	0.16	60,60,60,60	0
57	MG	2a	3110	1/1	0.87	0.35	63,63,63,63	0
57	MG	2A	3371	1/1	0.87	0.16	63,63,63,63	0
57	MG	2A	3375	1/1	0.87	0.11	57,57,57,57	0
57	MG	1a	3009	1/1	0.87	0.18	51,51,51,51	0
57	MG	1A	3403	1/1	0.87	0.07	14,14,14,14	0
57	MG	2A	3398	1/1	0.87	0.13	56,56,56,56	0
57	MG	1A	3419	1/1	0.87	0.17	64,64,64,64	0
57	MG	1A	3641	1/1	0.87	0.12	46,46,46,46	0
57	MG	1A	3642	1/1	0.87	0.15	35,35,35,35	0
57	MG	2A	3623	1/1	0.87	0.16	49,49,49,49	0
57	MG	1a	3034	1/1	0.87	0.21	47,47,47,47	0
57	MG	1A	3406	1/1	0.87	0.15	48,48,48,48	0
57	MG	2A	3633	1/1	0.87	0.18	70,70,70,70	0
57	MG	2A	3646	1/1	0.87	0.10	67,67,67,67	0
57	MG	1A	3479	1/1	0.87	0.08	18,18,18,18	0
57	MG	1A	3747	1/1	0.87	0.16	41,41,41,41	0
57	MG	1A	3373	1/1	0.88	0.12	41,41,41,41	0
57	MG	2A	3239	1/1	0.88	0.21	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1a	3201	1/1	0.88	0.10	59,59,59,59	0
57	MG	2A	3569	1/1	0.88	0.14	33,33,33,33	0
57	MG	2A	3254	1/1	0.88	0.26	58,58,58,58	0
57	MG	2A	3575	1/1	0.88	0.12	52,52,52,52	0
57	MG	1A	3574	1/1	0.88	0.08	26,26,26,26	0
57	MG	2A	3257	1/1	0.88	0.12	52,52,52,52	0
57	MG	2A	3589	1/1	0.88	0.13	41,41,41,41	0
57	MG	1A	3971	1/1	0.88	0.09	37,37,37,37	0
57	MG	2A	3600	1/1	0.88	0.12	59,59,59,59	0
57	MG	2A	3602	1/1	0.88	0.11	36,36,36,36	0
57	MG	2A	3271	1/1	0.88	0.09	44,44,44,44	0
57	MG	2A	3274	1/1	0.88	0.22	57,57,57,57	0
57	MG	1A	3392	1/1	0.88	0.07	27,27,27,27	0
57	MG	2A	3620	1/1	0.88	0.12	61,61,61,61	0
57	MG	1a	3216	1/1	0.88	0.18	67,67,67,67	0
57	MG	1A	3587	1/1	0.88	0.12	47,47,47,47	0
57	MG	1A	3842	1/1	0.88	0.08	41,41,41,41	0
57	MG	1A	3846	1/1	0.88	0.12	43,43,43,43	0
57	MG	1A	3458	1/1	0.88	0.15	38,38,38,38	0
57	MG	1A	3988	1/1	0.88	0.18	41,41,41,41	0
57	MG	1A	3460	1/1	0.88	0.10	36,36,36,36	0
57	MG	2A	3315	1/1	0.88	0.10	38,38,38,38	0
57	MG	2A	3320	1/1	0.88	0.11	53,53,53,53	0
57	MG	2A	3321	1/1	0.88	0.13	54,54,54,54	0
57	MG	2A	3664	1/1	0.88	0.09	58,58,58,58	0
57	MG	1A	3318	1/1	0.88	0.13	47,47,47,47	0
57	MG	2A	3669	1/1	0.88	0.12	58,58,58,58	0
57	MG	1a	3237	1/1	0.88	0.11	53,53,53,53	0
57	MG	2A	3335	1/1	0.88	0.12	32,32,32,32	0
57	MG	1A	3694	1/1	0.88	0.11	29,29,29,29	0
57	MG	1a	3079	1/1	0.88	0.26	53,53,53,53	0
57	MG	2A	3699	1/1	0.88	0.15	67,67,67,67	0
57	MG	1A	3521	1/1	0.88	0.10	46,46,46,46	0
57	MG	1A	3867	1/1	0.88	0.09	23,23,23,23	0
57	MG	1B	211	1/1	0.88	0.18	62,62,62,62	0
57	MG	1a	3265	1/1	0.88	0.16	56,56,56,56	0
57	MG	1a	3266	1/1	0.88	0.18	67,67,67,67	0
57	MG	2A	3385	1/1	0.88	0.11	71,71,71,71	0
57	MG	2A	3391	1/1	0.88	0.15	57,57,57,57	0
57	MG	1A	3612	1/1	0.88	0.10	48,48,48,48	0
57	MG	1y	201	1/1	0.88	0.16	67,67,67,67	0
57	MG	2B	201	1/1	0.88	0.17	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2B	204	1/1	0.88	0.15	69,69,69,69	0
57	MG	1y	202	1/1	0.88	0.12	61,61,61,61	0
57	MG	1A	3613	1/1	0.88	0.19	48,48,48,48	0
57	MG	2A	3403	1/1	0.88	0.11	41,41,41,41	0
57	MG	1A	3702	1/1	0.88	0.29	50,50,50,50	0
57	MG	2A	3016	1/1	0.88	0.18	63,63,63,63	0
57	MG	2A	3406	1/1	0.88	0.14	43,43,43,43	0
57	MG	2A	3019	1/1	0.88	0.21	41,41,41,41	0
57	MG	2A	3408	1/1	0.88	0.23	63,63,63,63	0
57	MG	2A	3031	1/1	0.88	0.20	63,63,63,63	0
57	MG	1A	3329	1/1	0.88	0.08	28,28,28,28	0
57	MG	2A	3052	1/1	0.88	0.17	62,62,62,62	0
57	MG	2A	3428	1/1	0.88	0.15	52,52,52,52	0
57	MG	2A	3430	1/1	0.88	0.38	48,48,48,48	0
57	MG	1a	3106	1/1	0.88	0.17	62,62,62,62	0
57	MG	2A	3434	1/1	0.88	0.10	44,44,44,44	0
57	MG	2A	3435	1/1	0.88	0.10	42,42,42,42	0
57	MG	2A	3055	1/1	0.88	0.18	49,49,49,49	0
57	MG	1a	3107	1/1	0.88	0.23	55,55,55,55	0
57	MG	1a	3114	1/1	0.88	0.10	68,68,68,68	0
57	MG	1a	3121	1/1	0.88	0.16	58,58,58,58	0
57	MG	1A	3087	1/1	0.88	0.21	48,48,48,48	0
57	MG	2A	3087	1/1	0.88	0.13	53,53,53,53	0
57	MG	2a	3040	1/1	0.88	0.17	56,56,56,56	0
57	MG	1a	3132	1/1	0.88	0.17	50,50,50,50	0
57	MG	1A	3472	1/1	0.88	0.12	43,43,43,43	0
57	MG	1A	3743	1/1	0.88	0.12	51,51,51,51	0
57	MG	2a	3061	1/1	0.88	0.35	69,69,69,69	0
57	MG	1A	3473	1/1	0.88	0.07	17,17,17,17	0
57	MG	2a	3077	1/1	0.88	0.25	54,54,54,54	0
57	MG	1A	3200	1/1	0.88	0.17	52,52,52,52	0
57	MG	1A	3758	1/1	0.88	0.17	43,43,43,43	0
57	MG	1a	3161	1/1	0.88	0.09	41,41,41,41	0
57	MG	2A	3160	1/1	0.88	0.16	52,52,52,52	0
57	MG	1a	3163	1/1	0.88	0.22	69,69,69,69	0
57	MG	1a	3171	1/1	0.88	0.14	58,58,58,58	0
57	MG	2A	3178	1/1	0.88	0.12	48,48,48,48	0
57	MG	1R	203	1/1	0.88	0.13	39,39,39,39	0
57	MG	1W	204	1/1	0.88	0.14	39,39,39,39	0
57	MG	1A	3155	1/1	0.88	0.18	38,38,38,38	0
57	MG	1A	3778	1/1	0.88	0.13	35,35,35,35	0
57	MG	1A	3484	1/1	0.88	0.09	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3510	1/1	0.88	0.15	54,54,54,54	0
57	MG	2a	3151	1/1	0.88	0.13	63,63,63,63	0
57	MG	1A	3286	1/1	0.88	0.12	63,63,63,63	0
57	MG	1a	3190	1/1	0.88	0.14	68,68,68,68	0
57	MG	1a	3028	1/1	0.88	0.24	55,55,55,55	0
57	MG	2A	3212	1/1	0.88	0.14	61,61,61,61	0
57	MG	2A	3531	1/1	0.88	0.12	53,53,53,53	0
57	MG	2A	3216	1/1	0.88	0.24	63,63,63,63	0
57	MG	2j	201	1/1	0.88	0.10	68,68,68,68	0
57	MG	2x	101	1/1	0.88	0.11	62,62,62,62	0
57	MG	1a	3194	1/1	0.88	0.12	65,65,65,65	0
57	MG	1A	3791	1/1	0.88	0.10	70,70,70,70	0
60	MPD	1T	207	8/8	0.88	0.18	56,60,62,64	0
57	MG	1A	3110	1/1	0.89	0.14	25,25,25,25	0
57	MG	1A	4013	1/1	0.89	0.18	57,57,57,57	0
57	MG	1a	3061	1/1	0.89	0.16	63,63,63,63	0
57	MG	2A	3429	1/1	0.89	0.12	47,47,47,47	0
57	MG	2A	3182	1/1	0.89	0.12	56,56,56,56	0
57	MG	1A	3907	1/1	0.89	0.16	56,56,56,56	0
57	MG	1A	4016	1/1	0.89	0.15	54,54,54,54	0
57	MG	1B	202	1/1	0.89	0.11	44,44,44,44	0
57	MG	1A	3338	1/1	0.89	0.11	51,51,51,51	0
57	MG	1a	3213	1/1	0.89	0.19	68,68,68,68	0
57	MG	1a	3074	1/1	0.89	0.10	54,54,54,54	0
57	MG	1A	3678	1/1	0.89	0.14	52,52,52,52	0
57	MG	1A	3011	1/1	0.89	0.09	42,42,42,42	0
57	MG	2A	3210	1/1	0.89	0.12	64,64,64,64	0
57	MG	2A	3720	1/1	0.89	0.14	52,52,52,52	0
57	MG	1a	3078	1/1	0.89	0.17	70,70,70,70	0
57	MG	1A	3691	1/1	0.89	0.17	54,54,54,54	0
57	MG	1a	3080	1/1	0.89	0.13	55,55,55,55	0
57	MG	2B	202	1/1	0.89	0.08	69,69,69,69	0
57	MG	1B	222	1/1	0.89	0.12	42,42,42,42	0
57	MG	1A	3933	1/1	0.89	0.09	50,50,50,50	0
57	MG	1A	3345	1/1	0.89	0.10	48,48,48,48	0
57	MG	1A	3353	1/1	0.89	0.08	30,30,30,30	0
57	MG	2A	3253	1/1	0.89	0.11	54,54,54,54	0
57	MG	1A	3549	1/1	0.89	0.10	30,30,30,30	0
57	MG	2D	307	1/1	0.89	0.10	53,53,53,53	0
57	MG	2A	3483	1/1	0.89	0.12	59,59,59,59	0
57	MG	1A	3844	1/1	0.89	0.10	25,25,25,25	0
57	MG	1F	317	1/1	0.89	0.11	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3953	1/1	0.89	0.12	48,48,48,48	0
57	MG	2A	3495	1/1	0.89	0.10	55,55,55,55	0
57	MG	1A	3010	1/1	0.89	0.17	57,57,57,57	0
57	MG	1a	3111	1/1	0.89	0.12	60,60,60,60	0
57	MG	1d	301	1/1	0.89	0.13	57,57,57,57	0
57	MG	1i	201	1/1	0.89	0.27	60,60,60,60	0
57	MG	2V	201	1/1	0.89	0.12	53,53,53,53	0
57	MG	1n	102	1/1	0.89	0.08	52,52,52,52	0
57	MG	21	102	1/1	0.89	0.14	48,48,48,48	0
57	MG	2A	3287	1/1	0.89	0.37	63,63,63,63	0
57	MG	2a	3007	1/1	0.89	0.12	53,53,53,53	0
57	MG	1N	205	1/1	0.89	0.07	46,46,46,46	0
57	MG	2A	3527	1/1	0.89	0.10	55,55,55,55	0
57	MG	1o	102	1/1	0.89	0.12	53,53,53,53	0
57	MG	2A	3529	1/1	0.89	0.14	70,70,70,70	0
57	MG	1a	3115	1/1	0.89	0.24	49,49,49,49	0
57	MG	1a	3118	1/1	0.89	0.19	55,55,55,55	0
57	MG	2a	3039	1/1	0.89	0.20	59,59,59,59	0
57	MG	1A	3555	1/1	0.89	0.15	43,43,43,43	0
57	MG	1A	3640	1/1	0.89	0.22	59,59,59,59	0
57	MG	2a	3049	1/1	0.89	0.28	61,61,61,61	0
57	MG	2a	3051	1/1	0.89	0.26	59,59,59,59	0
57	MG	2A	3006	1/1	0.89	0.10	54,54,54,54	0
57	MG	2A	3545	1/1	0.89	0.09	38,38,38,38	0
57	MG	1A	3209	1/1	0.89	0.29	67,67,67,67	0
57	MG	1W	205	1/1	0.89	0.08	48,48,48,48	0
57	MG	1A	3973	1/1	0.89	0.10	49,49,49,49	0
57	MG	1a	3147	1/1	0.89	0.12	54,54,54,54	0
57	MG	2A	3042	1/1	0.89	0.24	66,66,66,66	0
57	MG	10	108	1/1	0.89	0.09	51,51,51,51	0
57	MG	2a	3087	1/1	0.89	0.33	69,69,69,69	0
57	MG	1a	3007	1/1	0.89	0.11	56,56,56,56	0
57	MG	1A	3311	1/1	0.89	0.13	62,62,62,62	0
57	MG	2A	3363	1/1	0.89	0.08	50,50,50,50	0
57	MG	2A	3365	1/1	0.89	0.13	56,56,56,56	0
57	MG	1a	3018	1/1	0.89	0.09	56,56,56,56	0
57	MG	2a	3126	1/1	0.89	0.14	64,64,64,64	0
57	MG	1A	3312	1/1	0.89	0.12	37,37,37,37	0
57	MG	1A	3380	1/1	0.89	0.11	43,43,43,43	0
57	MG	2A	3380	1/1	0.89	0.09	49,49,49,49	0
57	MG	2A	3617	1/1	0.89	0.12	37,37,37,37	0
57	MG	2a	3138	1/1	0.89	0.15	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2a	3145	1/1	0.89	0.09	52,52,52,52	0
57	MG	2A	3079	1/1	0.89	0.14	50,50,50,50	0
57	MG	2a	3148	1/1	0.89	0.09	39,39,39,39	0
57	MG	1A	3386	1/1	0.89	0.07	20,20,20,20	0
57	MG	2a	3153	1/1	0.89	0.12	61,61,61,61	0
57	MG	1A	3190	1/1	0.89	0.14	52,52,52,52	0
57	MG	2A	3090	1/1	0.89	0.21	48,48,48,48	0
57	MG	2a	3181	1/1	0.89	0.17	62,62,62,62	0
57	MG	1a	3176	1/1	0.89	0.13	63,63,63,63	0
57	MG	1a	3032	1/1	0.89	0.13	43,43,43,43	0
57	MG	1A	3597	1/1	0.89	0.08	38,38,38,38	0
57	MG	1a	3184	1/1	0.89	0.19	56,56,56,56	0
57	MG	1A	3395	1/1	0.89	0.09	34,34,34,34	0
57	MG	2n	101	1/1	0.89	0.19	62,62,62,62	0
57	MG	1a	3041	1/1	0.89	0.17	43,43,43,43	0
57	MG	2A	3150	1/1	0.89	0.12	52,52,52,52	0
57	MG	1A	3779	1/1	0.89	0.12	39,39,39,39	0
57	MG	1A	4009	1/1	0.89	0.11	54,54,54,54	0
60	MPD	1a	3271	8/8	0.89	0.15	49,51,53,60	0
60	MPD	2B	218	8/8	0.89	0.18	44,53,60,60	0
57	MG	1a	3224	1/1	0.90	0.18	68,68,68,68	0
57	MG	1a	3090	1/1	0.90	0.18	54,54,54,54	0
57	MG	2A	3697	1/1	0.90	0.08	73,73,73,73	0
57	MG	2A	3432	1/1	0.90	0.22	44,44,44,44	0
57	MG	1A	3838	1/1	0.90	0.12	53,53,53,53	0
57	MG	2A	3705	1/1	0.90	0.13	55,55,55,55	0
57	MG	1F	313	1/1	0.90	0.36	37,37,37,37	0
57	MG	2A	3712	1/1	0.90	0.09	41,41,41,41	0
57	MG	1a	3230	1/1	0.90	0.14	52,52,52,52	0
57	MG	2A	3715	1/1	0.90	0.16	60,60,60,60	0
57	MG	1a	3098	1/1	0.90	0.17	57,57,57,57	0
57	MG	2A	3437	1/1	0.90	0.10	51,51,51,51	0
57	MG	1a	3100	1/1	0.90	0.17	61,61,61,61	0
57	MG	1A	3946	1/1	0.90	0.11	39,39,39,39	0
57	MG	1A	3948	1/1	0.90	0.11	53,53,53,53	0
57	MG	1A	3949	1/1	0.90	0.08	59,59,59,59	0
57	MG	1a	3243	1/1	0.90	0.13	53,53,53,53	0
57	MG	2A	3452	1/1	0.90	0.15	44,44,44,44	0
57	MG	2A	3215	1/1	0.90	0.13	52,52,52,52	0
57	MG	1a	3251	1/1	0.90	0.12	64,64,64,64	0
57	MG	1A	3096	1/1	0.90	0.20	43,43,43,43	0
57	MG	1O	201	1/1	0.90	0.08	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3468	1/1	0.90	0.09	44,44,44,44	0
57	MG	1A	3433	1/1	0.90	0.12	40,40,40,40	0
57	MG	2B	215	1/1	0.90	0.13	61,61,61,61	0
57	MG	1A	3954	1/1	0.90	0.10	49,49,49,49	0
57	MG	1a	3264	1/1	0.90	0.14	72,72,72,72	0
57	MG	1A	3602	1/1	0.90	0.09	24,24,24,24	0
57	MG	1A	3717	1/1	0.90	0.10	45,45,45,45	0
57	MG	1A	3396	1/1	0.90	0.09	28,28,28,28	0
57	MG	1d	302	1/1	0.90	0.09	61,61,61,61	0
57	MG	1a	3124	1/1	0.90	0.11	53,53,53,53	0
57	MG	1A	3854	1/1	0.90	0.08	30,30,30,30	0
57	MG	2R	201	1/1	0.90	0.12	55,55,55,55	0
57	MG	2A	3491	1/1	0.90	0.16	44,44,44,44	0
57	MG	17	104	1/1	0.90	0.13	33,33,33,33	0
57	MG	1a	3134	1/1	0.90	0.07	38,38,38,38	0
57	MG	1A	3856	1/1	0.90	0.11	46,46,46,46	0
57	MG	2A	3503	1/1	0.90	0.11	41,41,41,41	0
57	MG	1a	3142	1/1	0.90	0.12	62,62,62,62	0
57	MG	25	101	1/1	0.90	0.17	46,46,46,46	0
57	MG	28	101	1/1	0.90	0.13	46,46,46,46	0
57	MG	2A	3280	1/1	0.90	0.26	53,53,53,53	0
57	MG	2a	3005	1/1	0.90	0.22	64,64,64,64	0
57	MG	1y	203	1/1	0.90	0.24	59,59,59,59	0
57	MG	2A	3292	1/1	0.90	0.08	59,59,59,59	0
57	MG	1A	3607	1/1	0.90	0.18	24,24,24,24	0
57	MG	1A	3105	1/1	0.90	0.08	51,51,51,51	0
57	MG	2a	3026	1/1	0.90	0.24	64,64,64,64	0
57	MG	1A	3981	1/1	0.90	0.14	60,60,60,60	0
57	MG	2A	3307	1/1	0.90	0.14	41,41,41,41	0
57	MG	1A	3982	1/1	0.90	0.09	44,44,44,44	0
57	MG	1A	3865	1/1	0.90	0.07	32,32,32,32	0
57	MG	2A	3025	1/1	0.90	0.09	48,48,48,48	0
57	MG	1A	3302	1/1	0.90	0.20	58,58,58,58	0
57	MG	2a	3047	1/1	0.90	0.27	51,51,51,51	0
57	MG	1A	3569	1/1	0.90	0.12	39,39,39,39	0
57	MG	2A	3035	1/1	0.90	0.12	51,51,51,51	0
57	MG	2A	3554	1/1	0.90	0.08	43,43,43,43	0
57	MG	2A	3556	1/1	0.90	0.10	34,34,34,34	0
57	MG	1A	3871	1/1	0.90	0.08	34,34,34,34	0
57	MG	2a	3063	1/1	0.90	0.33	63,63,63,63	0
57	MG	2a	3065	1/1	0.90	0.10	69,69,69,69	0
57	MG	2a	3066	1/1	0.90	0.13	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3563	1/1	0.90	0.13	51,51,51,51	0
57	MG	1A	3761	1/1	0.90	0.12	52,52,52,52	0
57	MG	2a	3078	1/1	0.90	0.10	66,66,66,66	0
57	MG	1A	3995	1/1	0.90	0.20	61,61,61,61	0
57	MG	2A	3339	1/1	0.90	0.08	35,35,35,35	0
57	MG	1A	3671	1/1	0.90	0.09	53,53,53,53	0
57	MG	1A	3997	1/1	0.90	0.15	27,27,27,27	0
57	MG	1a	3052	1/1	0.90	0.12	50,50,50,50	0
57	MG	2A	3060	1/1	0.90	0.08	44,44,44,44	0
57	MG	2A	3364	1/1	0.90	0.07	36,36,36,36	0
57	MG	2a	3112	1/1	0.90	0.14	65,65,65,65	0
57	MG	2a	3114	1/1	0.90	0.11	45,45,45,45	0
57	MG	2a	3117	1/1	0.90	0.16	56,56,56,56	0
57	MG	1A	3157	1/1	0.90	0.19	54,54,54,54	0
57	MG	2A	3592	1/1	0.90	0.10	40,40,40,40	0
57	MG	2A	3073	1/1	0.90	0.16	56,56,56,56	0
57	MG	1A	3882	1/1	0.90	0.13	52,52,52,52	0
57	MG	2A	3608	1/1	0.90	0.07	32,32,32,32	0
57	MG	1A	3387	1/1	0.90	0.05	15,15,15,15	0
57	MG	1A	3689	1/1	0.90	0.08	40,40,40,40	0
57	MG	1A	3578	1/1	0.90	0.30	36,36,36,36	0
57	MG	2a	3140	1/1	0.90	0.12	54,54,54,54	0
57	MG	2a	3143	1/1	0.90	0.08	62,62,62,62	0
57	MG	1A	3899	1/1	0.90	0.12	21,21,21,21	0
57	MG	2A	3396	1/1	0.90	0.10	29,29,29,29	0
57	MG	2A	3095	1/1	0.90	0.14	48,48,48,48	0
57	MG	2A	3622	1/1	0.90	0.15	57,57,57,57	0
57	MG	2A	3104	1/1	0.90	0.30	54,54,54,54	0
57	MG	2A	3113	1/1	0.90	0.07	49,49,49,49	0
57	MG	1A	3905	1/1	0.90	0.11	37,37,37,37	0
57	MG	1A	3788	1/1	0.90	0.10	42,42,42,42	0
57	MG	2A	3642	1/1	0.90	0.14	46,46,46,46	0
57	MG	1A	3692	1/1	0.90	0.11	50,50,50,50	0
57	MG	1A	3792	1/1	0.90	0.07	34,34,34,34	0
57	MG	1A	3494	1/1	0.90	0.09	45,45,45,45	0
57	MG	1a	3207	1/1	0.90	0.10	63,63,63,63	0
57	MG	2l	201	1/1	0.90	0.13	60,60,60,60	0
57	MG	1A	3499	1/1	0.90	0.13	51,51,51,51	0
57	MG	1A	3593	1/1	0.90	0.12	30,30,30,30	0
57	MG	2A	3415	1/1	0.90	0.08	33,33,33,33	0
57	MG	1A	3829	1/1	0.90	0.10	41,41,41,41	0
57	MG	2A	3673	1/1	0.90	0.09	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3343	1/1	0.90	0.15	54,54,54,54	0
60	MPD	2A	3728	8/8	0.90	0.19	50,53,58,58	0
57	MG	1a	3221	1/1	0.90	0.16	62,62,62,62	0
57	MG	2A	3386	1/1	0.91	0.07	56,56,56,56	0
57	MG	1A	3972	1/1	0.91	0.07	45,45,45,45	0
57	MG	2A	3395	1/1	0.91	0.07	27,27,27,27	0
57	MG	2A	3677	1/1	0.91	0.12	33,33,33,33	0
57	MG	1A	3843	1/1	0.91	0.09	44,44,44,44	0
57	MG	2A	3685	1/1	0.91	0.13	38,38,38,38	0
57	MG	1A	3685	1/1	0.91	0.13	51,51,51,51	0
57	MG	1a	3178	1/1	0.91	0.09	51,51,51,51	0
57	MG	1A	3431	1/1	0.91	0.10	22,22,22,22	0
57	MG	2A	3086	1/1	0.91	0.10	44,44,44,44	0
57	MG	1a	3181	1/1	0.91	0.11	51,51,51,51	0
57	MG	1A	3599	1/1	0.91	0.10	39,39,39,39	0
57	MG	2A	3093	1/1	0.91	0.27	63,63,63,63	0
57	MG	1A	3080	1/1	0.91	0.17	37,37,37,37	0
57	MG	2A	3711	1/1	0.91	0.08	38,38,38,38	0
57	MG	1a	3036	1/1	0.91	0.20	58,58,58,58	0
57	MG	1a	3037	1/1	0.91	0.23	59,59,59,59	0
57	MG	1A	3120	1/1	0.91	0.11	38,38,38,38	0
57	MG	2A	3116	1/1	0.91	0.14	51,51,51,51	0
57	MG	2A	3418	1/1	0.91	0.15	51,51,51,51	0
57	MG	1a	3044	1/1	0.91	0.16	50,50,50,50	0
57	MG	2A	3425	1/1	0.91	0.07	41,41,41,41	0
57	MG	1A	3855	1/1	0.91	0.07	51,51,51,51	0
57	MG	2A	3129	1/1	0.91	0.18	57,57,57,57	0
57	MG	1A	3300	1/1	0.91	0.13	43,43,43,43	0
57	MG	2A	3140	1/1	0.91	0.20	60,60,60,60	0
57	MG	1A	3448	1/1	0.91	0.08	39,39,39,39	0
57	MG	1A	3530	1/1	0.91	0.17	24,24,24,24	0
57	MG	1A	3376	1/1	0.91	0.13	48,48,48,48	0
57	MG	2A	3158	1/1	0.91	0.10	44,44,44,44	0
57	MG	1A	3615	1/1	0.91	0.12	50,50,50,50	0
57	MG	2B	209	1/1	0.91	0.12	70,70,70,70	0
57	MG	1A	3196	1/1	0.91	0.08	40,40,40,40	0
57	MG	1A	4008	1/1	0.91	0.19	39,39,39,39	0
57	MG	2B	216	1/1	0.91	0.09	68,68,68,68	0
57	MG	2A	3440	1/1	0.91	0.08	60,60,60,60	0
57	MG	1a	3211	1/1	0.91	0.17	69,69,69,69	0
57	MG	1A	3303	1/1	0.91	0.13	76,76,76,76	0
57	MG	1A	3724	1/1	0.91	0.10	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3732	1/1	0.91	0.08	48,48,48,48	0
57	MG	2I	201	1/1	0.91	0.11	47,47,47,47	0
57	MG	1A	3126	1/1	0.91	0.13	34,34,34,34	0
57	MG	1a	3223	1/1	0.91	0.11	56,56,56,56	0
57	MG	1A	3545	1/1	0.91	0.20	46,46,46,46	0
57	MG	2A	3192	1/1	0.91	0.11	39,39,39,39	0
57	MG	2A	3462	1/1	0.91	0.12	48,48,48,48	0
57	MG	1A	3639	1/1	0.91	0.14	51,51,51,51	0
57	MG	1A	3148	1/1	0.91	0.12	48,48,48,48	0
57	MG	1A	3394	1/1	0.91	0.10	18,18,18,18	0
57	MG	2W	201	1/1	0.91	0.17	51,51,51,51	0
57	MG	2W	202	1/1	0.91	0.07	53,53,53,53	0
57	MG	2Y	201	1/1	0.91	0.24	56,56,56,56	0
57	MG	1A	3203	1/1	0.91	0.13	46,46,46,46	0
57	MG	1A	3902	1/1	0.91	0.11	18,18,18,18	0
57	MG	1a	3087	1/1	0.91	0.13	57,57,57,57	0
57	MG	25	102	1/1	0.91	0.14	41,41,41,41	0
57	MG	2A	3213	1/1	0.91	0.11	49,49,49,49	0
57	MG	1A	3763	1/1	0.91	0.07	46,46,46,46	0
57	MG	28	103	1/1	0.91	0.11	52,52,52,52	0
57	MG	1A	3041	1/1	0.91	0.14	46,46,46,46	0
57	MG	1a	3093	1/1	0.91	0.29	57,57,57,57	0
57	MG	2A	3223	1/1	0.91	0.13	57,57,57,57	0
57	MG	2A	3490	1/1	0.91	0.09	55,55,55,55	0
57	MG	1A	3397	1/1	0.91	0.08	29,29,29,29	0
57	MG	2A	3233	1/1	0.91	0.14	47,47,47,47	0
57	MG	2a	3028	1/1	0.91	0.14	59,59,59,59	0
57	MG	1A	3650	1/1	0.91	0.12	42,42,42,42	0
57	MG	1a	3099	1/1	0.91	0.10	60,60,60,60	0
57	MG	2a	3036	1/1	0.91	0.21	62,62,62,62	0
57	MG	2A	3502	1/1	0.91	0.11	57,57,57,57	0
57	MG	2a	3038	1/1	0.91	0.12	74,74,74,74	0
57	MG	1A	3227	1/1	0.91	0.17	47,47,47,47	0
57	MG	2A	3243	1/1	0.91	0.23	49,49,49,49	0
57	MG	2A	3508	1/1	0.91	0.08	43,43,43,43	0
57	MG	2a	3046	1/1	0.91	0.19	59,59,59,59	0
57	MG	2A	3249	1/1	0.91	0.12	49,49,49,49	0
57	MG	2A	3252	1/1	0.91	0.11	46,46,46,46	0
57	MG	1a	3260	1/1	0.91	0.08	62,62,62,62	0
57	MG	2A	3520	1/1	0.91	0.14	52,52,52,52	0
57	MG	1a	3101	1/1	0.91	0.29	58,58,58,58	0
57	MG	2a	3060	1/1	0.91	0.23	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3658	1/1	0.91	0.09	14,14,14,14	0
57	MG	1E	308	1/1	0.91	0.11	29,29,29,29	0
57	MG	2A	3262	1/1	0.91	0.22	47,47,47,47	0
57	MG	1F	304	1/1	0.91	0.19	27,27,27,27	0
57	MG	1A	3930	1/1	0.91	0.10	48,48,48,48	0
57	MG	1a	3267	1/1	0.91	0.08	52,52,52,52	0
57	MG	1a	3269	1/1	0.91	0.29	48,48,48,48	0
57	MG	1a	3270	1/1	0.91	0.11	46,46,46,46	0
57	MG	2a	3081	1/1	0.91	0.10	52,52,52,52	0
57	MG	1A	3787	1/1	0.91	0.11	49,49,49,49	0
57	MG	1A	3934	1/1	0.91	0.08	22,22,22,22	0
57	MG	2A	3285	1/1	0.91	0.16	54,54,54,54	0
57	MG	2a	3101	1/1	0.91	0.31	57,57,57,57	0
57	MG	2A	3286	1/1	0.91	0.23	61,61,61,61	0
57	MG	1f	201	1/1	0.91	0.23	55,55,55,55	0
57	MG	1g	202	1/1	0.91	0.09	64,64,64,64	0
57	MG	1A	3235	1/1	0.91	0.11	60,60,60,60	0
57	MG	1A	3251	1/1	0.91	0.09	39,39,39,39	0
57	MG	1A	3662	1/1	0.91	0.13	28,28,28,28	0
57	MG	2A	3302	1/1	0.91	0.07	43,43,43,43	0
57	MG	1A	3945	1/1	0.91	0.08	47,47,47,47	0
57	MG	1t	202	1/1	0.91	0.14	48,48,48,48	0
57	MG	1A	3057	1/1	0.91	0.15	44,44,44,44	0
57	MG	1T	201	1/1	0.91	0.08	40,40,40,40	0
57	MG	1a	3128	1/1	0.91	0.11	52,52,52,52	0
57	MG	1a	3131	1/1	0.91	0.09	43,43,43,43	0
57	MG	2A	3322	1/1	0.91	0.10	45,45,45,45	0
57	MG	2A	3604	1/1	0.91	0.12	72,72,72,72	0
57	MG	1W	201	1/1	0.91	0.13	45,45,45,45	0
57	MG	1A	3586	1/1	0.91	0.12	51,51,51,51	0
57	MG	2A	3012	1/1	0.91	0.14	50,50,50,50	0
57	MG	1a	3140	1/1	0.91	0.08	49,49,49,49	0
57	MG	1A	3804	1/1	0.91	0.14	15,15,15,15	0
57	MG	10	101	1/1	0.91	0.10	36,36,36,36	0
57	MG	1A	3417	1/1	0.91	0.10	14,14,14,14	0
57	MG	1A	3825	1/1	0.91	0.08	32,32,32,32	0
57	MG	2A	3360	1/1	0.91	0.18	77,77,77,77	0
57	MG	2A	3362	1/1	0.91	0.09	37,37,37,37	0
57	MG	1A	3826	1/1	0.91	0.10	42,42,42,42	0
57	MG	2A	3629	1/1	0.91	0.11	54,54,54,54	0
57	MG	2a	3189	1/1	0.91	0.09	51,51,51,51	0
57	MG	2A	3632	1/1	0.91	0.11	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3036	1/1	0.91	0.21	59,59,59,59	0
57	MG	2A	3641	1/1	0.91	0.12	60,60,60,60	0
57	MG	1A	3507	1/1	0.91	0.05	17,17,17,17	0
57	MG	2A	3370	1/1	0.91	0.12	44,44,44,44	0
57	MG	1A	3677	1/1	0.91	0.09	64,64,64,64	0
57	MG	1a	3159	1/1	0.91	0.15	64,64,64,64	0
57	MG	1a	3016	1/1	0.91	0.14	54,54,54,54	0
57	MG	1A	3162	1/1	0.91	0.07	37,37,37,37	0
57	MG	2A	3663	1/1	0.91	0.12	61,61,61,61	0
57	MG	1A	3014	1/1	0.91	0.12	46,46,46,46	0
57	MG	2A	3671	1/1	0.92	0.17	65,65,65,65	0
57	MG	2A	3672	1/1	0.92	0.07	60,60,60,60	0
57	MG	2A	3097	1/1	0.92	0.18	48,48,48,48	0
57	MG	1A	3857	1/1	0.92	0.07	41,41,41,41	0
57	MG	2A	3112	1/1	0.92	0.11	52,52,52,52	0
57	MG	1A	3135	1/1	0.92	0.18	35,35,35,35	0
57	MG	1a	3042	1/1	0.92	0.15	54,54,54,54	0
57	MG	2A	3119	1/1	0.92	0.07	38,38,38,38	0
57	MG	1A	3859	1/1	0.92	0.06	49,49,49,49	0
57	MG	1A	3862	1/1	0.92	0.12	44,44,44,44	0
57	MG	1a	3048	1/1	0.92	0.20	52,52,52,52	0
57	MG	2A	3132	1/1	0.92	0.17	54,54,54,54	0
57	MG	1A	3991	1/1	0.92	0.07	42,42,42,42	0
57	MG	2A	3137	1/1	0.92	0.26	55,55,55,55	0
57	MG	2A	3138	1/1	0.92	0.10	46,46,46,46	0
57	MG	1A	3992	1/1	0.92	0.08	48,48,48,48	0
57	MG	1A	3316	1/1	0.92	0.15	34,34,34,34	0
57	MG	1A	3245	1/1	0.92	0.23	48,48,48,48	0
57	MG	1A	3328	1/1	0.92	0.10	54,54,54,54	0
57	MG	1A	3249	1/1	0.92	0.09	54,54,54,54	0
57	MG	1A	3749	1/1	0.92	0.09	40,40,40,40	0
57	MG	2A	3431	1/1	0.92	0.10	45,45,45,45	0
57	MG	1A	3330	1/1	0.92	0.07	21,21,21,21	0
57	MG	2A	3164	1/1	0.92	0.23	53,53,53,53	0
57	MG	1a	3218	1/1	0.92	0.19	60,60,60,60	0
57	MG	1A	3754	1/1	0.92	0.09	26,26,26,26	0
57	MG	2A	3175	1/1	0.92	0.10	58,58,58,58	0
57	MG	1A	3880	1/1	0.92	0.06	35,35,35,35	0
57	MG	2A	3180	1/1	0.92	0.12	54,54,54,54	0
57	MG	1A	3647	1/1	0.92	0.09	58,58,58,58	0
57	MG	1A	4018	1/1	0.92	0.14	50,50,50,50	0
57	MG	1B	201	1/1	0.92	0.12	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2B	210	1/1	0.92	0.20	52,52,52,52	0
57	MG	2B	211	1/1	0.92	0.09	50,50,50,50	0
57	MG	2A	3443	1/1	0.92	0.17	48,48,48,48	0
57	MG	1A	3760	1/1	0.92	0.17	52,52,52,52	0
57	MG	1A	3033	1/1	0.92	0.09	30,30,30,30	0
57	MG	1A	3340	1/1	0.92	0.07	41,41,41,41	0
57	MG	1B	217	1/1	0.92	0.12	50,50,50,50	0
57	MG	2D	308	1/1	0.92	0.09	34,34,34,34	0
57	MG	2D	309	1/1	0.92	0.20	61,61,61,61	0
57	MG	1a	3234	1/1	0.92	0.10	48,48,48,48	0
57	MG	2E	306	1/1	0.92	0.08	40,40,40,40	0
57	MG	2G	201	1/1	0.92	0.15	63,63,63,63	0
57	MG	2A	3458	1/1	0.92	0.10	48,48,48,48	0
57	MG	1a	3086	1/1	0.92	0.13	50,50,50,50	0
57	MG	1A	3579	1/1	0.92	0.12	37,37,37,37	0
57	MG	1A	3254	1/1	0.92	0.11	41,41,41,41	0
57	MG	2A	3464	1/1	0.92	0.10	43,43,43,43	0
57	MG	2A	3465	1/1	0.92	0.16	50,50,50,50	0
57	MG	2A	3466	1/1	0.92	0.16	40,40,40,40	0
57	MG	2A	3467	1/1	0.92	0.09	60,60,60,60	0
57	MG	1A	3502	1/1	0.92	0.09	35,35,35,35	0
57	MG	1A	3082	1/1	0.92	0.07	34,34,34,34	0
57	MG	1a	3096	1/1	0.92	0.18	55,55,55,55	0
57	MG	1A	3591	1/1	0.92	0.10	49,49,49,49	0
57	MG	1a	3259	1/1	0.92	0.12	50,50,50,50	0
57	MG	2A	3222	1/1	0.92	0.08	40,40,40,40	0
57	MG	1B	231	1/1	0.92	0.09	60,60,60,60	0
57	MG	1A	3071	1/1	0.92	0.09	41,41,41,41	0
57	MG	1A	3351	1/1	0.92	0.07	30,30,30,30	0
57	MG	1A	3790	1/1	0.92	0.12	44,44,44,44	0
57	MG	2A	3237	1/1	0.92	0.11	52,52,52,52	0
57	MG	1A	3923	1/1	0.92	0.10	50,50,50,50	0
57	MG	2A	3492	1/1	0.92	0.08	47,47,47,47	0
57	MG	2a	3004	1/1	0.92	0.11	46,46,46,46	0
57	MG	1E	309	1/1	0.92	0.08	51,51,51,51	0
57	MG	1A	3352	1/1	0.92	0.13	53,53,53,53	0
57	MG	2A	3246	1/1	0.92	0.19	55,55,55,55	0
57	MG	2a	3014	1/1	0.92	0.18	55,55,55,55	0
57	MG	2a	3015	1/1	0.92	0.17	52,52,52,52	0
57	MG	2a	3018	1/1	0.92	0.16	44,44,44,44	0
57	MG	1A	3271	1/1	0.92	0.07	62,62,62,62	0
57	MG	1F	314	1/1	0.92	0.07	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1a	3110	1/1	0.92	0.18	56,56,56,56	0
57	MG	1A	3518	1/1	0.92	0.13	35,35,35,35	0
57	MG	1d	303	1/1	0.92	0.08	45,45,45,45	0
57	MG	1e	201	1/1	0.92	0.15	61,61,61,61	0
57	MG	1A	3124	1/1	0.92	0.10	46,46,46,46	0
57	MG	2A	3517	1/1	0.92	0.08	51,51,51,51	0
57	MG	1G	203	1/1	0.92	0.07	48,48,48,48	0
57	MG	1a	3116	1/1	0.92	0.16	51,51,51,51	0
57	MG	2A	3523	1/1	0.92	0.08	47,47,47,47	0
57	MG	1m	202	1/1	0.92	0.18	58,58,58,58	0
57	MG	2a	3044	1/1	0.92	0.15	61,61,61,61	0
57	MG	1n	101	1/1	0.92	0.36	64,64,64,64	0
57	MG	1A	3164	1/1	0.92	0.05	30,30,30,30	0
57	MG	1A	3814	1/1	0.92	0.11	22,22,22,22	0
57	MG	2a	3050	1/1	0.92	0.22	56,56,56,56	0
57	MG	1A	3815	1/1	0.92	0.10	28,28,28,28	0
57	MG	2a	3053	1/1	0.92	0.17	58,58,58,58	0
57	MG	2A	3283	1/1	0.92	0.23	53,53,53,53	0
57	MG	1a	3125	1/1	0.92	0.16	55,55,55,55	0
57	MG	1A	3819	1/1	0.92	0.08	54,54,54,54	0
57	MG	1A	3688	1/1	0.92	0.09	41,41,41,41	0
57	MG	2a	3062	1/1	0.92	0.20	56,56,56,56	0
57	MG	2A	3549	1/1	0.92	0.07	70,70,70,70	0
57	MG	2A	3552	1/1	0.92	0.08	48,48,48,48	0
57	MG	1A	3171	1/1	0.92	0.12	42,42,42,42	0
57	MG	2A	3294	1/1	0.92	0.13	56,56,56,56	0
57	MG	2a	3070	1/1	0.92	0.21	55,55,55,55	0
57	MG	2A	3295	1/1	0.92	0.10	53,53,53,53	0
57	MG	1T	204	1/1	0.92	0.11	52,52,52,52	0
57	MG	1A	3371	1/1	0.92	0.07	44,44,44,44	0
57	MG	1a	3139	1/1	0.92	0.14	62,62,62,62	0
57	MG	2a	3084	1/1	0.92	0.20	51,51,51,51	0
57	MG	2A	3008	1/1	0.92	0.08	36,36,36,36	0
57	MG	1A	3452	1/1	0.92	0.12	60,60,60,60	0
57	MG	1A	3951	1/1	0.92	0.14	36,36,36,36	0
57	MG	2a	3091	1/1	0.92	0.12	53,53,53,53	0
57	MG	2a	3092	1/1	0.92	0.22	47,47,47,47	0
57	MG	2a	3093	1/1	0.92	0.09	45,45,45,45	0
57	MG	2a	3099	1/1	0.92	0.34	46,46,46,46	0
57	MG	1A	3830	1/1	0.92	0.07	41,41,41,41	0
57	MG	2A	3580	1/1	0.92	0.09	36,36,36,36	0
57	MG	2A	3581	1/1	0.92	0.10	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3023	1/1	0.92	0.12	56,56,56,56	0
57	MG	1a	3143	1/1	0.92	0.12	56,56,56,56	0
57	MG	10	104	1/1	0.92	0.09	46,46,46,46	0
57	MG	1A	3211	1/1	0.92	0.08	45,45,45,45	0
57	MG	2a	3118	1/1	0.92	0.10	54,54,54,54	0
57	MG	2A	3594	1/1	0.92	0.11	54,54,54,54	0
57	MG	10	107	1/1	0.92	0.09	42,42,42,42	0
57	MG	2A	3601	1/1	0.92	0.08	32,32,32,32	0
57	MG	2a	3130	1/1	0.92	0.12	64,64,64,64	0
57	MG	2a	3131	1/1	0.92	0.15	54,54,54,54	0
57	MG	1A	3214	1/1	0.92	0.08	49,49,49,49	0
57	MG	2A	3603	1/1	0.92	0.07	37,37,37,37	0
57	MG	2A	3332	1/1	0.92	0.12	47,47,47,47	0
57	MG	1A	3960	1/1	0.92	0.06	46,46,46,46	0
57	MG	2A	3045	1/1	0.92	0.16	55,55,55,55	0
57	MG	1a	3005	1/1	0.92	0.08	58,58,58,58	0
57	MG	1a	3160	1/1	0.92	0.17	56,56,56,56	0
57	MG	2a	3144	1/1	0.92	0.08	64,64,64,64	0
57	MG	2A	3344	1/1	0.92	0.10	37,37,37,37	0
57	MG	1A	3840	1/1	0.92	0.08	44,44,44,44	0
57	MG	1A	3215	1/1	0.92	0.08	46,46,46,46	0
57	MG	1a	3164	1/1	0.92	0.14	55,55,55,55	0
57	MG	1a	3014	1/1	0.92	0.11	61,61,61,61	0
57	MG	2a	3164	1/1	0.92	0.10	61,61,61,61	0
57	MG	1A	3540	1/1	0.92	0.13	41,41,41,41	0
57	MG	2a	3170	1/1	0.92	0.17	49,49,49,49	0
57	MG	2a	3176	1/1	0.92	0.08	55,55,55,55	0
57	MG	2A	3625	1/1	0.92	0.11	46,46,46,46	0
57	MG	1A	3623	1/1	0.92	0.06	14,14,14,14	0
57	MG	2A	3076	1/1	0.92	0.10	45,45,45,45	0
57	MG	1A	3630	1/1	0.92	0.11	37,37,37,37	0
57	MG	2a	3186	1/1	0.92	0.09	52,52,52,52	0
57	MG	1A	3974	1/1	0.92	0.12	49,49,49,49	0
57	MG	2A	3636	1/1	0.92	0.12	52,52,52,52	0
57	MG	2A	3083	1/1	0.92	0.23	56,56,56,56	0
57	MG	1A	3464	1/1	0.92	0.08	54,54,54,54	0
57	MG	1A	3712	1/1	0.92	0.07	60,60,60,60	0
57	MG	2A	3382	1/1	0.92	0.20	61,61,61,61	0
57	MG	2A	3089	1/1	0.92	0.13	58,58,58,58	0
57	MG	1A	3978	1/1	0.92	0.11	36,36,36,36	0
57	MG	2A	3387	1/1	0.92	0.08	32,32,32,32	0
57	MG	2A	3389	1/1	0.92	0.09	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3715	1/1	0.92	0.07	29,29,29,29	0
57	MG	1A	3002	1/1	0.92	0.14	57,57,57,57	0
57	MG	1A	3718	1/1	0.92	0.13	30,30,30,30	0
57	MG	2A	3411	1/1	0.93	0.12	44,44,44,44	0
57	MG	2A	3700	1/1	0.93	0.12	46,46,46,46	0
57	MG	2A	3703	1/1	0.93	0.26	42,42,42,42	0
57	MG	2A	3133	1/1	0.93	0.20	58,58,58,58	0
57	MG	1A	3762	1/1	0.93	0.06	30,30,30,30	0
57	MG	1a	3059	1/1	0.93	0.10	50,50,50,50	0
57	MG	1A	3181	1/1	0.93	0.09	49,49,49,49	0
57	MG	1A	3388	1/1	0.93	0.06	23,23,23,23	0
57	MG	1A	3775	1/1	0.93	0.12	43,43,43,43	0
57	MG	1A	3188	1/1	0.93	0.11	41,41,41,41	0
57	MG	1a	3220	1/1	0.93	0.06	57,57,57,57	0
57	MG	2A	3154	1/1	0.93	0.16	45,45,45,45	0
57	MG	1A	3189	1/1	0.93	0.16	51,51,51,51	0
57	MG	1a	3222	1/1	0.93	0.08	75,75,75,75	0
57	MG	1A	3780	1/1	0.93	0.08	43,43,43,43	0
57	MG	2A	3722	1/1	0.93	0.16	54,54,54,54	0
57	MG	2A	3161	1/1	0.93	0.14	52,52,52,52	0
57	MG	2A	3724	1/1	0.93	0.08	50,50,50,50	0
57	MG	1B	204	1/1	0.93	0.11	42,42,42,42	0
57	MG	2A	3165	1/1	0.93	0.07	67,67,67,67	0
57	MG	1A	3324	1/1	0.93	0.10	34,34,34,34	0
57	MG	1B	216	1/1	0.93	0.10	43,43,43,43	0
57	MG	1A	3906	1/1	0.93	0.10	22,22,22,22	0
57	MG	1A	3485	1/1	0.93	0.07	39,39,39,39	0
57	MG	1a	3081	1/1	0.93	0.20	54,54,54,54	0
57	MG	1A	3912	1/1	0.93	0.07	53,53,53,53	0
57	MG	2A	3186	1/1	0.93	0.16	60,60,60,60	0
57	MG	1a	3084	1/1	0.93	0.08	46,46,46,46	0
57	MG	2A	3451	1/1	0.93	0.10	56,56,56,56	0
57	MG	1A	3580	1/1	0.93	0.09	37,37,37,37	0
57	MG	1B	225	1/1	0.93	0.11	47,47,47,47	0
57	MG	1A	3914	1/1	0.93	0.07	34,34,34,34	0
57	MG	1a	3089	1/1	0.93	0.06	43,43,43,43	0
57	MG	1a	3248	1/1	0.93	0.09	45,45,45,45	0
57	MG	2A	3461	1/1	0.93	0.10	53,53,53,53	0
57	MG	2A	3195	1/1	0.93	0.17	41,41,41,41	0
57	MG	1A	3916	1/1	0.93	0.11	52,52,52,52	0
57	MG	2A	3199	1/1	0.93	0.13	55,55,55,55	0
57	MG	2A	3202	1/1	0.93	0.21	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1B	230	1/1	0.93	0.08	44,44,44,44	0
57	MG	1A	3664	1/1	0.93	0.08	49,49,49,49	0
57	MG	1a	3094	1/1	0.93	0.10	57,57,57,57	0
57	MG	1A	3583	1/1	0.93	0.05	29,29,29,29	0
57	MG	2P	201	1/1	0.93	0.09	49,49,49,49	0
57	MG	1D	314	1/1	0.93	0.19	33,33,33,33	0
57	MG	2A	3214	1/1	0.93	0.20	51,51,51,51	0
57	MG	2R	202	1/1	0.93	0.12	47,47,47,47	0
57	MG	2A	3476	1/1	0.93	0.09	55,55,55,55	0
57	MG	1A	3486	1/1	0.93	0.08	20,20,20,20	0
57	MG	2A	3478	1/1	0.93	0.15	47,47,47,47	0
57	MG	1A	3004	1/1	0.93	0.11	40,40,40,40	0
57	MG	2A	3482	1/1	0.93	0.07	21,21,21,21	0
57	MG	1A	3927	1/1	0.93	0.09	52,52,52,52	0
57	MG	2A	3221	1/1	0.93	0.08	55,55,55,55	0
57	MG	1A	3929	1/1	0.93	0.17	45,45,45,45	0
57	MG	21	101	1/1	0.93	0.22	53,53,53,53	0
57	MG	1A	3674	1/1	0.93	0.07	43,43,43,43	0
57	MG	21	103	1/1	0.93	0.08	54,54,54,54	0
57	MG	1F	309	1/1	0.93	0.15	44,44,44,44	0
57	MG	2A	3228	1/1	0.93	0.24	51,51,51,51	0
57	MG	2A	3232	1/1	0.93	0.19	51,51,51,51	0
57	MG	1A	3932	1/1	0.93	0.07	50,50,50,50	0
57	MG	1A	3801	1/1	0.93	0.09	40,40,40,40	0
57	MG	2a	3002	1/1	0.93	0.22	57,57,57,57	0
57	MG	1A	3676	1/1	0.93	0.06	57,57,57,57	0
57	MG	1A	3130	1/1	0.93	0.10	47,47,47,47	0
57	MG	1d	304	1/1	0.93	0.06	55,55,55,55	0
57	MG	2A	3504	1/1	0.93	0.08	39,39,39,39	0
57	MG	2a	3010	1/1	0.93	0.16	61,61,61,61	0
57	MG	2a	3013	1/1	0.93	0.18	56,56,56,56	0
57	MG	1A	3808	1/1	0.93	0.06	32,32,32,32	0
57	MG	2A	3244	1/1	0.93	0.34	37,37,37,37	0
57	MG	1a	3112	1/1	0.93	0.21	53,53,53,53	0
57	MG	2a	3020	1/1	0.93	0.09	58,58,58,58	0
57	MG	2A	3248	1/1	0.93	0.12	50,50,50,50	0
57	MG	1f	202	1/1	0.93	0.13	45,45,45,45	0
57	MG	2A	3512	1/1	0.93	0.07	43,43,43,43	0
57	MG	2A	3515	1/1	0.93	0.08	67,67,67,67	0
57	MG	2a	3029	1/1	0.93	0.11	57,57,57,57	0
57	MG	2A	3516	1/1	0.93	0.12	61,61,61,61	0
57	MG	2a	3033	1/1	0.93	0.21	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1G	204	1/1	0.93	0.13	49,49,49,49	0
57	MG	1h	202	1/1	0.93	0.16	69,69,69,69	0
57	MG	1A	3053	1/1	0.93	0.25	31,31,31,31	0
57	MG	1A	3681	1/1	0.93	0.11	32,32,32,32	0
57	MG	1A	3263	1/1	0.93	0.10	37,37,37,37	0
57	MG	1A	3820	1/1	0.93	0.09	11,11,11,11	0
57	MG	1a	3122	1/1	0.93	0.14	56,56,56,56	0
57	MG	2A	3266	1/1	0.93	0.12	54,54,54,54	0
57	MG	1a	3123	1/1	0.93	0.08	45,45,45,45	0
57	MG	2A	3533	1/1	0.93	0.10	59,59,59,59	0
57	MG	2A	3534	1/1	0.93	0.14	61,61,61,61	0
57	MG	1P	204	1/1	0.93	0.07	59,59,59,59	0
57	MG	1A	3022	1/1	0.93	0.09	43,43,43,43	0
57	MG	2a	3052	1/1	0.93	0.17	51,51,51,51	0
57	MG	1A	3409	1/1	0.93	0.06	18,18,18,18	0
57	MG	2a	3054	1/1	0.93	0.18	53,53,53,53	0
57	MG	2A	3544	1/1	0.93	0.07	36,36,36,36	0
57	MG	1A	3270	1/1	0.93	0.11	51,51,51,51	0
57	MG	2a	3059	1/1	0.93	0.20	53,53,53,53	0
57	MG	1V	204	1/1	0.93	0.09	46,46,46,46	0
57	MG	1A	3510	1/1	0.93	0.06	14,14,14,14	0
57	MG	1a	3133	1/1	0.93	0.13	61,61,61,61	0
57	MG	1A	3103	1/1	0.93	0.14	34,34,34,34	0
57	MG	2A	3557	1/1	0.93	0.09	54,54,54,54	0
57	MG	1A	3955	1/1	0.93	0.10	42,42,42,42	0
57	MG	2a	3068	1/1	0.93	0.09	60,60,60,60	0
57	MG	2A	3291	1/1	0.93	0.17	33,33,33,33	0
57	MG	1A	3060	1/1	0.93	0.11	47,47,47,47	0
57	MG	2a	3071	1/1	0.93	0.13	58,58,58,58	0
57	MG	2a	3073	1/1	0.93	0.17	58,58,58,58	0
57	MG	1A	3348	1/1	0.93	0.10	43,43,43,43	0
57	MG	1A	3424	1/1	0.93	0.12	30,30,30,30	0
57	MG	2A	3024	1/1	0.93	0.10	58,58,58,58	0
57	MG	2a	3080	1/1	0.93	0.11	47,47,47,47	0
57	MG	1A	3427	1/1	0.93	0.08	22,22,22,22	0
57	MG	2a	3083	1/1	0.93	0.25	54,54,54,54	0
57	MG	1A	3158	1/1	0.93	0.12	52,52,52,52	0
57	MG	2A	3032	1/1	0.93	0.21	51,51,51,51	0
57	MG	2A	3304	1/1	0.93	0.10	37,37,37,37	0
57	MG	1A	3285	1/1	0.93	0.11	29,29,29,29	0
57	MG	2a	3089	1/1	0.93	0.10	54,54,54,54	0
57	MG	1A	3706	1/1	0.93	0.15	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3616	1/1	0.93	0.07	32,32,32,32	0
57	MG	2A	3038	1/1	0.93	0.19	46,46,46,46	0
57	MG	2a	3094	1/1	0.93	0.19	60,60,60,60	0
57	MG	2a	3095	1/1	0.93	0.18	67,67,67,67	0
57	MG	1A	3851	1/1	0.93	0.11	15,15,15,15	0
57	MG	2A	3595	1/1	0.93	0.07	61,61,61,61	0
57	MG	2a	3103	1/1	0.93	0.39	61,61,61,61	0
57	MG	2a	3104	1/1	0.93	0.30	48,48,48,48	0
57	MG	1a	3010	1/1	0.93	0.27	63,63,63,63	0
57	MG	2A	3047	1/1	0.93	0.09	52,52,52,52	0
57	MG	2a	3109	1/1	0.93	0.31	50,50,50,50	0
57	MG	1A	3034	1/1	0.93	0.12	47,47,47,47	0
57	MG	2A	3053	1/1	0.93	0.18	58,58,58,58	0
57	MG	1a	3015	1/1	0.93	0.12	59,59,59,59	0
57	MG	2A	3607	1/1	0.93	0.07	42,42,42,42	0
57	MG	1A	3292	1/1	0.93	0.10	37,37,37,37	0
57	MG	1A	3299	1/1	0.93	0.13	27,27,27,27	0
57	MG	1a	3170	1/1	0.93	0.08	49,49,49,49	0
57	MG	2a	3125	1/1	0.93	0.10	49,49,49,49	0
57	MG	1A	3035	1/1	0.93	0.07	32,32,32,32	0
57	MG	2a	3129	1/1	0.93	0.09	67,67,67,67	0
57	MG	2A	3061	1/1	0.93	0.08	43,43,43,43	0
57	MG	2A	3348	1/1	0.93	0.07	45,45,45,45	0
57	MG	1A	3301	1/1	0.93	0.14	53,53,53,53	0
57	MG	2A	3065	1/1	0.93	0.07	45,45,45,45	0
57	MG	1a	3024	1/1	0.93	0.10	51,51,51,51	0
57	MG	2A	3075	1/1	0.93	0.10	48,48,48,48	0
57	MG	1A	3985	1/1	0.93	0.11	35,35,35,35	0
57	MG	2a	3139	1/1	0.93	0.09	60,60,60,60	0
57	MG	2A	3626	1/1	0.93	0.07	67,67,67,67	0
57	MG	2A	3077	1/1	0.93	0.08	43,43,43,43	0
57	MG	1A	3632	1/1	0.93	0.08	40,40,40,40	0
57	MG	1A	3038	1/1	0.93	0.10	32,32,32,32	0
57	MG	2A	3081	1/1	0.93	0.09	51,51,51,51	0
57	MG	2A	3373	1/1	0.93	0.07	44,44,44,44	0
57	MG	2a	3150	1/1	0.93	0.09	45,45,45,45	0
57	MG	1a	3180	1/1	0.93	0.24	60,60,60,60	0
57	MG	1A	3224	1/1	0.93	0.11	29,29,29,29	0
57	MG	2a	3159	1/1	0.93	0.11	56,56,56,56	0
57	MG	1A	3377	1/1	0.93	0.09	49,49,49,49	0
57	MG	2a	3165	1/1	0.93	0.17	58,58,58,58	0
57	MG	1a	3183	1/1	0.93	0.09	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3652	1/1	0.93	0.12	31,31,31,31	0
57	MG	1A	3306	1/1	0.93	0.08	35,35,35,35	0
57	MG	2a	3177	1/1	0.93	0.07	64,64,64,64	0
57	MG	2a	3178	1/1	0.93	0.13	62,62,62,62	0
57	MG	1A	3554	1/1	0.93	0.06	32,32,32,32	0
57	MG	1a	3040	1/1	0.93	0.14	58,58,58,58	0
57	MG	1a	3189	1/1	0.93	0.06	58,58,58,58	0
57	MG	2a	3184	1/1	0.93	0.24	59,59,59,59	0
57	MG	1A	3643	1/1	0.93	0.10	52,52,52,52	0
57	MG	2A	3099	1/1	0.93	0.14	47,47,47,47	0
57	MG	2A	3103	1/1	0.93	0.16	47,47,47,47	0
57	MG	1A	3868	1/1	0.93	0.08	41,41,41,41	0
57	MG	1A	3125	1/1	0.93	0.12	29,29,29,29	0
57	MG	1A	3759	1/1	0.93	0.08	33,33,33,33	0
57	MG	1A	3560	1/1	0.93	0.08	52,52,52,52	0
57	MG	1A	4010	1/1	0.93	0.18	39,39,39,39	0
57	MG	1A	4011	1/1	0.93	0.17	64,64,64,64	0
57	MG	2A	3688	1/1	0.93	0.09	49,49,49,49	0
57	MG	2A	3123	1/1	0.93	0.10	33,33,33,33	0
57	MG	1A	3563	1/1	0.93	0.07	34,34,34,34	0
57	MG	1a	3205	1/1	0.93	0.13	59,59,59,59	0
57	MG	1a	3056	1/1	0.93	0.14	51,51,51,51	0
57	MG	2A	3698	1/1	0.93	0.09	63,63,63,63	0
61	ZN	24	501	1/1	0.93	0.17	127,127,127,127	0
57	MG	1a	3006	1/1	0.94	0.10	59,59,59,59	0
57	MG	2A	3706	1/1	0.94	0.08	33,33,33,33	0
57	MG	2A	3707	1/1	0.94	0.07	35,35,35,35	0
57	MG	2A	3088	1/1	0.94	0.10	40,40,40,40	0
57	MG	1A	3562	1/1	0.94	0.17	56,56,56,56	0
57	MG	1A	3182	1/1	0.94	0.09	49,49,49,49	0
57	MG	1A	3670	1/1	0.94	0.15	33,33,33,33	0
57	MG	1A	3824	1/1	0.94	0.09	41,41,41,41	0
57	MG	1A	3564	1/1	0.94	0.09	50,50,50,50	0
57	MG	1A	3673	1/1	0.94	0.09	36,36,36,36	0
57	MG	1A	3566	1/1	0.94	0.07	15,15,15,15	0
57	MG	1A	3360	1/1	0.94	0.12	45,45,45,45	0
57	MG	1A	3976	1/1	0.94	0.07	48,48,48,48	0
57	MG	2A	3109	1/1	0.94	0.15	42,42,42,42	0
57	MG	1A	3222	1/1	0.94	0.15	33,33,33,33	0
57	MG	2A	3412	1/1	0.94	0.06	30,30,30,30	0
57	MG	1a	3026	1/1	0.94	0.21	53,53,53,53	0
57	MG	2A	3115	1/1	0.94	0.20	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3416	1/1	0.94	0.07	49,49,49,49	0
57	MG	2B	203	1/1	0.94	0.17	54,54,54,54	0
57	MG	1a	3193	1/1	0.94	0.08	47,47,47,47	0
57	MG	2A	3419	1/1	0.94	0.05	28,28,28,28	0
57	MG	2A	3117	1/1	0.94	0.25	47,47,47,47	0
57	MG	1A	3834	1/1	0.94	0.08	34,34,34,34	0
57	MG	2A	3120	1/1	0.94	0.31	47,47,47,47	0
57	MG	1a	3195	1/1	0.94	0.13	52,52,52,52	0
57	MG	1A	3570	1/1	0.94	0.09	39,39,39,39	0
57	MG	1a	3030	1/1	0.94	0.12	38,38,38,38	0
57	MG	1A	3462	1/1	0.94	0.10	46,46,46,46	0
57	MG	2A	3131	1/1	0.94	0.18	52,52,52,52	0
57	MG	2D	303	1/1	0.94	0.14	44,44,44,44	0
57	MG	2D	305	1/1	0.94	0.10	30,30,30,30	0
57	MG	1a	3202	1/1	0.94	0.07	57,57,57,57	0
57	MG	1A	3983	1/1	0.94	0.06	16,16,16,16	0
57	MG	1A	3363	1/1	0.94	0.07	42,42,42,42	0
57	MG	1A	3370	1/1	0.94	0.09	38,38,38,38	0
57	MG	1A	3686	1/1	0.94	0.10	54,54,54,54	0
57	MG	1a	3038	1/1	0.94	0.10	56,56,56,56	0
57	MG	1A	3467	1/1	0.94	0.06	41,41,41,41	0
57	MG	1a	3212	1/1	0.94	0.07	64,64,64,64	0
57	MG	2A	3149	1/1	0.94	0.13	44,44,44,44	0
57	MG	1A	3183	1/1	0.94	0.19	63,63,63,63	0
57	MG	1a	3215	1/1	0.94	0.09	44,44,44,44	0
57	MG	2A	3157	1/1	0.94	0.11	57,57,57,57	0
57	MG	1A	3581	1/1	0.94	0.08	33,33,33,33	0
57	MG	1A	3226	1/1	0.94	0.09	38,38,38,38	0
57	MG	2A	3453	1/1	0.94	0.10	49,49,49,49	0
57	MG	1A	3187	1/1	0.94	0.08	47,47,47,47	0
57	MG	2T	201	1/1	0.94	0.18	51,51,51,51	0
57	MG	1A	3476	1/1	0.94	0.06	24,24,24,24	0
57	MG	2T	203	1/1	0.94	0.07	55,55,55,55	0
57	MG	1A	3305	1/1	0.94	0.20	25,25,25,25	0
57	MG	1A	3378	1/1	0.94	0.06	26,26,26,26	0
57	MG	2A	3460	1/1	0.94	0.07	55,55,55,55	0
57	MG	2V	203	1/1	0.94	0.15	53,53,53,53	0
57	MG	2A	3166	1/1	0.94	0.12	59,59,59,59	0
57	MG	1a	3053	1/1	0.94	0.07	57,57,57,57	0
57	MG	1A	3999	1/1	0.94	0.08	39,39,39,39	0
57	MG	2A	3169	1/1	0.94	0.24	49,49,49,49	0
57	MG	1A	3481	1/1	0.94	0.07	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3114	1/1	0.94	0.15	28,28,28,28	0
57	MG	1A	3861	1/1	0.94	0.07	32,32,32,32	0
57	MG	1A	3595	1/1	0.94	0.09	54,54,54,54	0
57	MG	2A	3183	1/1	0.94	0.12	48,48,48,48	0
57	MG	27	101	1/1	0.94	0.10	49,49,49,49	0
57	MG	1A	3237	1/1	0.94	0.17	47,47,47,47	0
57	MG	1A	3069	1/1	0.94	0.20	27,27,27,27	0
57	MG	2A	3475	1/1	0.94	0.10	48,48,48,48	0
57	MG	2A	3188	1/1	0.94	0.13	48,48,48,48	0
57	MG	2a	3003	1/1	0.94	0.10	52,52,52,52	0
57	MG	1a	3066	1/1	0.94	0.12	45,45,45,45	0
57	MG	1a	3068	1/1	0.94	0.08	53,53,53,53	0
57	MG	1A	3489	1/1	0.94	0.08	53,53,53,53	0
57	MG	1A	4015	1/1	0.94	0.09	52,52,52,52	0
57	MG	1a	3241	1/1	0.94	0.08	49,49,49,49	0
57	MG	1A	3600	1/1	0.94	0.10	50,50,50,50	0
57	MG	1a	3244	1/1	0.94	0.09	56,56,56,56	0
57	MG	1a	3245	1/1	0.94	0.07	52,52,52,52	0
57	MG	2A	3200	1/1	0.94	0.12	57,57,57,57	0
57	MG	1A	3314	1/1	0.94	0.06	32,32,32,32	0
57	MG	2a	3021	1/1	0.94	0.23	58,58,58,58	0
57	MG	2A	3203	1/1	0.94	0.06	40,40,40,40	0
57	MG	2A	3204	1/1	0.94	0.19	43,43,43,43	0
57	MG	2a	3025	1/1	0.94	0.12	57,57,57,57	0
57	MG	1a	3249	1/1	0.94	0.12	51,51,51,51	0
57	MG	1A	4020	1/1	0.94	0.13	48,48,48,48	0
57	MG	1A	3869	1/1	0.94	0.07	20,20,20,20	0
57	MG	1a	3254	1/1	0.94	0.15	45,45,45,45	0
57	MG	1A	3722	1/1	0.94	0.07	35,35,35,35	0
57	MG	1A	3723	1/1	0.94	0.09	39,39,39,39	0
57	MG	1A	3123	1/1	0.94	0.07	64,64,64,64	0
57	MG	1B	207	1/1	0.94	0.15	50,50,50,50	0
57	MG	2A	3217	1/1	0.94	0.09	49,49,49,49	0
57	MG	1a	3083	1/1	0.94	0.15	52,52,52,52	0
57	MG	2A	3220	1/1	0.94	0.13	57,57,57,57	0
57	MG	2a	3041	1/1	0.94	0.27	65,65,65,65	0
57	MG	1B	208	1/1	0.94	0.25	48,48,48,48	0
57	MG	1B	210	1/1	0.94	0.09	46,46,46,46	0
57	MG	1A	3729	1/1	0.94	0.11	42,42,42,42	0
57	MG	2A	3518	1/1	0.94	0.07	58,58,58,58	0
57	MG	2a	3048	1/1	0.94	0.11	58,58,58,58	0
57	MG	1A	3730	1/1	0.94	0.10	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3521	1/1	0.94	0.08	49,49,49,49	0
57	MG	1A	3605	1/1	0.94	0.19	43,43,43,43	0
57	MG	2A	3230	1/1	0.94	0.08	43,43,43,43	0
57	MG	2A	3524	1/1	0.94	0.13	50,50,50,50	0
57	MG	1A	3741	1/1	0.94	0.08	47,47,47,47	0
57	MG	2a	3056	1/1	0.94	0.19	49,49,49,49	0
57	MG	1A	3191	1/1	0.94	0.15	53,53,53,53	0
57	MG	2A	3234	1/1	0.94	0.11	40,40,40,40	0
57	MG	1A	3321	1/1	0.94	0.14	48,48,48,48	0
57	MG	2A	3236	1/1	0.94	0.12	38,38,38,38	0
57	MG	2A	3532	1/1	0.94	0.06	53,53,53,53	0
57	MG	1A	3896	1/1	0.94	0.07	36,36,36,36	0
57	MG	1A	3323	1/1	0.94	0.06	26,26,26,26	0
57	MG	2A	3535	1/1	0.94	0.09	47,47,47,47	0
57	MG	1d	305	1/1	0.94	0.07	75,75,75,75	0
57	MG	2a	3067	1/1	0.94	0.20	57,57,57,57	0
57	MG	2A	3241	1/1	0.94	0.21	51,51,51,51	0
57	MG	2A	3541	1/1	0.94	0.09	48,48,48,48	0
57	MG	1A	3192	1/1	0.94	0.19	27,27,27,27	0
57	MG	1A	3751	1/1	0.94	0.06	37,37,37,37	0
57	MG	2A	3245	1/1	0.94	0.10	43,43,43,43	0
57	MG	1A	3400	1/1	0.94	0.06	11,11,11,11	0
57	MG	1D	308	1/1	0.94	0.19	44,44,44,44	0
57	MG	1A	3325	1/1	0.94	0.07	46,46,46,46	0
57	MG	1A	3911	1/1	0.94	0.07	52,52,52,52	0
57	MG	1i	202	1/1	0.94	0.13	55,55,55,55	0
57	MG	2A	3558	1/1	0.94	0.10	52,52,52,52	0
57	MG	1l	201	1/1	0.94	0.13	56,56,56,56	0
57	MG	2A	3255	1/1	0.94	0.18	54,54,54,54	0
57	MG	1l	202	1/1	0.94	0.11	64,64,64,64	0
57	MG	1A	3756	1/1	0.94	0.11	48,48,48,48	0
57	MG	2A	3259	1/1	0.94	0.08	43,43,43,43	0
57	MG	1D	316	1/1	0.94	0.07	49,49,49,49	0
57	MG	1A	3327	1/1	0.94	0.14	24,24,24,24	0
57	MG	1E	305	1/1	0.94	0.07	40,40,40,40	0
57	MG	2A	3267	1/1	0.94	0.14	48,48,48,48	0
57	MG	1o	101	1/1	0.94	0.14	49,49,49,49	0
57	MG	2a	3096	1/1	0.94	0.07	55,55,55,55	0
57	MG	1E	307	1/1	0.94	0.08	44,44,44,44	0
57	MG	1A	3093	1/1	0.94	0.07	56,56,56,56	0
57	MG	1A	3915	1/1	0.94	0.08	47,47,47,47	0
57	MG	1A	3517	1/1	0.94	0.07	16,16,16,16	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3032	1/1	0.94	0.17	45,45,45,45	0
57	MG	2A	3002	1/1	0.94	0.06	38,38,38,38	0
57	MG	2A	3597	1/1	0.94	0.08	53,53,53,53	0
57	MG	1A	3040	1/1	0.94	0.10	47,47,47,47	0
57	MG	1a	3117	1/1	0.94	0.19	36,36,36,36	0
57	MG	1A	3269	1/1	0.94	0.06	23,23,23,23	0
57	MG	2a	3116	1/1	0.94	0.08	47,47,47,47	0
57	MG	1a	3119	1/1	0.94	0.32	55,55,55,55	0
57	MG	1A	3168	1/1	0.94	0.17	43,43,43,43	0
57	MG	2a	3119	1/1	0.94	0.10	60,60,60,60	0
57	MG	2a	3121	1/1	0.94	0.14	54,54,54,54	0
57	MG	2A	3014	1/1	0.94	0.09	51,51,51,51	0
57	MG	1F	318	1/1	0.94	0.08	41,41,41,41	0
57	MG	1A	3926	1/1	0.94	0.12	35,35,35,35	0
57	MG	1A	3127	1/1	0.94	0.27	42,42,42,42	0
57	MG	1A	3422	1/1	0.94	0.09	19,19,19,19	0
57	MG	1N	203	1/1	0.94	0.08	45,45,45,45	0
57	MG	1a	3127	1/1	0.94	0.19	52,52,52,52	0
57	MG	1A	3276	1/1	0.94	0.10	56,56,56,56	0
57	MG	1A	3532	1/1	0.94	0.09	46,46,46,46	0
57	MG	1A	3207	1/1	0.94	0.16	30,30,30,30	0
57	MG	1A	3173	1/1	0.94	0.07	48,48,48,48	0
57	MG	1A	3349	1/1	0.94	0.08	44,44,44,44	0
57	MG	1a	3137	1/1	0.94	0.09	61,61,61,61	0
57	MG	2A	3043	1/1	0.94	0.09	39,39,39,39	0
57	MG	1A	3434	1/1	0.94	0.10	52,52,52,52	0
57	MG	2A	3327	1/1	0.94	0.14	38,38,38,38	0
57	MG	1A	3942	1/1	0.94	0.06	25,25,25,25	0
57	MG	2a	3146	1/1	0.94	0.09	56,56,56,56	0
57	MG	2A	3634	1/1	0.94	0.10	48,48,48,48	0
57	MG	2A	3049	1/1	0.94	0.18	54,54,54,54	0
57	MG	2A	3050	1/1	0.94	0.06	47,47,47,47	0
57	MG	1A	3543	1/1	0.94	0.12	45,45,45,45	0
57	MG	1T	205	1/1	0.94	0.08	50,50,50,50	0
57	MG	1V	203	1/1	0.94	0.08	31,31,31,31	0
57	MG	2a	3160	1/1	0.94	0.12	52,52,52,52	0
57	MG	1A	3653	1/1	0.94	0.28	42,42,42,42	0
57	MG	1A	3436	1/1	0.94	0.09	44,44,44,44	0
57	MG	2A	3654	1/1	0.94	0.06	29,29,29,29	0
57	MG	2a	3168	1/1	0.94	0.06	45,45,45,45	0
57	MG	1A	3656	1/1	0.94	0.07	17,17,17,17	0
57	MG	2a	3173	1/1	0.94	0.09	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3353	1/1	0.94	0.10	54,54,54,54	0
57	MG	1A	3798	1/1	0.94	0.06	46,46,46,46	0
57	MG	1A	3210	1/1	0.94	0.19	26,26,26,26	0
57	MG	2A	3062	1/1	0.94	0.12	40,40,40,40	0
57	MG	2A	3063	1/1	0.94	0.20	43,43,43,43	0
57	MG	1A	3012	1/1	0.94	0.09	32,32,32,32	0
57	MG	1A	3553	1/1	0.94	0.10	49,49,49,49	0
57	MG	2A	3072	1/1	0.94	0.10	44,44,44,44	0
57	MG	1A	3287	1/1	0.94	0.09	48,48,48,48	0
57	MG	1A	3066	1/1	0.94	0.05	32,32,32,32	0
57	MG	2a	3188	1/1	0.94	0.19	57,57,57,57	0
57	MG	2A	3680	1/1	0.94	0.14	39,39,39,39	0
57	MG	13	102	1/1	0.94	0.10	51,51,51,51	0
57	MG	1a	3165	1/1	0.94	0.10	53,53,53,53	0
57	MG	2A	3689	1/1	0.94	0.12	62,62,62,62	0
57	MG	2A	3078	1/1	0.94	0.13	43,43,43,43	0
57	MG	2p	101	1/1	0.94	0.17	49,49,49,49	0
57	MG	2t	201	1/1	0.94	0.13	40,40,40,40	0
57	MG	15	105	1/1	0.94	0.11	25,25,25,25	0
58	CLM	2A	3727	20/20	0.94	0.10	33,38,57,59	0
57	MG	15	108	1/1	0.94	0.07	34,34,34,34	0
57	MG	15	109	1/1	0.94	0.07	46,46,46,46	0
57	MG	1A	3455	1/1	0.94	0.07	41,41,41,41	0
57	MG	2A	3388	1/1	0.94	0.10	49,49,49,49	0
57	MG	2A	3084	1/1	0.94	0.07	35,35,35,35	0
57	MG	1A	3958	1/1	0.94	0.16	37,37,37,37	0
61	ZN	14	501	1/1	0.94	0.11	104,104,104,104	0
57	MG	2A	3393	1/1	0.94	0.08	51,51,51,51	0
57	MG	1B	212	1/1	0.95	0.07	45,45,45,45	0
57	MG	1a	3225	1/1	0.95	0.12	60,60,60,60	0
57	MG	1a	3226	1/1	0.95	0.11	49,49,49,49	0
57	MG	1a	3064	1/1	0.95	0.23	57,57,57,57	0
57	MG	1A	3261	1/1	0.95	0.08	40,40,40,40	0
57	MG	2A	3146	1/1	0.95	0.18	45,45,45,45	0
57	MG	1A	3771	1/1	0.95	0.07	12,12,12,12	0
57	MG	1A	3772	1/1	0.95	0.07	37,37,37,37	0
57	MG	1A	3557	1/1	0.95	0.14	58,58,58,58	0
57	MG	2A	3153	1/1	0.95	0.10	37,37,37,37	0
57	MG	1a	3072	1/1	0.95	0.17	46,46,46,46	0
57	MG	2A	3417	1/1	0.95	0.06	38,38,38,38	0
57	MG	2A	3155	1/1	0.95	0.05	30,30,30,30	0
57	MG	1A	3381	1/1	0.95	0.07	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3383	1/1	0.95	0.06	39,39,39,39	0
57	MG	1B	226	1/1	0.95	0.06	35,35,35,35	0
57	MG	1a	3238	1/1	0.95	0.08	54,54,54,54	0
57	MG	1A	3109	1/1	0.95	0.11	31,31,31,31	0
57	MG	2A	3163	1/1	0.95	0.16	35,35,35,35	0
57	MG	1A	3781	1/1	0.95	0.07	46,46,46,46	0
57	MG	1a	3242	1/1	0.95	0.13	52,52,52,52	0
57	MG	1A	3202	1/1	0.95	0.12	38,38,38,38	0
57	MG	1A	3028	1/1	0.95	0.16	26,26,26,26	0
57	MG	1D	306	1/1	0.95	0.07	45,45,45,45	0
57	MG	1A	3389	1/1	0.95	0.05	22,22,22,22	0
57	MG	2A	3172	1/1	0.95	0.08	34,34,34,34	0
57	MG	2A	3174	1/1	0.95	0.06	44,44,44,44	0
57	MG	2B	213	1/1	0.95	0.08	54,54,54,54	0
57	MG	2A	3438	1/1	0.95	0.06	30,30,30,30	0
57	MG	1A	3111	1/1	0.95	0.11	36,36,36,36	0
57	MG	1A	3029	1/1	0.95	0.10	36,36,36,36	0
57	MG	1A	3020	1/1	0.95	0.25	33,33,33,33	0
57	MG	2A	3181	1/1	0.95	0.09	45,45,45,45	0
57	MG	1A	3573	1/1	0.95	0.08	21,21,21,21	0
57	MG	1A	3482	1/1	0.95	0.12	27,27,27,27	0
57	MG	1a	3256	1/1	0.95	0.09	55,55,55,55	0
57	MG	2A	3450	1/1	0.95	0.06	48,48,48,48	0
57	MG	2E	303	1/1	0.95	0.07	36,36,36,36	0
57	MG	1a	3088	1/1	0.95	0.16	46,46,46,46	0
57	MG	2F	303	1/1	0.95	0.11	43,43,43,43	0
57	MG	1A	3795	1/1	0.95	0.07	44,44,44,44	0
57	MG	1A	3672	1/1	0.95	0.09	52,52,52,52	0
57	MG	1A	3935	1/1	0.95	0.07	42,42,42,42	0
57	MG	1A	3936	1/1	0.95	0.10	36,36,36,36	0
57	MG	2N	201	1/1	0.95	0.06	59,59,59,59	0
57	MG	1A	3577	1/1	0.95	0.11	43,43,43,43	0
57	MG	1A	3074	1/1	0.95	0.07	33,33,33,33	0
57	MG	1A	3941	1/1	0.95	0.07	19,19,19,19	0
57	MG	2Q	201	1/1	0.95	0.14	51,51,51,51	0
57	MG	1a	3268	1/1	0.95	0.14	47,47,47,47	0
57	MG	2A	3198	1/1	0.95	0.06	41,41,41,41	0
57	MG	1A	3334	1/1	0.95	0.05	28,28,28,28	0
57	MG	1F	316	1/1	0.95	0.12	35,35,35,35	0
57	MG	1b	301	1/1	0.95	0.19	52,52,52,52	0
57	MG	1A	3806	1/1	0.95	0.09	22,22,22,22	0
57	MG	1A	3281	1/1	0.95	0.07	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3487	1/1	0.95	0.06	19,19,19,19	0
57	MG	2A	3470	1/1	0.95	0.08	60,60,60,60	0
57	MG	2V	202	1/1	0.95	0.17	49,49,49,49	0
57	MG	1A	3046	1/1	0.95	0.11	44,44,44,44	0
57	MG	2A	3209	1/1	0.95	0.09	49,49,49,49	0
57	MG	1A	3341	1/1	0.95	0.06	32,32,32,32	0
57	MG	1A	3079	1/1	0.95	0.19	35,35,35,35	0
57	MG	20	101	1/1	0.95	0.08	41,41,41,41	0
57	MG	1A	3497	1/1	0.95	0.09	40,40,40,40	0
57	MG	1a	3109	1/1	0.95	0.21	46,46,46,46	0
57	MG	1A	3589	1/1	0.95	0.07	16,16,16,16	0
57	MG	1A	3052	1/1	0.95	0.14	33,33,33,33	0
57	MG	1A	3500	1/1	0.95	0.08	38,38,38,38	0
57	MG	1a	3113	1/1	0.95	0.27	45,45,45,45	0
57	MG	25	103	1/1	0.95	0.08	48,48,48,48	0
57	MG	1A	3827	1/1	0.95	0.08	45,45,45,45	0
57	MG	27	102	1/1	0.95	0.21	37,37,37,37	0
57	MG	27	103	1/1	0.95	0.17	38,38,38,38	0
57	MG	2A	3485	1/1	0.95	0.07	54,54,54,54	0
57	MG	1Q	201	1/1	0.95	0.09	27,27,27,27	0
57	MG	1A	3021	1/1	0.95	0.10	30,30,30,30	0
57	MG	1A	3415	1/1	0.95	0.07	40,40,40,40	0
57	MG	2A	3224	1/1	0.95	0.07	44,44,44,44	0
57	MG	1T	202	1/1	0.95	0.09	43,43,43,43	0
57	MG	1A	3961	1/1	0.95	0.10	40,40,40,40	0
57	MG	2a	3006	1/1	0.95	0.07	54,54,54,54	0
57	MG	2A	3229	1/1	0.95	0.06	27,27,27,27	0
57	MG	2A	3497	1/1	0.95	0.10	40,40,40,40	0
57	MG	2a	3009	1/1	0.95	0.23	54,54,54,54	0
57	MG	2A	3498	1/1	0.95	0.05	36,36,36,36	0
57	MG	1A	3596	1/1	0.95	0.06	27,27,27,27	0
57	MG	1U	207	1/1	0.95	0.07	37,37,37,37	0
57	MG	1A	3968	1/1	0.95	0.04	21,21,21,21	0
57	MG	2a	3016	1/1	0.95	0.06	50,50,50,50	0
57	MG	2a	3017	1/1	0.95	0.10	46,46,46,46	0
57	MG	1A	3832	1/1	0.95	0.05	33,33,33,33	0
57	MG	2a	3019	1/1	0.95	0.06	64,64,64,64	0
57	MG	1V	205	1/1	0.95	0.06	41,41,41,41	0
57	MG	1A	3833	1/1	0.95	0.10	40,40,40,40	0
57	MG	2A	3001	1/1	0.95	0.22	49,49,49,49	0
57	MG	1A	3085	1/1	0.95	0.06	38,38,38,38	0
57	MG	1A	3699	1/1	0.95	0.07	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1Y	201	1/1	0.95	0.06	41,41,41,41	0
57	MG	2A	3242	1/1	0.95	0.15	50,50,50,50	0
57	MG	1A	3291	1/1	0.95	0.10	51,51,51,51	0
57	MG	10	102	1/1	0.95	0.08	31,31,31,31	0
57	MG	2a	3032	1/1	0.95	0.19	55,55,55,55	0
57	MG	2A	3011	1/1	0.95	0.06	27,27,27,27	0
57	MG	10	103	1/1	0.95	0.05	37,37,37,37	0
57	MG	1A	3003	1/1	0.95	0.06	20,20,20,20	0
57	MG	1A	3703	1/1	0.95	0.07	44,44,44,44	0
57	MG	1A	3511	1/1	0.95	0.06	36,36,36,36	0
57	MG	2A	3022	1/1	0.95	0.25	44,44,44,44	0
57	MG	2A	3525	1/1	0.95	0.05	27,27,27,27	0
57	MG	1A	3421	1/1	0.95	0.08	50,50,50,50	0
57	MG	11	101	1/1	0.95	0.13	42,42,42,42	0
57	MG	11	104	1/1	0.95	0.11	47,47,47,47	0
57	MG	1A	3979	1/1	0.95	0.07	53,53,53,53	0
57	MG	1a	3145	1/1	0.95	0.07	55,55,55,55	0
57	MG	1A	3228	1/1	0.95	0.24	24,24,24,24	0
57	MG	2A	3263	1/1	0.95	0.09	20,20,20,20	0
57	MG	1A	3849	1/1	0.95	0.06	50,50,50,50	0
57	MG	2A	3265	1/1	0.95	0.33	45,45,45,45	0
57	MG	2A	3536	1/1	0.95	0.06	49,49,49,49	0
57	MG	2A	3538	1/1	0.95	0.11	46,46,46,46	0
57	MG	1A	3229	1/1	0.95	0.27	31,31,31,31	0
57	MG	1a	3151	1/1	0.95	0.09	61,61,61,61	0
57	MG	2A	3040	1/1	0.95	0.12	33,33,33,33	0
57	MG	2A	3542	1/1	0.95	0.05	40,40,40,40	0
57	MG	2A	3272	1/1	0.95	0.12	53,53,53,53	0
57	MG	2A	3273	1/1	0.95	0.26	51,51,51,51	0
57	MG	1a	3152	1/1	0.95	0.10	45,45,45,45	0
57	MG	2A	3546	1/1	0.95	0.11	25,25,25,25	0
57	MG	17	102	1/1	0.95	0.14	26,26,26,26	0
57	MG	2a	3064	1/1	0.95	0.13	47,47,47,47	0
57	MG	2A	3550	1/1	0.95	0.07	51,51,51,51	0
57	MG	1a	3156	1/1	0.95	0.11	39,39,39,39	0
57	MG	2A	3553	1/1	0.95	0.05	39,39,39,39	0
57	MG	1A	3058	1/1	0.95	0.09	21,21,21,21	0
57	MG	2A	3555	1/1	0.95	0.06	65,65,65,65	0
57	MG	18	102	1/1	0.95	0.12	32,32,32,32	0
57	MG	1a	3002	1/1	0.95	0.12	49,49,49,49	0
57	MG	1a	3162	1/1	0.95	0.18	55,55,55,55	0
57	MG	2a	3076	1/1	0.95	0.10	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3716	1/1	0.95	0.09	21,21,21,21	0
57	MG	2A	3560	1/1	0.95	0.07	33,33,33,33	0
57	MG	1A	3236	1/1	0.95	0.21	47,47,47,47	0
57	MG	2A	3290	1/1	0.95	0.15	47,47,47,47	0
57	MG	2A	3565	1/1	0.95	0.07	56,56,56,56	0
57	MG	1A	3520	1/1	0.95	0.08	20,20,20,20	0
57	MG	1a	3167	1/1	0.95	0.16	62,62,62,62	0
57	MG	2A	3571	1/1	0.95	0.09	37,37,37,37	0
57	MG	2A	3293	1/1	0.95	0.06	46,46,46,46	0
57	MG	1a	3169	1/1	0.95	0.06	43,43,43,43	0
57	MG	1a	3008	1/1	0.95	0.19	46,46,46,46	0
57	MG	1A	3720	1/1	0.95	0.06	62,62,62,62	0
57	MG	1A	3150	1/1	0.95	0.27	38,38,38,38	0
57	MG	1a	3173	1/1	0.95	0.09	44,44,44,44	0
57	MG	2A	3585	1/1	0.95	0.05	38,38,38,38	0
57	MG	2A	3586	1/1	0.95	0.12	48,48,48,48	0
57	MG	2A	3300	1/1	0.95	0.12	45,45,45,45	0
57	MG	1a	3013	1/1	0.95	0.08	49,49,49,49	0
57	MG	1A	3304	1/1	0.95	0.26	39,39,39,39	0
57	MG	2A	3306	1/1	0.95	0.09	36,36,36,36	0
57	MG	1A	3435	1/1	0.95	0.07	47,47,47,47	0
57	MG	2A	3308	1/1	0.95	0.16	68,68,68,68	0
57	MG	1A	3151	1/1	0.95	0.08	24,24,24,24	0
57	MG	1a	3017	1/1	0.95	0.09	51,51,51,51	0
57	MG	1A	3364	1/1	0.95	0.07	13,13,13,13	0
57	MG	2A	3317	1/1	0.95	0.07	28,28,28,28	0
57	MG	1A	3444	1/1	0.95	0.17	26,26,26,26	0
57	MG	2a	3115	1/1	0.95	0.11	42,42,42,42	0
57	MG	2A	3605	1/1	0.95	0.11	42,42,42,42	0
57	MG	2A	3606	1/1	0.95	0.07	49,49,49,49	0
57	MG	1a	3021	1/1	0.95	0.09	44,44,44,44	0
57	MG	1A	3733	1/1	0.95	0.08	20,20,20,20	0
57	MG	2A	3323	1/1	0.95	0.06	34,34,34,34	0
57	MG	1A	4000	1/1	0.95	0.08	42,42,42,42	0
57	MG	2A	3613	1/1	0.95	0.08	40,40,40,40	0
57	MG	2A	3615	1/1	0.95	0.12	26,26,26,26	0
57	MG	2A	3616	1/1	0.95	0.10	55,55,55,55	0
57	MG	2a	3128	1/1	0.95	0.07	53,53,53,53	0
57	MG	2A	3325	1/1	0.95	0.16	55,55,55,55	0
57	MG	1A	4004	1/1	0.95	0.07	49,49,49,49	0
57	MG	2A	3082	1/1	0.95	0.13	43,43,43,43	0
57	MG	1A	4007	1/1	0.95	0.06	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3334	1/1	0.95	0.05	37,37,37,37	0
57	MG	2a	3134	1/1	0.95	0.12	60,60,60,60	0
57	MG	1A	3625	1/1	0.95	0.08	45,45,45,45	0
57	MG	2a	3136	1/1	0.95	0.06	43,43,43,43	0
57	MG	1A	3368	1/1	0.95	0.06	22,22,22,22	0
57	MG	2A	3337	1/1	0.95	0.07	40,40,40,40	0
57	MG	1a	3192	1/1	0.95	0.16	56,56,56,56	0
57	MG	2A	3340	1/1	0.95	0.11	49,49,49,49	0
57	MG	1A	3008	1/1	0.95	0.08	25,25,25,25	0
57	MG	2A	3342	1/1	0.95	0.07	44,44,44,44	0
57	MG	1A	3450	1/1	0.95	0.07	20,20,20,20	0
57	MG	1A	3748	1/1	0.95	0.10	48,48,48,48	0
57	MG	2A	3349	1/1	0.95	0.07	38,38,38,38	0
57	MG	2A	3091	1/1	0.95	0.07	44,44,44,44	0
57	MG	1A	3250	1/1	0.95	0.13	50,50,50,50	0
57	MG	2A	3644	1/1	0.95	0.14	50,50,50,50	0
57	MG	2a	3152	1/1	0.95	0.10	55,55,55,55	0
57	MG	1a	3198	1/1	0.95	0.10	65,65,65,65	0
57	MG	1A	3879	1/1	0.95	0.07	31,31,31,31	0
57	MG	2A	3651	1/1	0.95	0.08	40,40,40,40	0
57	MG	1A	3061	1/1	0.95	0.12	36,36,36,36	0
57	MG	1a	3039	1/1	0.95	0.08	58,58,58,58	0
57	MG	2A	3101	1/1	0.95	0.10	41,41,41,41	0
57	MG	2A	3102	1/1	0.95	0.14	40,40,40,40	0
57	MG	2a	3169	1/1	0.95	0.13	52,52,52,52	0
57	MG	2A	3366	1/1	0.95	0.13	33,33,33,33	0
57	MG	1A	3752	1/1	0.95	0.05	27,27,27,27	0
57	MG	2a	3174	1/1	0.95	0.09	62,62,62,62	0
57	MG	1A	4017	1/1	0.95	0.07	38,38,38,38	0
57	MG	2A	3108	1/1	0.95	0.15	56,56,56,56	0
57	MG	1A	3544	1/1	0.95	0.05	33,33,33,33	0
57	MG	2A	3670	1/1	0.95	0.09	49,49,49,49	0
57	MG	1A	3253	1/1	0.95	0.12	47,47,47,47	0
57	MG	1A	3548	1/1	0.95	0.16	22,22,22,22	0
57	MG	2A	3114	1/1	0.95	0.09	53,53,53,53	0
57	MG	2A	3674	1/1	0.95	0.09	36,36,36,36	0
57	MG	2A	3383	1/1	0.95	0.17	56,56,56,56	0
57	MG	2A	3384	1/1	0.95	0.10	50,50,50,50	0
57	MG	1A	3459	1/1	0.95	0.04	17,17,17,17	0
57	MG	2A	3681	1/1	0.95	0.06	55,55,55,55	0
57	MG	2A	3684	1/1	0.95	0.06	35,35,35,35	0
57	MG	1A	3065	1/1	0.95	0.08	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3551	1/1	0.95	0.14	42,42,42,42	0
57	MG	1a	3214	1/1	0.95	0.10	59,59,59,59	0
57	MG	1B	206	1/1	0.95	0.05	36,36,36,36	0
57	MG	2A	3691	1/1	0.95	0.09	57,57,57,57	0
57	MG	1A	3900	1/1	0.95	0.06	26,26,26,26	0
57	MG	1A	3259	1/1	0.95	0.22	32,32,32,32	0
57	MG	2A	3696	1/1	0.95	0.11	65,65,65,65	0
59	ARG	1B	232	12/12	0.95	0.09	26,36,46,51	0
57	MG	2A	3394	1/1	0.95	0.07	45,45,45,45	0
57	MG	1a	3057	1/1	0.95	0.10	55,55,55,55	0
60	MPD	18	103	8/8	0.95	0.11	25,28,37,43	0
57	MG	2A	3127	1/1	0.95	0.21	41,41,41,41	0
57	MG	1B	209	1/1	0.95	0.09	45,45,45,45	0
57	MG	1A	3648	1/1	0.95	0.08	31,31,31,31	0
57	MG	1a	3060	1/1	0.95	0.09	51,51,51,51	0
57	MG	1A	3379	1/1	0.95	0.08	44,44,44,44	0
57	MG	1R	202	1/1	0.96	0.08	37,37,37,37	0
57	MG	1A	3618	1/1	0.96	0.05	20,20,20,20	0
57	MG	1A	3140	1/1	0.96	0.07	21,21,21,21	0
57	MG	1A	3621	1/1	0.96	0.07	40,40,40,40	0
57	MG	1T	203	1/1	0.96	0.06	39,39,39,39	0
57	MG	2A	3368	1/1	0.96	0.05	34,34,34,34	0
57	MG	1A	3622	1/1	0.96	0.10	35,35,35,35	0
57	MG	1A	3141	1/1	0.96	0.11	47,47,47,47	0
57	MG	2A	3372	1/1	0.96	0.14	43,43,43,43	0
57	MG	1T	206	1/1	0.96	0.06	47,47,47,47	0
57	MG	1U	201	1/1	0.96	0.18	28,28,28,28	0
57	MG	2A	3702	1/1	0.96	0.08	61,61,61,61	0
57	MG	1a	3158	1/1	0.96	0.05	41,41,41,41	0
57	MG	1U	205	1/1	0.96	0.16	34,34,34,34	0
57	MG	2A	3381	1/1	0.96	0.09	47,47,47,47	0
57	MG	1U	206	1/1	0.96	0.10	29,29,29,29	0
57	MG	1A	3757	1/1	0.96	0.10	56,56,56,56	0
57	MG	1A	3184	1/1	0.96	0.06	24,24,24,24	0
57	MG	1A	3626	1/1	0.96	0.05	30,30,30,30	0
57	MG	2A	3096	1/1	0.96	0.07	44,44,44,44	0
57	MG	1A	3356	1/1	0.96	0.09	17,17,17,17	0
57	MG	2A	3098	1/1	0.96	0.07	47,47,47,47	0
57	MG	1A	3118	1/1	0.96	0.06	24,24,24,24	0
57	MG	2A	3100	1/1	0.96	0.10	40,40,40,40	0
57	MG	1W	202	1/1	0.96	0.05	30,30,30,30	0
57	MG	1A	3149	1/1	0.96	0.19	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3937	1/1	0.96	0.06	29,29,29,29	0
57	MG	2A	3721	1/1	0.96	0.08	39,39,39,39	0
57	MG	1X	101	1/1	0.96	0.07	32,32,32,32	0
57	MG	2A	3105	1/1	0.96	0.06	46,46,46,46	0
57	MG	1A	3633	1/1	0.96	0.09	35,35,35,35	0
57	MG	1A	3764	1/1	0.96	0.10	46,46,46,46	0
57	MG	1A	3297	1/1	0.96	0.17	30,30,30,30	0
57	MG	2A	3402	1/1	0.96	0.09	40,40,40,40	0
57	MG	1a	3175	1/1	0.96	0.08	43,43,43,43	0
57	MG	1A	3766	1/1	0.96	0.04	30,30,30,30	0
57	MG	2B	205	1/1	0.96	0.11	50,50,50,50	0
57	MG	1a	3177	1/1	0.96	0.06	50,50,50,50	0
57	MG	1A	3943	1/1	0.96	0.14	18,18,18,18	0
57	MG	10	105	1/1	0.96	0.07	43,43,43,43	0
57	MG	1A	3768	1/1	0.96	0.06	20,20,20,20	0
57	MG	2A	3410	1/1	0.96	0.07	33,33,33,33	0
57	MG	1A	3637	1/1	0.96	0.15	40,40,40,40	0
57	MG	1A	3119	1/1	0.96	0.21	45,45,45,45	0
57	MG	1A	3774	1/1	0.96	0.05	24,24,24,24	0
57	MG	2A	3125	1/1	0.96	0.12	42,42,42,42	0
57	MG	11	103	1/1	0.96	0.06	37,37,37,37	0
57	MG	2D	301	1/1	0.96	0.08	25,25,25,25	0
57	MG	1a	3185	1/1	0.96	0.06	58,58,58,58	0
57	MG	2D	304	1/1	0.96	0.07	44,44,44,44	0
57	MG	1a	3186	1/1	0.96	0.09	53,53,53,53	0
57	MG	1A	3441	1/1	0.96	0.06	25,25,25,25	0
57	MG	2A	3422	1/1	0.96	0.10	39,39,39,39	0
57	MG	2A	3423	1/1	0.96	0.10	58,58,58,58	0
57	MG	1A	3776	1/1	0.96	0.13	33,33,33,33	0
57	MG	15	102	1/1	0.96	0.06	27,27,27,27	0
57	MG	2A	3134	1/1	0.96	0.07	48,48,48,48	0
57	MG	2E	305	1/1	0.96	0.16	43,43,43,43	0
57	MG	2A	3427	1/1	0.96	0.06	34,34,34,34	0
57	MG	2E	307	1/1	0.96	0.07	48,48,48,48	0
57	MG	2F	302	1/1	0.96	0.05	33,33,33,33	0
57	MG	1A	3777	1/1	0.96	0.06	41,41,41,41	0
57	MG	1A	3442	1/1	0.96	0.08	56,56,56,56	0
57	MG	1A	3232	1/1	0.96	0.13	30,30,30,30	0
57	MG	15	110	1/1	0.96	0.06	57,57,57,57	0
57	MG	2A	3142	1/1	0.96	0.06	42,42,42,42	0
57	MG	1A	3537	1/1	0.96	0.07	34,34,34,34	0
57	MG	2A	3144	1/1	0.96	0.09	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	17	103	1/1	0.96	0.14	31,31,31,31	0
57	MG	2A	3147	1/1	0.96	0.10	43,43,43,43	0
57	MG	2P	202	1/1	0.96	0.07	56,56,56,56	0
57	MG	1A	3538	1/1	0.96	0.05	17,17,17,17	0
57	MG	2Q	202	1/1	0.96	0.23	52,52,52,52	0
57	MG	17	105	1/1	0.96	0.07	39,39,39,39	0
57	MG	18	101	1/1	0.96	0.07	32,32,32,32	0
57	MG	1a	3200	1/1	0.96	0.07	54,54,54,54	0
57	MG	1A	3645	1/1	0.96	0.11	28,28,28,28	0
57	MG	1a	3001	1/1	0.96	0.10	52,52,52,52	0
57	MG	1A	3959	1/1	0.96	0.08	42,42,42,42	0
57	MG	1a	3004	1/1	0.96	0.14	49,49,49,49	0
57	MG	1A	3784	1/1	0.96	0.07	48,48,48,48	0
57	MG	2A	3449	1/1	0.96	0.06	44,44,44,44	0
57	MG	1A	3445	1/1	0.96	0.05	46,46,46,46	0
57	MG	1a	3209	1/1	0.96	0.08	45,45,45,45	0
57	MG	2A	3162	1/1	0.96	0.16	32,32,32,32	0
57	MG	1A	3963	1/1	0.96	0.09	25,25,25,25	0
57	MG	1A	3366	1/1	0.96	0.11	50,50,50,50	0
57	MG	1A	3043	1/1	0.96	0.07	23,23,23,23	0
57	MG	2A	3457	1/1	0.96	0.07	50,50,50,50	0
57	MG	1A	3122	1/1	0.96	0.15	37,37,37,37	0
57	MG	1a	3011	1/1	0.96	0.11	26,26,26,26	0
57	MG	1a	3012	1/1	0.96	0.12	52,52,52,52	0
57	MG	23	101	1/1	0.96	0.12	42,42,42,42	0
57	MG	1A	3652	1/1	0.96	0.11	46,46,46,46	0
57	MG	1A	3451	1/1	0.96	0.07	19,19,19,19	0
57	MG	1A	3068	1/1	0.96	0.10	38,38,38,38	0
57	MG	1a	3219	1/1	0.96	0.13	56,56,56,56	0
57	MG	1A	3372	1/1	0.96	0.06	40,40,40,40	0
57	MG	1A	3796	1/1	0.96	0.05	32,32,32,32	0
57	MG	1A	3797	1/1	0.96	0.12	41,41,41,41	0
57	MG	1A	3456	1/1	0.96	0.12	49,49,49,49	0
57	MG	1A	3800	1/1	0.96	0.06	35,35,35,35	0
57	MG	29	101	1/1	0.96	0.19	53,53,53,53	0
57	MG	2a	3001	1/1	0.96	0.07	46,46,46,46	0
57	MG	1A	3240	1/1	0.96	0.15	43,43,43,43	0
57	MG	1a	3023	1/1	0.96	0.10	42,42,42,42	0
57	MG	1A	3802	1/1	0.96	0.17	36,36,36,36	0
57	MG	1A	3193	1/1	0.96	0.18	36,36,36,36	0
57	MG	1A	3051	1/1	0.96	0.13	31,31,31,31	0
57	MG	1A	3310	1/1	0.96	0.15	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3556	1/1	0.96	0.12	47,47,47,47	0
57	MG	1A	3811	1/1	0.96	0.09	42,42,42,42	0
57	MG	2A	3480	1/1	0.96	0.07	45,45,45,45	0
57	MG	2a	3011	1/1	0.96	0.20	49,49,49,49	0
57	MG	1A	3812	1/1	0.96	0.05	37,37,37,37	0
57	MG	1a	3235	1/1	0.96	0.09	64,64,64,64	0
57	MG	1A	3195	1/1	0.96	0.07	45,45,45,45	0
57	MG	1a	3035	1/1	0.96	0.10	38,38,38,38	0
57	MG	1A	3989	1/1	0.96	0.12	30,30,30,30	0
57	MG	2A	3201	1/1	0.96	0.07	45,45,45,45	0
57	MG	1A	3559	1/1	0.96	0.07	37,37,37,37	0
57	MG	1a	3240	1/1	0.96	0.17	56,56,56,56	0
57	MG	1A	3816	1/1	0.96	0.06	29,29,29,29	0
57	MG	2A	3493	1/1	0.96	0.10	46,46,46,46	0
57	MG	1A	3463	1/1	0.96	0.07	46,46,46,46	0
57	MG	1A	3993	1/1	0.96	0.15	54,54,54,54	0
57	MG	1A	3994	1/1	0.96	0.11	42,42,42,42	0
57	MG	1A	3081	1/1	0.96	0.07	24,24,24,24	0
57	MG	1A	3313	1/1	0.96	0.06	30,30,30,30	0
57	MG	2A	3500	1/1	0.96	0.07	53,53,53,53	0
57	MG	1A	3823	1/1	0.96	0.06	15,15,15,15	0
57	MG	1A	3062	1/1	0.96	0.07	35,35,35,35	0
57	MG	1A	3468	1/1	0.96	0.04	27,27,27,27	0
57	MG	2A	3506	1/1	0.96	0.07	41,41,41,41	0
57	MG	1A	3675	1/1	0.96	0.11	46,46,46,46	0
57	MG	1A	3469	1/1	0.96	0.06	33,33,33,33	0
57	MG	1A	3384	1/1	0.96	0.11	33,33,33,33	0
57	MG	1a	3258	1/1	0.96	0.06	44,44,44,44	0
57	MG	1A	3198	1/1	0.96	0.09	42,42,42,42	0
57	MG	2a	3042	1/1	0.96	0.24	48,48,48,48	0
57	MG	1A	3680	1/1	0.96	0.06	37,37,37,37	0
57	MG	2A	3514	1/1	0.96	0.07	58,58,58,58	0
57	MG	2a	3045	1/1	0.96	0.22	54,54,54,54	0
57	MG	1A	3255	1/1	0.96	0.07	66,66,66,66	0
57	MG	1A	3682	1/1	0.96	0.09	43,43,43,43	0
57	MG	2A	3225	1/1	0.96	0.06	44,44,44,44	0
57	MG	1A	3683	1/1	0.96	0.06	29,29,29,29	0
57	MG	2A	3227	1/1	0.96	0.17	38,38,38,38	0
57	MG	1A	3835	1/1	0.96	0.06	29,29,29,29	0
57	MG	1a	3062	1/1	0.96	0.15	47,47,47,47	0
57	MG	1A	3258	1/1	0.96	0.16	35,35,35,35	0
57	MG	2A	3231	1/1	0.96	0.18	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3199	1/1	0.96	0.15	32,32,32,32	0
57	MG	1A	3576	1/1	0.96	0.10	32,32,32,32	0
57	MG	1A	3687	1/1	0.96	0.10	36,36,36,36	0
57	MG	1a	3067	1/1	0.96	0.17	64,64,64,64	0
57	MG	1A	3390	1/1	0.96	0.08	38,38,38,38	0
57	MG	1A	3480	1/1	0.96	0.05	35,35,35,35	0
57	MG	2A	3238	1/1	0.96	0.09	50,50,50,50	0
57	MG	1a	3070	1/1	0.96	0.06	41,41,41,41	0
57	MG	1A	3847	1/1	0.96	0.08	41,41,41,41	0
57	MG	1A	3690	1/1	0.96	0.13	39,39,39,39	0
57	MG	1A	3260	1/1	0.96	0.09	25,25,25,25	0
57	MG	1B	205	1/1	0.96	0.08	37,37,37,37	0
57	MG	1A	3165	1/1	0.96	0.09	43,43,43,43	0
57	MG	1g	201	1/1	0.96	0.19	49,49,49,49	0
57	MG	1A	3483	1/1	0.96	0.06	22,22,22,22	0
57	MG	2A	3247	1/1	0.96	0.10	28,28,28,28	0
57	MG	2a	3072	1/1	0.96	0.09	56,56,56,56	0
57	MG	1A	3695	1/1	0.96	0.12	35,35,35,35	0
57	MG	2a	3074	1/1	0.96	0.22	47,47,47,47	0
57	MG	1A	3582	1/1	0.96	0.09	38,38,38,38	0
57	MG	1A	3326	1/1	0.96	0.11	39,39,39,39	0
57	MG	1A	3166	1/1	0.96	0.10	39,39,39,39	0
57	MG	1A	3167	1/1	0.96	0.05	21,21,21,21	0
57	MG	1B	215	1/1	0.96	0.07	41,41,41,41	0
57	MG	1A	3266	1/1	0.96	0.05	39,39,39,39	0
57	MG	1A	3588	1/1	0.96	0.12	46,46,46,46	0
57	MG	1A	3204	1/1	0.96	0.18	38,38,38,38	0
57	MG	2A	3260	1/1	0.96	0.13	48,48,48,48	0
57	MG	1A	3590	1/1	0.96	0.12	40,40,40,40	0
57	MG	1A	3708	1/1	0.96	0.07	34,34,34,34	0
57	MG	2a	3088	1/1	0.96	0.13	50,50,50,50	0
57	MG	1t	201	1/1	0.96	0.09	48,48,48,48	0
57	MG	1B	224	1/1	0.96	0.06	38,38,38,38	0
57	MG	1a	3091	1/1	0.96	0.15	39,39,39,39	0
57	MG	1A	3490	1/1	0.96	0.06	23,23,23,23	0
57	MG	2A	3268	1/1	0.96	0.19	49,49,49,49	0
57	MG	2A	3269	1/1	0.96	0.13	43,43,43,43	0
57	MG	1A	3711	1/1	0.96	0.07	28,28,28,28	0
57	MG	2a	3098	1/1	0.96	0.24	42,42,42,42	0
57	MG	1A	3404	1/1	0.96	0.03	16,16,16,16	0
57	MG	2A	3570	1/1	0.96	0.07	51,51,51,51	0
57	MG	1a	3095	1/1	0.96	0.09	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1B	228	1/1	0.96	0.08	48,48,48,48	0
57	MG	1A	3405	1/1	0.96	0.14	40,40,40,40	0
57	MG	2A	3276	1/1	0.96	0.30	50,50,50,50	0
57	MG	2a	3108	1/1	0.96	0.23	50,50,50,50	0
57	MG	2A	3577	1/1	0.96	0.06	52,52,52,52	0
57	MG	1A	3268	1/1	0.96	0.05	37,37,37,37	0
57	MG	2a	3111	1/1	0.96	0.07	33,33,33,33	0
57	MG	1A	3872	1/1	0.96	0.05	29,29,29,29	0
57	MG	2a	3113	1/1	0.96	0.13	50,50,50,50	0
57	MG	1D	305	1/1	0.96	0.15	28,28,28,28	0
57	MG	2A	3583	1/1	0.96	0.09	50,50,50,50	0
57	MG	2A	3584	1/1	0.96	0.07	47,47,47,47	0
57	MG	2A	3281	1/1	0.96	0.15	41,41,41,41	0
57	MG	1A	3874	1/1	0.96	0.10	53,53,53,53	0
57	MG	1A	3083	1/1	0.96	0.17	29,29,29,29	0
57	MG	2a	3120	1/1	0.96	0.09	44,44,44,44	0
57	MG	2A	3015	1/1	0.96	0.08	31,31,31,31	0
57	MG	1a	3103	1/1	0.96	0.24	44,44,44,44	0
57	MG	2a	3123	1/1	0.96	0.07	42,42,42,42	0
57	MG	2A	3289	1/1	0.96	0.19	45,45,45,45	0
57	MG	2A	3017	1/1	0.96	0.08	48,48,48,48	0
57	MG	2A	3596	1/1	0.96	0.08	56,56,56,56	0
57	MG	2a	3127	1/1	0.96	0.07	53,53,53,53	0
57	MG	2A	3018	1/1	0.96	0.16	34,34,34,34	0
57	MG	1A	3877	1/1	0.96	0.06	38,38,38,38	0
57	MG	1A	3169	1/1	0.96	0.14	21,21,21,21	0
57	MG	1A	3129	1/1	0.96	0.16	32,32,32,32	0
57	MG	1A	3721	1/1	0.96	0.05	25,25,25,25	0
57	MG	2A	3296	1/1	0.96	0.04	30,30,30,30	0
57	MG	1A	3503	1/1	0.96	0.08	20,20,20,20	0
57	MG	2A	3026	1/1	0.96	0.04	24,24,24,24	0
57	MG	1A	3414	1/1	0.96	0.05	26,26,26,26	0
57	MG	1A	3506	1/1	0.96	0.09	43,43,43,43	0
57	MG	1A	3726	1/1	0.96	0.09	49,49,49,49	0
57	MG	2A	3610	1/1	0.96	0.06	53,53,53,53	0
57	MG	1A	3273	1/1	0.96	0.05	32,32,32,32	0
57	MG	2a	3142	1/1	0.96	0.07	60,60,60,60	0
57	MG	1A	3894	1/1	0.96	0.08	45,45,45,45	0
57	MG	2A	3037	1/1	0.96	0.07	39,39,39,39	0
57	MG	1F	307	1/1	0.96	0.15	19,19,19,19	0
57	MG	1A	3072	1/1	0.96	0.09	24,24,24,24	0
57	MG	1F	311	1/1	0.96	0.14	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3313	1/1	0.96	0.07	42,42,42,42	0
57	MG	1F	312	1/1	0.96	0.05	24,24,24,24	0
57	MG	2A	3316	1/1	0.96	0.06	34,34,34,34	0
57	MG	1A	3606	1/1	0.96	0.08	24,24,24,24	0
57	MG	2A	3318	1/1	0.96	0.08	28,28,28,28	0
57	MG	2a	3156	1/1	0.96	0.09	52,52,52,52	0
57	MG	2a	3157	1/1	0.96	0.07	54,54,54,54	0
57	MG	2a	3158	1/1	0.96	0.09	57,57,57,57	0
57	MG	2A	3046	1/1	0.96	0.07	53,53,53,53	0
57	MG	1a	3120	1/1	0.96	0.28	50,50,50,50	0
57	MG	2a	3161	1/1	0.96	0.08	51,51,51,51	0
57	MG	1A	3279	1/1	0.96	0.12	21,21,21,21	0
57	MG	1F	315	1/1	0.96	0.09	43,43,43,43	0
57	MG	2A	3630	1/1	0.96	0.07	37,37,37,37	0
57	MG	2A	3631	1/1	0.96	0.09	58,58,58,58	0
57	MG	1A	3736	1/1	0.96	0.05	35,35,35,35	0
57	MG	1A	3737	1/1	0.96	0.08	39,39,39,39	0
57	MG	2a	3171	1/1	0.96	0.13	47,47,47,47	0
57	MG	1A	3738	1/1	0.96	0.06	32,32,32,32	0
57	MG	1G	201	1/1	0.96	0.06	63,63,63,63	0
57	MG	2A	3330	1/1	0.96	0.08	39,39,39,39	0
57	MG	2A	3331	1/1	0.96	0.14	43,43,43,43	0
57	MG	1A	3059	1/1	0.96	0.10	35,35,35,35	0
57	MG	2a	3179	1/1	0.96	0.08	56,56,56,56	0
57	MG	1A	3512	1/1	0.96	0.06	42,42,42,42	0
57	MG	2A	3647	1/1	0.96	0.05	40,40,40,40	0
57	MG	1a	3129	1/1	0.96	0.16	48,48,48,48	0
57	MG	2a	3183	1/1	0.96	0.07	65,65,65,65	0
57	MG	1a	3130	1/1	0.96	0.08	47,47,47,47	0
57	MG	1A	3513	1/1	0.96	0.07	10,10,10,10	0
57	MG	2A	3338	1/1	0.96	0.08	35,35,35,35	0
57	MG	1H	201	1/1	0.96	0.10	42,42,42,42	0
57	MG	2A	3656	1/1	0.96	0.06	24,24,24,24	0
57	MG	1H	202	1/1	0.96	0.06	40,40,40,40	0
57	MG	1A	3745	1/1	0.96	0.10	25,25,25,25	0
57	MG	2f	201	1/1	0.96	0.11	50,50,50,50	0
57	MG	2A	3068	1/1	0.96	0.11	47,47,47,47	0
57	MG	2A	3343	1/1	0.96	0.05	27,27,27,27	0
57	MG	2l	202	1/1	0.96	0.18	52,52,52,52	0
57	MG	2A	3070	1/1	0.96	0.13	46,46,46,46	0
57	MG	1A	3746	1/1	0.96	0.07	14,14,14,14	0
57	MG	1A	3136	1/1	0.96	0.10	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3216	1/1	0.96	0.12	21,21,21,21	0
58	CLM	1A	4022	20/20	0.96	0.08	18,30,47,48	0
57	MG	2A	3351	1/1	0.96	0.11	40,40,40,40	0
57	MG	2A	3352	1/1	0.96	0.14	42,42,42,42	0
57	MG	1A	3423	1/1	0.96	0.08	27,27,27,27	0
57	MG	2A	3675	1/1	0.96	0.06	43,43,43,43	0
57	MG	2A	3354	1/1	0.96	0.07	27,27,27,27	0
57	MG	2A	3355	1/1	0.96	0.05	34,34,34,34	0
57	MG	2A	3357	1/1	0.96	0.13	56,56,56,56	0
57	MG	1A	3750	1/1	0.96	0.08	33,33,33,33	0
57	MG	1A	3922	1/1	0.96	0.05	30,30,30,30	0
57	MG	2A	3361	1/1	0.96	0.14	35,35,35,35	0
61	ZN	2Y	202	1/1	0.96	0.06	81,81,81,81	0
57	MG	2A	3687	1/1	0.96	0.08	47,47,47,47	0
57	MG	1A	3128	1/1	0.97	0.17	24,24,24,24	0
57	MG	1A	3809	1/1	0.97	0.05	30,30,30,30	0
57	MG	2A	3420	1/1	0.97	0.05	42,42,42,42	0
57	MG	2A	3726	1/1	0.97	0.06	43,43,43,43	0
57	MG	1A	3536	1/1	0.97	0.14	20,20,20,20	0
57	MG	1A	3179	1/1	0.97	0.08	36,36,36,36	0
57	MG	1A	3813	1/1	0.97	0.08	45,45,45,45	0
57	MG	1A	3247	1/1	0.97	0.08	26,26,26,26	0
57	MG	1A	3667	1/1	0.97	0.07	36,36,36,36	0
57	MG	1a	3025	1/1	0.97	0.05	45,45,45,45	0
57	MG	1A	3668	1/1	0.97	0.05	33,33,33,33	0
57	MG	1A	3817	1/1	0.97	0.17	26,26,26,26	0
57	MG	1A	3539	1/1	0.97	0.04	17,17,17,17	0
57	MG	1A	3248	1/1	0.97	0.09	43,43,43,43	0
57	MG	1A	3541	1/1	0.97	0.06	30,30,30,30	0
57	MG	2A	3170	1/1	0.97	0.09	37,37,37,37	0
57	MG	2A	3171	1/1	0.97	0.07	48,48,48,48	0
57	MG	1A	3024	1/1	0.97	0.05	15,15,15,15	0
57	MG	1a	3231	1/1	0.97	0.07	42,42,42,42	0
57	MG	2B	217	1/1	0.97	0.09	53,53,53,53	0
57	MG	1A	3098	1/1	0.97	0.05	44,44,44,44	0
57	MG	2D	302	1/1	0.97	0.40	40,40,40,40	0
57	MG	1A	3998	1/1	0.97	0.09	12,12,12,12	0
57	MG	2A	3179	1/1	0.97	0.07	55,55,55,55	0
57	MG	1A	3425	1/1	0.97	0.07	21,21,21,21	0
57	MG	1A	3132	1/1	0.97	0.09	23,23,23,23	0
57	MG	1A	4001	1/1	0.97	0.07	30,30,30,30	0
57	MG	1A	3546	1/1	0.97	0.12	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3444	1/1	0.97	0.06	27,27,27,27	0
57	MG	2A	3445	1/1	0.97	0.09	49,49,49,49	0
57	MG	2A	3185	1/1	0.97	0.10	44,44,44,44	0
57	MG	2A	3447	1/1	0.97	0.05	23,23,23,23	0
57	MG	1A	4006	1/1	0.97	0.07	38,38,38,38	0
57	MG	1A	3133	1/1	0.97	0.05	34,34,34,34	0
57	MG	2F	301	1/1	0.97	0.22	38,38,38,38	0
57	MG	1A	3331	1/1	0.97	0.12	33,33,33,33	0
57	MG	1a	3043	1/1	0.97	0.12	41,41,41,41	0
57	MG	1A	3185	1/1	0.97	0.14	33,33,33,33	0
57	MG	1A	3335	1/1	0.97	0.10	9,9,9,9	0
57	MG	1a	3047	1/1	0.97	0.12	44,44,44,44	0
57	MG	2A	3455	1/1	0.97	0.04	46,46,46,46	0
57	MG	2A	3193	1/1	0.97	0.06	56,56,56,56	0
57	MG	1A	3552	1/1	0.97	0.07	33,33,33,33	0
57	MG	1a	3247	1/1	0.97	0.06	45,45,45,45	0
57	MG	1A	3099	1/1	0.97	0.14	25,25,25,25	0
57	MG	2A	3197	1/1	0.97	0.07	42,42,42,42	0
57	MG	1a	3051	1/1	0.97	0.14	52,52,52,52	0
57	MG	1a	3250	1/1	0.97	0.13	42,42,42,42	0
57	MG	1A	3256	1/1	0.97	0.06	35,35,35,35	0
57	MG	1A	3837	1/1	0.97	0.13	46,46,46,46	0
57	MG	1A	3439	1/1	0.97	0.15	46,46,46,46	0
57	MG	1a	3055	1/1	0.97	0.18	36,36,36,36	0
57	MG	1A	3102	1/1	0.97	0.10	25,25,25,25	0
57	MG	1A	3841	1/1	0.97	0.05	41,41,41,41	0
57	MG	1A	3342	1/1	0.97	0.07	25,25,25,25	0
57	MG	2A	3471	1/1	0.97	0.05	36,36,36,36	0
57	MG	1A	4019	1/1	0.97	0.07	43,43,43,43	0
57	MG	1A	3558	1/1	0.97	0.05	31,31,31,31	0
57	MG	2A	3211	1/1	0.97	0.09	37,37,37,37	0
57	MG	1A	3138	1/1	0.97	0.09	35,35,35,35	0
57	MG	1a	3263	1/1	0.97	0.09	49,49,49,49	0
57	MG	1A	3054	1/1	0.97	0.13	25,25,25,25	0
57	MG	1A	3104	1/1	0.97	0.11	30,30,30,30	0
57	MG	1A	3447	1/1	0.97	0.07	35,35,35,35	0
57	MG	1A	3347	1/1	0.97	0.08	22,22,22,22	0
57	MG	2A	3481	1/1	0.97	0.05	50,50,50,50	0
57	MG	1A	3850	1/1	0.97	0.06	33,33,33,33	0
57	MG	2A	3219	1/1	0.97	0.05	39,39,39,39	0
57	MG	1A	3449	1/1	0.97	0.08	41,41,41,41	0
57	MG	1A	3567	1/1	0.97	0.05	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3853	1/1	0.97	0.09	31,31,31,31	0
57	MG	25	104	1/1	0.97	0.05	40,40,40,40	0
57	MG	1A	3142	1/1	0.97	0.07	45,45,45,45	0
57	MG	1a	3071	1/1	0.97	0.14	56,56,56,56	0
57	MG	1A	3143	1/1	0.97	0.05	30,30,30,30	0
57	MG	1A	3350	1/1	0.97	0.04	20,20,20,20	0
57	MG	1A	3453	1/1	0.97	0.04	50,50,50,50	0
57	MG	1A	3454	1/1	0.97	0.07	36,36,36,36	0
57	MG	1A	3144	1/1	0.97	0.09	64,64,64,64	0
57	MG	1A	3575	1/1	0.97	0.06	20,20,20,20	0
57	MG	1A	3145	1/1	0.97	0.12	41,41,41,41	0
57	MG	1A	3146	1/1	0.97	0.21	32,32,32,32	0
57	MG	1g	203	1/1	0.97	0.08	55,55,55,55	0
57	MG	2A	3501	1/1	0.97	0.07	49,49,49,49	0
57	MG	1h	201	1/1	0.97	0.15	42,42,42,42	0
57	MG	1A	3864	1/1	0.97	0.08	38,38,38,38	0
57	MG	1A	3147	1/1	0.97	0.06	22,22,22,22	0
57	MG	1A	3075	1/1	0.97	0.10	32,32,32,32	0
57	MG	1A	3713	1/1	0.97	0.23	29,29,29,29	0
57	MG	1A	3714	1/1	0.97	0.20	36,36,36,36	0
57	MG	2a	3012	1/1	0.97	0.12	45,45,45,45	0
57	MG	1A	3358	1/1	0.97	0.04	14,14,14,14	0
57	MG	1A	3870	1/1	0.97	0.06	30,30,30,30	0
57	MG	1A	3106	1/1	0.97	0.13	28,28,28,28	0
57	MG	1D	301	1/1	0.97	0.05	38,38,38,38	0
57	MG	1D	303	1/1	0.97	0.11	24,24,24,24	0
57	MG	1A	3108	1/1	0.97	0.09	33,33,33,33	0
57	MG	1A	3274	1/1	0.97	0.20	33,33,33,33	0
57	MG	1D	307	1/1	0.97	0.05	31,31,31,31	0
57	MG	1A	3275	1/1	0.97	0.04	26,26,26,26	0
57	MG	2a	3022	1/1	0.97	0.06	46,46,46,46	0
57	MG	1D	311	1/1	0.97	0.15	28,28,28,28	0
57	MG	2A	3251	1/1	0.97	0.06	47,47,47,47	0
57	MG	1A	3585	1/1	0.97	0.07	42,42,42,42	0
57	MG	1A	3063	1/1	0.97	0.07	31,31,31,31	0
57	MG	1A	3277	1/1	0.97	0.06	19,19,19,19	0
57	MG	1A	3367	1/1	0.97	0.09	23,23,23,23	0
57	MG	2A	3004	1/1	0.97	0.04	39,39,39,39	0
57	MG	1D	317	1/1	0.97	0.09	38,38,38,38	0
57	MG	1A	3278	1/1	0.97	0.09	30,30,30,30	0
57	MG	1A	3471	1/1	0.97	0.06	37,37,37,37	0
57	MG	2A	3261	1/1	0.97	0.12	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1E	306	1/1	0.97	0.08	15,15,15,15	0
57	MG	1A	3369	1/1	0.97	0.05	23,23,23,23	0
57	MG	1A	3884	1/1	0.97	0.13	23,23,23,23	0
57	MG	1A	3885	1/1	0.97	0.06	29,29,29,29	0
57	MG	1F	302	1/1	0.97	0.13	25,25,25,25	0
57	MG	2A	3537	1/1	0.97	0.06	44,44,44,44	0
57	MG	1a	3108	1/1	0.97	0.05	37,37,37,37	0
57	MG	1A	3154	1/1	0.97	0.11	19,19,19,19	0
57	MG	1F	306	1/1	0.97	0.05	23,23,23,23	0
57	MG	2A	3270	1/1	0.97	0.05	36,36,36,36	0
57	MG	1A	3891	1/1	0.97	0.06	24,24,24,24	0
57	MG	1A	3892	1/1	0.97	0.04	37,37,37,37	0
57	MG	1A	3475	1/1	0.97	0.06	13,13,13,13	0
57	MG	1A	3734	1/1	0.97	0.07	44,44,44,44	0
57	MG	1A	3895	1/1	0.97	0.07	44,44,44,44	0
57	MG	2A	3548	1/1	0.97	0.06	35,35,35,35	0
57	MG	2A	3027	1/1	0.97	0.07	39,39,39,39	0
57	MG	2A	3277	1/1	0.97	0.14	33,33,33,33	0
57	MG	2a	3055	1/1	0.97	0.08	53,53,53,53	0
57	MG	2A	3029	1/1	0.97	0.05	31,31,31,31	0
57	MG	1A	3064	1/1	0.97	0.05	46,46,46,46	0
57	MG	1A	3897	1/1	0.97	0.09	22,22,22,22	0
57	MG	1A	3898	1/1	0.97	0.04	14,14,14,14	0
57	MG	2A	3282	1/1	0.97	0.16	45,45,45,45	0
57	MG	2A	3034	1/1	0.97	0.11	45,45,45,45	0
57	MG	2A	3284	1/1	0.97	0.26	51,51,51,51	0
57	MG	1A	3282	1/1	0.97	0.11	40,40,40,40	0
57	MG	1A	3055	1/1	0.97	0.07	21,21,21,21	0
57	MG	1A	3739	1/1	0.97	0.17	44,44,44,44	0
57	MG	2A	3288	1/1	0.97	0.08	37,37,37,37	0
57	MG	1A	3904	1/1	0.97	0.04	11,11,11,11	0
57	MG	1A	3740	1/1	0.97	0.05	47,47,47,47	0
57	MG	1A	3374	1/1	0.97	0.10	27,27,27,27	0
57	MG	1A	3375	1/1	0.97	0.06	29,29,29,29	0
57	MG	2A	3044	1/1	0.97	0.09	44,44,44,44	0
57	MG	1A	3208	1/1	0.97	0.25	27,27,27,27	0
57	MG	1A	3601	1/1	0.97	0.05	45,45,45,45	0
57	MG	1A	3047	1/1	0.97	0.08	18,18,18,18	0
57	MG	2a	3075	1/1	0.97	0.07	43,43,43,43	0
57	MG	1A	3603	1/1	0.97	0.15	20,20,20,20	0
57	MG	1A	3160	1/1	0.97	0.06	35,35,35,35	0
57	MG	2A	3051	1/1	0.97	0.07	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3161	1/1	0.97	0.04	19,19,19,19	0
57	MG	2A	3301	1/1	0.97	0.04	26,26,26,26	0
57	MG	1A	3917	1/1	0.97	0.07	57,57,57,57	0
57	MG	2a	3082	1/1	0.97	0.27	46,46,46,46	0
57	MG	1A	3918	1/1	0.97	0.05	38,38,38,38	0
57	MG	1Q	203	1/1	0.97	0.06	31,31,31,31	0
57	MG	2A	3588	1/1	0.97	0.05	50,50,50,50	0
57	MG	2A	3056	1/1	0.97	0.07	29,29,29,29	0
57	MG	1a	3136	1/1	0.97	0.13	44,44,44,44	0
57	MG	2A	3310	1/1	0.97	0.07	35,35,35,35	0
57	MG	1R	201	1/1	0.97	0.09	26,26,26,26	0
57	MG	2a	3090	1/1	0.97	0.21	50,50,50,50	0
57	MG	1a	3138	1/1	0.97	0.07	36,36,36,36	0
57	MG	1A	3288	1/1	0.97	0.10	16,16,16,16	0
57	MG	1A	3290	1/1	0.97	0.08	38,38,38,38	0
57	MG	2A	3599	1/1	0.97	0.05	29,29,29,29	0
57	MG	1A	3610	1/1	0.97	0.10	32,32,32,32	0
57	MG	1A	3382	1/1	0.97	0.08	45,45,45,45	0
57	MG	2a	3097	1/1	0.97	0.23	51,51,51,51	0
57	MG	1A	3067	1/1	0.97	0.04	24,24,24,24	0
57	MG	2A	3319	1/1	0.97	0.11	49,49,49,49	0
57	MG	2a	3100	1/1	0.97	0.21	37,37,37,37	0
57	MG	2A	3066	1/1	0.97	0.05	34,34,34,34	0
57	MG	1A	3925	1/1	0.97	0.12	27,27,27,27	0
57	MG	2A	3069	1/1	0.97	0.26	41,41,41,41	0
57	MG	2a	3105	1/1	0.97	0.36	51,51,51,51	0
57	MG	1A	3755	1/1	0.97	0.12	22,22,22,22	0
57	MG	1A	3049	1/1	0.97	0.11	28,28,28,28	0
57	MG	1a	3148	1/1	0.97	0.07	35,35,35,35	0
57	MG	2A	3326	1/1	0.97	0.09	42,42,42,42	0
57	MG	1A	3294	1/1	0.97	0.05	36,36,36,36	0
57	MG	2A	3612	1/1	0.97	0.09	31,31,31,31	0
57	MG	1U	204	1/1	0.97	0.14	24,24,24,24	0
57	MG	1A	3295	1/1	0.97	0.12	35,35,35,35	0
57	MG	1A	3931	1/1	0.97	0.04	41,41,41,41	0
57	MG	1a	3153	1/1	0.97	0.05	47,47,47,47	0
57	MG	1A	3296	1/1	0.97	0.08	42,42,42,42	0
57	MG	2A	3619	1/1	0.97	0.08	44,44,44,44	0
57	MG	1A	3036	1/1	0.97	0.06	23,23,23,23	0
57	MG	1A	3218	1/1	0.97	0.09	22,22,22,22	0
57	MG	1A	3391	1/1	0.97	0.04	26,26,26,26	0
57	MG	1A	3220	1/1	0.97	0.14	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3085	1/1	0.97	0.21	40,40,40,40	0
57	MG	1A	3505	1/1	0.97	0.05	44,44,44,44	0
57	MG	1A	3938	1/1	0.97	0.06	32,32,32,32	0
57	MG	1A	3624	1/1	0.97	0.06	39,39,39,39	0
57	MG	1A	3221	1/1	0.97	0.08	32,32,32,32	0
57	MG	1A	3086	1/1	0.97	0.07	22,22,22,22	0
57	MG	2A	3345	1/1	0.97	0.06	31,31,31,31	0
57	MG	2A	3346	1/1	0.97	0.13	42,42,42,42	0
57	MG	2A	3347	1/1	0.97	0.04	24,24,24,24	0
57	MG	1a	3166	1/1	0.97	0.05	48,48,48,48	0
57	MG	2A	3635	1/1	0.97	0.07	54,54,54,54	0
57	MG	2A	3092	1/1	0.97	0.11	41,41,41,41	0
57	MG	1Z	301	1/1	0.97	0.09	51,51,51,51	0
57	MG	1a	3168	1/1	0.97	0.05	41,41,41,41	0
57	MG	1A	3769	1/1	0.97	0.05	32,32,32,32	0
57	MG	2A	3645	1/1	0.97	0.06	38,38,38,38	0
57	MG	1A	3627	1/1	0.97	0.05	33,33,33,33	0
57	MG	1A	3508	1/1	0.97	0.07	15,15,15,15	0
57	MG	1A	3773	1/1	0.97	0.07	21,21,21,21	0
57	MG	2a	3141	1/1	0.97	0.15	53,53,53,53	0
57	MG	1A	3070	1/1	0.97	0.09	24,24,24,24	0
57	MG	1A	3225	1/1	0.97	0.12	31,31,31,31	0
57	MG	1A	3092	1/1	0.97	0.07	36,36,36,36	0
57	MG	1A	3401	1/1	0.97	0.11	14,14,14,14	0
57	MG	1A	3635	1/1	0.97	0.04	28,28,28,28	0
57	MG	2A	3657	1/1	0.97	0.05	58,58,58,58	0
57	MG	1A	3952	1/1	0.97	0.07	54,54,54,54	0
57	MG	1A	3636	1/1	0.97	0.11	21,21,21,21	0
57	MG	2A	3661	1/1	0.97	0.06	50,50,50,50	0
57	MG	2A	3107	1/1	0.97	0.09	30,30,30,30	0
57	MG	13	101	1/1	0.97	0.16	28,28,28,28	0
57	MG	2a	3154	1/1	0.97	0.12	32,32,32,32	0
57	MG	2A	3666	1/1	0.97	0.05	42,42,42,42	0
57	MG	1A	3025	1/1	0.97	0.09	27,27,27,27	0
57	MG	2A	3369	1/1	0.97	0.04	21,21,21,21	0
57	MG	2A	3110	1/1	0.97	0.06	45,45,45,45	0
57	MG	13	103	1/1	0.97	0.05	37,37,37,37	0
57	MG	1A	3638	1/1	0.97	0.09	37,37,37,37	0
57	MG	2a	3162	1/1	0.97	0.06	49,49,49,49	0
57	MG	1A	3170	1/1	0.97	0.14	23,23,23,23	0
57	MG	15	106	1/1	0.97	0.09	30,30,30,30	0
57	MG	2a	3166	1/1	0.97	0.07	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3376	1/1	0.97	0.12	49,49,49,49	0
57	MG	2A	3676	1/1	0.97	0.04	37,37,37,37	0
57	MG	15	107	1/1	0.97	0.18	24,24,24,24	0
57	MG	1A	3515	1/1	0.97	0.04	38,38,38,38	0
57	MG	2A	3118	1/1	0.97	0.09	47,47,47,47	0
57	MG	2a	3172	1/1	0.97	0.05	50,50,50,50	0
57	MG	1A	3094	1/1	0.97	0.04	23,23,23,23	0
57	MG	1A	3231	1/1	0.97	0.09	35,35,35,35	0
57	MG	17	101	1/1	0.97	0.10	23,23,23,23	0
57	MG	1A	3407	1/1	0.97	0.07	28,28,28,28	0
57	MG	1A	3789	1/1	0.97	0.06	55,55,55,55	0
57	MG	1A	3965	1/1	0.97	0.05	34,34,34,34	0
57	MG	1A	3172	1/1	0.97	0.16	26,26,26,26	0
57	MG	1A	3967	1/1	0.97	0.04	19,19,19,19	0
57	MG	2A	3692	1/1	0.97	0.08	36,36,36,36	0
57	MG	1A	3095	1/1	0.97	0.10	43,43,43,43	0
57	MG	2A	3694	1/1	0.97	0.06	44,44,44,44	0
57	MG	19	101	1/1	0.97	0.11	41,41,41,41	0
57	MG	1A	3411	1/1	0.97	0.17	36,36,36,36	0
57	MG	1A	3970	1/1	0.97	0.04	39,39,39,39	0
57	MG	2A	3135	1/1	0.97	0.08	23,23,23,23	0
57	MG	1a	3003	1/1	0.97	0.06	45,45,45,45	0
57	MG	1A	3522	1/1	0.97	0.04	29,29,29,29	0
57	MG	2A	3701	1/1	0.97	0.05	55,55,55,55	0
57	MG	1A	3524	1/1	0.97	0.22	21,21,21,21	0
57	MG	1A	3412	1/1	0.97	0.04	15,15,15,15	0
57	MG	2A	3401	1/1	0.97	0.05	30,30,30,30	0
57	MG	1A	3174	1/1	0.97	0.17	39,39,39,39	0
57	MG	1A	3529	1/1	0.97	0.05	41,41,41,41	0
57	MG	1a	3208	1/1	0.97	0.07	48,48,48,48	0
57	MG	1A	3799	1/1	0.97	0.07	47,47,47,47	0
57	MG	2A	3709	1/1	0.97	0.11	42,42,42,42	0
57	MG	2A	3710	1/1	0.97	0.07	44,44,44,44	0
57	MG	1A	3317	1/1	0.97	0.12	44,44,44,44	0
57	MG	1A	3175	1/1	0.97	0.11	19,19,19,19	0
57	MG	1A	3416	1/1	0.97	0.07	21,21,21,21	0
57	MG	1A	3980	1/1	0.97	0.07	32,32,32,32	0
57	MG	2A	3151	1/1	0.97	0.05	41,41,41,41	0
57	MG	2A	3152	1/1	0.97	0.06	53,53,53,53	0
57	MG	1A	3238	1/1	0.97	0.22	29,29,29,29	0
57	MG	2A	3414	1/1	0.97	0.04	49,49,49,49	0
57	MG	1A	3534	1/1	0.97	0.08	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3661	1/1	0.97	0.04	35,35,35,35	0
57	MG	2A	3156	1/1	0.97	0.21	46,46,46,46	0
57	MG	2A	3519	1/1	0.98	0.07	48,48,48,48	0
57	MG	1A	3910	1/1	0.98	0.07	26,26,26,26	0
57	MG	1A	3307	1/1	0.98	0.09	8,8,8,8	0
57	MG	1A	3309	1/1	0.98	0.26	29,29,29,29	0
57	MG	1A	3152	1/1	0.98	0.23	35,35,35,35	0
57	MG	1a	3046	1/1	0.98	0.17	34,34,34,34	0
57	MG	1A	3015	1/1	0.98	0.06	29,29,29,29	0
57	MG	2A	3526	1/1	0.98	0.05	39,39,39,39	0
57	MG	1A	3782	1/1	0.98	0.04	15,15,15,15	0
57	MG	2A	3106	1/1	0.98	0.04	31,31,31,31	0
57	MG	2A	3309	1/1	0.98	0.13	36,36,36,36	0
57	MG	1A	3666	1/1	0.98	0.04	30,30,30,30	0
57	MG	1a	3050	1/1	0.98	0.05	36,36,36,36	0
57	MG	1D	310	1/1	0.98	0.04	41,41,41,41	0
57	MG	1A	3050	1/1	0.98	0.32	37,37,37,37	0
57	MG	2A	3314	1/1	0.98	0.04	34,34,34,34	0
57	MG	2A	3111	1/1	0.98	0.06	42,42,42,42	0
57	MG	1A	3565	1/1	0.98	0.08	29,29,29,29	0
57	MG	1A	3786	1/1	0.98	0.09	27,27,27,27	0
57	MG	1A	3385	1/1	0.98	0.06	15,15,15,15	0
57	MG	1A	3156	1/1	0.98	0.12	29,29,29,29	0
57	MG	1A	3016	1/1	0.98	0.09	28,28,28,28	0
57	MG	1D	318	1/1	0.98	0.05	38,38,38,38	0
57	MG	1E	301	1/1	0.98	0.11	27,27,27,27	0
57	MG	1E	302	1/1	0.98	0.08	26,26,26,26	0
57	MG	1A	3315	1/1	0.98	0.15	24,24,24,24	0
57	MG	1E	304	1/1	0.98	0.08	33,33,33,33	0
57	MG	2A	3122	1/1	0.98	0.08	41,41,41,41	0
57	MG	1A	3474	1/1	0.98	0.05	31,31,31,31	0
57	MG	1A	3121	1/1	0.98	0.05	31,31,31,31	0
57	MG	2A	3329	1/1	0.98	0.06	47,47,47,47	0
57	MG	2A	3551	1/1	0.98	0.04	46,46,46,46	0
57	MG	1A	3793	1/1	0.98	0.06	23,23,23,23	0
57	MG	1A	3572	1/1	0.98	0.06	45,45,45,45	0
57	MG	2A	3128	1/1	0.98	0.09	37,37,37,37	0
57	MG	2A	3333	1/1	0.98	0.07	44,44,44,44	0
57	MG	1A	3159	1/1	0.98	0.06	23,23,23,23	0
57	MG	2A	3130	1/1	0.98	0.13	38,38,38,38	0
57	MG	1F	301	1/1	0.98	0.05	21,21,21,21	0
57	MG	1A	3477	1/1	0.98	0.04	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1F	303	1/1	0.98	0.17	28,28,28,28	0
57	MG	2A	3561	1/1	0.98	0.04	18,18,18,18	0
57	MG	1A	3257	1/1	0.98	0.06	35,35,35,35	0
57	MG	1F	305	1/1	0.98	0.06	28,28,28,28	0
57	MG	1A	3679	1/1	0.98	0.06	15,15,15,15	0
57	MG	2A	3567	1/1	0.98	0.08	49,49,49,49	0
57	MG	1A	3319	1/1	0.98	0.07	37,37,37,37	0
57	MG	1a	3075	1/1	0.98	0.07	40,40,40,40	0
57	MG	2A	3139	1/1	0.98	0.04	33,33,33,33	0
57	MG	1a	3246	1/1	0.98	0.05	55,55,55,55	0
57	MG	2A	3141	1/1	0.98	0.14	43,43,43,43	0
57	MG	2A	3574	1/1	0.98	0.07	33,33,33,33	0
57	MG	1F	308	1/1	0.98	0.08	26,26,26,26	0
57	MG	1A	3393	1/1	0.98	0.08	12,12,12,12	0
57	MG	1F	310	1/1	0.98	0.10	27,27,27,27	0
57	MG	2A	3578	1/1	0.98	0.04	40,40,40,40	0
57	MG	2A	3579	1/1	0.98	0.06	41,41,41,41	0
57	MG	2A	3145	1/1	0.98	0.12	29,29,29,29	0
57	MG	1A	3320	1/1	0.98	0.05	22,22,22,22	0
57	MG	1A	3088	1/1	0.98	0.10	25,25,25,25	0
57	MG	1A	3322	1/1	0.98	0.08	17,17,17,17	0
57	MG	1A	3201	1/1	0.98	0.16	34,34,34,34	0
57	MG	1A	3805	1/1	0.98	0.04	33,33,33,33	0
57	MG	2a	3027	1/1	0.98	0.07	52,52,52,52	0
57	MG	2A	3356	1/1	0.98	0.08	32,32,32,32	0
57	MG	1A	3398	1/1	0.98	0.03	14,14,14,14	0
57	MG	2a	3030	1/1	0.98	0.12	42,42,42,42	0
57	MG	2A	3358	1/1	0.98	0.07	34,34,34,34	0
57	MG	2A	3590	1/1	0.98	0.09	38,38,38,38	0
57	MG	1a	3257	1/1	0.98	0.06	25,25,25,25	0
57	MG	1A	3399	1/1	0.98	0.06	17,17,17,17	0
57	MG	2a	3035	1/1	0.98	0.07	31,31,31,31	0
57	MG	1A	3089	1/1	0.98	0.15	21,21,21,21	0
57	MG	1A	3810	1/1	0.98	0.07	24,24,24,24	0
57	MG	1A	3090	1/1	0.98	0.06	32,32,32,32	0
57	MG	1A	3163	1/1	0.98	0.20	23,23,23,23	0
57	MG	2A	3598	1/1	0.98	0.04	36,36,36,36	0
57	MG	1A	3947	1/1	0.98	0.10	46,46,46,46	0
57	MG	1A	3205	1/1	0.98	0.07	33,33,33,33	0
57	MG	2A	3367	1/1	0.98	0.08	40,40,40,40	0
57	MG	1A	3493	1/1	0.98	0.04	39,39,39,39	0
57	MG	1A	3693	1/1	0.98	0.14	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3264	1/1	0.98	0.16	29,29,29,29	0
57	MG	1A	3495	1/1	0.98	0.08	21,21,21,21	0
57	MG	1A	3818	1/1	0.98	0.14	19,19,19,19	0
57	MG	1P	201	1/1	0.98	0.15	28,28,28,28	0
57	MG	1P	202	1/1	0.98	0.13	26,26,26,26	0
57	MG	1A	3496	1/1	0.98	0.06	28,28,28,28	0
57	MG	1A	3265	1/1	0.98	0.22	24,24,24,24	0
57	MG	1A	3498	1/1	0.98	0.06	38,38,38,38	0
57	MG	1Q	202	1/1	0.98	0.05	33,33,33,33	0
57	MG	1A	3822	1/1	0.98	0.06	25,25,25,25	0
57	MG	2A	3614	1/1	0.98	0.04	21,21,21,21	0
57	MG	1Q	204	1/1	0.98	0.06	33,33,33,33	0
57	MG	2A	3173	1/1	0.98	0.04	40,40,40,40	0
57	MG	1A	3206	1/1	0.98	0.07	28,28,28,28	0
57	MG	1A	3026	1/1	0.98	0.15	27,27,27,27	0
57	MG	2A	3176	1/1	0.98	0.05	43,43,43,43	0
57	MG	2A	3177	1/1	0.98	0.08	33,33,33,33	0
57	MG	1A	3333	1/1	0.98	0.06	18,18,18,18	0
57	MG	1A	3704	1/1	0.98	0.04	18,18,18,18	0
57	MG	1A	3037	1/1	0.98	0.05	32,32,32,32	0
57	MG	1A	3828	1/1	0.98	0.09	34,34,34,34	0
57	MG	1A	3018	1/1	0.98	0.12	18,18,18,18	0
57	MG	1A	3707	1/1	0.98	0.08	28,28,28,28	0
57	MG	2A	3184	1/1	0.98	0.06	51,51,51,51	0
57	MG	2A	3628	1/1	0.98	0.07	47,47,47,47	0
57	MG	1A	3337	1/1	0.98	0.07	26,26,26,26	0
57	MG	1A	3709	1/1	0.98	0.10	15,15,15,15	0
57	MG	1U	202	1/1	0.98	0.05	30,30,30,30	0
57	MG	1m	201	1/1	0.98	0.05	60,60,60,60	0
57	MG	1A	3039	1/1	0.98	0.11	29,29,29,29	0
57	MG	1A	3339	1/1	0.98	0.05	22,22,22,22	0
57	MG	1A	3056	1/1	0.98	0.07	34,34,34,34	0
57	MG	1A	3836	1/1	0.98	0.05	36,36,36,36	0
57	MG	2A	3639	1/1	0.98	0.07	55,55,55,55	0
57	MG	2A	3640	1/1	0.98	0.05	47,47,47,47	0
57	MG	1V	201	1/1	0.98	0.10	24,24,24,24	0
57	MG	1V	202	1/1	0.98	0.12	20,20,20,20	0
57	MG	1A	3272	1/1	0.98	0.07	41,41,41,41	0
57	MG	2A	3409	1/1	0.98	0.06	38,38,38,38	0
57	MG	1A	3212	1/1	0.98	0.03	12,12,12,12	0
57	MG	1A	3097	1/1	0.98	0.11	21,21,21,21	0
57	MG	2A	3648	1/1	0.98	0.06	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3420	1/1	0.98	0.04	23,23,23,23	0
57	MG	2A	3650	1/1	0.98	0.08	36,36,36,36	0
57	MG	1A	3608	1/1	0.98	0.11	26,26,26,26	0
57	MG	1A	3609	1/1	0.98	0.12	22,22,22,22	0
57	MG	1A	3073	1/1	0.98	0.06	30,30,30,30	0
57	MG	1A	3845	1/1	0.98	0.05	36,36,36,36	0
57	MG	2A	3655	1/1	0.98	0.07	32,32,32,32	0
57	MG	1A	3007	1/1	0.98	0.09	24,24,24,24	0
57	MG	1A	3346	1/1	0.98	0.06	43,43,43,43	0
57	MG	2A	3658	1/1	0.98	0.05	42,42,42,42	0
57	MG	2A	3205	1/1	0.98	0.07	39,39,39,39	0
57	MG	2A	3206	1/1	0.98	0.09	39,39,39,39	0
57	MG	2A	3421	1/1	0.98	0.04	36,36,36,36	0
57	MG	2A	3662	1/1	0.98	0.05	37,37,37,37	0
57	MG	2a	3102	1/1	0.98	0.24	52,52,52,52	0
57	MG	1A	3217	1/1	0.98	0.06	43,43,43,43	0
57	MG	2A	3007	1/1	0.98	0.04	36,36,36,36	0
57	MG	2A	3665	1/1	0.98	0.05	52,52,52,52	0
57	MG	1A	3614	1/1	0.98	0.05	26,26,26,26	0
57	MG	2A	3667	1/1	0.98	0.04	35,35,35,35	0
57	MG	2A	3010	1/1	0.98	0.07	51,51,51,51	0
57	MG	1A	3134	1/1	0.98	0.05	32,32,32,32	0
57	MG	1a	3135	1/1	0.98	0.07	29,29,29,29	0
57	MG	2A	3013	1/1	0.98	0.05	19,19,19,19	0
57	MG	1A	3727	1/1	0.98	0.04	16,16,16,16	0
57	MG	1A	3728	1/1	0.98	0.03	27,27,27,27	0
57	MG	1A	3426	1/1	0.98	0.06	23,23,23,23	0
57	MG	1A	3219	1/1	0.98	0.06	43,43,43,43	0
57	MG	1A	3428	1/1	0.98	0.05	16,16,16,16	0
57	MG	1A	3429	1/1	0.98	0.05	29,29,29,29	0
57	MG	2A	3020	1/1	0.98	0.14	37,37,37,37	0
57	MG	2A	3021	1/1	0.98	0.05	33,33,33,33	0
57	MG	11	102	1/1	0.98	0.08	42,42,42,42	0
57	MG	2A	3682	1/1	0.98	0.09	37,37,37,37	0
57	MG	2A	3683	1/1	0.98	0.04	37,37,37,37	0
57	MG	1A	3430	1/1	0.98	0.09	44,44,44,44	0
57	MG	1A	3735	1/1	0.98	0.07	15,15,15,15	0
57	MG	2A	3686	1/1	0.98	0.07	45,45,45,45	0
57	MG	11	105	1/1	0.98	0.05	39,39,39,39	0
57	MG	1a	3146	1/1	0.98	0.07	29,29,29,29	0
57	MG	1A	3280	1/1	0.98	0.11	34,34,34,34	0
57	MG	2A	3028	1/1	0.98	0.03	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3860	1/1	0.98	0.04	30,30,30,30	0
57	MG	2A	3030	1/1	0.98	0.09	22,22,22,22	0
57	MG	1A	3432	1/1	0.98	0.05	27,27,27,27	0
57	MG	15	101	1/1	0.98	0.07	29,29,29,29	0
57	MG	1A	3526	1/1	0.98	0.04	26,26,26,26	0
57	MG	15	103	1/1	0.98	0.11	34,34,34,34	0
57	MG	1A	3100	1/1	0.98	0.23	27,27,27,27	0
57	MG	1a	3154	1/1	0.98	0.05	47,47,47,47	0
57	MG	1A	3013	1/1	0.98	0.09	21,21,21,21	0
57	MG	1A	4002	1/1	0.98	0.17	42,42,42,42	0
57	MG	2A	3039	1/1	0.98	0.13	34,34,34,34	0
57	MG	1a	3157	1/1	0.98	0.04	49,49,49,49	0
57	MG	2A	3041	1/1	0.98	0.03	21,21,21,21	0
57	MG	1A	4003	1/1	0.98	0.03	27,27,27,27	0
57	MG	1A	3076	1/1	0.98	0.16	24,24,24,24	0
57	MG	1A	4005	1/1	0.98	0.05	38,38,38,38	0
57	MG	1A	3628	1/1	0.98	0.04	16,16,16,16	0
57	MG	1A	3629	1/1	0.98	0.05	49,49,49,49	0
57	MG	1A	3223	1/1	0.98	0.19	27,27,27,27	0
57	MG	2a	3149	1/1	0.98	0.06	45,45,45,45	0
57	MG	2A	3048	1/1	0.98	0.06	42,42,42,42	0
57	MG	1A	3176	1/1	0.98	0.07	24,24,24,24	0
57	MG	1A	3438	1/1	0.98	0.03	9,9,9,9	0
57	MG	2A	3713	1/1	0.98	0.06	40,40,40,40	0
57	MG	1A	3177	1/1	0.98	0.41	35,35,35,35	0
57	MG	2a	3155	1/1	0.98	0.07	57,57,57,57	0
57	MG	1A	3440	1/1	0.98	0.06	21,21,21,21	0
57	MG	1A	3139	1/1	0.98	0.06	27,27,27,27	0
57	MG	19	102	1/1	0.98	0.05	44,44,44,44	0
57	MG	1A	3077	1/1	0.98	0.12	25,25,25,25	0
57	MG	1A	3289	1/1	0.98	0.05	8,8,8,8	0
57	MG	2A	3258	1/1	0.98	0.09	41,41,41,41	0
57	MG	1A	3362	1/1	0.98	0.03	10,10,10,10	0
57	MG	1A	3042	1/1	0.98	0.07	16,16,16,16	0
57	MG	1A	3030	1/1	0.98	0.04	31,31,31,31	0
57	MG	1A	3365	1/1	0.98	0.04	18,18,18,18	0
57	MG	1A	3107	1/1	0.98	0.11	23,23,23,23	0
57	MG	1A	4021	1/1	0.98	0.04	41,41,41,41	0
57	MG	1A	3293	1/1	0.98	0.06	27,27,27,27	0
57	MG	1A	3044	1/1	0.98	0.07	14,14,14,14	0
57	MG	1A	3233	1/1	0.98	0.17	27,27,27,27	0
57	MG	2A	3067	1/1	0.98	0.11	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3886	1/1	0.98	0.04	30,30,30,30	0
57	MG	1A	3887	1/1	0.98	0.03	34,34,34,34	0
57	MG	1A	3888	1/1	0.98	0.06	34,34,34,34	0
57	MG	1A	3547	1/1	0.98	0.09	33,33,33,33	0
57	MG	2A	3489	1/1	0.98	0.04	37,37,37,37	0
57	MG	1A	3006	1/1	0.98	0.04	16,16,16,16	0
57	MG	2A	3074	1/1	0.98	0.12	39,39,39,39	0
57	MG	1A	3186	1/1	0.98	0.06	41,41,41,41	0
57	MG	1A	3649	1/1	0.98	0.10	48,48,48,48	0
57	MG	2B	214	1/1	0.98	0.06	51,51,51,51	0
57	MG	2A	3494	1/1	0.98	0.03	47,47,47,47	0
57	MG	1A	3023	1/1	0.98	0.17	19,19,19,19	0
57	MG	1a	3020	1/1	0.98	0.08	43,43,43,43	0
57	MG	1A	3651	1/1	0.98	0.05	34,34,34,34	0
57	MG	1B	213	1/1	0.98	0.06	33,33,33,33	0
57	MG	1B	214	1/1	0.98	0.04	32,32,32,32	0
57	MG	1A	3048	1/1	0.98	0.07	42,42,42,42	0
57	MG	1A	3457	1/1	0.98	0.12	40,40,40,40	0
57	MG	1A	3770	1/1	0.98	0.03	28,28,28,28	0
57	MG	1a	3027	1/1	0.98	0.22	55,55,55,55	0
57	MG	1A	3239	1/1	0.98	0.18	32,32,32,32	0
57	MG	2A	3505	1/1	0.98	0.03	38,38,38,38	0
57	MG	1A	3112	1/1	0.98	0.08	28,28,28,28	0
57	MG	2E	302	1/1	0.98	0.05	35,35,35,35	0
57	MG	1B	220	1/1	0.98	0.07	22,22,22,22	0
57	MG	2E	304	1/1	0.98	0.09	37,37,37,37	0
57	MG	1B	221	1/1	0.98	0.06	28,28,28,28	0
57	MG	1A	3901	1/1	0.98	0.03	49,49,49,49	0
57	MG	1B	223	1/1	0.98	0.04	37,37,37,37	0
57	MG	1A	3657	1/1	0.98	0.09	45,45,45,45	0
57	MG	1A	3903	1/1	0.98	0.05	27,27,27,27	0
57	MG	2A	3513	1/1	0.98	0.04	49,49,49,49	0
57	MG	2F	304	1/1	0.98	0.16	38,38,38,38	0
57	MG	1A	3244	1/1	0.98	0.15	28,28,28,28	0
57	MG	1A	3084	1/1	0.98	0.19	34,34,34,34	0
57	MG	1A	3115	1/1	0.98	0.06	16,16,16,16	0
61	ZN	1n	104	1/1	0.98	0.04	66,66,66,66	0
57	MG	1A	3117	1/1	0.98	0.04	26,26,26,26	0
57	MG	1A	3909	1/1	0.98	0.05	40,40,40,40	0
62	SF4	1d	306	8/8	0.98	0.05	52,62,71,75	0
62	SF4	2d	501	8/8	0.98	0.05	58,67,74,76	0
57	MG	1A	3956	1/1	0.99	0.04	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1V	206	1/1	0.99	0.05	34,34,34,34	0
57	MG	1A	3017	1/1	0.99	0.18	33,33,33,33	0
57	MG	2A	3643	1/1	0.99	0.04	31,31,31,31	0
57	MG	2A	3303	1/1	0.99	0.06	52,52,52,52	0
57	MG	1A	3153	1/1	0.99	0.08	22,22,22,22	0
57	MG	2A	3305	1/1	0.99	0.04	28,28,28,28	0
57	MG	2A	3469	1/1	0.99	0.05	24,24,24,24	0
57	MG	1W	203	1/1	0.99	0.10	16,16,16,16	0
57	MG	1A	3213	1/1	0.99	0.03	15,15,15,15	0
57	MG	1A	3298	1/1	0.99	0.12	31,31,31,31	0
57	MG	2A	3390	1/1	0.99	0.09	29,29,29,29	0
57	MG	1A	3410	1/1	0.99	0.04	35,35,35,35	0
57	MG	2A	3392	1/1	0.99	0.04	38,38,38,38	0
57	MG	1a	3031	1/1	0.99	0.04	33,33,33,33	0
57	MG	2A	3562	1/1	0.99	0.04	42,42,42,42	0
57	MG	2A	3009	1/1	0.99	0.07	34,34,34,34	0
57	MG	1A	3962	1/1	0.99	0.05	30,30,30,30	0
57	MG	1A	3252	1/1	0.99	0.07	25,25,25,25	0
57	MG	2A	3566	1/1	0.99	0.04	41,41,41,41	0
57	MG	1A	3964	1/1	0.99	0.08	36,36,36,36	0
57	MG	1A	3443	1/1	0.99	0.02	21,21,21,21	0
57	MG	1A	3908	1/1	0.99	0.03	9,9,9,9	0
57	MG	1A	3807	1/1	0.99	0.11	47,47,47,47	0
57	MG	1A	3230	1/1	0.99	0.04	27,27,27,27	0
57	MG	1A	3116	1/1	0.99	0.09	26,26,26,26	0
57	MG	2E	308	1/1	0.99	0.05	24,24,24,24	0
57	MG	2A	3573	1/1	0.99	0.06	43,43,43,43	0
57	MG	1A	3354	1/1	0.99	0.03	15,15,15,15	0
57	MG	1A	3001	1/1	0.99	0.02	31,31,31,31	0
57	MG	2A	3488	1/1	0.99	0.04	34,34,34,34	0
57	MG	1A	3592	1/1	0.99	0.04	33,33,33,33	0
57	MG	1A	3019	1/1	0.99	0.17	22,22,22,22	0
57	MG	1A	3357	1/1	0.99	0.08	20,20,20,20	0
57	MG	1A	3719	1/1	0.99	0.03	35,35,35,35	0
57	MG	1A	3234	1/1	0.99	0.10	25,25,25,25	0
57	MG	1a	3253	1/1	0.99	0.12	44,44,44,44	0
57	MG	2A	3250	1/1	0.99	0.09	33,33,33,33	0
57	MG	1A	3091	1/1	0.99	0.02	12,12,12,12	0
57	MG	2A	3678	1/1	0.99	0.03	33,33,33,33	0
57	MG	1A	3131	1/1	0.99	0.14	23,23,23,23	0
57	MG	1A	3332	1/1	0.99	0.05	23,23,23,23	0
57	MG	2A	3587	1/1	0.99	0.03	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3523	1/1	0.99	0.03	23,23,23,23	0
57	MG	1A	3725	1/1	0.99	0.06	19,19,19,19	0
57	MG	2a	3163	1/1	0.99	0.02	48,48,48,48	0
57	MG	1A	3561	1/1	0.99	0.04	31,31,31,31	0
57	MG	15	104	1/1	0.99	0.16	25,25,25,25	0
57	MG	1A	3009	1/1	0.99	0.04	23,23,23,23	0
57	MG	2A	3593	1/1	0.99	0.06	30,30,30,30	0
57	MG	1A	3873	1/1	0.99	0.04	23,23,23,23	0
57	MG	1A	3928	1/1	0.99	0.06	36,36,36,36	0
57	MG	1N	201	1/1	0.99	0.03	31,31,31,31	0
57	MG	1N	202	1/1	0.99	0.10	26,26,26,26	0
57	MG	1A	3488	1/1	0.99	0.03	26,26,26,26	0
57	MG	1a	3196	1/1	0.99	0.10	40,40,40,40	0
57	MG	1A	3875	1/1	0.99	0.06	32,32,32,32	0
57	MG	2a	3175	1/1	0.99	0.06	42,42,42,42	0
57	MG	1A	3308	1/1	0.99	0.06	30,30,30,30	0
57	MG	1A	3527	1/1	0.99	0.03	17,17,17,17	0
57	MG	1A	3731	1/1	0.99	0.08	24,24,24,24	0
57	MG	1A	3101	1/1	0.99	0.09	23,23,23,23	0
57	MG	1A	3336	1/1	0.99	0.06	35,35,35,35	0
57	MG	1A	3031	1/1	0.99	0.03	25,25,25,25	0
57	MG	1A	3005	1/1	0.99	0.07	18,18,18,18	0
57	MG	1A	3241	1/1	0.99	0.14	26,26,26,26	0
57	MG	1a	3206	1/1	0.99	0.06	51,51,51,51	0
57	MG	2A	3124	1/1	0.99	0.03	33,33,33,33	0
57	MG	1A	3242	1/1	0.99	0.13	36,36,36,36	0
57	MG	1D	302	1/1	0.99	0.16	25,25,25,25	0
57	MG	1A	3243	1/1	0.99	0.23	35,35,35,35	0
57	MG	1D	304	1/1	0.99	0.06	40,40,40,40	0
57	MG	1A	3113	1/1	0.99	0.10	31,31,31,31	0
57	MG	1A	3137	1/1	0.99	0.03	17,17,17,17	0
57	MG	1A	3654	1/1	0.99	0.03	25,25,25,25	0
57	MG	1A	3465	1/1	0.99	0.03	37,37,37,37	0
57	MG	1D	309	1/1	0.99	0.02	13,13,13,13	0
57	MG	2A	3059	1/1	0.99	0.06	41,41,41,41	0
57	MG	1A	3890	1/1	0.99	0.03	34,34,34,34	0
57	MG	1A	3839	1/1	0.99	0.03	14,14,14,14	0
57	MG	1A	3501	1/1	0.99	0.04	36,36,36,36	0
57	MG	1D	313	1/1	0.99	0.13	18,18,18,18	0
57	MG	1U	203	1/1	0.99	0.10	30,30,30,30	0
57	MG	1A	3744	1/1	0.99	0.05	16,16,16,16	0
57	MG	1A	3698	1/1	0.99	0.06	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3402	1/1	0.99	0.02	11,11,11,11	0
57	MG	1A	3246	1/1	0.99	0.10	24,24,24,24	0
57	MG	1A	3701	1/1	0.99	0.04	31,31,31,31	0
57	MG	2A	3374	1/1	0.99	0.08	38,38,38,38	0
57	MG	1A	3045	1/1	0.99	0.08	14,14,14,14	0
57	MG	2A	3071	1/1	0.99	0.04	20,20,20,20	0
61	ZN	1Y	202	1/1	0.99	0.03	52,52,52,52	0
57	MG	1A	3619	1/1	0.99	0.07	20,20,20,20	0
61	ZN	15	111	1/1	0.99	0.02	37,37,37,37	0
61	ZN	16	501	1/1	0.99	0.04	35,35,35,35	0
61	ZN	19	103	1/1	0.99	0.03	37,37,37,37	0
57	MG	2A	3379	1/1	0.99	0.05	28,28,28,28	0
57	MG	1A	3180	1/1	0.99	0.17	32,32,32,32	0
57	MG	2A	3637	1/1	0.99	0.07	39,39,39,39	0
61	ZN	25	105	1/1	0.99	0.03	47,47,47,47	0
61	ZN	26	501	1/1	0.99	0.03	56,56,56,56	0
61	ZN	29	102	1/1	0.99	0.04	63,63,63,63	0
61	ZN	2n	102	1/1	0.99	0.03	73,73,73,73	0
57	MG	2A	3638	1/1	0.99	0.04	29,29,29,29	0
57	MG	2A	3547	1/1	0.99	0.03	44,44,44,44	0
57	MG	1A	3920	1/1	1.00	0.04	41,41,41,41	0
57	MG	2A	3378	1/1	1.00	0.03	22,22,22,22	0
57	MG	1A	3491	1/1	1.00	0.03	22,22,22,22	0
57	MG	1A	3767	1/1	1.00	0.02	31,31,31,31	0

6.5 Other polymers (i)

There are no such residues in this entry.