wwPDB X-ray Structure Validation Summary Report (i)

Apr 19, 2026 – 08:36 AM UTC

PDB ID	:	7RQE / pdb_00007rqe
Title	:	Crystal structure of the Thermus thermophilus 70S ribosome in complex with protein Y, A-site deacylated tRNA analog CACCA, P-site MAI-tripeptidyl-tRNA analog ACCA-IAM, and chloramphenicol at 2.40A resolution
Authors	:	Syroegin, E.A.; Flemmich, L.; Klepacki, D.; Vazquez-Laslop, N.; Micura, R.; Polikanov, Y.S.
Deposited on	:	2021-08-06
Resolution	:	2.40 Å(reported)

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

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

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

The following versions of software and data (see references ①) were used in the production of this report:

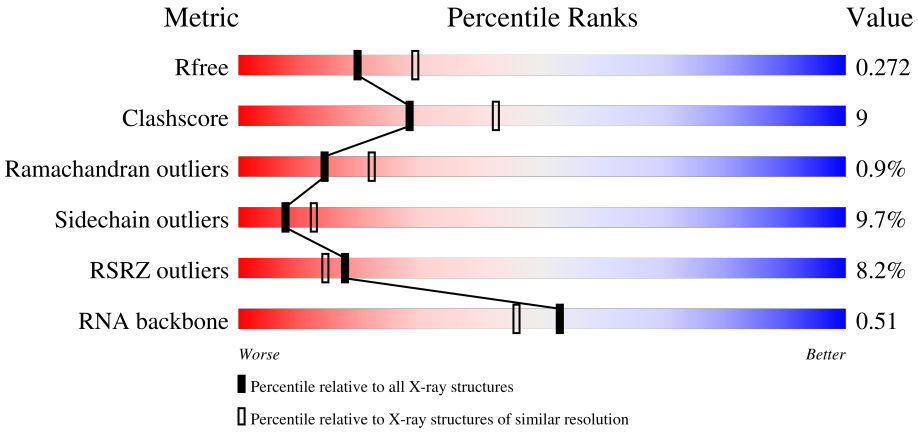
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)
RNA backbone	3983	1155 (2.70-2.10)

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

Mol	Chain	Length	Quality of chain
1	1A	2915	5% 65% 28% 6%
1	2A	2915	5% 59% 32% 7%
2	1B	121	2% 69% 26%
2	2B	121	3% 55% 40% 5%

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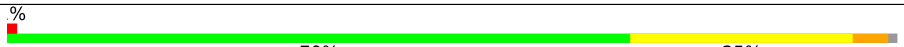
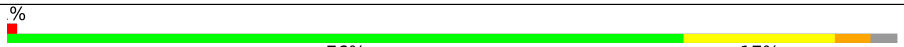
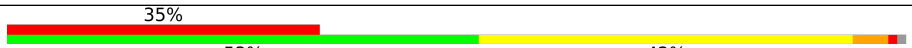
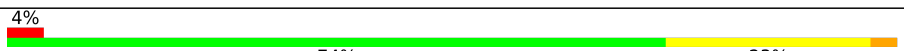
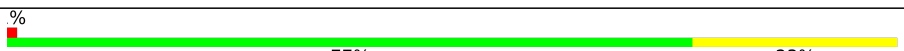
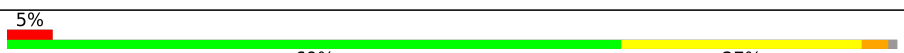
Mol	Chain	Length	Quality of chain
3	1D	276	
3	2D	276	
4	1E	206	
4	2E	206	
5	1F	210	
5	2F	210	
6	1G	182	
6	2G	182	
7	1H	180	
7	2H	180	
8	1I	148	
8	2I	148	
9	1N	140	
9	2N	140	
10	1O	122	
10	2O	122	
11	1P	150	
11	2P	150	
12	1Q	141	
12	2Q	141	
13	1R	118	
13	2R	118	
14	1S	112	
14	2S	112	
15	1T	146	

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Mol	Chain	Length	Quality of chain
15	2T	146	2% 64% 23% 10%
16	1U	118	% 81% 15%
16	2U	118	3% 70% 25%
17	1V	101	% 78% 19%
17	2V	101	4% 64% 29% 6%
18	1W	113	% 81% 17%
18	2W	113	3% 78% 20%
19	1X	96	2% 77% 21%
19	2X	96	8% 77% 21%
20	1Y	110	2% 72% 23%
20	2Y	110	11% 56% 33% 8%
21	1Z	206	2% 72% 23%
21	2Z	206	15% 62% 31% 5%
22	10	85	7% 79% 16%
22	20	85	9% 74% 22%
23	11	98	% 73% 22%
23	21	98	% 58% 35% 6%
24	12	72	3% 68% 28%
24	22	72	8% 68% 26%
25	13	60	67% 28%
25	23	60	5% 67% 30%
26	14	71	24% 54% 35% 8%
26	24	71	54% 42% 44% 10%
27	15	60	2% 72% 22% 5%
27	25	60	2% 80% 15%

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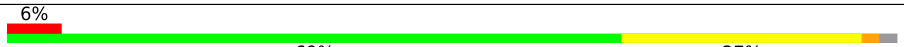
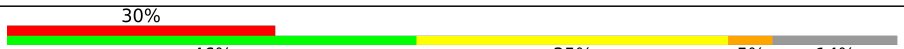
Mol	Chain	Length	Quality of chain
28	16	54	
28	26	54	
29	17	49	
29	27	49	
30	18	65	
30	28	65	
31	19	37	
31	29	37	
32	1a	1521	
32	2a	1521	
33	1b	256	
33	2b	256	
34	1c	239	
34	2c	239	
35	1d	209	
35	2d	209	
36	1e	162	
36	2e	162	
37	1f	101	
37	2f	101	
38	1g	156	
38	2g	156	
39	1h	138	
39	2h	138	
40	1i	128	

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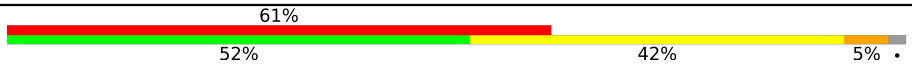
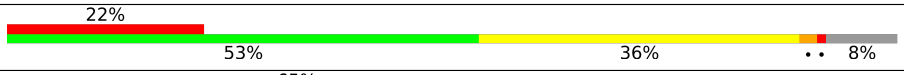
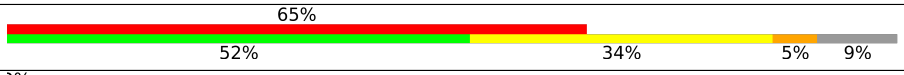
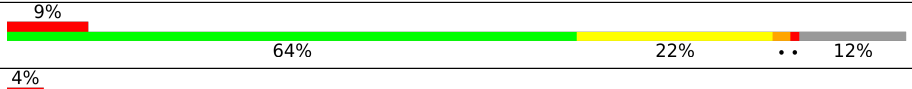
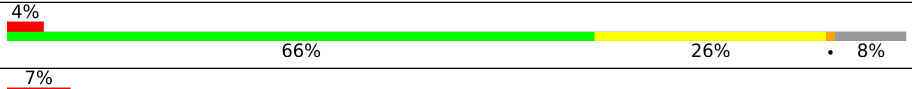
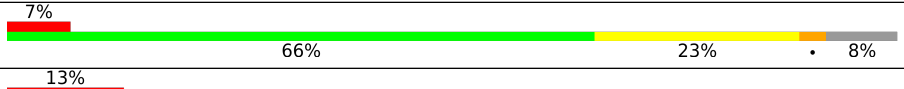
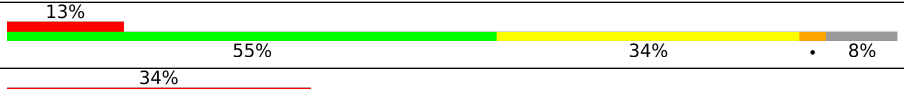
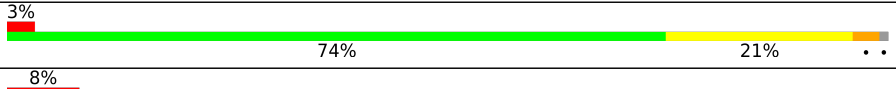
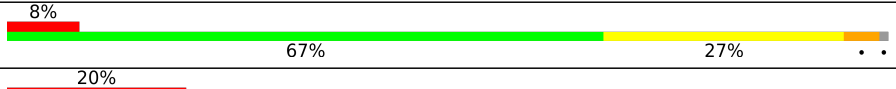
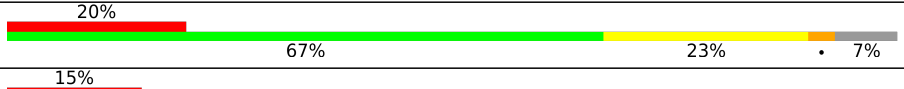
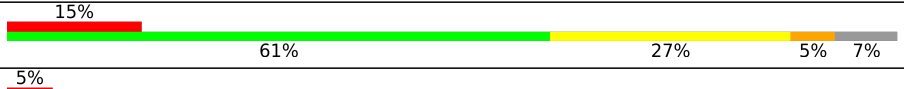
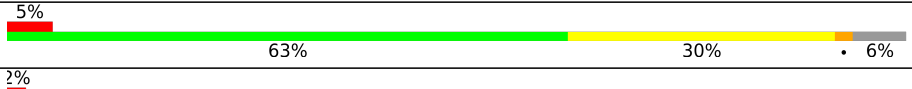
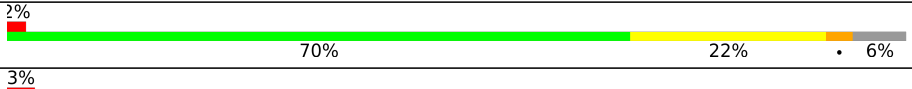
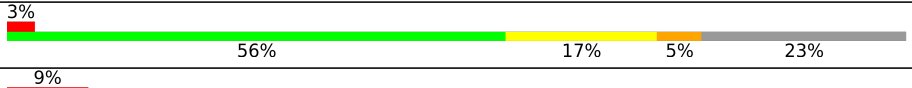
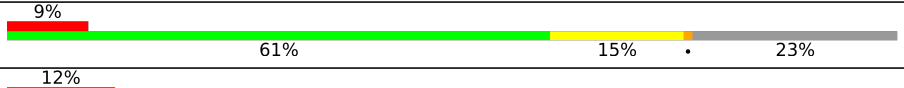
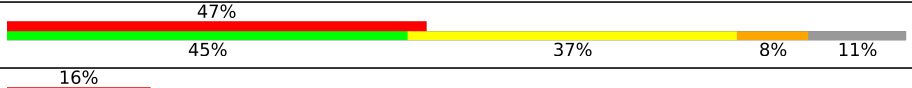
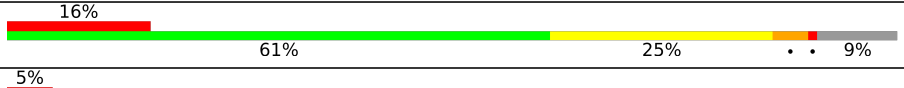
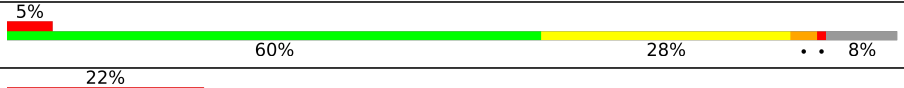
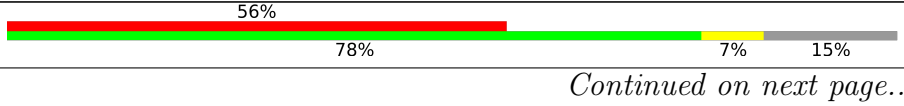
Mol	Chain	Length	Quality of chain
40	2i	128	
41	1j	105	
41	2j	105	
42	1k	129	
42	2k	129	
43	1l	132	
43	2l	132	
44	1m	126	
44	2m	126	
45	1n	61	
45	2n	61	
46	1o	89	
46	2o	89	
47	1p	88	
47	2p	88	
48	1q	105	
48	2q	105	
49	1r	88	
49	2r	88	
50	1s	93	
50	2s	93	
51	1t	106	
51	2t	106	
52	1u	27	
52	2u	27	

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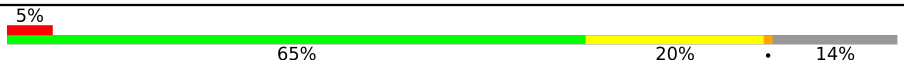
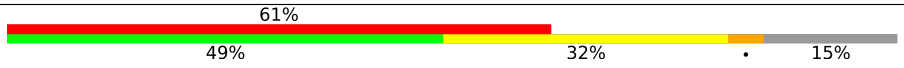
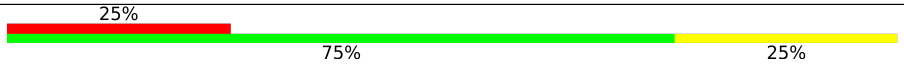
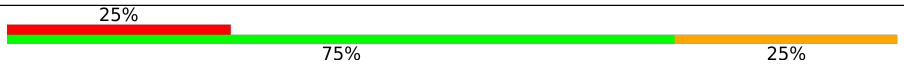
Mol	Chain	Length	Quality of chain
53	1y	113	
53	2y	113	
54	1w	5	
54	2w	5	
55	1x	4	
55	2x	4	
56	1v	3	
56	2v	3	

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
57	MG	1A	3323	-	-	-	X
57	MG	2a	3050	-	-	-	X

2 Entry composition (i)

There are 63 unique types of molecules in this entry. The entry contains 297868 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
			21	14	3	3	1			
56	2v	3	Total	C	N	O	S	0	0	0
			21	14	3	3	1			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	1A	1016	Total	Mg	0	0
			1016	1016		
57	1B	30	Total	Mg	0	0
			30	30		
57	1D	21	Total	Mg	0	0
			21	21		
57	1E	8	Total	Mg	0	0
			8	8		
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	4	Total Mg 4 4	0	0
57	1O	1	Total Mg 1 1	0	0
57	1P	5	Total Mg 5 5	0	0
57	1Q	5	Total Mg 5 5	0	0
57	1R	5	Total Mg 5 5	0	0
57	1T	7	Total Mg 7 7	0	0
57	1U	6	Total Mg 6 6	0	0
57	1V	7	Total Mg 7 7	0	0
57	1W	3	Total Mg 3 3	0	0
57	1X	1	Total Mg 1 1	0	0
57	1Y	2	Total Mg 2 2	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	7	Total Mg 7 7	0	0
57	17	5	Total Mg 5 5	0	0
57	18	3	Total Mg 3 3	0	0
57	19	3	Total Mg 3 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	1a	266	Total Mg 266 266	0	0
57	1b	1	Total Mg 1 1	0	0
57	1d	4	Total Mg 4 4	0	0
57	1e	2	Total Mg 2 2	0	0
57	1f	2	Total Mg 2 2	0	0
57	1g	2	Total Mg 2 2	0	0
57	1h	2	Total Mg 2 2	0	0
57	1i	1	Total Mg 1 1	0	0
57	1l	2	Total Mg 2 2	0	0
57	1m	1	Total Mg 1 1	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	2	Total Mg 2 2	0	0
57	1x	2	Total Mg 2 2	0	0
57	2A	746	Total Mg 746 746	0	0
57	2B	19	Total Mg 19 19	0	0
57	2D	8	Total Mg 8 8	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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	2I	1	Total Mg 1 1	0	0
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	3	Total Mg 3 3	0	0
57	2X	1	Total Mg 1 1	0	0
57	2Y	1	Total Mg 1 1	0	0
57	20	2	Total Mg 2 2	0	0
57	21	1	Total Mg 1 1	0	0
57	23	1	Total Mg 1 1	0	0
57	25	3	Total Mg 3 3	0	0
57	27	1	Total Mg 1 1	0	0
57	28	2	Total Mg 2 2	0	0
57	2a	190	Total Mg 190 190	0	0
57	2e	1	Total Mg 1 1	0	0
57	2f	1	Total Mg 1 1	0	0

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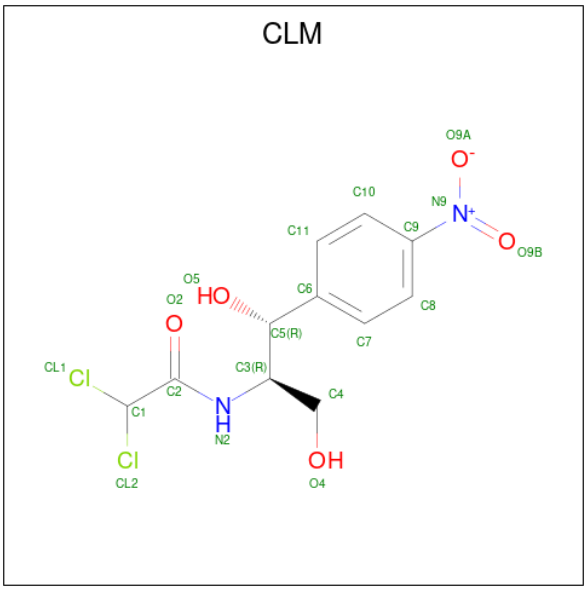
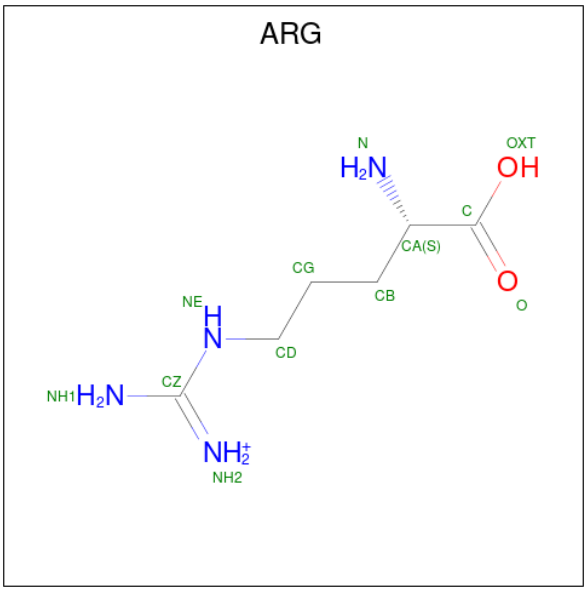
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	2j	2	Total Mg 2 2	0	0
57	2r	1	Total Mg 1 1	0	0
57	2t	1	Total Mg 1 1	0	0
57	2x	1	Total Mg 1 1	0	0

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



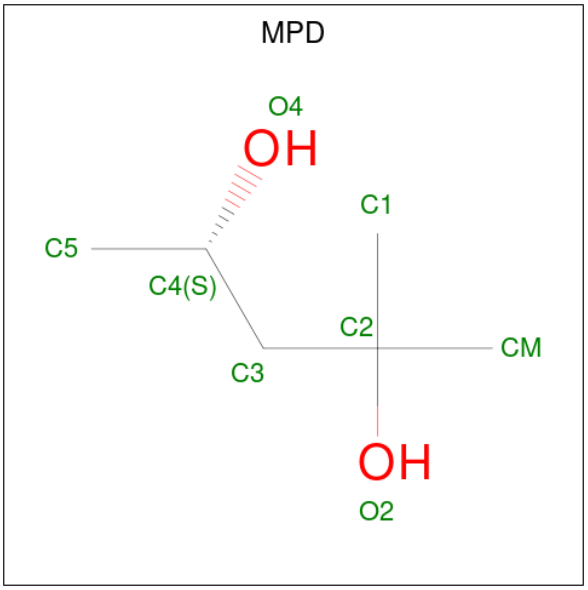
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	1A	1	Total C Cl N O 20 11 2 2 5	0	0
58	2A	1	Total C Cl N O 20 11 2 2 5	0	0

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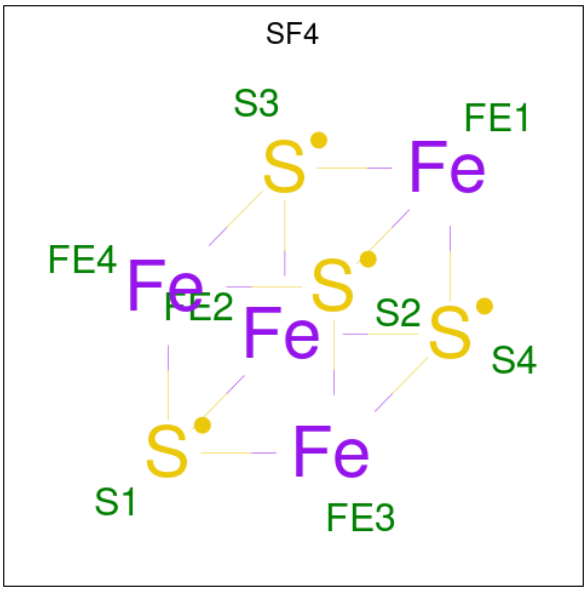
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	18	1	Total C O 8 6 2	0	0
60	1a	1	Total C O 8 6 2	0	0
60	2A	1	Total C O 8 6 2	0	0
60	2B	1	Total C O 8 6 2	0	0

- 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	4023	Total O 4023 4023	0	0
63	1B	93	Total O 93 93	0	0
63	1D	112	Total O 112 112	0	0
63	1E	81	Total O 81 81	0	0
63	1F	61	Total O 61 61	0	0
63	1G	20	Total O 20 20	0	0
63	1H	12	Total O 12 12	0	0
63	1I	6	Total O 6 6	0	0
63	1N	51	Total O 51 51	0	0
63	1O	24	Total O 24 24	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
63	1P	71	Total O 71 71	0	0
63	1Q	41	Total O 41 41	0	0
63	1R	33	Total O 33 33	0	0
63	1S	16	Total O 16 16	0	0
63	1T	34	Total O 34 34	0	0
63	1U	54	Total O 54 54	0	0
63	1V	42	Total O 42 42	0	0
63	1W	29	Total O 29 29	0	0
63	1X	23	Total O 23 23	0	0
63	1Y	16	Total O 16 16	0	0
63	1Z	12	Total O 12 12	0	0
63	10	25	Total O 25 25	0	0
63	11	22	Total O 22 22	0	0
63	12	13	Total O 13 13	0	0
63	13	21	Total O 21 21	0	0
63	14	2	Total O 2 2	0	0
63	15	26	Total O 26 26	0	0
63	16	20	Total O 20 20	0	0
63	17	16	Total O 16 16	0	0
63	18	30	Total O 30 30	0	0
63	19	6	Total O 6 6	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
63	1a	378	Total O 378 378	0	0
63	1b	1	Total O 1 1	0	0
63	1d	3	Total O 3 3	0	0
63	1e	3	Total O 3 3	0	0
63	1f	2	Total O 2 2	0	0
63	1h	1	Total O 1 1	0	0
63	1j	1	Total O 1 1	0	0
63	1l	6	Total O 6 6	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	2	Total O 2 2	0	0
63	1w	5	Total O 5 5	0	0
63	1x	3	Total O 3 3	0	0
63	2A	2284	Total O 2284 2284	0	0
63	2B	46	Total O 46 46	0	0
63	2D	57	Total O 57 57	0	0
63	2E	32	Total O 32 32	0	0
63	2F	27	Total O 27 27	0	0
63	2G	6	Total O 6 6	0	0
63	2H	3	Total O 3 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
63	2I	4	Total O 4 4	0	0
63	2N	6	Total O 6 6	0	0
63	2O	21	Total O 21 21	0	0
63	2P	24	Total O 24 24	0	0
63	2Q	17	Total O 17 17	0	0
63	2R	16	Total O 16 16	0	0
63	2S	5	Total O 5 5	0	0
63	2T	13	Total O 13 13	0	0
63	2U	16	Total O 16 16	0	0
63	2V	5	Total O 5 5	0	0
63	2W	17	Total O 17 17	0	0
63	2X	8	Total O 8 8	0	0
63	2Y	5	Total O 5 5	0	0
63	2Z	11	Total O 11 11	0	0
63	20	11	Total O 11 11	0	0
63	21	20	Total O 20 20	0	0
63	22	1	Total O 1 1	0	0
63	23	3	Total O 3 3	0	0
63	25	13	Total O 13 13	0	0
63	26	5	Total O 5 5	0	0
63	27	9	Total O 9 9	0	0

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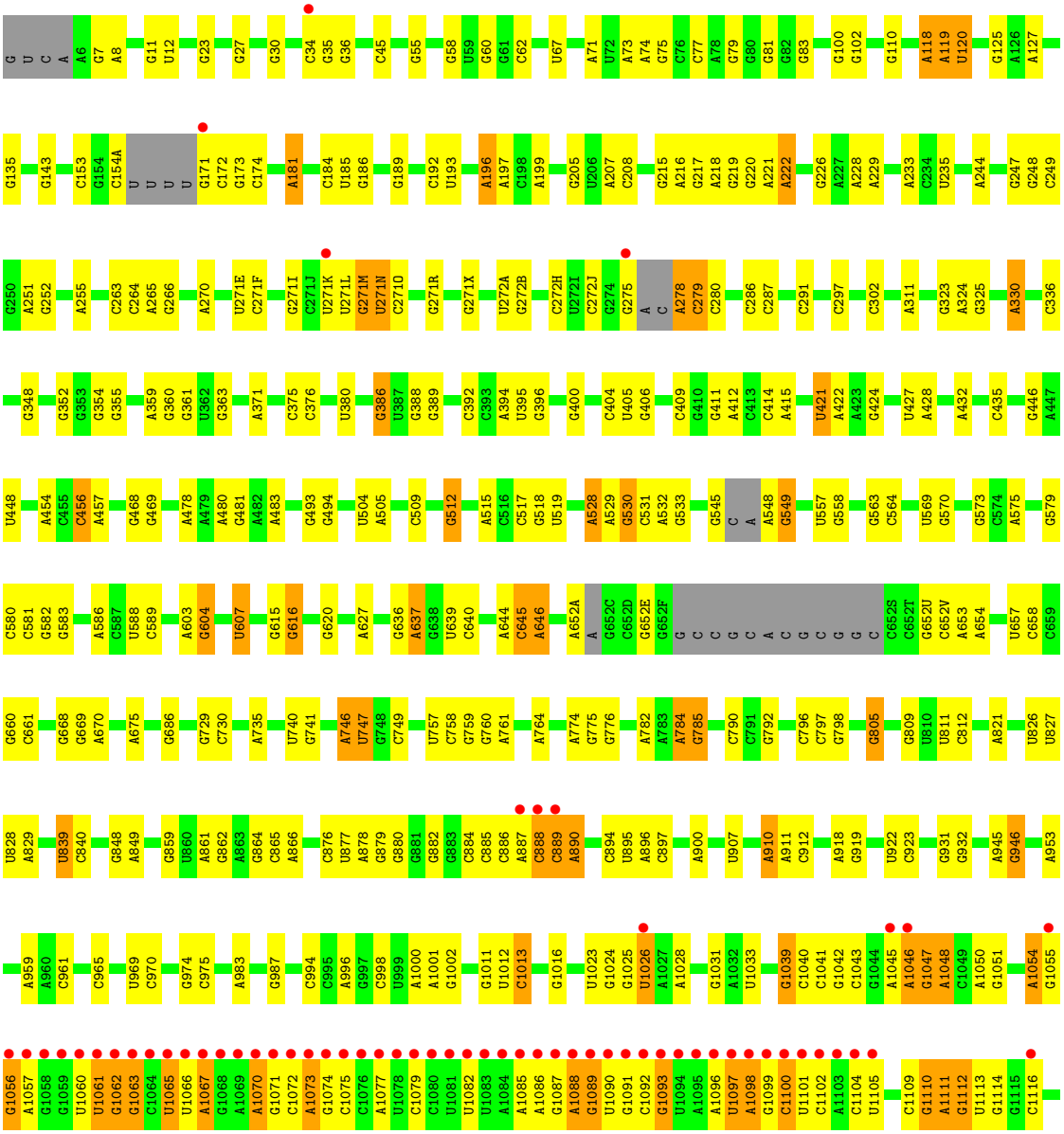
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
63	28	11	Total O 11 11	0	0
63	29	2	Total O 2 2	0	0
63	2a	317	Total O 317 317	0	0
63	2d	2	Total O 2 2	0	0
63	2e	1	Total O 1 1	0	0
63	2f	3	Total O 3 3	0	0
63	2j	2	Total O 2 2	0	0
63	2l	2	Total O 2 2	0	0
63	2n	2	Total O 2 2	0	0
63	2o	4	Total O 4 4	0	0
63	2p	2	Total O 2 2	0	0
63	2r	3	Total O 3 3	0	0
63	2t	2	Total O 2 2	0	0
63	2y	3	Total O 3 3	0	0
63	2w	3	Total O 3 3	0	0
63	2x	3	Total O 3 3	0	0

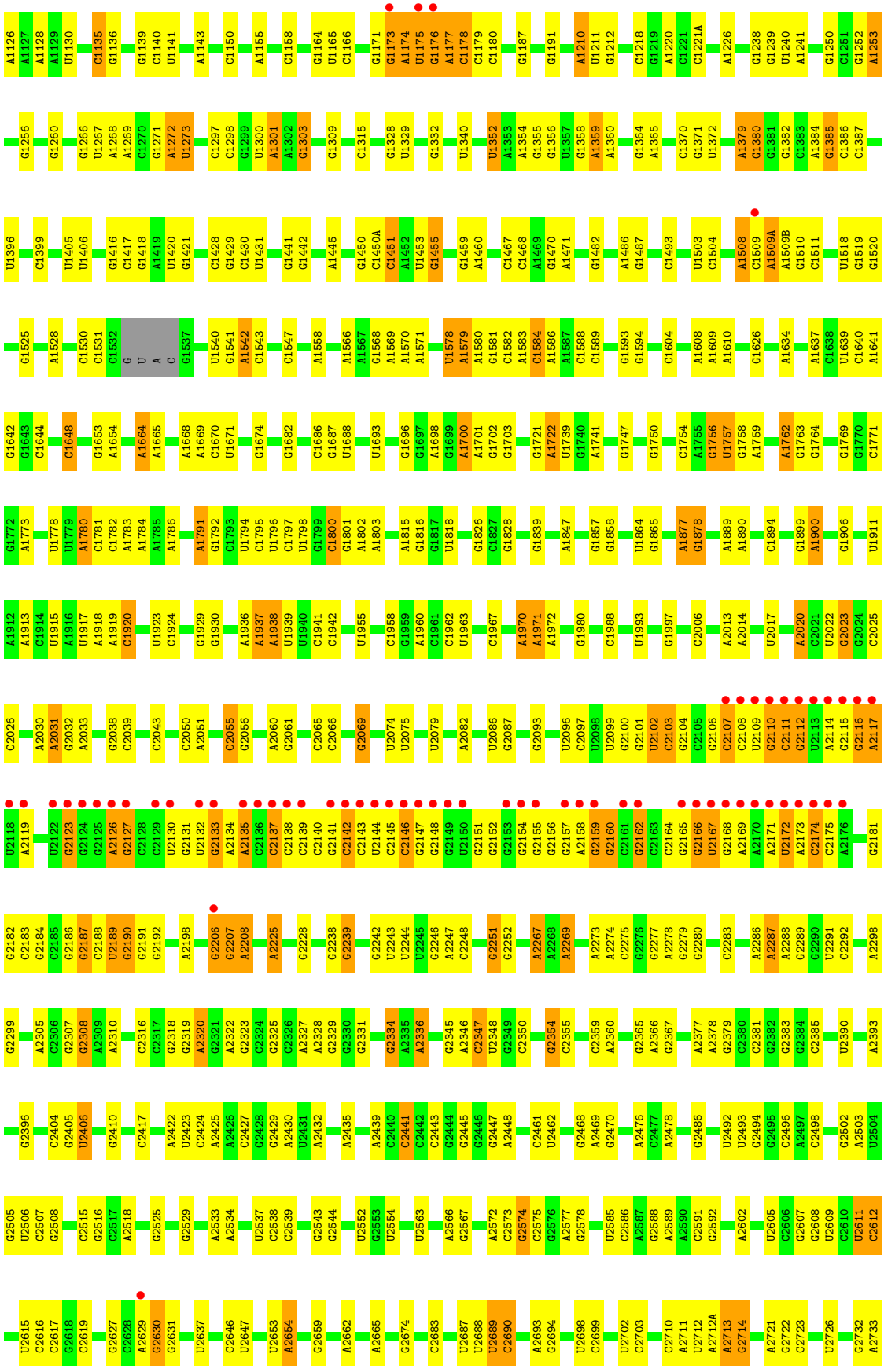
3 Residue-property plots (i)

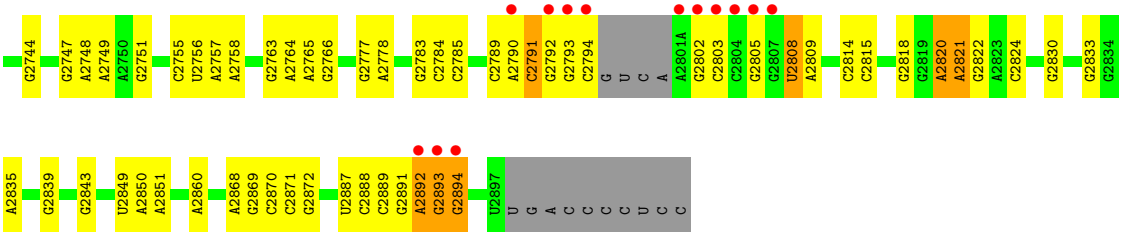
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: 23S Ribosomal RNA

Chain 1A:

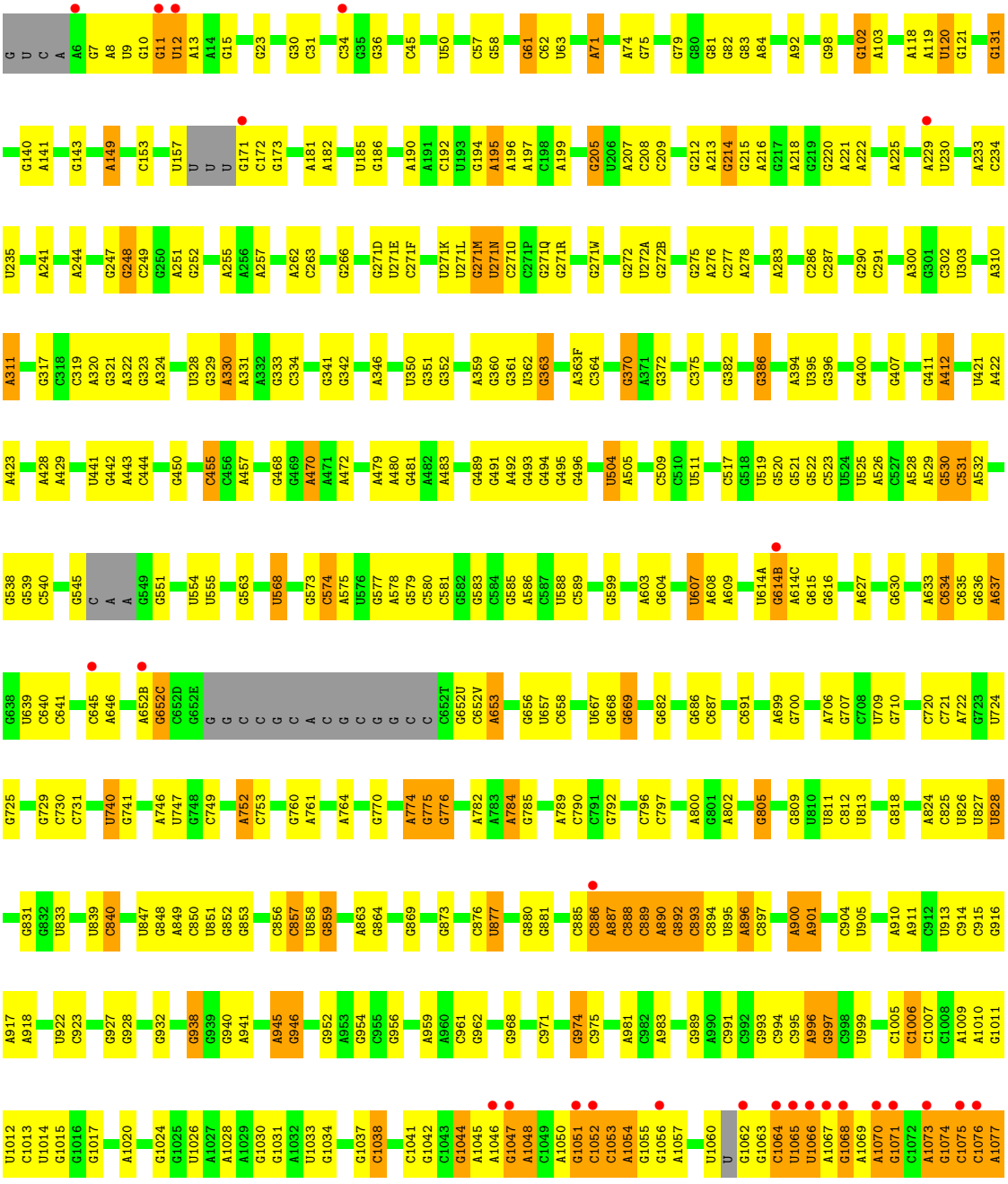


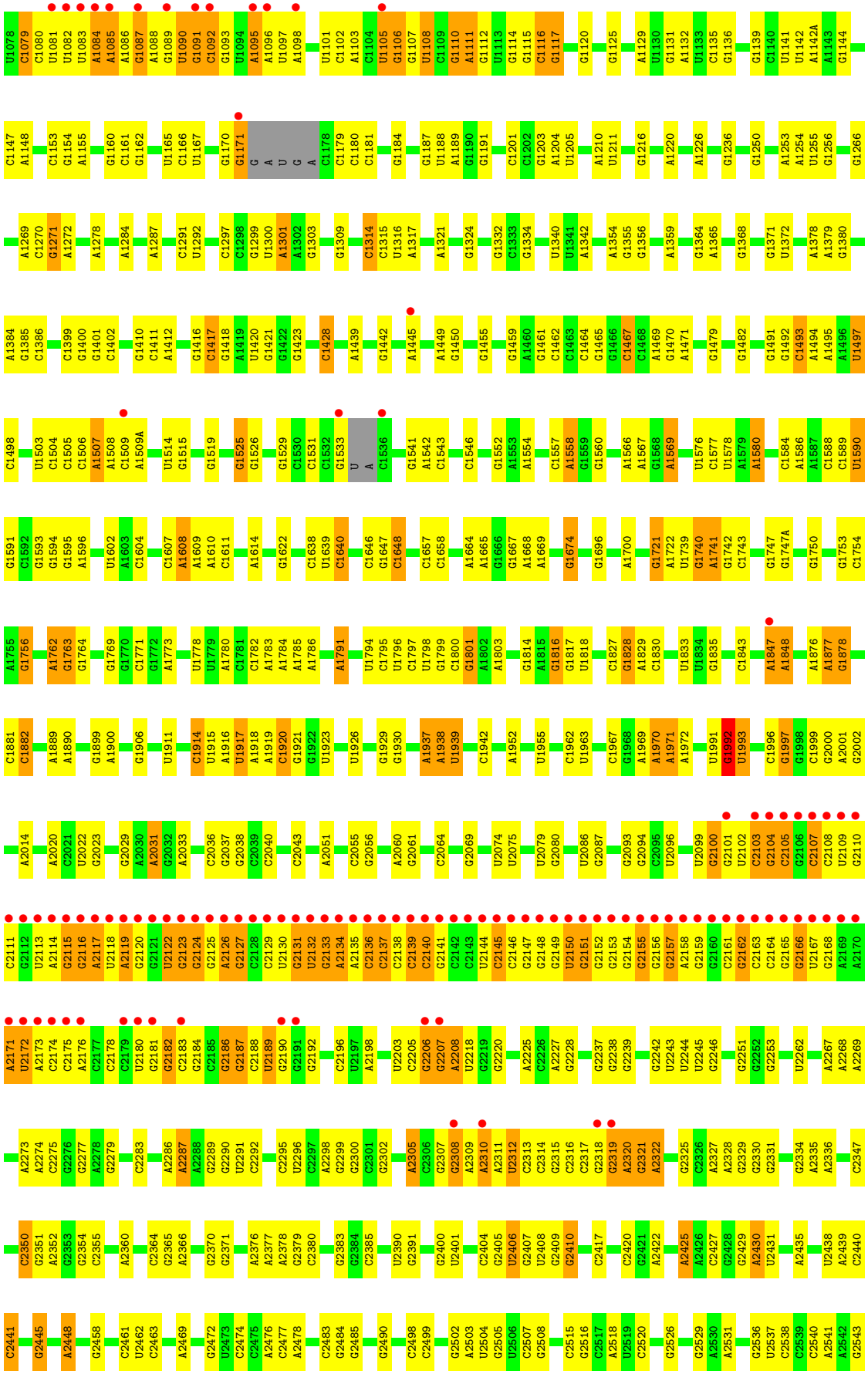

A1126 A1127 A1128 A1129 U1130 C1135 G1136 G1139 C1140 U1141 A1143 C1150 A1155 C1158 G1164 U1165 C1166 G1171 G1173 A1174 U1175 G1176 A1177 C1178 C1179 C1180 G1187 G1191 A1210 U1211 G1212 C1218 G1219 A1220 C1221 C1221A A1226 G1238 G1239 U1240 A1241 G1250 C1251 G1252 A1253
G1256 G1260 G1266 U1267 A1268 A1269 C1270 G1271 A1272 U1273 C1297 C1298 G1299 U1300 A1301 A1302 G1303 G1309 C1315 G1328 U1329 G1332 U1340 U1352 A1353 A1354 G1355 G1356 U1357 G1358 A1359 A1360 G1364 A1365 C1370 G1371 U1372 A1379 G1380 G1381 G1382 C1383 A1384 G1385 C1386 C1387
U1396 C1399 U1405 U1406 G1416 C1417 G1418 A1419 U1420 G1421 C1428 G1429 C1430 U1431 G1441 G1442 A1445 G1450 C1450A C1451 A1452 U1453 G1455 G1459 A1460 C1467 C1468 A1469 G1470 A1471 G1482 A1486 G1487 C1493 U1503 C1504 A1508 C1509 A1509A A1509B G1510 C1511 U1518 G1519 G1520
G1525 A1528 C1530 C1531 C1532 G U A C G1537 U1540 G1541 A1542 C1543 C1547 A1558 A1566 A1567 G1568 A1569 A1570 A1571 U1578 A1579 A1580 G1581 C1582 A1583 C1584 A1586 A1587 C1588 C1589 G1593 G1594 C1604 A1608 A1609 A1610 G1626 A1634 A1637 C1638 U1639 C1640 A1641
G1642 G1643 C1644 C1648 G1653 A1654 A1664 A1665 A1668 A1669 C1670 U1671 G1674 G1682 C1686 G1687 U1688 U1693 G1696 G1697 A1698 G1699 A1700 A1701 G1702 G1703 G1721 A1722 U1739 G1740 A1741 G1747 G1750 C1754 A1755 G1756 U1757 G1758 A1759 A1762 G1763 G1764 G1769 G1770 C1771
G1772 A1773 U1778 U1779 A1780 C1781 C1782 A1783 A1784 A1785 A1786 A1791 G1792 C1793 U1794 C1795 U1796 C1797 U1798 G1799 C1800 G1801 A1802 A1803 A1815 G1816 C1817 U1818 G1826 C1827 G1828 G1839 A1847 G1857 G1858 U1864 G1865 A1877 G1878 A1889 A1890 C1894 G1899 A1900 G1906 U1911
A1912 A1913 C1914 U1915 A1916 U1917 A1918 A1919 C1920 U1923 C1924 G1929 G1930 A1936 A1937 A1938 U1939 U1940 C1941 C1942 U1955 C1958 G1959 A1960 C1961 C1962 U1963 C1967 A1970 A1971 A1972 G1980 C1988 U1993 G1997 C2006 A2013 A2014 U2017 A2020 C2021 U2022 G2023 G2024 C2025
C2026 A2030 A2031 G2032 A2033 G2038 C2039 C2043 C2050 A2051 C2055 G2056 A2060 G2061 C2065 C2066 G2069 U2074 U2075 U2079 A2082 U2086 G2087 G2093 U2096 C2097 U2098 U2099 G2100 G2101 U2102 C2103 G2104 C2105 G2106 C2107 C2108 G2110 C2111 C2112 U2113 A2114 C2115 G2116 A2117
U2118 A2119 U2122 G2123 G2124 G2125 A2126 G2127 C2128 C2129 U2130 G2131 U2132 G2133 A2134 A2135 C2136 C2137 C2138 C2139 C2140 G2141 C2142 C2143 U2144 C2145 C2146 G2147 G2148 G2149 U2150 G2151 G2152 G2153 G2154 G2155 G2156 G2157 A2158 G2159 G2160 C2161 G2162 C2163 C2164 G2165 G2166 U2167 G2168 A2169 A2170 A2171 U2172 A2173 C2174 C2175 A2176 G2181
G2182 C2183 G2184 C2185 G2186 G2187 C2188 U2189 G2190 G2191 G2192 A2198 G2206 G2207 A2208 A2225 G2228 G2238 G2239 G2242 U2243 U2244 U2245 C2246 A2247 C2248 G2251 G2252 A2267 A2268 A2269 A2273 A2274 C2275 G2276 G2277 A2278 G2279 G2280 C2283 A2286 A2287 A2288 G2289 G2290 U2291 C2292 A2298
G2299 A2305 C2306 G2307 G2308 A2309 A2310 C2316 C2317 G2318 G2319 A2320 G2321 A2322 G2323 C2324 G2325 C2326 A2327 A2328 G2329 G2330 G2331 G2334 A2335 A2336 G2345 A2346 C2347 U2348 G2349 C2350 G2354 C2355 C2359 A2360 G2365 A2366 G2367 A2377 A2378 G2379 C2380 C2381 G2382 G2383 G2384 C2385 U2390 A2393
G2396 C2404 G2405 U2406 G2410 C2417 A2422 U2423 C2424 A2425 A2426 C2427 G2428 G2429 A2430 U2431 A2432 A2435 A2439 C2440 C2441 C2442 C2443 G2444 G2445 G2446 G2447 A2448 C2461 U2462 G2468 A2469 G2470 A2476 C2477 A2478 G2486 U2492 U2493 G2494 G2496 C2496 A2497 C2498 G2502 A2503 U2504
G2505 U2506 C2507 G2508 C2515 G2516 C2517 A2518 G2525 G2529 A2533 A2534 U2537 C2538 C2539 G2543 G2544 U2552 G2553 U2554 U2563 A2566 G2567 A2572 C2573 G2574 C2575 G2576 A2577 G2578 U2585 C2586 A2587 G2588 A2589 A2590 C2591 G2592 A2602 U2605 C2606 G2607 G2608 U2609 C2610 U2611 C2612
U2615 C2616 C2617 G2618 C2619 G2627 C2628 A2629 G2630 G2631 U2637 C2646 U2647 U2653 A2654 G2659 A2662 A2665 G2674 C2683 U2687 U2688 U2689 C2690 A2693 G2694 U2698 C2699 U2702 C2703 C2710 A2711 U2712 A2712A A2713 G2714 A2721 G2722 C2723 U2726 G2732 A2733

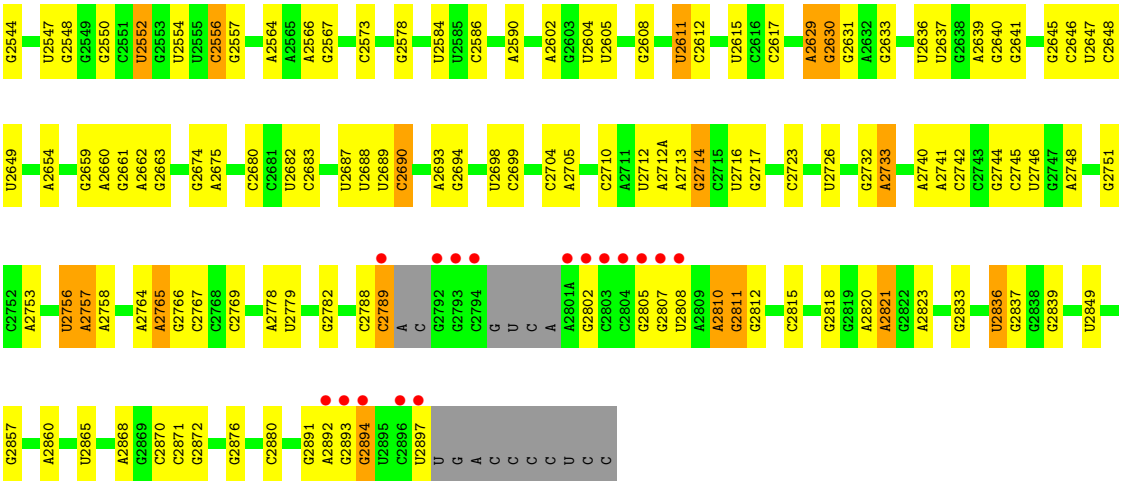


• Molecule 1: 23S Ribosomal RNA

Chain 2A:

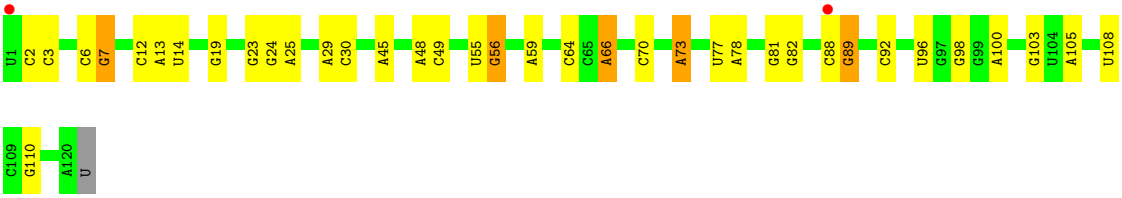






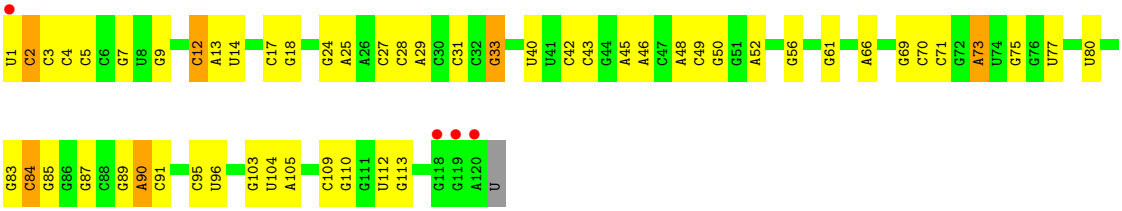
• Molecule 2: 5S Ribosomal RNA

Chain 1B:



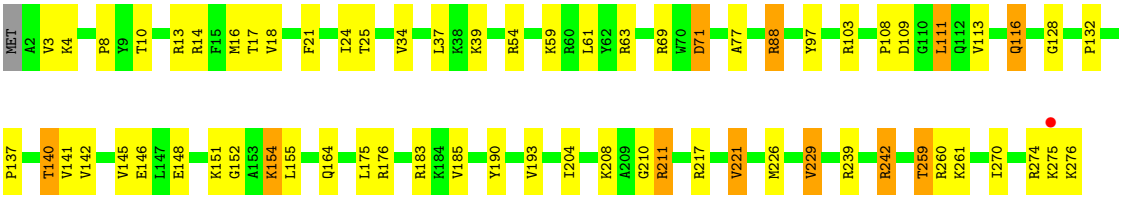
• Molecule 2: 5S Ribosomal RNA

Chain 2B:



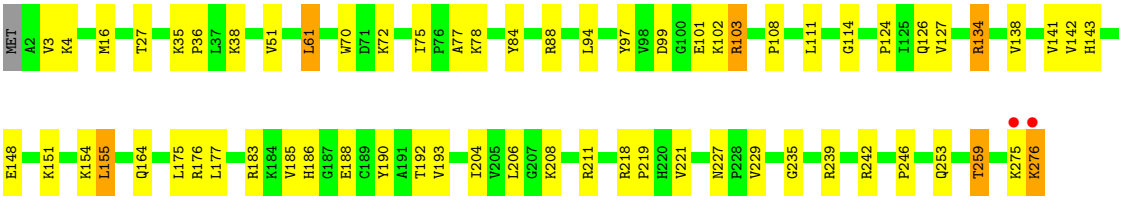
• Molecule 3: 50S ribosomal protein L2

Chain 1D:



• Molecule 3: 50S ribosomal protein L2

Chain 2D:

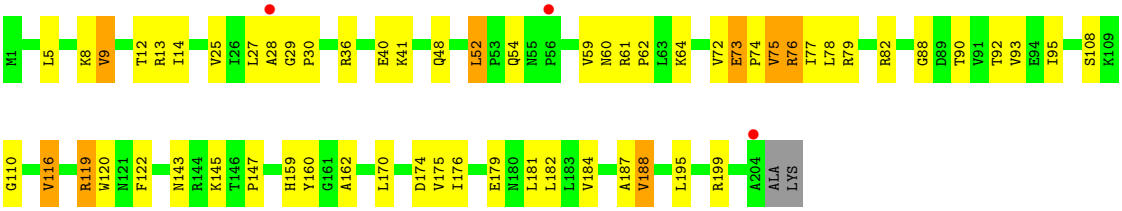


• Molecule 4: 50S ribosomal protein L3

Chain 1E:

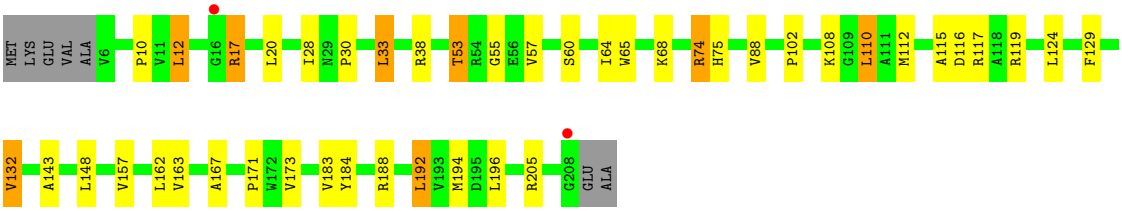
• Molecule 4: 50S ribosomal protein L3

Chain 2E:



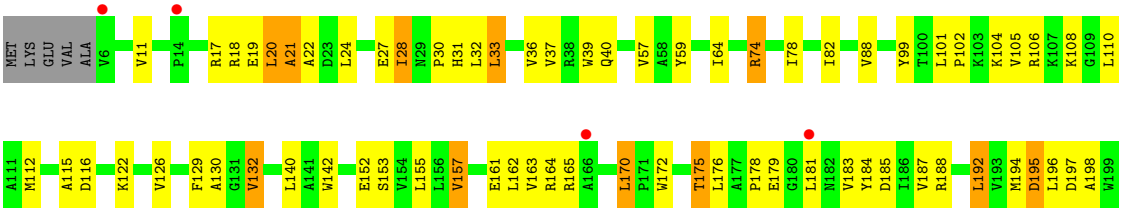
• Molecule 5: 50S ribosomal protein L4

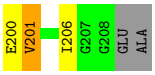
Chain 1F:



• Molecule 5: 50S ribosomal protein L4

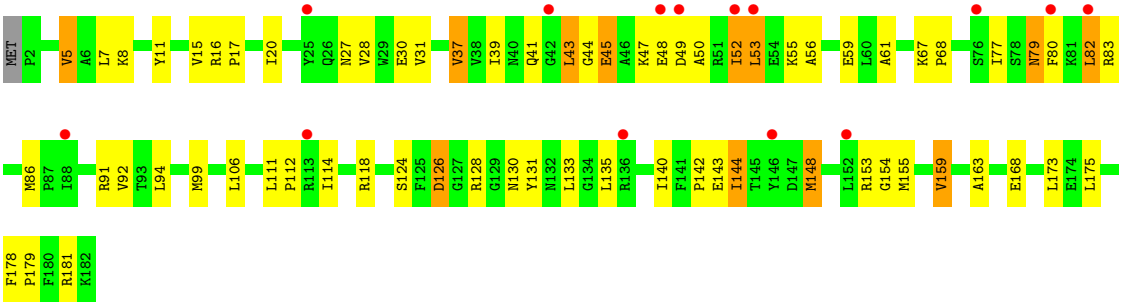
Chain 2F:





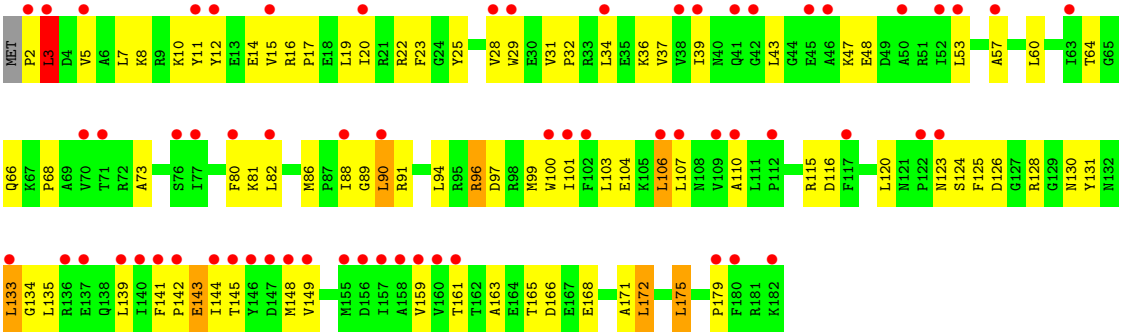
• Molecule 6: 50S ribosomal protein L5

Chain 1G:



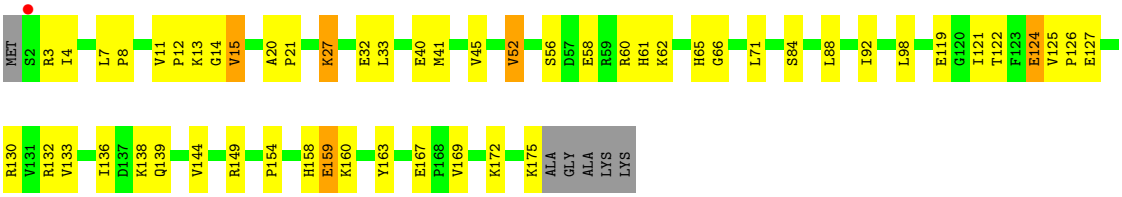
• Molecule 6: 50S ribosomal protein L5

Chain 2G:



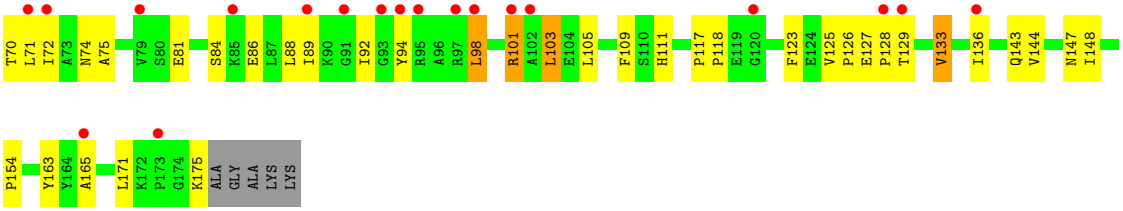
• Molecule 7: 50S ribosomal protein L6

Chain 1H:



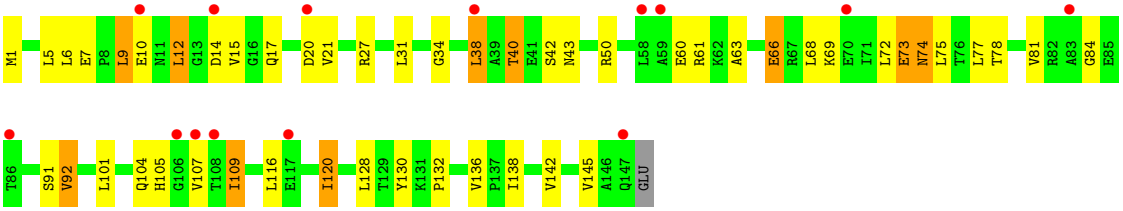
• Molecule 7: 50S ribosomal protein L6

Chain 2H:



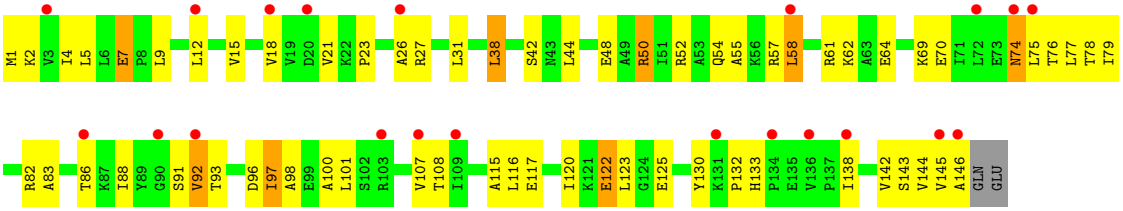
• Molecule 8: 50S ribosomal protein L9

Chain 1I:



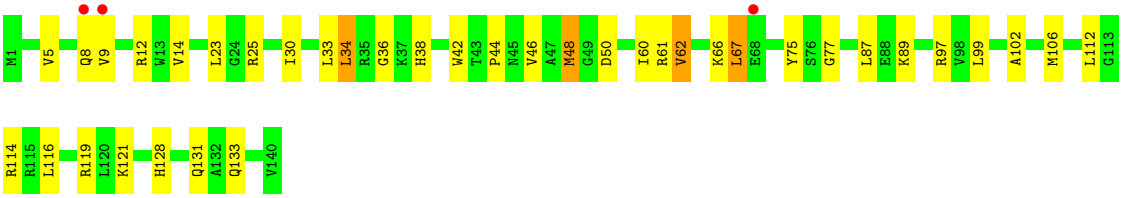
• Molecule 8: 50S ribosomal protein L9

Chain 2I:



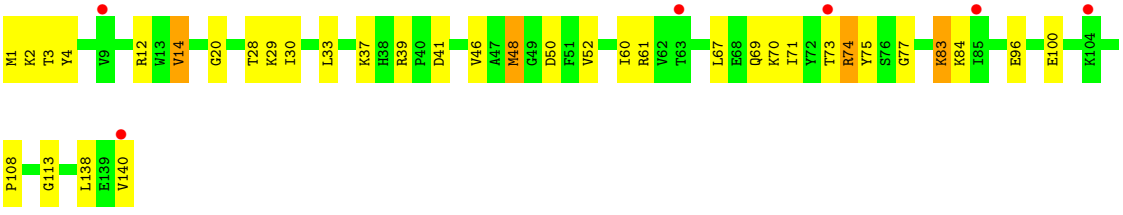
• Molecule 9: 50S ribosomal protein L13

Chain 1N:



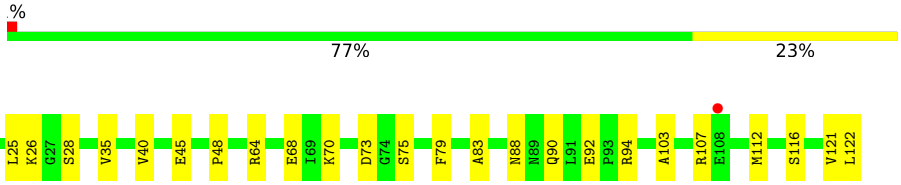
• Molecule 9: 50S ribosomal protein L13

Chain 2N:



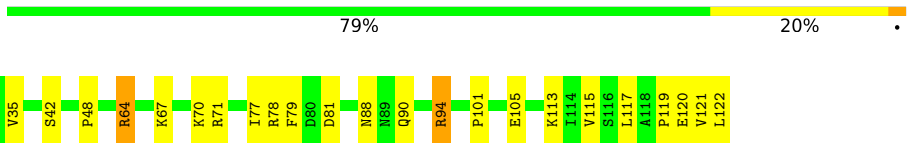
• Molecule 10: 50S ribosomal protein L14

Chain 1O:



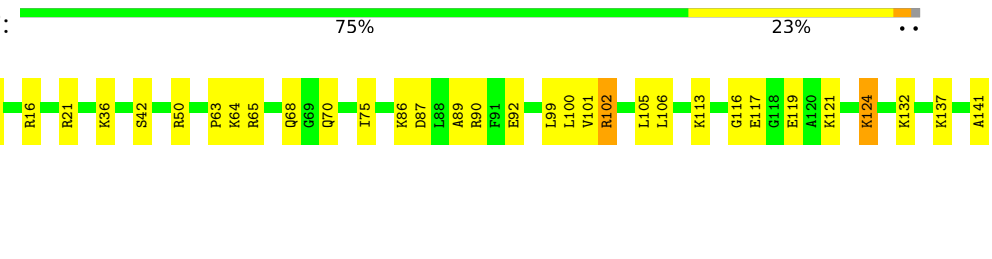
• Molecule 10: 50S ribosomal protein L14

Chain 2O:



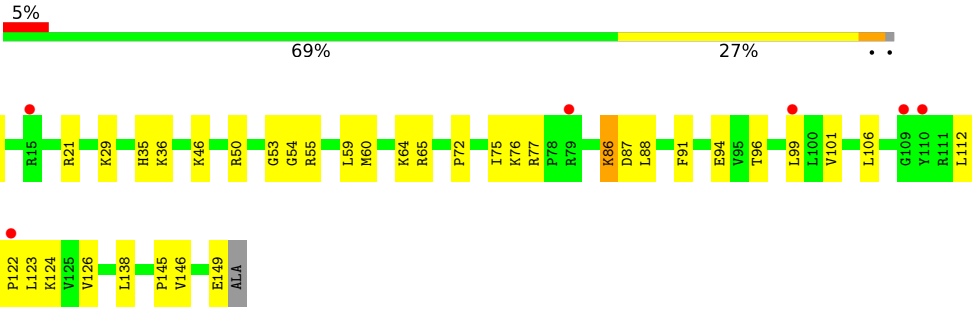
• Molecule 11: 50S ribosomal protein L15

Chain 1P:



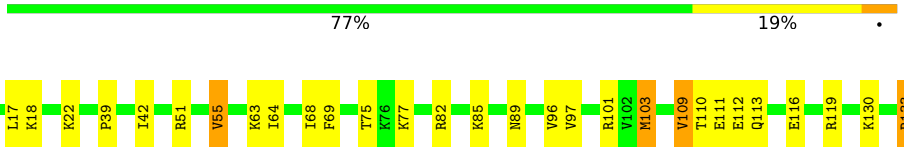
• Molecule 11: 50S ribosomal protein L15

Chain 2P:



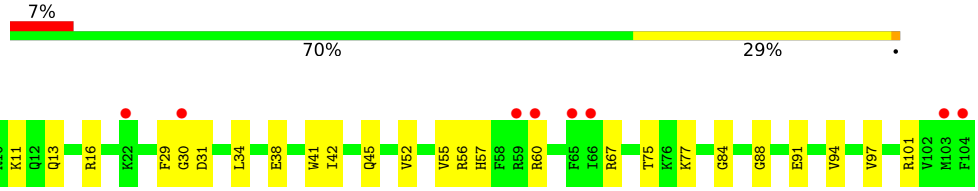
• Molecule 12: 50S ribosomal protein L16

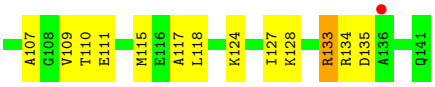
Chain 1Q:



• Molecule 12: 50S ribosomal protein L16

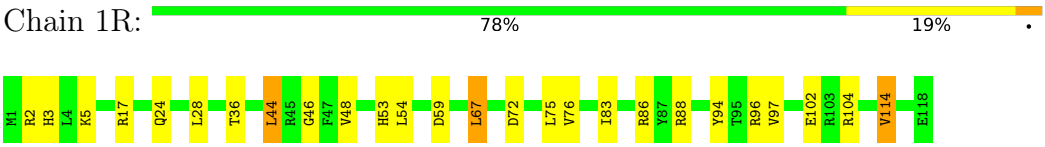
Chain 2Q:





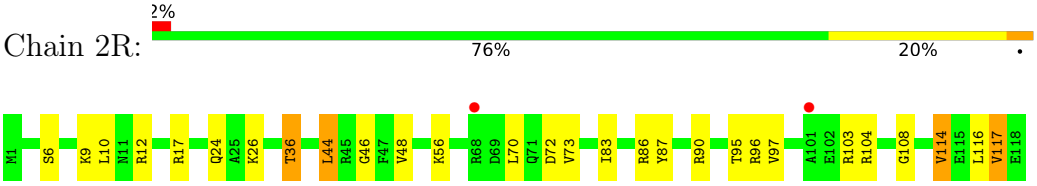
• Molecule 13: 50S ribosomal protein L17

Chain 1R:



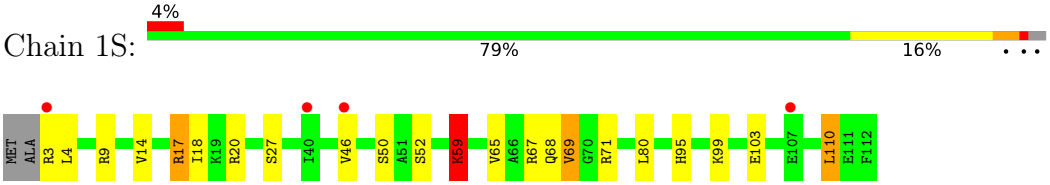
• Molecule 13: 50S ribosomal protein L17

Chain 2R:



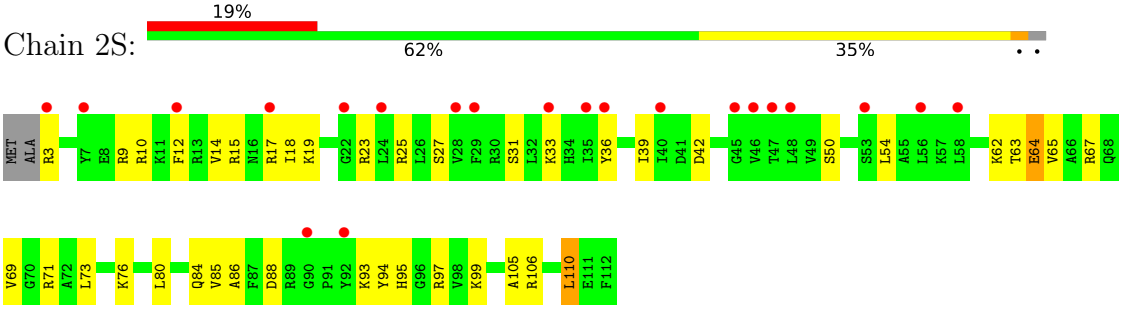
• Molecule 14: 50S ribosomal protein L18

Chain 1S:



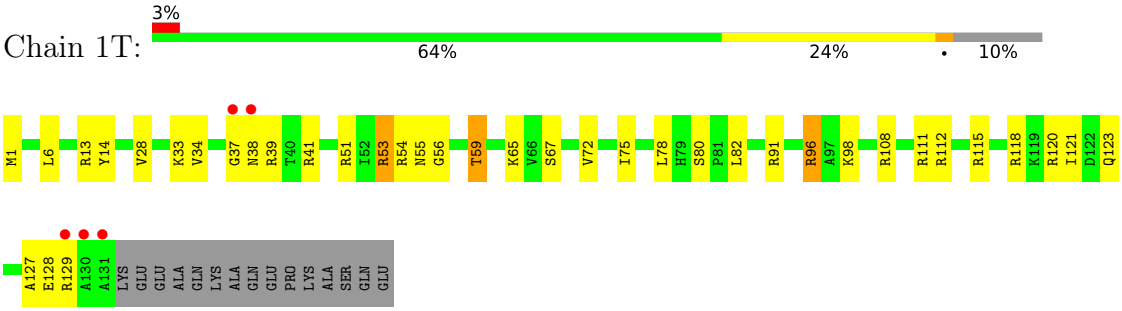
• Molecule 14: 50S ribosomal protein L18

Chain 2S:



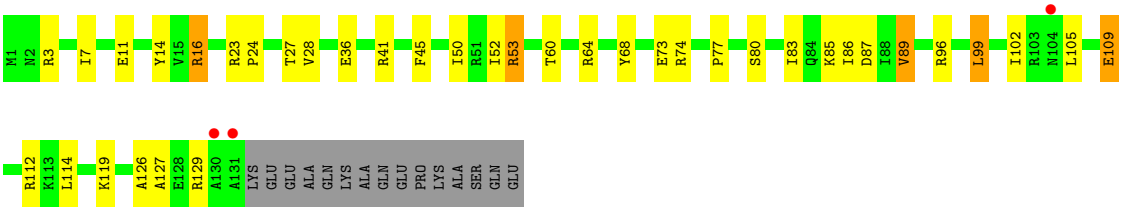
• Molecule 15: 50S ribosomal protein L19

Chain 1T:



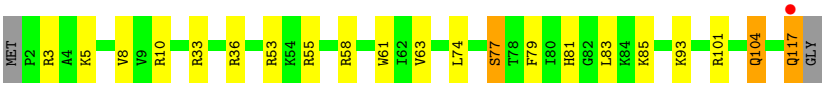
• Molecule 15: 50S ribosomal protein L19

Chain 2T:



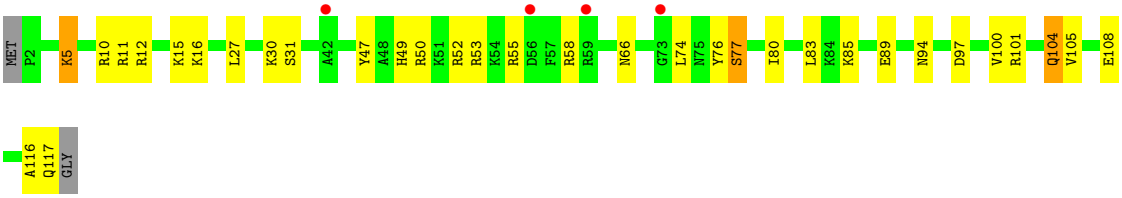
• Molecule 16: 50S ribosomal protein L20

Chain 1U:



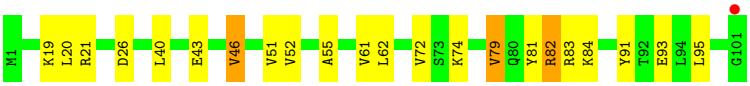
• Molecule 16: 50S ribosomal protein L20

Chain 2U:



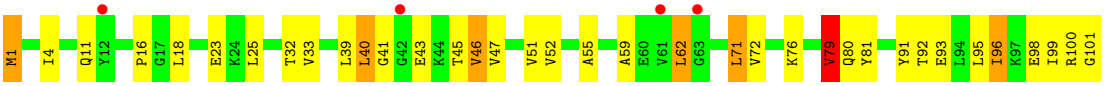
• Molecule 17: 50S ribosomal protein L21

Chain 1V:



• Molecule 17: 50S ribosomal protein L21

Chain 2V:

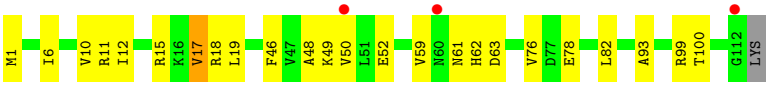


• Molecule 18: 50S ribosomal protein L22

Chain 1W:

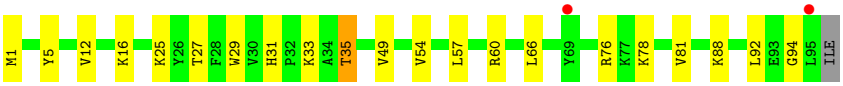
• Molecule 18: 50S ribosomal protein L22

Chain 2W:



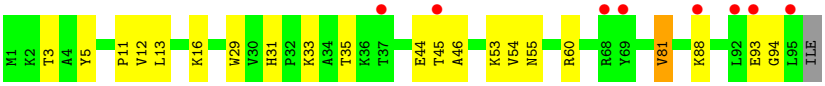
• Molecule 19: 50S ribosomal protein L23

Chain 1X:



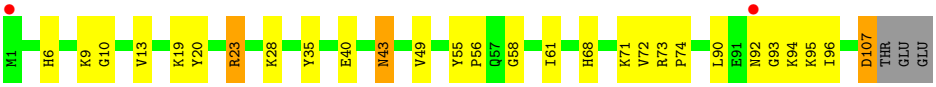
• Molecule 19: 50S ribosomal protein L23

Chain 2X:



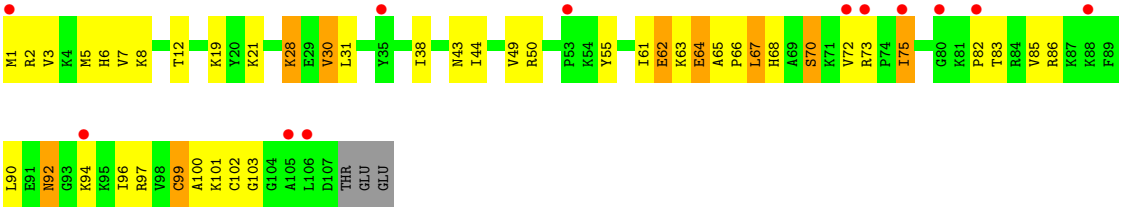
• Molecule 20: 50S ribosomal protein L24

Chain 1Y:



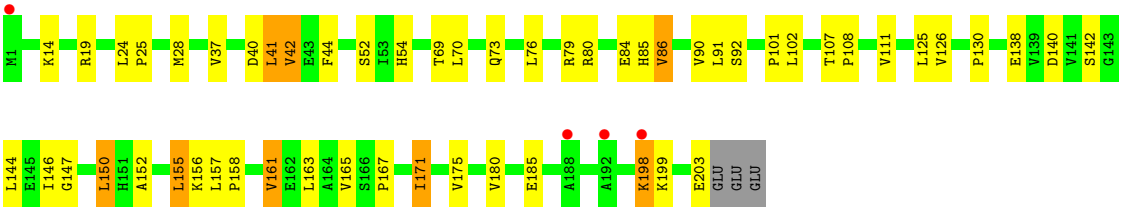
• Molecule 20: 50S ribosomal protein L24

Chain 2Y:



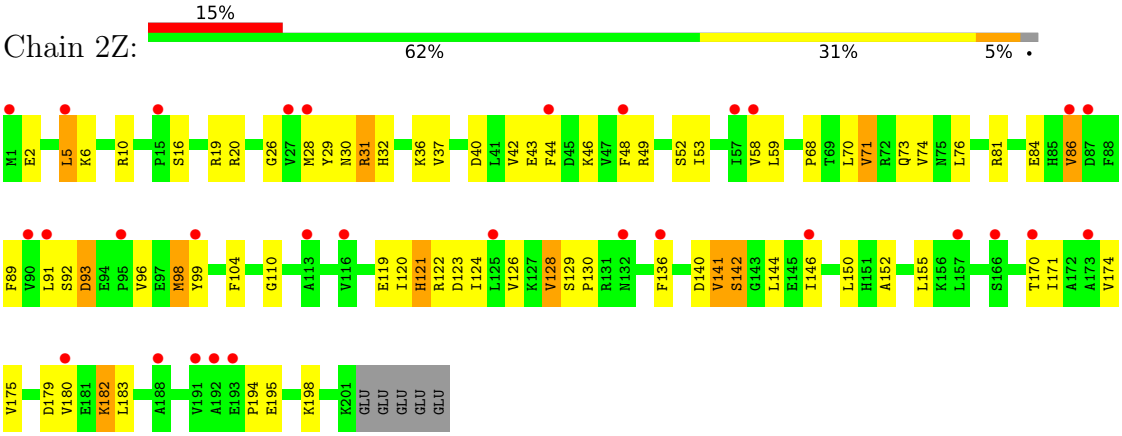
• Molecule 21: 50S ribosomal protein L25

Chain 1Z:



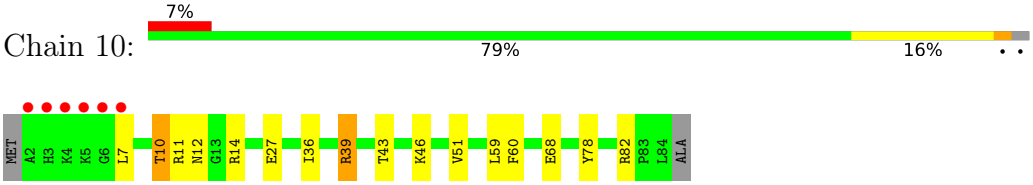
• Molecule 21: 50S ribosomal protein L25

Chain 2Z:



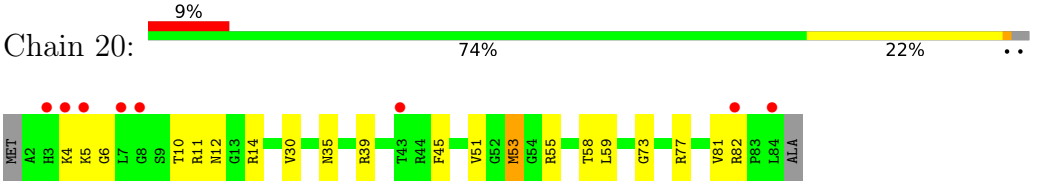
• Molecule 22: 50S ribosomal protein L27

Chain 10:



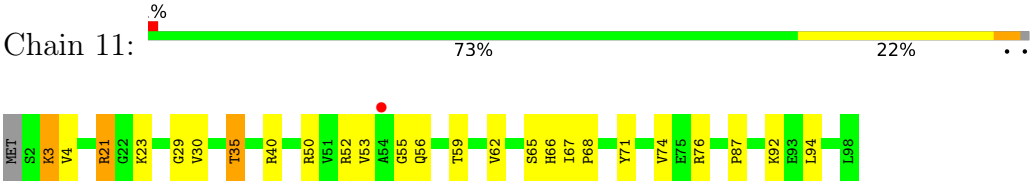
• Molecule 22: 50S ribosomal protein L27

Chain 20:



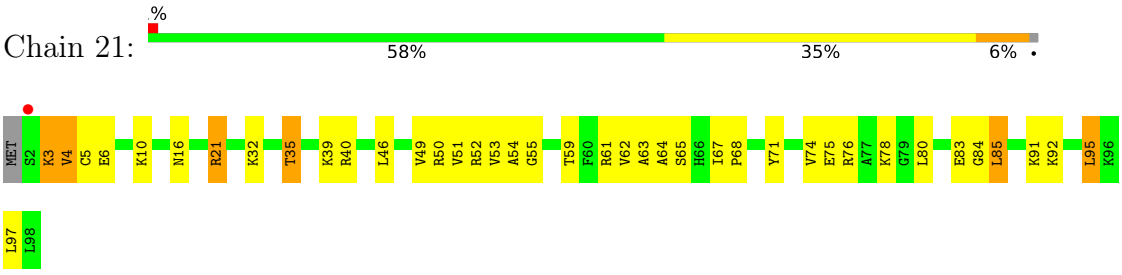
• Molecule 23: 50S ribosomal protein L28

Chain 11:



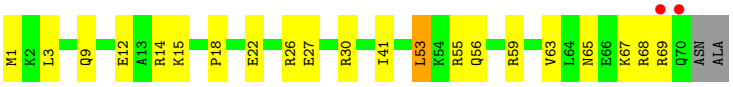
• Molecule 23: 50S ribosomal protein L28

Chain 21:



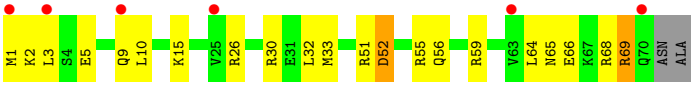
• Molecule 24: 50S ribosomal protein L29

Chain 12:



• Molecule 24: 50S ribosomal protein L29

Chain 22:

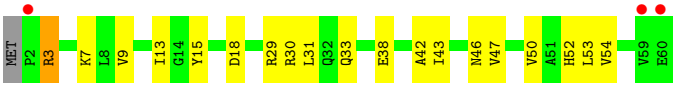


• Molecule 25: 50S ribosomal protein L30

Chain 13:

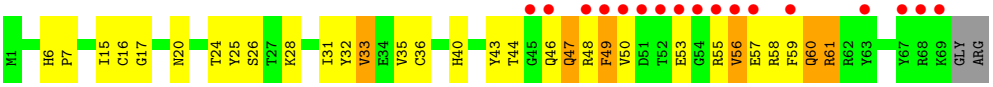
• Molecule 25: 50S ribosomal protein L30

Chain 23:



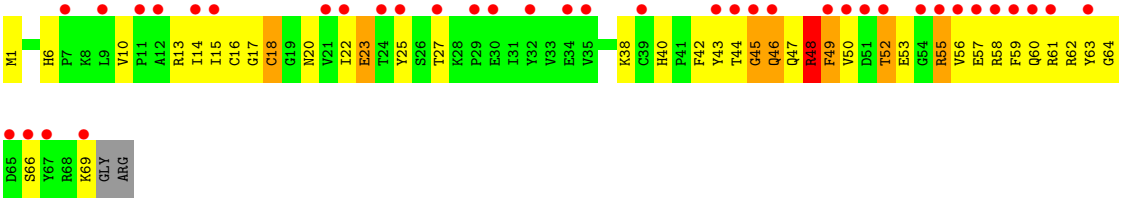
• Molecule 26: 50S ribosomal protein L31

Chain 14:



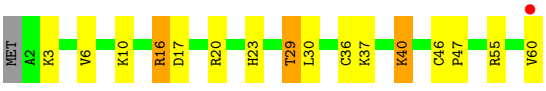
• Molecule 26: 50S ribosomal protein L31

Chain 24:



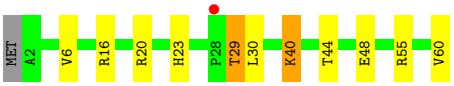
• Molecule 27: 50S ribosomal protein L32

Chain 15:



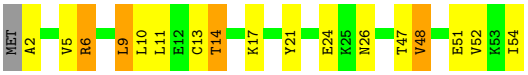
• Molecule 27: 50S ribosomal protein L32

Chain 25:



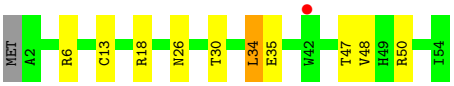
• Molecule 28: 50S ribosomal protein L33

Chain 16:



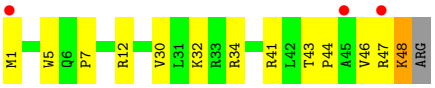
• Molecule 28: 50S ribosomal protein L33

Chain 26:



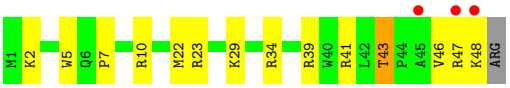
• Molecule 29: 50S ribosomal protein L34

Chain 17:



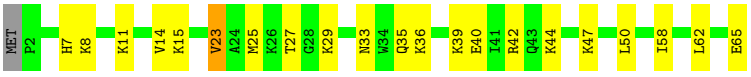
• Molecule 29: 50S ribosomal protein L34

Chain 27:



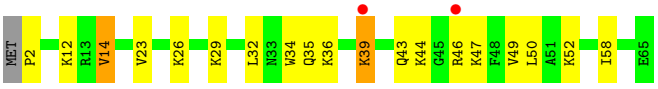
• Molecule 30: 50S ribosomal protein L35

Chain 18:



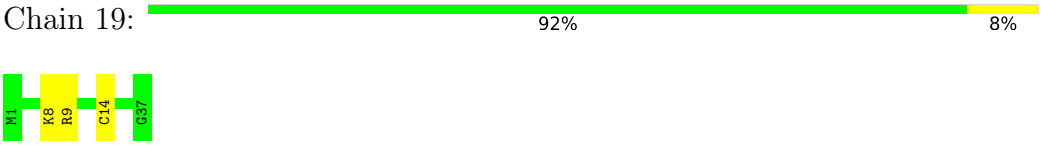
• Molecule 30: 50S ribosomal protein L35

Chain 28:



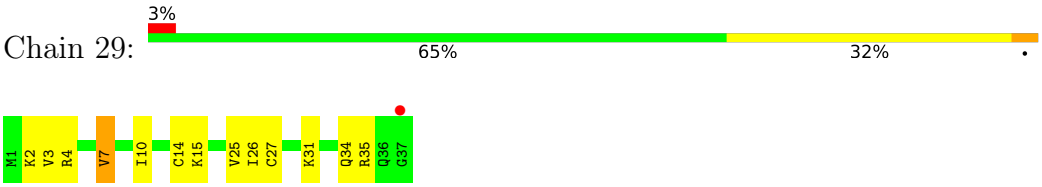
• Molecule 31: 50S ribosomal protein L36

Chain 19:



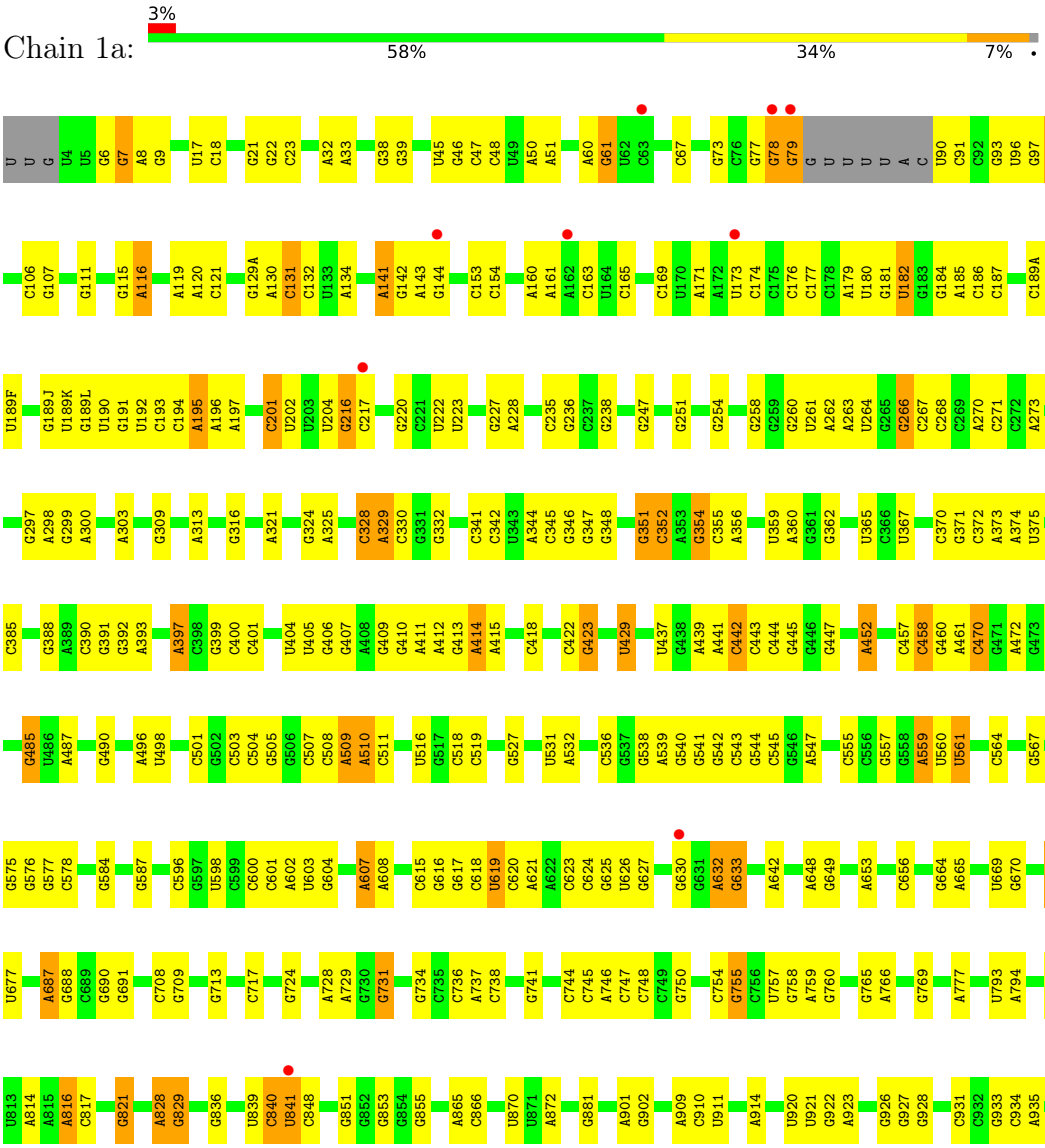
• Molecule 31: 50S ribosomal protein L36

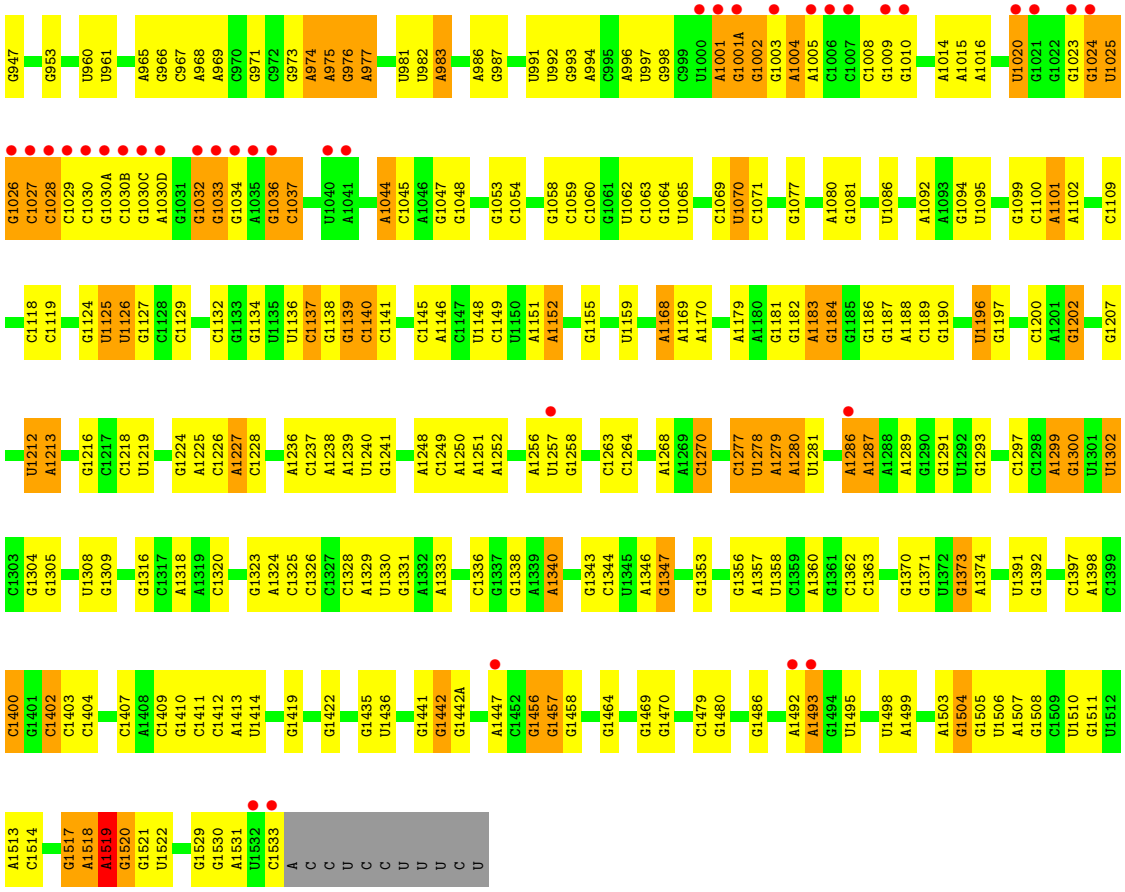
Chain 29:



• Molecule 32: 16S Ribosomal RNA

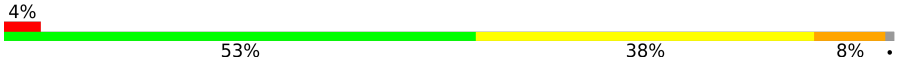
Chain 1a:

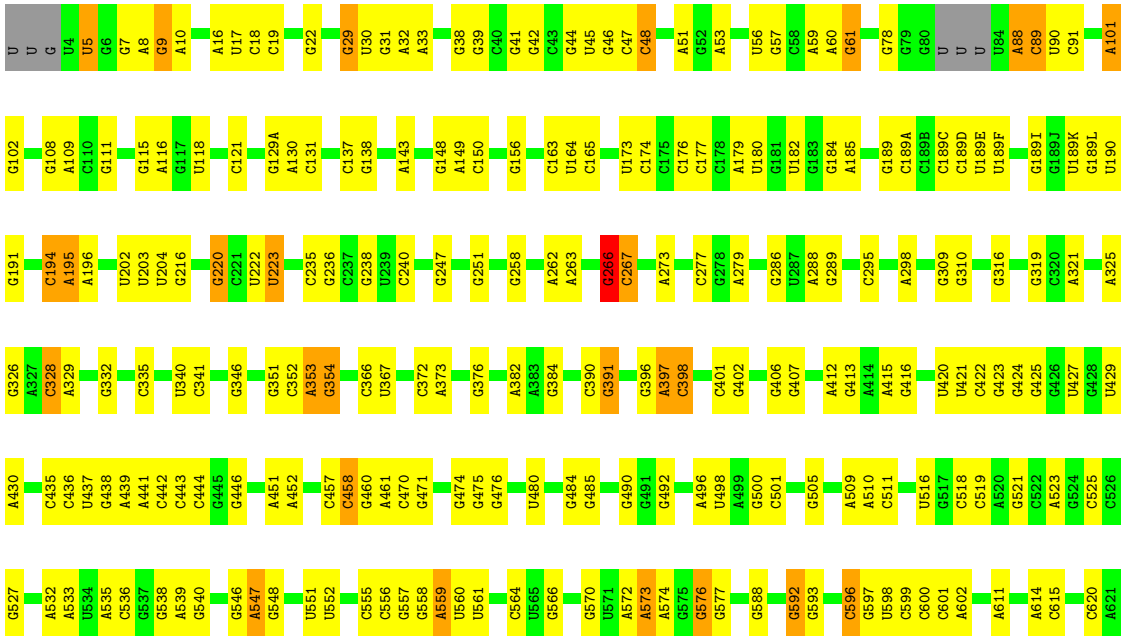


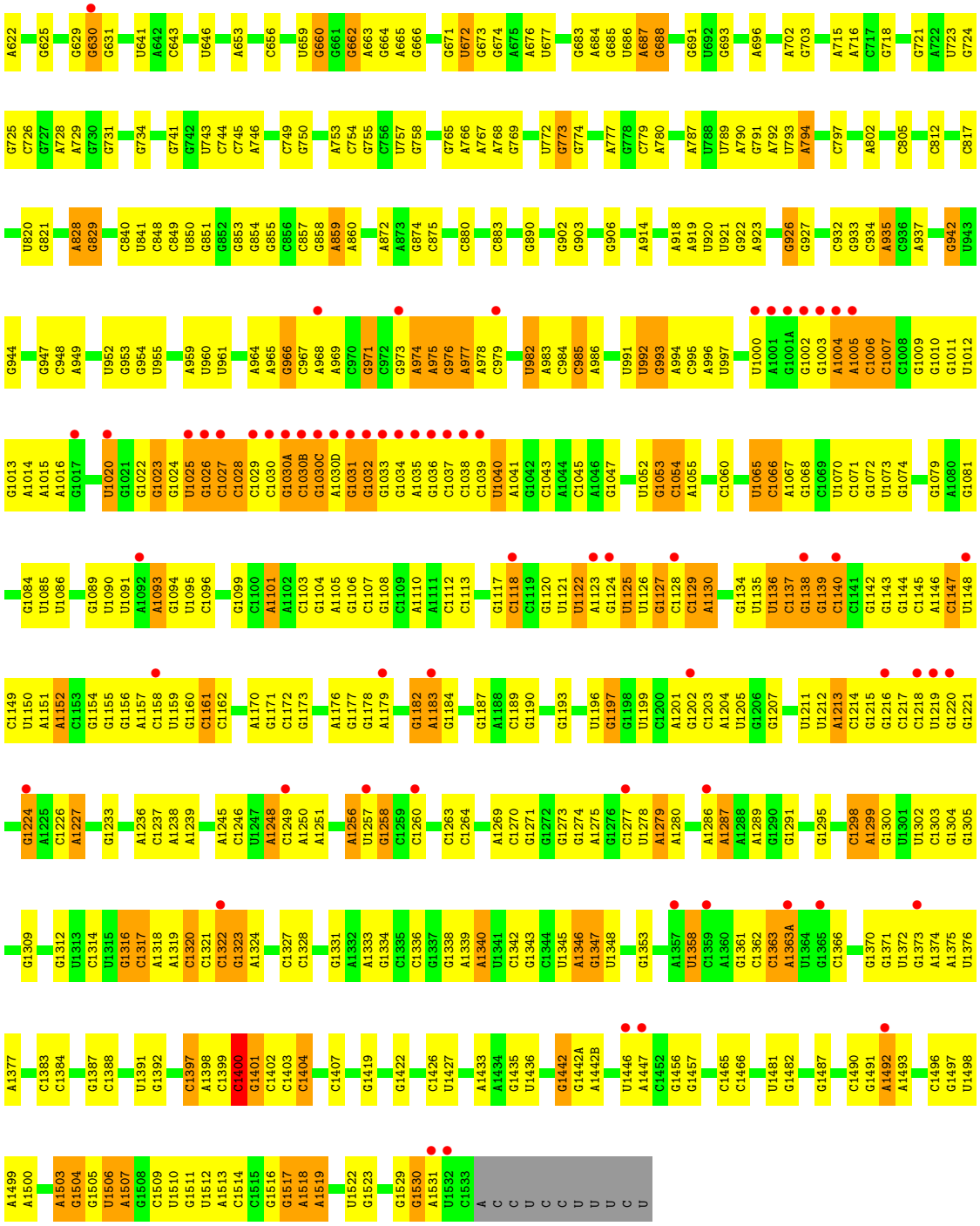


• Molecule 32: 16S Ribosomal RNA

Chain 2a:

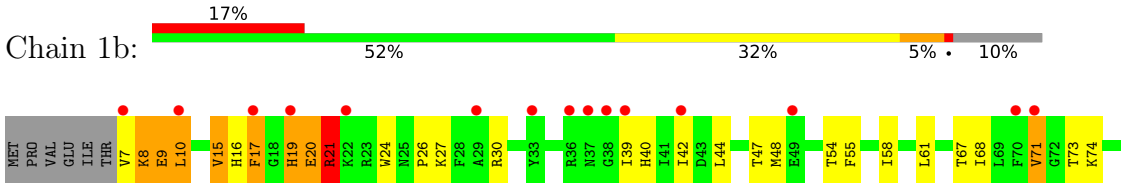


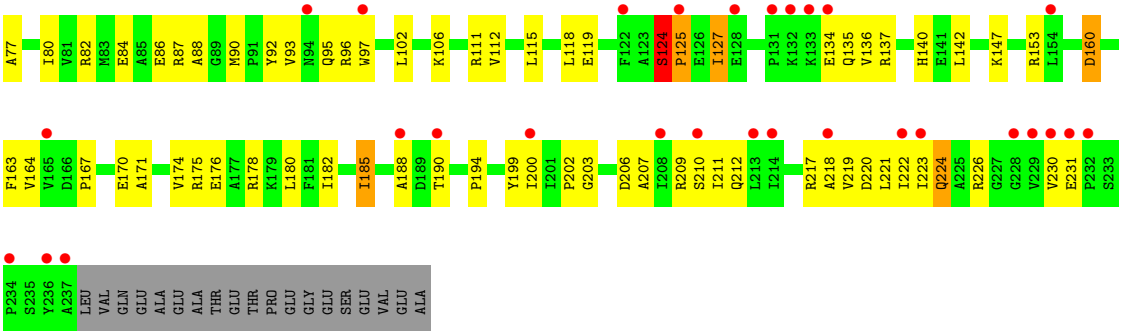




• Molecule 33: 30S ribosomal protein S2

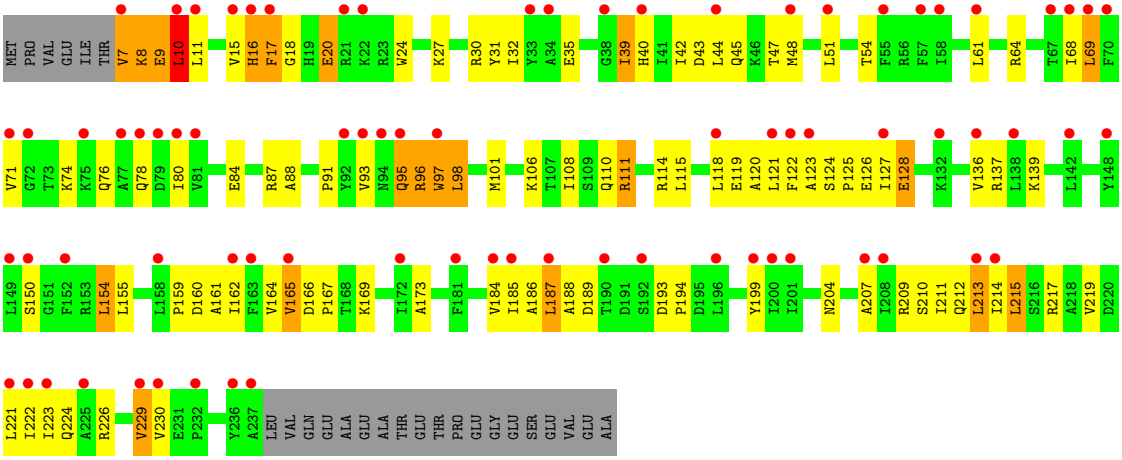
Chain 1b:





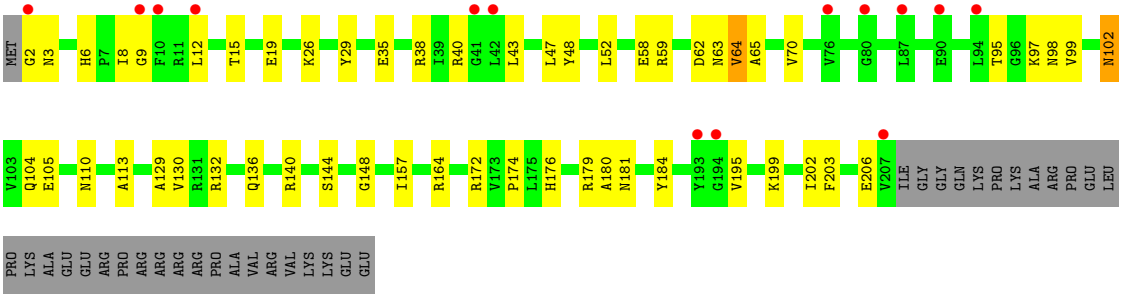
• Molecule 33: 30S ribosomal protein S2

Chain 2b:



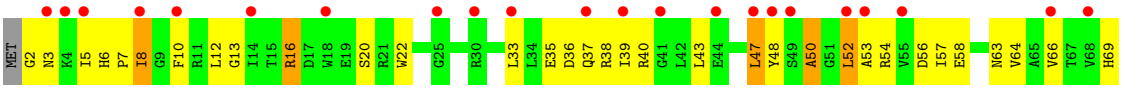
• Molecule 34: 30S ribosomal protein S3

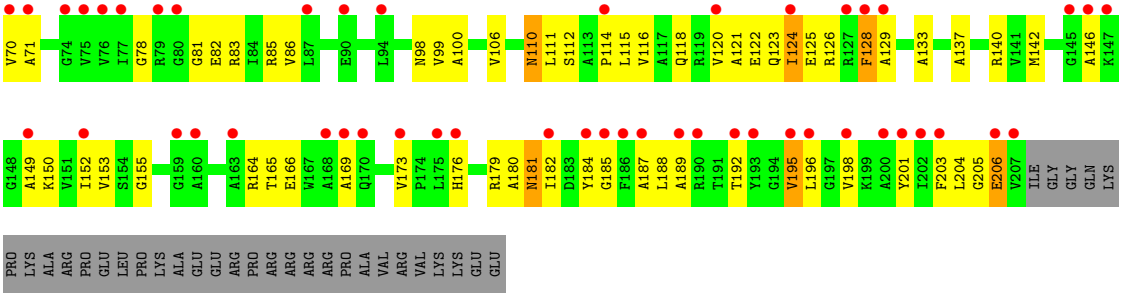
Chain 1c:



• Molecule 34: 30S ribosomal protein S3

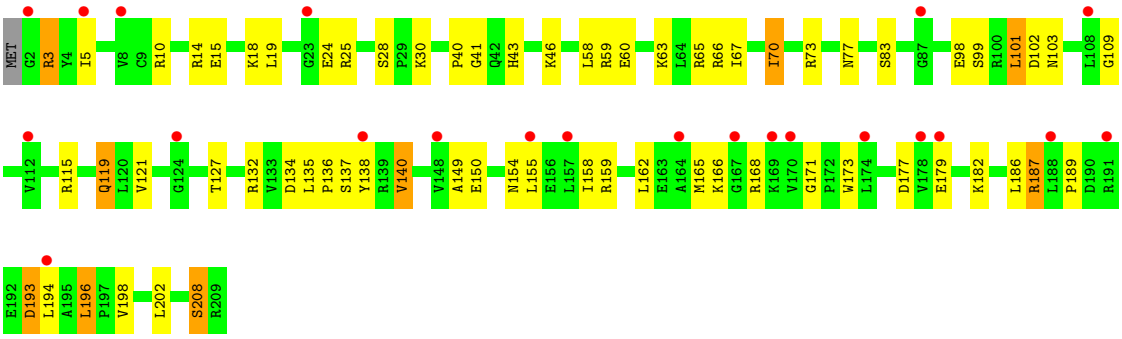
Chain 2c:





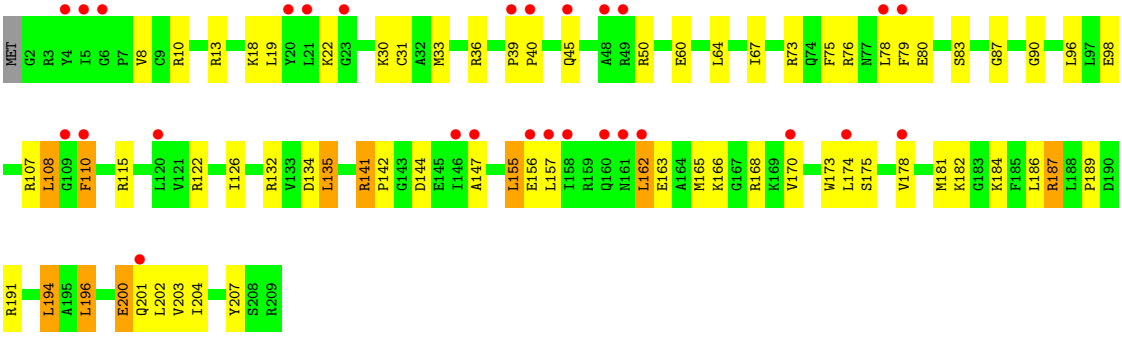
• Molecule 35: 30S ribosomal protein S4

Chain 1d:



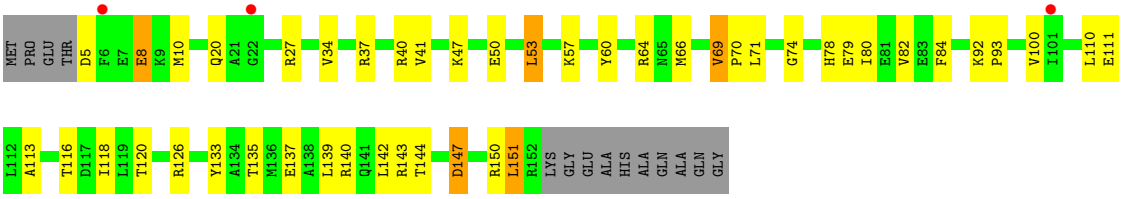
• Molecule 35: 30S ribosomal protein S4

Chain 2d:



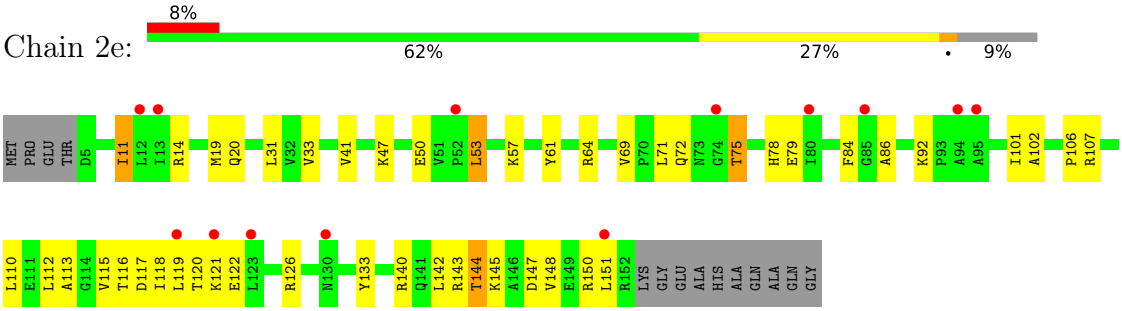
• Molecule 36: 30S ribosomal protein S5

Chain 1e:



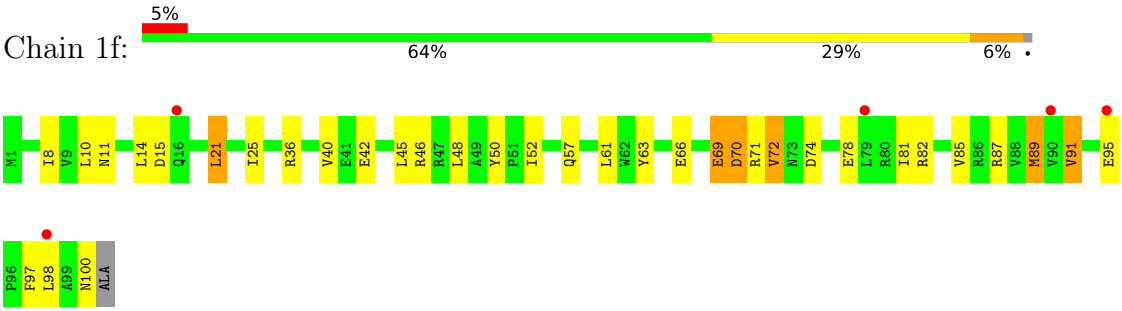
• Molecule 36: 30S ribosomal protein S5

Chain 2e:



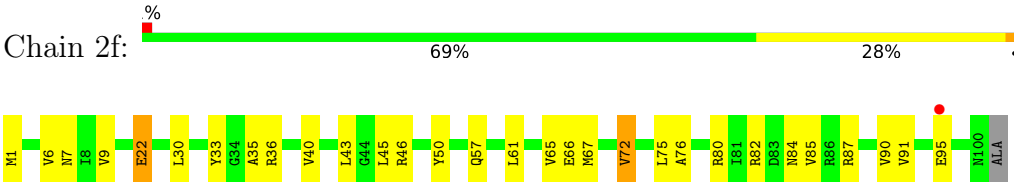
• Molecule 37: 30S ribosomal protein S6

Chain 1f:



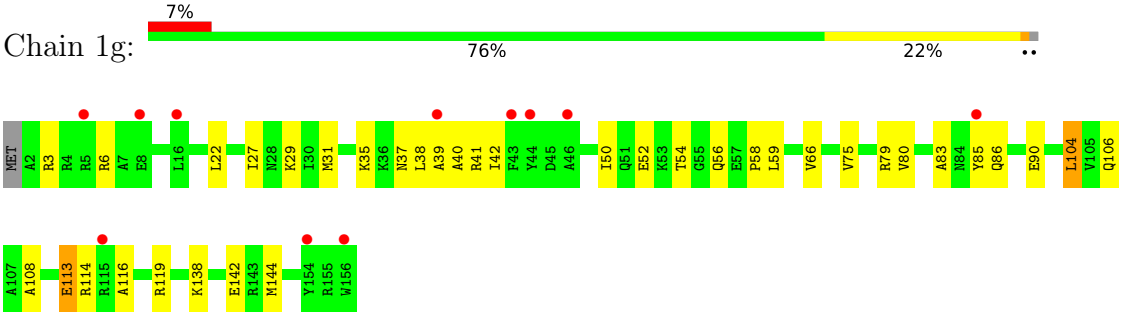
• Molecule 37: 30S ribosomal protein S6

Chain 2f:



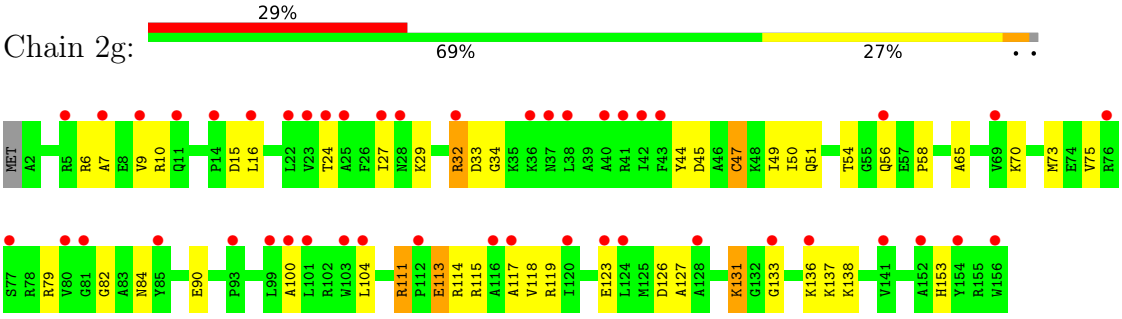
• Molecule 38: 30S ribosomal protein S7

Chain 1g:



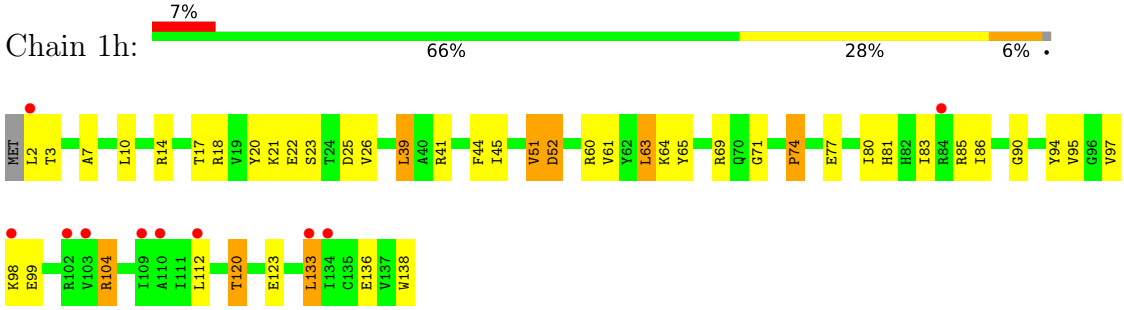
• Molecule 38: 30S ribosomal protein S7

Chain 2g:



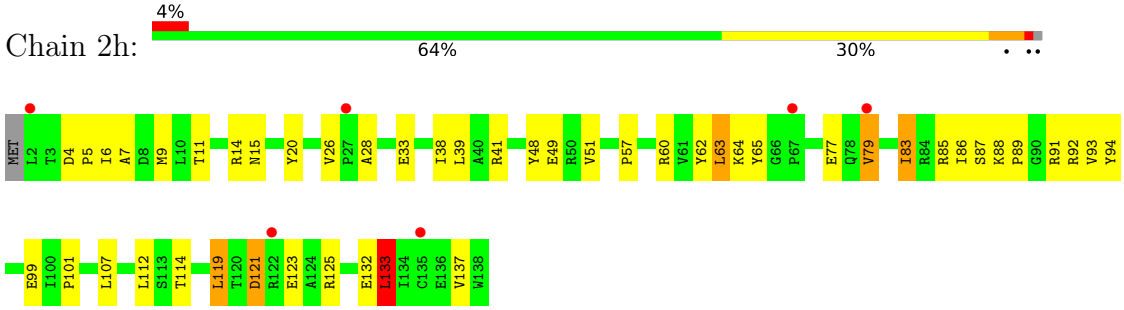
• Molecule 39: 30S ribosomal protein S8

Chain 1h:



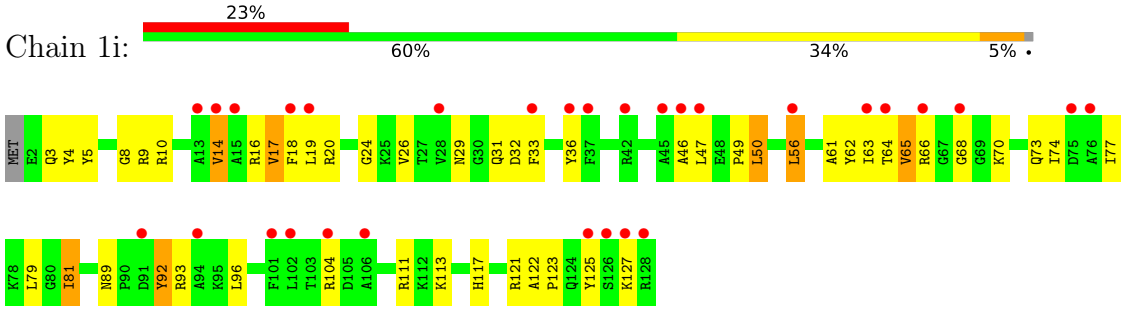
• Molecule 39: 30S ribosomal protein S8

Chain 2h:



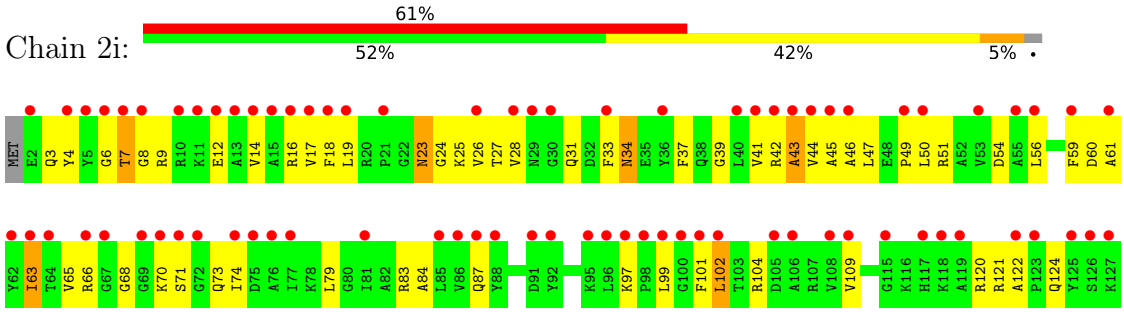
• Molecule 40: 30S ribosomal protein S9

Chain 1i:



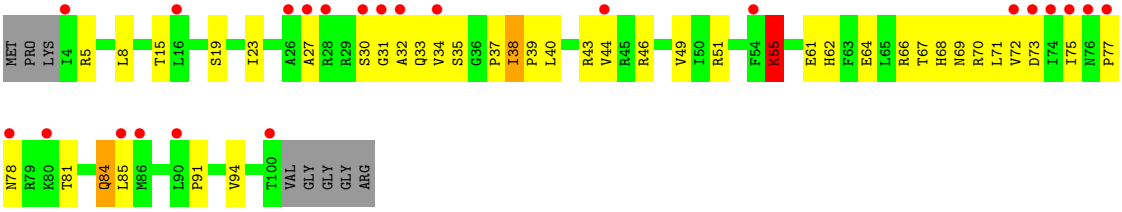
• Molecule 40: 30S ribosomal protein S9

Chain 2i:



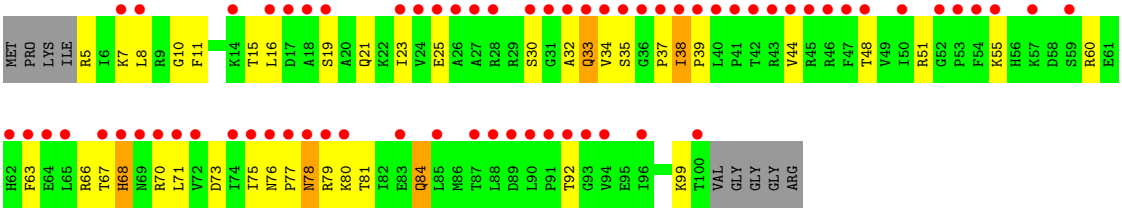
• Molecule 41: 30S ribosomal protein S10

Chain 1j:



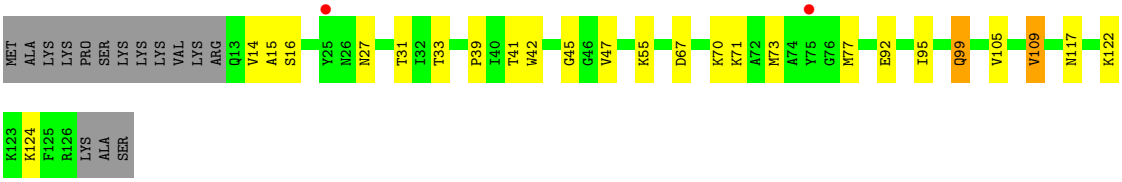
• Molecule 41: 30S ribosomal protein S10

Chain 2j:



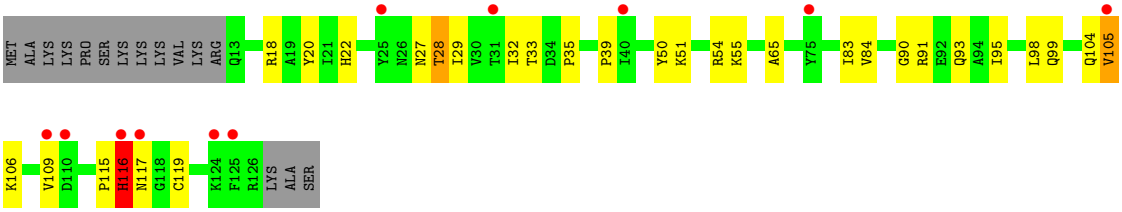
• Molecule 42: 30S ribosomal protein S11

Chain 1k:



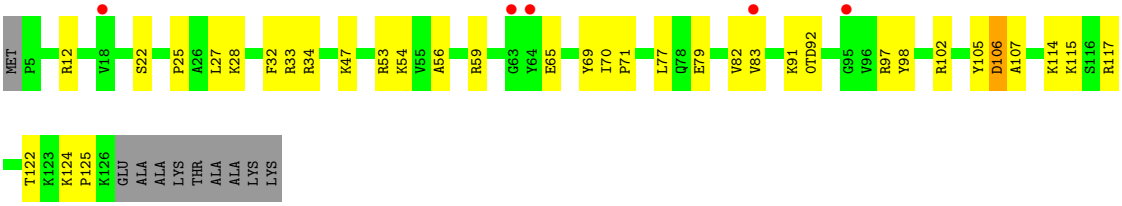
• Molecule 42: 30S ribosomal protein S11

Chain 2k:



• Molecule 43: 30S ribosomal protein S12

Chain 1l:

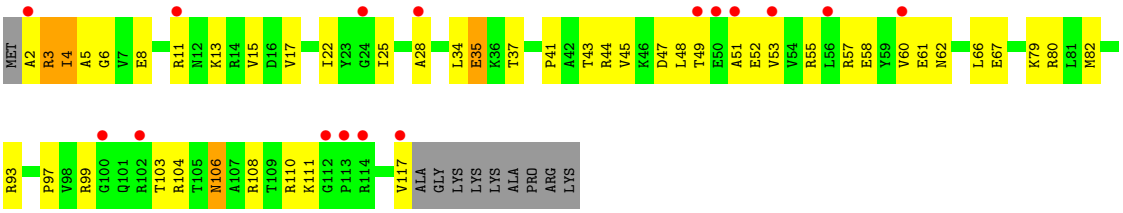


• Molecule 43: 30S ribosomal protein S12

Chain 2l:

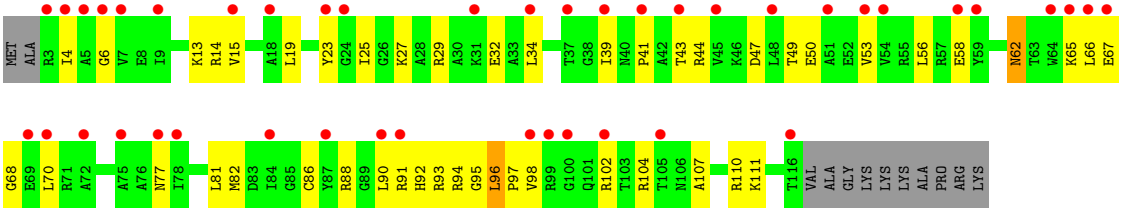
• Molecule 44: 30S ribosomal protein S13

Chain 1m:



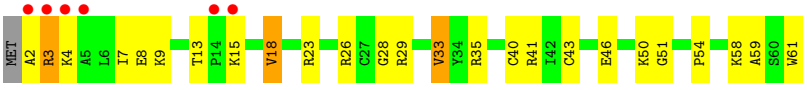
• Molecule 44: 30S ribosomal protein S13

Chain 2m:



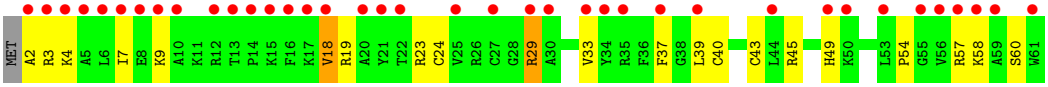
• Molecule 45: 30S ribosomal protein S14 type Z

Chain 1n:



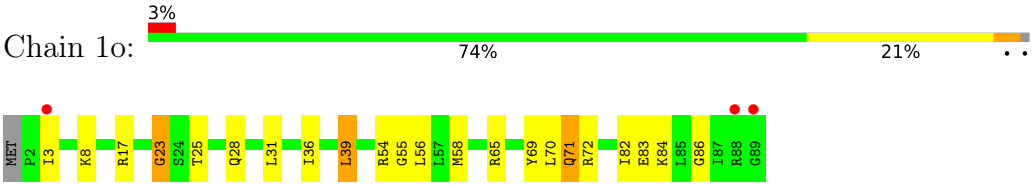
• Molecule 45: 30S ribosomal protein S14 type Z

Chain 2n:



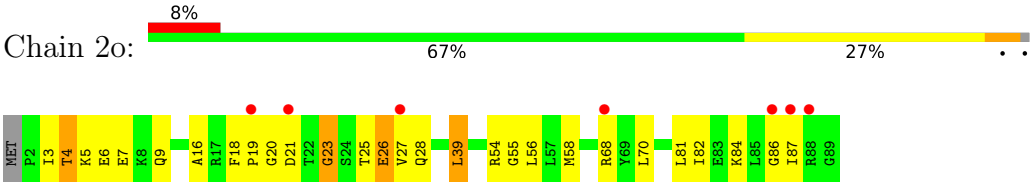
• Molecule 46: 30S ribosomal protein S15

Chain 1o:



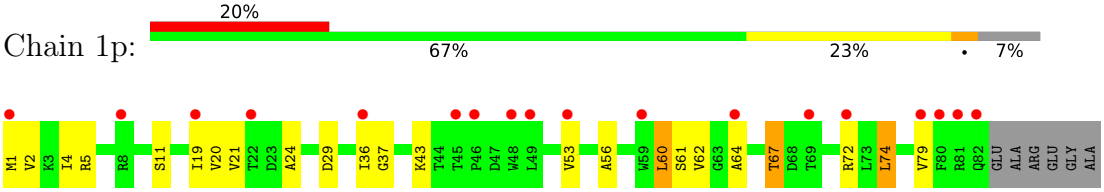
• Molecule 46: 30S ribosomal protein S15

Chain 2o:



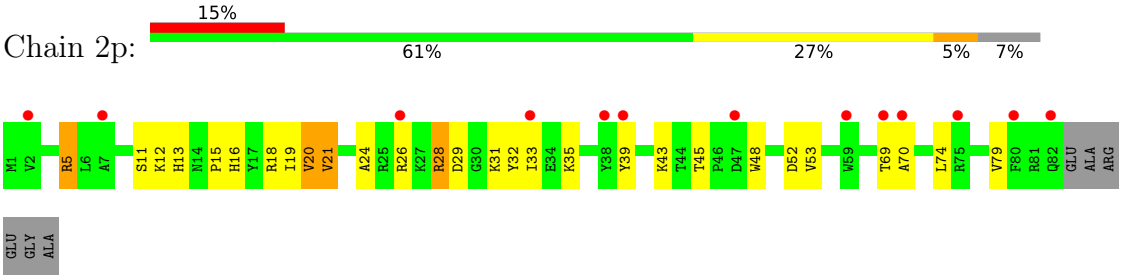
• Molecule 47: 30S ribosomal protein S16

Chain 1p:



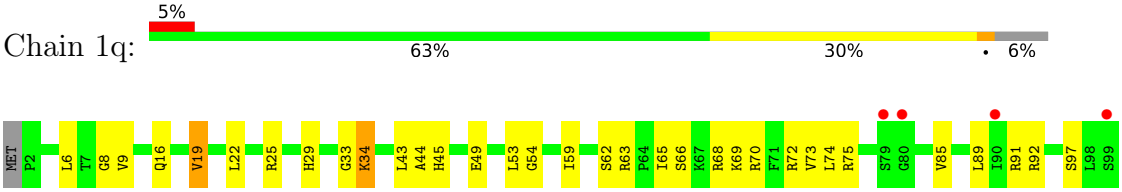
• Molecule 47: 30S ribosomal protein S16

Chain 2p:



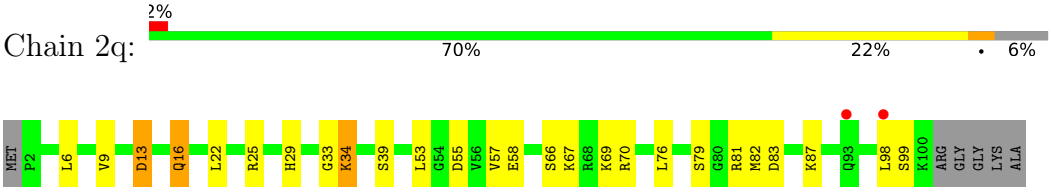
• Molecule 48: 30S ribosomal protein S17

Chain 1q:



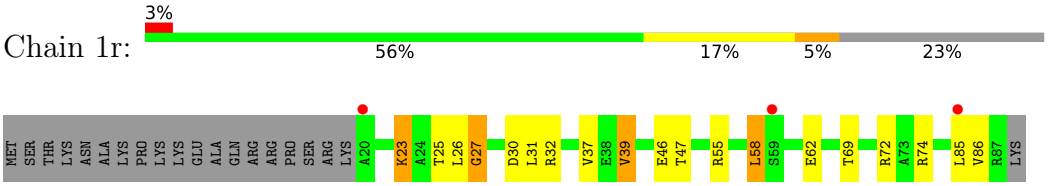
• Molecule 48: 30S ribosomal protein S17

Chain 2q:



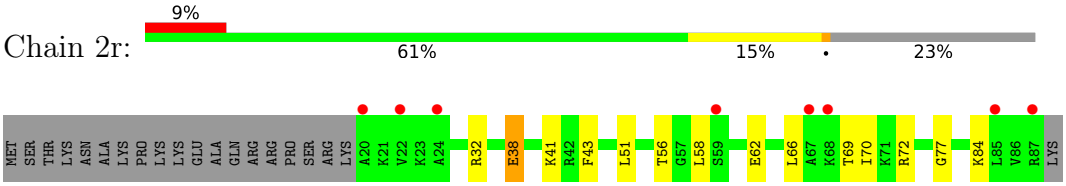
• Molecule 49: 30S ribosomal protein S18

Chain 1r:



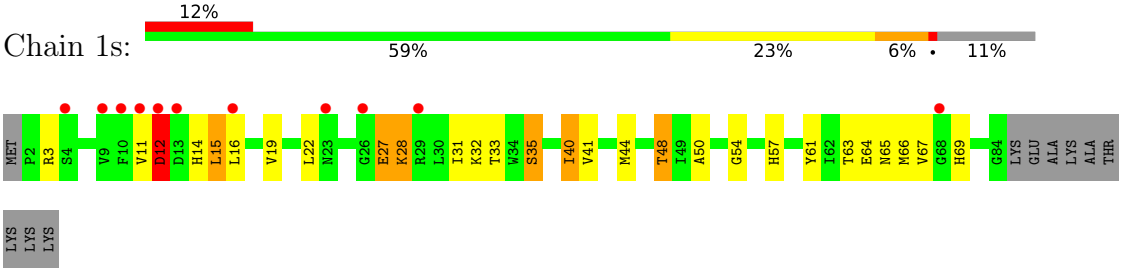
• Molecule 49: 30S ribosomal protein S18

Chain 2r:



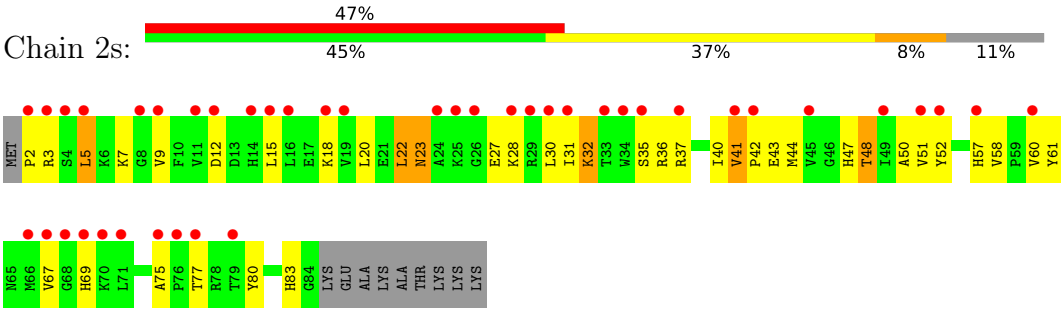
• Molecule 50: 30S ribosomal protein S19

Chain 1s:



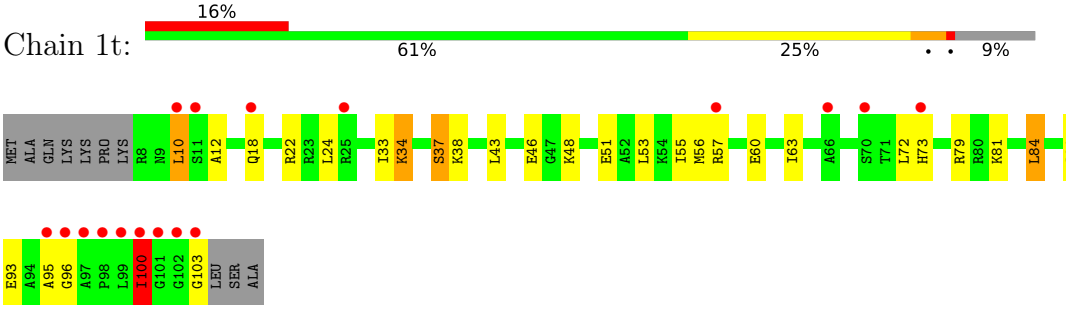
• Molecule 50: 30S ribosomal protein S19

Chain 2s:



• Molecule 51: 30S ribosomal protein S20

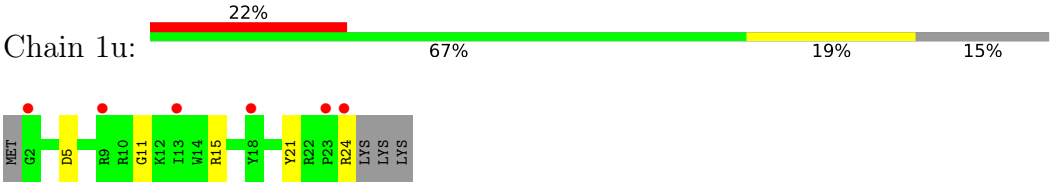
Chain 1t:



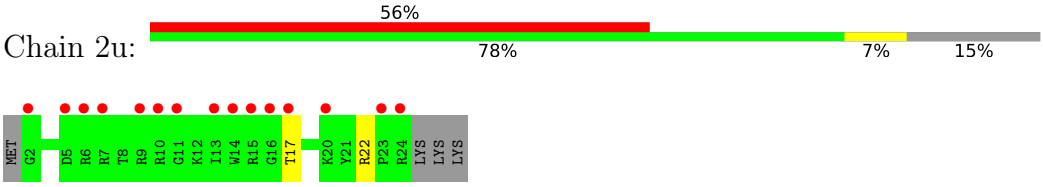
• Molecule 51: 30S ribosomal protein S20

Chain 2t:

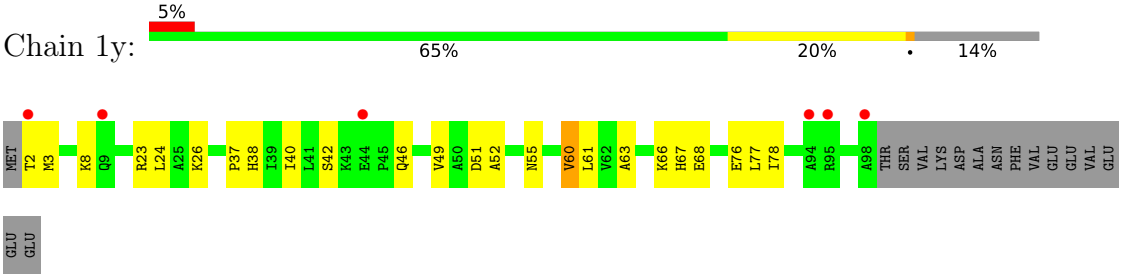
• Molecule 52: 30S ribosomal protein Thx



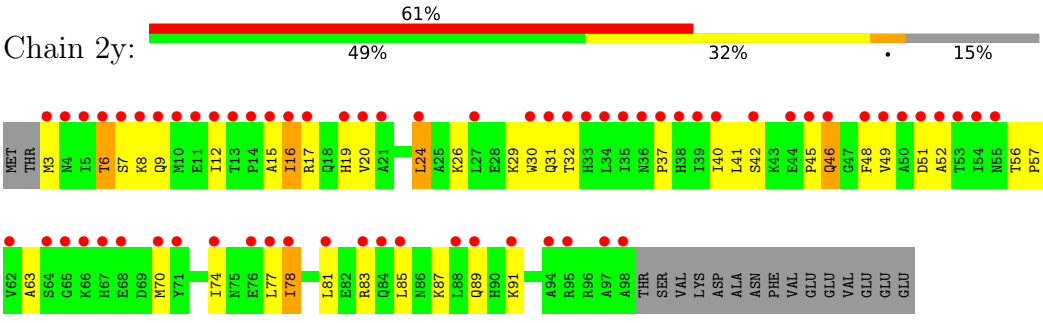
• Molecule 52: 30S ribosomal protein Thx



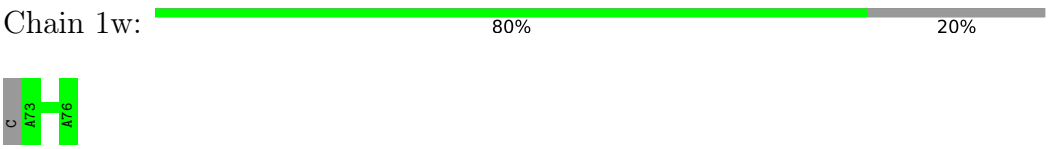
• Molecule 53: Ribosome-associated inhibitor A



• Molecule 53: Ribosome-associated inhibitor A

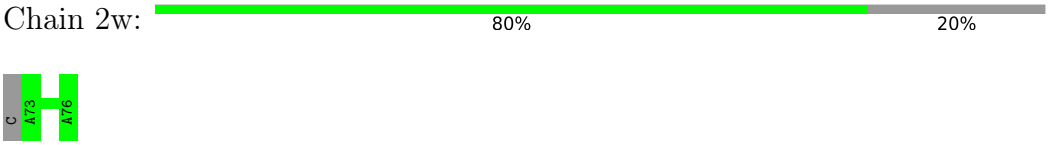


• Molecule 54: A-site Deacylated tRNA Analog



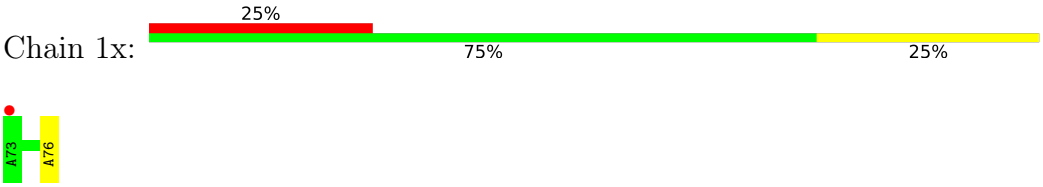
• Molecule 54: A-site Deacylated tRNA Analog

Chain 2w:



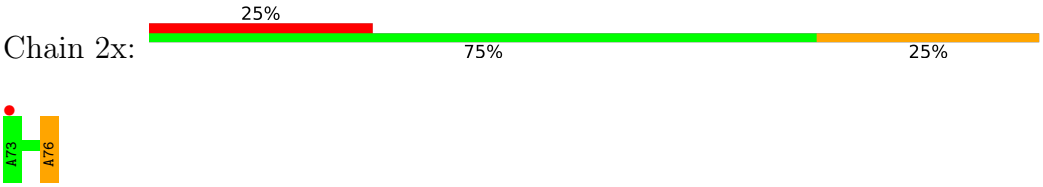
• Molecule 55: P-site Peptidyl-tRNA Analog RNA

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:

There are no outlier residues recorded for this chain.

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	209.81Å 449.56Å 621.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	211.38 – 2.40 211.38 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.7 (211.38-2.40) 99.7 (211.38-2.40)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.12 (at 2.40Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.225 , 0.269 0.228 , 0.272	Depositor DCC
R_{free} test set	112792 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	44.8	Xtriage
Anisotropy	0.136	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 62.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.38$, $< L^2 > = 0.20$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	297868	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.59% 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: 0TD, 5MC, G7M, MPD, 2MG, 2MA, 4OC, OMG, MA6, OMC, SF4, UR3, ZN, CLM, MG, PSU, 5MU, 8AN, OMU, M2G

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	1A	0.28	1/69031 (0.0%)	0.48	4/107754 (0.0%)
1	2A	0.22	0/68903	0.42	3/107552 (0.0%)
2	1B	0.23	0/2876	0.43	0/4486
2	2B	0.19	0/2878	0.36	0/4490
3	1D	0.27	0/2181	0.53	0/2940
3	2D	0.22	0/2186	0.47	0/2944
4	1E	0.26	0/1592	0.48	0/2149
4	2E	0.21	0/1592	0.43	0/2149
5	1F	0.25	0/1619	0.47	0/2193
5	2F	0.21	0/1615	0.47	2/2188 (0.1%)
6	1G	0.21	0/1451	0.45	0/1961
6	2G	0.20	0/1449	0.44	0/1957
7	1H	0.21	0/1356	0.41	0/1834
7	2H	0.20	0/1350	0.42	0/1826
8	1I	0.19	0/1109	0.47	1/1512 (0.1%)
8	2I	0.19	0/1091	0.41	0/1490
9	1N	0.24	0/1148	0.47	0/1547
9	2N	0.19	0/1144	0.38	0/1543
10	1O	0.24	0/943	0.46	0/1269
10	2O	0.21	0/943	0.40	0/1269
11	1P	0.26	0/1152	0.50	0/1533
11	2P	0.22	0/1152	0.47	0/1533
12	1Q	0.26	0/1143	0.48	0/1527
12	2Q	0.21	0/1143	0.43	0/1527
13	1R	0.27	0/982	0.50	0/1312
13	2R	0.21	0/982	0.47	0/1312
14	1S	0.22	0/887	0.49	0/1180
14	2S	0.20	0/880	0.43	0/1172
15	1T	0.25	0/1105	0.49	0/1477
15	2T	0.21	0/1097	0.44	0/1468
16	1U	0.29	0/977	0.50	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
16	2U	0.19	0/977	0.39	0/1301
17	1V	0.29	0/786	0.49	0/1053
17	2V	0.19	0/782	0.40	0/1049
18	1W	0.29	0/897	0.47	0/1205
18	2W	0.20	0/897	0.41	0/1205
19	1X	0.27	0/764	0.49	0/1025
19	2X	0.20	0/764	0.42	0/1025
20	1Y	0.23	0/823	0.50	0/1099
20	2Y	0.19	0/823	0.44	0/1100
21	1Z	0.21	0/1620	0.44	0/2200
21	2Z	0.19	0/1590	0.43	0/2162
22	10	0.27	0/662	0.49	0/881
22	20	0.21	0/659	0.49	0/877
23	11	0.25	0/761	0.43	0/1013
23	21	0.22	0/766	0.44	0/1018
24	12	0.22	0/590	0.46	0/781
24	22	0.22	0/594	0.47	0/785
25	13	0.25	0/474	0.49	0/635
25	23	0.17	0/469	0.39	0/630
26	14	0.23	0/559	0.59	0/754
26	24	0.27	0/549	0.67	0/741
27	15	0.27	0/473	0.52	0/639
27	25	0.21	0/469	0.43	0/635
28	16	0.24	0/460	0.46	0/613
28	26	0.20	0/456	0.40	0/608
29	17	0.30	0/426	0.54	0/561
29	27	0.24	0/426	0.46	0/561
30	18	0.26	0/525	0.51	0/691
30	28	0.20	0/525	0.38	0/691
31	19	0.28	0/310	0.49	0/407
31	29	0.21	0/310	0.45	0/407
32	1a	0.20	0/35795	0.38	0/55864
32	2a	0.19	0/35890	0.38	2/56012 (0.0%)
33	1b	0.22	0/1876	0.47	0/2533
33	2b	0.23	0/1860	0.52	0/2518
34	1c	0.19	0/1582	0.42	0/2137
34	2c	0.20	0/1566	0.40	0/2119
35	1d	0.20	0/1695	0.46	0/2274
35	2d	0.19	0/1698	0.45	0/2277
36	1e	0.20	0/1149	0.43	0/1548
36	2e	0.20	0/1149	0.41	0/1548
37	1f	0.19	0/827	0.39	0/1120
37	2f	0.18	0/829	0.39	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
38	1g	0.19	0/1254	0.40	0/1683
38	2g	0.20	0/1248	0.38	0/1676
39	1h	0.18	0/1118	0.42	0/1506
39	2h	0.17	0/1108	0.40	0/1494
40	1i	0.19	0/1005	0.43	0/1351
40	2i	0.24	0/985	0.50	0/1329
41	1j	0.19	0/732	0.39	0/993
41	2j	0.22	0/723	0.45	0/984
42	1k	0.19	0/849	0.44	0/1150
42	2k	0.19	0/848	0.48	2/1149 (0.2%)
43	1l	0.20	0/937	0.46	0/1260
43	2l	0.19	0/937	0.41	0/1260
44	1m	0.21	0/924	0.46	0/1242
44	2m	0.22	0/905	0.46	0/1217
45	1n	0.18	0/501	0.40	0/664
45	2n	0.21	0/501	0.41	0/664
46	1o	0.18	0/739	0.36	0/985
46	2o	0.18	0/739	0.37	0/985
47	1p	0.22	0/697	0.50	0/939
47	2p	0.20	0/693	0.43	0/935
48	1q	0.19	0/836	0.41	0/1117
48	2q	0.18	0/836	0.42	0/1117
49	1r	0.19	0/560	0.42	0/746
49	2r	0.19	0/560	0.42	0/746
50	1s	0.17	0/663	0.44	0/895
50	2s	0.24	0/660	0.46	0/893
51	1t	0.19	0/734	0.43	0/969
51	2t	0.20	0/736	0.44	0/976
52	1u	0.19	0/203	0.40	0/266
52	2u	0.21	0/203	0.45	0/266
53	1y	0.18	0/776	0.37	0/1048
53	2y	0.22	0/761	0.43	0/1030
54	1w	0.30	0/69	0.57	0/106
54	2w	0.18	0/69	0.30	0/106
55	1x	0.29	0/44	0.54	0/67
55	2x	0.20	0/44	0.44	0/67
56	1v	0.31	0/20	0.33	0/25
56	2v	0.18	0/20	0.31	0/25
All	All	0.23	1/310296 (0.0%)	0.43	14/463751 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a

sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
21	2Z	0	1
26	24	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	2552	OMU	O3'-P	5.09	1.61	1.56

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1A	1042	G	OP1-P-O3'	-9.51	79.46	108.00
1	1A	1042	G	OP2-P-O3'	-6.82	87.55	108.00
1	2A	752	A	C2'-C3'-O3'	6.32	118.98	109.50
1	2A	1992	G	C2'-C3'-O3'	6.16	118.74	109.50
1	1A	2689	U	C4'-C3'-O3'	5.68	117.92	109.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
26	24	18	CYS	Peptide
21	2Z	136	PHE	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	31205	608	0
1	2A	61758	0	31153	738	0
2	1B	2572	0	1305	29	0
2	2B	2573	0	1306	41	0
3	1D	2131	0	2207	47	0
3	2D	2136	0	2218	46	0
4	1E	1559	0	1618	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	2E	1559	0	1618	37	0
5	1F	1584	0	1625	29	0
5	2F	1580	0	1619	51	0
6	1G	1426	0	1445	49	0
6	2G	1424	0	1441	56	0
7	1H	1330	0	1407	31	0
7	2H	1324	0	1402	37	0
8	1I	1094	0	1127	27	0
8	2I	1076	0	1094	35	0
9	1N	1121	0	1195	23	0
9	2N	1117	0	1184	23	0
10	1O	933	0	996	21	0
10	2O	933	0	996	20	0
11	1P	1135	0	1212	28	0
11	2P	1135	0	1212	34	0
12	1Q	1122	0	1177	28	0
12	2Q	1122	0	1177	29	0
13	1R	968	0	1033	14	0
13	2R	968	0	1033	19	0
14	1S	877	0	938	17	0
14	2S	870	0	923	31	0
15	1T	1091	0	1151	29	0
15	2T	1083	0	1136	28	0
16	1U	959	0	1019	15	0
16	2U	959	0	1019	25	0
17	1V	775	0	841	12	0
17	2V	771	0	830	20	0
18	1W	886	0	940	11	0
18	2W	886	0	940	13	0
19	1X	750	0	814	15	0
19	2X	750	0	814	15	0
20	1Y	810	0	892	23	0
20	2Y	810	0	887	27	0
21	1Z	1587	0	1598	35	0
21	2Z	1557	0	1564	49	0
22	10	653	0	674	17	0
22	20	650	0	665	13	0
23	11	754	0	823	16	0
23	21	759	0	837	33	0
24	12	588	0	643	14	0
24	22	592	0	654	14	0
25	13	469	0	518	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	23	464	0	514	16	0
26	14	546	0	522	25	0
26	24	536	0	514	27	0
27	15	459	0	476	9	0
27	25	455	0	465	7	0
28	16	453	0	473	12	0
28	26	449	0	469	5	0
29	17	418	0	467	13	0
29	27	418	0	467	10	0
30	18	517	0	582	14	0
30	28	517	0	582	13	0
31	19	307	0	335	2	0
31	29	307	0	335	9	0
32	1a	32246	0	16293	396	0
32	2a	32331	0	16337	449	0
33	1b	1842	0	1862	59	0
33	2b	1825	0	1828	67	0
34	1c	1558	0	1557	32	0
34	2c	1542	0	1517	63	0
35	1d	1665	0	1687	45	0
35	2d	1668	0	1703	43	0
36	1e	1133	0	1191	28	0
36	2e	1133	0	1191	32	0
37	1f	814	0	808	23	0
37	2f	816	0	808	19	0
38	1g	1235	0	1249	22	0
38	2g	1229	0	1238	27	0
39	1h	1098	0	1143	31	0
39	2h	1088	0	1126	30	0
40	1i	986	0	990	43	0
40	2i	966	0	953	51	0
41	1j	719	0	672	28	0
41	2j	710	0	661	33	0
42	1k	834	0	838	15	0
42	2k	833	0	836	17	0
43	1l	932	0	981	22	0
43	2l	932	0	981	20	0
44	1m	914	0	954	33	0
44	2m	895	0	920	25	0
45	1n	492	0	529	21	0
45	2n	492	0	529	22	0
46	1o	728	0	760	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
46	2o	728	0	760	15	0
47	1p	681	0	697	11	0
47	2p	677	0	686	16	0
48	1q	823	0	891	21	0
48	2q	823	0	891	17	0
49	1r	555	0	618	16	0
49	2r	555	0	618	10	0
50	1s	648	0	658	23	0
50	2s	645	0	635	29	0
51	1t	732	0	809	21	0
51	2t	733	0	795	18	0
52	1u	199	0	208	5	0
52	2u	199	0	208	1	0
53	1y	764	0	786	15	0
53	2y	749	0	757	30	0
54	1w	63	0	34	0	0
54	2w	63	0	34	0	0
55	1x	63	0	33	0	0
55	2x	63	0	33	1	0
56	1v	21	0	27	0	0
56	2v	21	0	27	0	0
57	10	8	0	0	0	0
57	11	5	0	0	0	0
57	13	3	0	0	0	0
57	15	7	0	0	0	0
57	17	5	0	0	0	0
57	18	3	0	0	0	0
57	19	3	0	0	0	0
57	1A	1016	0	0	0	0
57	1B	30	0	0	0	0
57	1D	21	0	0	0	0
57	1E	8	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	4	0	0	0	0
57	1O	1	0	0	0	0
57	1P	5	0	0	0	0
57	1Q	5	0	0	0	0
57	1R	5	0	0	0	0
57	1T	7	0	0	0	0
57	1U	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	1V	7	0	0	0	0
57	1W	3	0	0	0	0
57	1X	1	0	0	0	0
57	1Y	2	0	0	0	0
57	1Z	1	0	0	0	0
57	1a	266	0	0	0	0
57	1b	1	0	0	0	0
57	1d	4	0	0	0	0
57	1e	2	0	0	0	0
57	1f	2	0	0	0	0
57	1g	2	0	0	0	0
57	1h	2	0	0	0	0
57	1i	1	0	0	0	0
57	1l	2	0	0	0	0
57	1m	1	0	0	0	0
57	1n	3	0	0	0	0
57	1o	2	0	0	0	0
57	1t	2	0	0	0	0
57	1x	2	0	0	0	0
57	1y	2	0	0	0	0
57	20	2	0	0	0	0
57	21	1	0	0	0	0
57	23	1	0	0	0	0
57	25	3	0	0	0	0
57	27	1	0	0	0	0
57	28	2	0	0	0	0
57	2A	746	0	0	0	0
57	2B	19	0	0	0	0
57	2D	8	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
57	2T	4	0	0	0	0
57	2U	1	0	0	0	0
57	2V	3	0	0	0	0
57	2W	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	2X	1	0	0	0	0
57	2Y	1	0	0	0	0
57	2a	190	0	0	0	0
57	2e	1	0	0	0	0
57	2f	1	0	0	0	0
57	2j	2	0	0	0	0
57	2r	1	0	0	0	0
57	2t	1	0	0	0	0
57	2x	1	0	0	0	0
58	1A	20	0	11	0	0
58	2A	20	0	11	0	0
59	1A	12	0	12	2	0
59	1B	12	0	12	2	0
60	18	8	0	14	1	0
60	1A	8	0	14	1	0
60	1T	8	0	14	0	0
60	1a	8	0	11	5	0
60	2A	8	0	14	0	0
60	2B	8	0	14	1	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	0	0
62	2d	8	0	0	0	0
63	10	25	0	0	0	0
63	11	22	0	0	0	0
63	12	13	0	0	2	0
63	13	21	0	0	1	0
63	14	2	0	0	0	0
63	15	26	0	0	1	0
63	16	20	0	0	2	0
63	17	16	0	0	2	0
63	18	30	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
63	19	6	0	0	0	0
63	1A	4023	0	0	127	0
63	1B	93	0	0	6	0
63	1D	112	0	0	5	0
63	1E	81	0	0	2	0
63	1F	61	0	0	0	0
63	1G	20	0	0	0	0
63	1H	12	0	0	1	0
63	1I	6	0	0	0	0
63	1N	51	0	0	1	0
63	1O	24	0	0	3	0
63	1P	71	0	0	5	0
63	1Q	41	0	0	4	0
63	1R	33	0	0	1	0
63	1S	16	0	0	0	0
63	1T	34	0	0	2	0
63	1U	54	0	0	6	0
63	1V	42	0	0	1	0
63	1W	29	0	0	1	0
63	1X	23	0	0	1	0
63	1Y	16	0	0	1	0
63	1Z	12	0	0	1	0
63	1a	378	0	0	13	0
63	1b	1	0	0	0	0
63	1d	3	0	0	0	0
63	1e	3	0	0	1	0
63	1f	2	0	0	0	0
63	1h	1	0	0	0	0
63	1j	1	0	0	0	0
63	1l	6	0	0	1	0
63	1o	2	0	0	1	0
63	1p	3	0	0	0	0
63	1t	1	0	0	0	0
63	1w	5	0	0	0	0
63	1x	3	0	0	0	0
63	1y	2	0	0	0	0
63	20	11	0	0	0	0
63	21	20	0	0	3	0
63	22	1	0	0	0	0
63	23	3	0	0	1	0
63	25	13	0	0	0	0
63	26	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
63	27	9	0	0	1	0
63	28	11	0	0	1	0
63	29	2	0	0	0	0
63	2A	2284	0	0	124	0
63	2B	46	0	0	3	0
63	2D	57	0	0	3	0
63	2E	32	0	0	3	0
63	2F	27	0	0	0	0
63	2G	6	0	0	1	0
63	2H	3	0	0	0	0
63	2I	4	0	0	2	0
63	2N	6	0	0	0	0
63	2O	21	0	0	2	0
63	2P	24	0	0	3	0
63	2Q	17	0	0	2	0
63	2R	16	0	0	3	0
63	2S	5	0	0	2	0
63	2T	13	0	0	0	0
63	2U	16	0	0	3	0
63	2V	5	0	0	1	0
63	2W	17	0	0	0	0
63	2X	8	0	0	1	0
63	2Y	5	0	0	0	0
63	2Z	11	0	0	3	0
63	2a	317	0	0	26	0
63	2d	2	0	0	0	0
63	2e	1	0	0	0	0
63	2f	3	0	0	0	0
63	2j	2	0	0	0	0
63	2l	2	0	0	0	0
63	2n	2	0	0	0	0
63	2o	4	0	0	1	0
63	2p	2	0	0	0	0
63	2r	3	0	0	0	0
63	2t	2	0	0	0	0
63	2w	3	0	0	0	0
63	2x	3	0	0	1	0
63	2y	3	0	0	0	0
All	All	297868	0	194800	4145	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

The worst 5 of 4145 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1082:U:H3	1:1A:1086:A:N6	1.35	1.24
1:2A:2139:C:H42	1:2A:2152:G:H1	0.96	0.96
1:1A:1082:U:O4	1:1A:1086:A:N1	1.99	0.94
1:1A:2137:C:N4	1:1A:2154:G:H1	1.67	0.93
1:2A:2319:G:H22	14:2S:3:ARG:HD3	1.34	0.92

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	1D	273/276 (99%)	261 (96%)	12 (4%)	0	100 100
3	2D	273/276 (99%)	255 (93%)	18 (7%)	0	100 100
4	1E	202/206 (98%)	192 (95%)	9 (4%)	1 (0%)	24 37
4	2E	202/206 (98%)	193 (96%)	8 (4%)	1 (0%)	24 37
5	1F	201/210 (96%)	195 (97%)	6 (3%)	0	100 100
5	2F	201/210 (96%)	187 (93%)	13 (6%)	1 (0%)	24 37
6	1G	179/182 (98%)	155 (87%)	22 (12%)	2 (1%)	11 18
6	2G	179/182 (98%)	157 (88%)	18 (10%)	4 (2%)	5 6
7	1H	172/180 (96%)	164 (95%)	5 (3%)	3 (2%)	7 10
7	2H	171/180 (95%)	150 (88%)	17 (10%)	4 (2%)	5 6
8	1I	145/148 (98%)	126 (87%)	18 (12%)	1 (1%)	18 28
8	2I	144/148 (97%)	128 (89%)	14 (10%)	2 (1%)	9 13
9	1N	138/140 (99%)	134 (97%)	4 (3%)	0	100 100
9	2N	138/140 (99%)	132 (96%)	6 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
10	1O	120/122 (98%)	114 (95%)	6 (5%)	0	100 100
10	2O	120/122 (98%)	112 (93%)	8 (7%)	0	100 100
11	1P	147/150 (98%)	139 (95%)	8 (5%)	0	100 100
11	2P	147/150 (98%)	138 (94%)	6 (4%)	3 (2%)	6 7
12	1Q	139/141 (99%)	132 (95%)	7 (5%)	0	100 100
12	2Q	139/141 (99%)	131 (94%)	8 (6%)	0	100 100
13	1R	116/118 (98%)	114 (98%)	2 (2%)	0	100 100
13	2R	116/118 (98%)	113 (97%)	3 (3%)	0	100 100
14	1S	108/112 (96%)	98 (91%)	9 (8%)	1 (1%)	14 22
14	2S	108/112 (96%)	99 (92%)	9 (8%)	0	100 100
15	1T	129/146 (88%)	125 (97%)	4 (3%)	0	100 100
15	2T	129/146 (88%)	123 (95%)	6 (5%)	0	100 100
16	1U	114/118 (97%)	114 (100%)	0	0	100 100
16	2U	114/118 (97%)	111 (97%)	3 (3%)	0	100 100
17	1V	99/101 (98%)	94 (95%)	4 (4%)	1 (1%)	12 20
17	2V	99/101 (98%)	88 (89%)	9 (9%)	2 (2%)	6 7
18	1W	110/113 (97%)	109 (99%)	1 (1%)	0	100 100
18	2W	110/113 (97%)	110 (100%)	0	0	100 100
19	1X	93/96 (97%)	89 (96%)	3 (3%)	1 (1%)	11 18
19	2X	93/96 (97%)	89 (96%)	3 (3%)	1 (1%)	11 18
20	1Y	105/110 (96%)	96 (91%)	9 (9%)	0	100 100
20	2Y	105/110 (96%)	98 (93%)	7 (7%)	0	100 100
21	1Z	201/206 (98%)	186 (92%)	14 (7%)	1 (0%)	24 37
21	2Z	199/206 (97%)	179 (90%)	19 (10%)	1 (0%)	24 37
22	10	81/85 (95%)	78 (96%)	3 (4%)	0	100 100
22	20	81/85 (95%)	76 (94%)	5 (6%)	0	100 100
23	11	95/98 (97%)	92 (97%)	2 (2%)	1 (1%)	11 18
23	21	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	11 18
24	12	68/72 (94%)	68 (100%)	0	0	100 100
24	22	68/72 (94%)	67 (98%)	0	1 (2%)	8 12
25	13	57/60 (95%)	55 (96%)	2 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
25	23	57/60 (95%)	54 (95%)	3 (5%)	0	100 100
26	14	67/71 (94%)	51 (76%)	13 (19%)	3 (4%)	2 1
26	24	67/71 (94%)	49 (73%)	12 (18%)	6 (9%)	0 0
27	15	57/60 (95%)	56 (98%)	1 (2%)	0	100 100
27	25	57/60 (95%)	54 (95%)	3 (5%)	0	100 100
28	16	51/54 (94%)	49 (96%)	2 (4%)	0	100 100
28	26	51/54 (94%)	49 (96%)	2 (4%)	0	100 100
29	17	46/49 (94%)	46 (100%)	0	0	100 100
29	27	46/49 (94%)	46 (100%)	0	0	100 100
30	18	62/65 (95%)	61 (98%)	1 (2%)	0	100 100
30	28	62/65 (95%)	62 (100%)	0	0	100 100
31	19	35/37 (95%)	35 (100%)	0	0	100 100
31	29	35/37 (95%)	32 (91%)	3 (9%)	0	100 100
33	1b	229/256 (90%)	183 (80%)	39 (17%)	7 (3%)	3 3
33	2b	229/256 (90%)	185 (81%)	34 (15%)	10 (4%)	2 1
34	1c	204/239 (85%)	180 (88%)	24 (12%)	0	100 100
34	2c	204/239 (85%)	175 (86%)	25 (12%)	4 (2%)	6 7
35	1d	206/209 (99%)	189 (92%)	17 (8%)	0	100 100
35	2d	206/209 (99%)	185 (90%)	19 (9%)	2 (1%)	12 20
36	1e	146/162 (90%)	143 (98%)	2 (1%)	1 (1%)	18 28
36	2e	146/162 (90%)	135 (92%)	11 (8%)	0	100 100
37	1f	98/101 (97%)	94 (96%)	4 (4%)	0	100 100
37	2f	98/101 (97%)	94 (96%)	4 (4%)	0	100 100
38	1g	153/156 (98%)	144 (94%)	9 (6%)	0	100 100
38	2g	153/156 (98%)	136 (89%)	13 (8%)	4 (3%)	4 4
39	1h	135/138 (98%)	127 (94%)	7 (5%)	1 (1%)	18 28
39	2h	135/138 (98%)	122 (90%)	11 (8%)	2 (2%)	8 12
40	1i	125/128 (98%)	114 (91%)	11 (9%)	0	100 100
40	2i	124/128 (97%)	110 (89%)	11 (9%)	3 (2%)	4 5
41	1j	95/105 (90%)	82 (86%)	9 (10%)	4 (4%)	2 2
41	2j	94/105 (90%)	79 (84%)	11 (12%)	4 (4%)	2 1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
42	1k	112/129 (87%)	100 (89%)	12 (11%)	0	100 100
42	2k	112/129 (87%)	101 (90%)	9 (8%)	2 (2%)	6 9
43	1l	119/132 (90%)	110 (92%)	8 (7%)	1 (1%)	16 25
43	2l	119/132 (90%)	108 (91%)	10 (8%)	1 (1%)	16 25
44	1m	114/126 (90%)	104 (91%)	8 (7%)	2 (2%)	6 9
44	2m	112/126 (89%)	94 (84%)	17 (15%)	1 (1%)	14 22
45	1n	58/61 (95%)	57 (98%)	1 (2%)	0	100 100
45	2n	58/61 (95%)	55 (95%)	3 (5%)	0	100 100
46	1o	86/89 (97%)	80 (93%)	5 (6%)	1 (1%)	10 16
46	2o	86/89 (97%)	79 (92%)	5 (6%)	2 (2%)	5 6
47	1p	80/88 (91%)	71 (89%)	9 (11%)	0	100 100
47	2p	80/88 (91%)	70 (88%)	9 (11%)	1 (1%)	9 14
48	1q	97/105 (92%)	88 (91%)	8 (8%)	1 (1%)	12 20
48	2q	97/105 (92%)	89 (92%)	7 (7%)	1 (1%)	12 20
49	1r	66/88 (75%)	62 (94%)	3 (4%)	1 (2%)	8 12
49	2r	66/88 (75%)	60 (91%)	6 (9%)	0	100 100
50	1s	81/93 (87%)	73 (90%)	6 (7%)	2 (2%)	4 5
50	2s	81/93 (87%)	66 (82%)	15 (18%)	0	100 100
51	1t	94/106 (89%)	83 (88%)	10 (11%)	1 (1%)	11 18
51	2t	96/106 (91%)	86 (90%)	6 (6%)	4 (4%)	2 2
52	1u	21/27 (78%)	20 (95%)	1 (5%)	0	100 100
52	2u	21/27 (78%)	19 (90%)	2 (10%)	0	100 100
53	1y	95/113 (84%)	90 (95%)	5 (5%)	0	100 100
53	2y	94/113 (83%)	82 (87%)	11 (12%)	1 (1%)	11 18
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%)	10729 (92%)	808 (7%)	106 (1%)	14 22

5 of 106 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	1G	49	ASP
14	1S	59	LYS

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Mol	Chain	Res	Type
26	14	61	ARG
33	1b	21	ARG
33	1b	124	SER

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	1D	214/218 (98%)	194 (91%)	20 (9%)	8 14
3	2D	215/218 (99%)	196 (91%)	19 (9%)	9 15
4	1E	164/166 (99%)	156 (95%)	8 (5%)	22 39
4	2E	164/166 (99%)	150 (92%)	14 (8%)	10 16
5	1F	160/166 (96%)	145 (91%)	15 (9%)	8 13
5	2F	159/166 (96%)	137 (86%)	22 (14%)	3 4
6	1G	144/156 (92%)	128 (89%)	16 (11%)	6 9
6	2G	142/156 (91%)	126 (89%)	16 (11%)	5 8
7	1H	144/148 (97%)	129 (90%)	15 (10%)	7 10
7	2H	143/148 (97%)	128 (90%)	15 (10%)	6 10
8	1I	111/124 (90%)	92 (83%)	19 (17%)	2 2
8	2I	108/124 (87%)	86 (80%)	22 (20%)	1 1
9	1N	119/119 (100%)	104 (87%)	15 (13%)	4 6
9	2N	118/119 (99%)	110 (93%)	8 (7%)	14 25
10	1O	100/100 (100%)	97 (97%)	3 (3%)	36 58
10	2O	100/100 (100%)	96 (96%)	4 (4%)	28 47
11	1P	115/116 (99%)	109 (95%)	6 (5%)	21 36
11	2P	115/116 (99%)	107 (93%)	8 (7%)	14 24
12	1Q	111/111 (100%)	100 (90%)	11 (10%)	7 11
12	2Q	111/111 (100%)	104 (94%)	7 (6%)	16 29
13	1R	101/101 (100%)	92 (91%)	9 (9%)	9 15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
13	2R	101/101 (100%)	94 (93%)	7 (7%)	14 24
14	1S	87/88 (99%)	78 (90%)	9 (10%)	7 11
14	2S	85/88 (97%)	80 (94%)	5 (6%)	18 31
15	1T	115/127 (91%)	105 (91%)	10 (9%)	9 16
15	2T	113/127 (89%)	107 (95%)	6 (5%)	20 36
16	1U	93/94 (99%)	86 (92%)	7 (8%)	12 21
16	2U	93/94 (99%)	87 (94%)	6 (6%)	15 27
17	1V	81/82 (99%)	72 (89%)	9 (11%)	6 9
17	2V	80/82 (98%)	68 (85%)	12 (15%)	3 3
18	1W	90/92 (98%)	85 (94%)	5 (6%)	19 33
18	2W	90/92 (98%)	83 (92%)	7 (8%)	11 20
19	1X	77/78 (99%)	73 (95%)	4 (5%)	21 36
19	2X	77/78 (99%)	75 (97%)	2 (3%)	40 63
20	1Y	86/91 (94%)	82 (95%)	4 (5%)	23 41
20	2Y	86/91 (94%)	71 (83%)	15 (17%)	2 2
21	1Z	169/179 (94%)	153 (90%)	16 (10%)	8 13
21	2Z	165/179 (92%)	141 (86%)	24 (14%)	3 4
22	10	65/67 (97%)	61 (94%)	4 (6%)	16 29
22	20	64/67 (96%)	60 (94%)	4 (6%)	16 29
23	11	79/83 (95%)	73 (92%)	6 (8%)	12 21
23	21	81/83 (98%)	73 (90%)	8 (10%)	7 11
24	12	65/67 (97%)	60 (92%)	5 (8%)	12 20
24	22	66/67 (98%)	63 (96%)	3 (4%)	24 42
25	13	51/52 (98%)	45 (88%)	6 (12%)	5 7
25	23	50/52 (96%)	47 (94%)	3 (6%)	17 31
26	14	58/63 (92%)	52 (90%)	6 (10%)	7 11
26	24	54/63 (86%)	44 (82%)	10 (18%)	1 2
27	15	51/52 (98%)	44 (86%)	7 (14%)	3 5
27	25	50/52 (96%)	45 (90%)	5 (10%)	7 11
28	16	51/52 (98%)	45 (88%)	6 (12%)	5 7
28	26	50/52 (96%)	47 (94%)	3 (6%)	17 31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
29	17	41/42 (98%)	38 (93%)	3 (7%)	13 22
29	27	41/42 (98%)	37 (90%)	4 (10%)	7 12
30	18	54/55 (98%)	48 (89%)	6 (11%)	6 9
30	28	54/55 (98%)	49 (91%)	5 (9%)	8 14
31	19	34/34 (100%)	34 (100%)	0	100 100
31	29	34/34 (100%)	31 (91%)	3 (9%)	9 15
33	1b	191/220 (87%)	168 (88%)	23 (12%)	5 7
33	2b	187/220 (85%)	160 (86%)	27 (14%)	3 4
34	1c	144/188 (77%)	134 (93%)	10 (7%)	14 24
34	2c	140/188 (74%)	119 (85%)	21 (15%)	3 3
35	1d	171/181 (94%)	147 (86%)	24 (14%)	3 4
35	2d	172/181 (95%)	152 (88%)	20 (12%)	5 8
36	1e	114/123 (93%)	101 (89%)	13 (11%)	5 8
36	2e	114/123 (93%)	103 (90%)	11 (10%)	8 12
37	1f	85/90 (94%)	71 (84%)	14 (16%)	2 3
37	2f	85/90 (94%)	77 (91%)	8 (9%)	8 13
38	1g	120/127 (94%)	111 (92%)	9 (8%)	12 21
38	2g	119/127 (94%)	107 (90%)	12 (10%)	7 11
39	1h	116/119 (98%)	103 (89%)	13 (11%)	6 9
39	2h	114/119 (96%)	101 (89%)	13 (11%)	5 8
40	1i	91/99 (92%)	82 (90%)	9 (10%)	7 11
40	2i	88/99 (89%)	79 (90%)	9 (10%)	7 11
41	1j	68/92 (74%)	59 (87%)	9 (13%)	4 5
41	2j	68/92 (74%)	61 (90%)	7 (10%)	7 11
42	1k	83/99 (84%)	78 (94%)	5 (6%)	17 31
42	2k	83/99 (84%)	78 (94%)	5 (6%)	17 31
43	1l	96/108 (89%)	92 (96%)	4 (4%)	26 45
43	2l	96/108 (89%)	86 (90%)	10 (10%)	7 10
44	1m	90/101 (89%)	84 (93%)	6 (7%)	15 26
44	2m	87/101 (86%)	74 (85%)	13 (15%)	3 3
45	1n	49/50 (98%)	42 (86%)	7 (14%)	3 4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
45	2n	49/50 (98%)	45 (92%)	4 (8%)	10 18
46	1o	78/80 (98%)	74 (95%)	4 (5%)	21 37
46	2o	78/80 (98%)	71 (91%)	7 (9%)	9 15
47	1p	69/74 (93%)	59 (86%)	10 (14%)	3 4
47	2p	68/74 (92%)	61 (90%)	7 (10%)	7 11
48	1q	94/97 (97%)	89 (95%)	5 (5%)	20 36
48	2q	94/97 (97%)	89 (95%)	5 (5%)	20 36
49	1r	59/77 (77%)	54 (92%)	5 (8%)	10 16
49	2r	59/77 (77%)	57 (97%)	2 (3%)	32 54
50	1s	68/80 (85%)	60 (88%)	8 (12%)	5 7
50	2s	67/80 (84%)	54 (81%)	13 (19%)	1 2
51	1t	71/82 (87%)	64 (90%)	7 (10%)	7 11
51	2t	70/82 (85%)	60 (86%)	10 (14%)	3 4
52	1u	18/22 (82%)	18 (100%)	0	100 100
52	2u	18/22 (82%)	18 (100%)	0	100 100
53	1y	82/98 (84%)	75 (92%)	7 (8%)	10 16
53	2y	79/98 (81%)	70 (89%)	9 (11%)	5 8
56	1v	2/2 (100%)	1 (50%)	1 (50%)	0 0
56	2v	2/2 (100%)	2 (100%)	0	100 100
All	All	9535/10264 (93%)	8612 (90%)	923 (10%)	8 12

5 of 923 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	2E	27	LEU
48	2q	16	GLN
12	2Q	60	ARG
47	2p	5	ARG
38	2g	15	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 142 such sidechains are listed below:

Mol	Chain	Res	Type
36	2e	130	ASN

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Mol	Chain	Res	Type
38	2g	64	GLN
43	2l	99	HIS
38	1g	56	GLN
38	1g	37	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2865/2915 (98%)	413 (14%)	30 (1%)
1	2A	2858/2915 (98%)	476 (16%)	29 (1%)
2	1B	119/121 (98%)	11 (9%)	0
2	2B	119/121 (98%)	11 (9%)	0
32	1a	1497/1521 (98%)	248 (16%)	0
32	2a	1501/1521 (98%)	289 (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%)	1448 (16%)	59 (0%)

5 of 1448 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	23	G
1	1A	34	C
1	1A	45	C
1	1A	71	A
1	1A	74	A

5 of 59 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	2756	U
1	2A	2172	U
1	2A	752	A
1	2A	2171	A
1	2A	1420	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	OMC	2A	1920	1	19,22,23	0.82	0	25,31,34	1.08	2 (8%)
1	2MA	1A	2503	1,57	22,25,26	1.49	5 (22%)	32,37,40	2.33	8 (25%)
1	PSU	1A	1917	1	18,21,22	1.36	2 (11%)	21,30,33	2.02	3 (14%)
32	G7M	1a	527	57,32	23,26,27	1.52	3 (13%)	34,39,42	1.65	5 (14%)
32	5MC	2a	967	32	19,22,23	1.75	3 (15%)	26,32,35	1.09	3 (11%)
32	UR3	1a	1498	32	19,22,23	0.99	1 (5%)	26,32,35	1.77	4 (15%)
32	UR3	2a	1498	32	19,22,23	1.02	2 (10%)	26,32,35	1.64	2 (7%)
32	PSU	1a	516	32	18,21,22	1.36	2 (11%)	21,30,33	1.94	5 (23%)
1	PSU	1A	2605	1	18,21,22	1.47	4 (22%)	21,30,33	1.99	4 (19%)
1	OMC	1A	1920	1	19,22,23	0.83	0	25,31,34	0.98	1 (4%)
1	5MU	2A	1915	1	19,22,23	1.44	4 (21%)	27,32,35	2.12	8 (29%)
1	OMG	1A	2251	1,57,55	23,26,27	1.23	3 (13%)	32,38,41	2.06	6 (18%)
1	PSU	2A	1917	1,57	18,21,22	1.37	2 (11%)	21,30,33	2.01	3 (14%)
32	5MC	2a	1407	32	19,22,23	1.62	2 (10%)	26,32,35	1.12	3 (11%)
1	5MC	2A	1942	1	19,22,23	1.69	3 (15%)	26,32,35	1.15	2 (7%)
32	MA6	1a	1519	32	23,26,27	0.43	0	33,38,41	2.02	9 (27%)
32	5MC	2a	1404	32	19,22,23	1.77	3 (15%)	26,32,35	1.23	4 (15%)
32	M2G	2a	966	57,32	24,27,28	1.33	3 (12%)	33,40,43	1.82	5 (15%)
32	5MC	1a	1400	32	19,22,23	1.70	3 (15%)	26,32,35	1.11	2 (7%)
32	MA6	2a	1519	32	23,26,27	0.45	0	33,38,41	2.14	10 (30%)
32	5MC	2a	1400	32	19,22,23	1.53	2 (10%)	26,32,35	1.27	3 (11%)
1	5MC	2A	1962	1,57	19,22,23	1.69	3 (15%)	26,32,35	1.12	2 (7%)
55	8AN	2x	76	57,55	21,24,25	1.38	3 (14%)	26,35,38	2.29	10 (38%)
1	5MC	1A	1962	1,57	19,22,23	1.64	3 (15%)	26,32,35	1.13	4 (15%)
1	OMU	1A	2552	1,57	19,22,23	1.31	3 (15%)	25,31,34	1.83	6 (24%)
43	0TD	1l	92	43	8,9,10	4.61	2 (25%)	6,11,13	2.73	3 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	PSU	2A	1911	1	18,21,22	1.39	2 (11%)	21,30,33	2.02	4 (19%)
1	OMG	2A	2251	1,57,55	23,26,27	1.22	3 (13%)	32,38,41	1.98	7 (21%)
32	PSU	2a	516	57,32	18,21,22	1.33	2 (11%)	21,30,33	2.10	5 (23%)
1	5MC	1A	1942	1	19,22,23	1.42	3 (15%)	26,32,35	1.10	2 (7%)
32	M2G	1a	966	32	24,27,28	1.29	3 (12%)	33,40,43	1.84	5 (15%)
32	4OC	1a	1402	32	20,23,24	0.75	0	25,32,35	1.01	1 (4%)
32	G7M	2a	527	32	23,26,27	1.49	3 (13%)	34,39,42	1.69	5 (14%)
43	0TD	2l	92	43	8,9,10	4.54	1 (12%)	6,11,13	5.96	3 (50%)
32	4OC	2a	1402	32	20,23,24	0.76	0	25,32,35	0.96	0
55	8AN	1x	76	57,55	21,24,25	1.38	3 (14%)	26,35,38	2.40	9 (34%)
1	5MU	2A	1939	1	19,22,23	1.48	5 (26%)	27,32,35	2.16	8 (29%)
1	PSU	2A	2605	1	18,21,22	1.35	2 (11%)	21,30,33	1.92	4 (19%)
32	5MC	1a	967	32	19,22,23	1.65	3 (15%)	26,32,35	1.12	2 (7%)
32	5MC	1a	1407	32	19,22,23	1.72	2 (10%)	26,32,35	1.17	3 (11%)
1	PSU	1A	1911	1	18,21,22	1.38	2 (11%)	21,30,33	2.10	5 (23%)
1	2MA	2A	2503	1,57	22,25,26	1.47	4 (18%)	32,37,40	2.36	9 (28%)
32	MA6	2a	1518	32	23,26,27	0.39	0	33,38,41	2.08	9 (27%)
1	5MU	1A	1915	1	19,22,23	1.44	4 (21%)	27,32,35	2.19	9 (33%)
1	OMU	2A	2552	1,57	19,22,23	1.23	3 (15%)	25,31,34	1.91	6 (24%)
1	5MU	1A	1939	1,57	19,22,23	1.43	5 (26%)	27,32,35	2.19	8 (29%)
32	MA6	1a	1518	32	23,26,27	0.38	0	33,38,41	2.00	10 (30%)
32	5MC	1a	1404	32	19,22,23	1.66	3 (15%)	26,32,35	1.13	2 (7%)
32	2MG	1a	1207	32	23,26,27	1.26	3 (13%)	33,38,41	2.18	6 (18%)
32	2MG	2a	1207	32	23,26,27	1.23	3 (13%)	33,38,41	2.15	8 (24%)

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	OMC	2A	1920	1	-	1/9/27/28	0/2/2/2
1	2MA	1A	2503	1,57	-	1/7/25/26	0/3/3/3
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
32	G7M	1a	527	57,32	-	2/7/25/26	0/3/3/3
32	5MC	2a	967	32	-	0/7/25/26	0/2/2/2
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	UR3	2a	1498	32	-	0/7/25/26	0/2/2/2
32	PSU	1a	516	32	-	1/7/25/26	0/2/2/2
1	PSU	1A	2605	1	-	0/7/25/26	0/2/2/2
1	OMC	1A	1920	1	-	1/9/27/28	0/2/2/2
1	5MU	2A	1915	1	-	2/7/25/26	0/2/2/2
1	OMG	1A	2251	1,57,55	-	0/9/27/28	0/3/3/3
1	PSU	2A	1917	1,57	-	0/7/25/26	0/2/2/2
32	5MC	2a	1407	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	1519	32	-	2/11/29/30	0/3/3/3
32	5MC	2a	1404	32	-	0/7/25/26	0/2/2/2
32	M2G	2a	966	57,32	-	0/11/29/30	0/3/3/3
32	5MC	1a	1400	32	-	0/7/25/26	0/2/2/2
32	MA6	2a	1519	32	-	2/11/29/30	0/3/3/3
32	5MC	2a	1400	32	-	0/7/25/26	0/2/2/2
1	5MC	2A	1962	1,57	-	0/7/25/26	0/2/2/2
55	8AN	2x	76	57,55	-	1/7/25/26	0/3/3/3
1	5MC	1A	1962	1,57	-	0/7/25/26	0/2/2/2
1	OMU	1A	2552	1,57	-	0/9/27/28	0/2/2/2
43	0TD	1l	92	43	-	2/7/12/14	-
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
1	OMG	2A	2251	1,57,55	-	0/9/27/28	0/3/3/3
32	PSU	2a	516	57,32	-	0/7/25/26	0/2/2/2
1	5MC	1A	1942	1	-	0/7/25/26	0/2/2/2
32	M2G	1a	966	32	-	0/11/29/30	0/3/3/3
32	4OC	1a	1402	32	-	2/9/29/30	0/2/2/2
32	G7M	2a	527	32	-	2/7/25/26	0/3/3/3
43	0TD	2l	92	43	-	2/7/12/14	-
32	4OC	2a	1402	32	-	0/9/29/30	0/2/2/2
55	8AN	1x	76	57,55	-	1/7/25/26	0/3/3/3
1	5MU	2A	1939	1	-	0/7/25/26	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
32	5MC	1a	967	32	-	0/7/25/26	0/2/2/2
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
1	2MA	2A	2503	1,57	-	1/7/25/26	0/3/3/3
32	MA6	2a	1518	32	-	0/11/29/30	0/3/3/3
1	5MU	1A	1915	1	-	2/7/25/26	0/2/2/2
1	OMU	2A	2552	1,57	-	0/9/27/28	0/2/2/2
1	5MU	1A	1939	1,57	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	MA6	1a	1518	32	-	0/11/29/30	0/3/3/3
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
32	2MG	1a	1207	32	-	0/9/27/28	0/3/3/3
32	2MG	2a	1207	32	-	2/9/27/28	0/3/3/3

The worst 5 of 120 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	1l	92	0TD	CB-SB	-12.34	1.69	1.82
43	2l	92	0TD	CB-SB	-12.33	1.69	1.82
32	2a	1404	5MC	C5-C4	6.49	1.49	1.44
32	2a	967	5MC	C5-C4	6.44	1.49	1.44
32	1a	1407	5MC	C5-C4	6.29	1.48	1.44

The worst 5 of 247 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	2l	92	0TD	CSB-SB-CB	-13.86	77.44	102.36
1	2A	2503	2MA	C5-C4-N3	-8.11	118.64	127.18
1	1A	2503	2MA	C5-C4-N3	-7.81	118.95	127.18
32	1a	1498	UR3	C4-N3-C2	-7.19	118.79	124.58
32	1a	1207	2MG	C2-N3-C4	7.13	120.92	112.00

There are no chirality outliers.

5 of 27 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1A	1915	5MU	O4'-C1'-N1-C2
1	1A	1915	5MU	O4'-C1'-N1-C6
43	1l	92	0TD	CG-CB-SB-CSB
1	2A	1915	5MU	O4'-C1'-N1-C2
1	2A	1915	5MU	O4'-C1'-N1-C6

There are no ring outliers.

17 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	2A	1920	OMC	1	0
1	1A	1920	OMC	1	0
1	1A	2251	OMG	1	0
1	2A	1917	PSU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	1a	1519	MA6	1	0
32	2a	1404	5MC	1	0
32	1a	1400	5MC	2	0
32	2a	1519	MA6	2	0
32	2a	1400	5MC	3	0
55	2x	76	8AN	1	0
32	1a	1402	4OC	3	0
43	2l	92	0TD	2	0
32	2a	1402	4OC	1	0
1	2A	1939	5MU	2	0
32	2a	1518	MA6	1	0
1	2A	2552	OMU	1	0
32	1a	1518	MA6	2	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2517 ligands modelled in this entry, 2505 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	$\#\|Z\| > 2$
58	CLM	2A	3747	-	20,20,20	0.85	0	23,27,27	1.25	2 (8%)
58	CLM	1A	4017	-	20,20,20	1.10	2 (10%)	23,27,27	1.96	7 (30%)
59	ARG	1A	4018	57	10,11,11	0.76	1 (10%)	9,13,13	0.90	1 (11%)
60	MPD	2B	220	-	7,7,7	0.31	0	9,10,10	0.19	0
60	MPD	1T	208	-	7,7,7	0.31	0	9,10,10	0.24	0
60	MPD	1A	4019	-	7,7,7	0.31	0	9,10,10	0.16	0
59	ARG	1B	231	-	10,11,11	0.78	1 (10%)	9,13,13	1.01	1 (11%)
62	SF4	2d	501	35	0,12,12	-	-	-		
62	SF4	1d	305	35	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
60	MPD	18	104	-	7,7,7	0.29	0	9,10,10	0.22	0
60	MPD	1a	1867	-	7,7,7	0.37	0	9,10,10	0.41	0
60	MPD	2A	3748	-	7,7,7	0.29	0	9,10,10	0.18	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	CLM	2A	3747	-	-	0/20/22/22	0/1/1/1
58	CLM	1A	4017	-	-	2/20/22/22	0/1/1/1
59	ARG	1A	4018	57	-	2/11/11/11	-
60	MPD	2B	220	-	-	4/5/5/5	-
60	MPD	1T	208	-	-	1/5/5/5	-
60	MPD	1A	4019	-	-	3/5/5/5	-
59	ARG	1B	231	-	-	3/11/11/11	-
62	SF4	2d	501	35	-	-	0/6/5/5
62	SF4	1d	305	35	-	-	0/6/5/5
60	MPD	18	104	-	-	1/5/5/5	-
60	MPD	1a	1867	-	-	4/5/5/5	-
60	MPD	2A	3748	-	-	2/5/5/5	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	1A	4017	CLM	C6-C5	-2.97	1.47	1.51
58	1A	4017	CLM	C9-N9	-2.47	1.39	1.45
59	1B	231	ARG	OXT-C	-2.26	1.23	1.30
59	1A	4018	ARG	OXT-C	-2.15	1.23	1.30

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
58	1A	4017	CLM	C8-C9-N9	4.57	123.33	119.34
58	1A	4017	CLM	C10-C9-N9	-4.56	115.35	119.34
58	1A	4017	CLM	C6-C5-C3	3.44	117.89	111.72
58	2A	3747	CLM	C6-C5-C3	3.04	117.17	111.72
58	1A	4017	CLM	O5-C5-C6	-2.72	105.30	111.20

There are no chirality outliers.

5 of 22 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
59	1B	231	ARG	O-C-CA-N
60	1A	4019	MPD	C2-C3-C4-O4
60	1A	4019	MPD	C2-C3-C4-C5
60	2B	220	MPD	C2-C3-C4-C5
59	1B	231	ARG	CA-CB-CG-CD

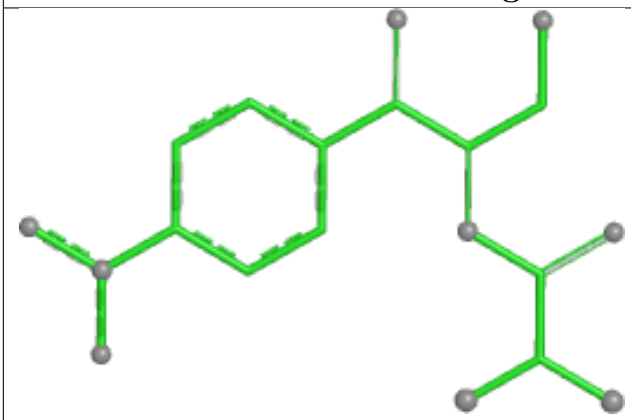
There are no ring outliers.

6 monomers are involved in 12 short contacts:

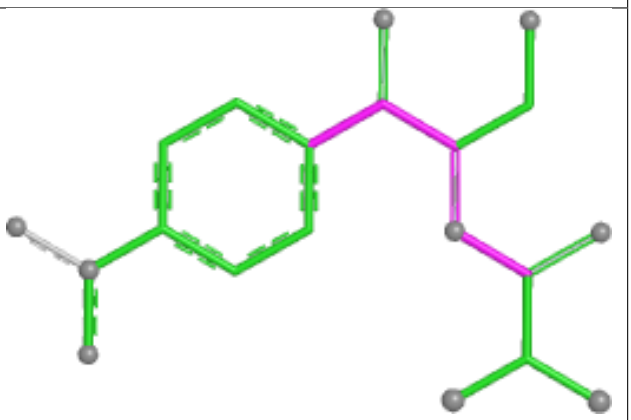
Mol	Chain	Res	Type	Clashes	Symm-Clashes
59	1A	4018	ARG	2	0
60	2B	220	MPD	1	0
60	1A	4019	MPD	1	0
59	1B	231	ARG	2	0
60	18	104	MPD	1	0
60	1a	1867	MPD	5	0

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.

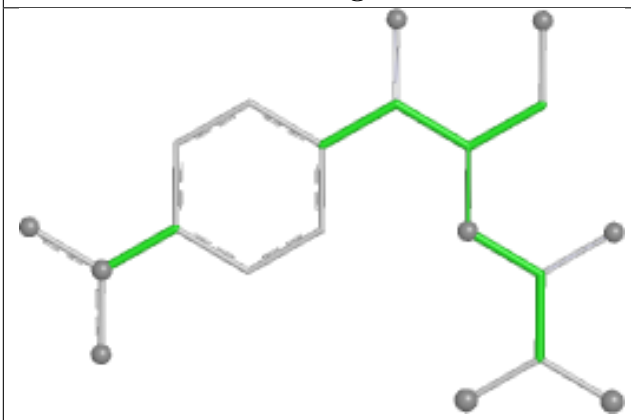
Ligand CLM 2A 3747



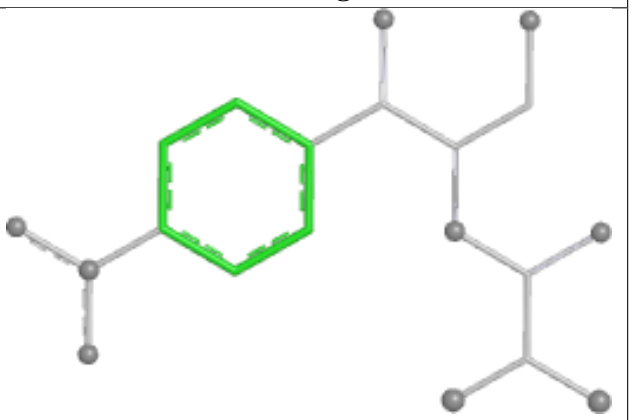
Bond lengths



Bond angles

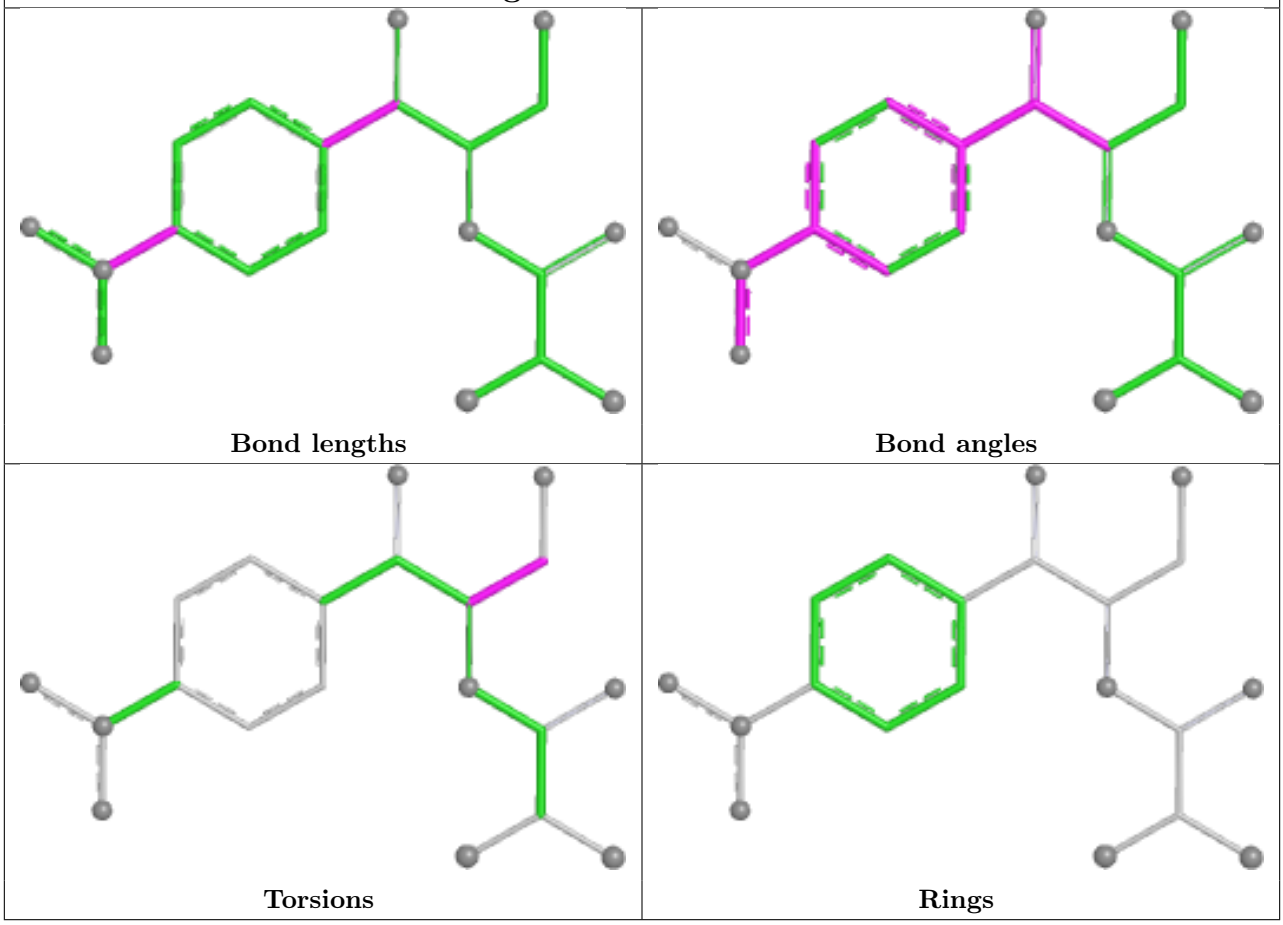


Torsions



Rings

Ligand CLM 1A 4017



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	1A	2861/2915 (98%)	-0.49	139 (4%) 35 31	19, 36, 84, 95	0
1	2A	2856/2915 (97%)	0.04	148 (5%) 33 29	32, 53, 85, 95	0
2	1B	120/121 (99%)	-0.25	2 (1%) 69 65	30, 48, 62, 74	0
2	2B	120/121 (99%)	0.76	4 (3%) 49 45	58, 70, 78, 82	0
3	1D	275/276 (99%)	-0.11	1 (0%) 88 86	21, 36, 49, 61	0
3	2D	275/276 (99%)	0.27	2 (0%) 84 81	29, 48, 60, 71	0
4	1E	204/206 (99%)	-0.05	0 100 100	18, 40, 57, 66	0
4	2E	204/206 (99%)	0.42	3 (1%) 72 68	32, 53, 66, 75	0
5	1F	203/210 (96%)	0.05	2 (0%) 79 76	19, 41, 64, 77	0
5	2F	203/210 (96%)	0.70	4 (1%) 65 60	31, 62, 71, 78	0
6	1G	181/182 (99%)	0.88	14 (7%) 19 16	45, 59, 70, 79	0
6	2G	181/182 (99%)	1.76	63 (34%) 1 1	63, 73, 80, 84	0
7	1H	174/180 (96%)	0.39	1 (0%) 85 83	37, 52, 62, 66	0
7	2H	173/180 (96%)	1.41	35 (20%) 3 2	58, 71, 77, 80	0
8	1I	147/148 (99%)	1.04	14 (9%) 14 11	41, 66, 73, 78	0
8	2I	146/148 (98%)	1.30	21 (14%) 6 4	54, 68, 77, 84	0
9	1N	140/140 (100%)	0.04	3 (2%) 63 59	25, 38, 57, 72	0
9	2N	140/140 (100%)	0.75	6 (4%) 40 36	44, 60, 69, 71	0
10	1O	122/122 (100%)	-0.06	1 (0%) 82 80	28, 41, 56, 64	0
10	2O	122/122 (100%)	0.46	0 100 100	42, 51, 62, 68	0
11	1P	149/150 (99%)	0.09	0 100 100	19, 45, 65, 74	0
11	2P	149/150 (99%)	0.70	8 (5%) 31 28	37, 61, 72, 78	0
12	1Q	141/141 (100%)	0.02	0 100 100	25, 39, 50, 60	0
12	2Q	141/141 (100%)	0.97	10 (7%) 22 18	43, 60, 68, 72	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	1R	118/118 (100%)	-0.17	0 100 100	25, 34, 48, 54	0
13	2R	118/118 (100%)	0.33	2 (1%) 69 65	37, 49, 58, 65	0
14	1S	110/112 (98%)	0.47	4 (3%) 46 42	37, 48, 59, 63	0
14	2S	110/112 (98%)	1.48	21 (19%) 3 2	59, 66, 71, 71	0
15	1T	131/146 (89%)	0.22	5 (3%) 44 40	33, 45, 64, 80	0
15	2T	131/146 (89%)	0.53	3 (2%) 61 57	42, 55, 68, 77	0
16	1U	116/118 (98%)	-0.28	1 (0%) 81 78	21, 30, 45, 59	0
16	2U	116/118 (98%)	0.68	4 (3%) 48 44	40, 56, 67, 72	0
17	1V	101/101 (100%)	0.03	1 (0%) 79 76	22, 40, 55, 63	0
17	2V	101/101 (100%)	0.87	4 (3%) 42 38	40, 64, 71, 77	0
18	1W	112/113 (99%)	-0.18	1 (0%) 81 78	24, 31, 50, 72	0
18	2W	112/113 (99%)	0.48	3 (2%) 56 52	35, 49, 63, 81	0
19	1X	95/96 (98%)	0.03	2 (2%) 63 59	27, 38, 57, 64	0
19	2X	95/96 (98%)	0.91	8 (8%) 17 14	45, 56, 68, 75	0
20	1Y	107/110 (97%)	0.31	2 (1%) 66 62	34, 47, 59, 71	0
20	2Y	107/110 (97%)	1.20	12 (11%) 10 7	55, 65, 73, 78	0
21	1Z	203/206 (98%)	0.65	4 (1%) 65 60	39, 55, 67, 75	0
21	2Z	201/206 (97%)	1.40	30 (14%) 5 4	61, 69, 76, 80	0
22	10	83/85 (97%)	0.18	6 (7%) 21 18	27, 36, 55, 69	0
22	20	83/85 (97%)	1.15	8 (9%) 13 10	45, 58, 68, 70	0
23	11	97/98 (98%)	0.19	1 (1%) 79 76	27, 43, 63, 68	0
23	21	97/98 (98%)	0.53	1 (1%) 79 76	38, 52, 68, 73	0
24	12	70/72 (97%)	0.29	2 (2%) 53 50	37, 48, 58, 68	0
24	22	70/72 (97%)	1.06	6 (8%) 16 13	55, 64, 69, 71	0
25	13	59/60 (98%)	0.00	0 100 100	24, 35, 57, 63	0
25	23	59/60 (98%)	0.67	3 (5%) 33 30	53, 58, 70, 76	0
26	14	69/71 (97%)	1.34	17 (24%) 2 1	54, 70, 80, 85	0
26	24	69/71 (97%)	2.22	38 (55%) 0 0	72, 78, 82, 84	0
27	15	59/60 (98%)	-0.26	1 (1%) 69 65	22, 32, 45, 54	0
27	25	59/60 (98%)	0.20	1 (1%) 69 65	33, 48, 60, 66	0
28	16	53/54 (98%)	-0.00	0 100 100	33, 42, 52, 57	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
28	26	53/54 (98%)	0.58	1 (1%) 66 62	47, 56, 63, 67	0
29	17	48/49 (97%)	-0.19	3 (6%) 26 22	21, 28, 52, 61	0
29	27	48/49 (97%)	0.07	3 (6%) 26 22	34, 39, 60, 66	0
30	18	64/65 (98%)	-0.21	0 100 100	27, 34, 40, 54	0
30	28	64/65 (98%)	0.57	2 (3%) 51 47	40, 51, 58, 63	0
31	19	37/37 (100%)	-0.00	0 100 100	30, 39, 51, 58	0
31	29	37/37 (100%)	1.03	1 (2%) 56 52	51, 60, 71, 71	0
32	1a	1488/1521 (97%)	0.32	45 (3%) 52 48	35, 64, 82, 95	0
32	2a	1492/1521 (98%)	0.62	64 (4%) 40 36	44, 69, 84, 95	0
33	1b	231/256 (90%)	1.40	44 (19%) 3 2	60, 70, 77, 82	0
33	2b	231/256 (90%)	1.69	77 (33%) 1 1	66, 75, 80, 84	0
34	1c	206/239 (86%)	1.01	14 (6%) 23 20	56, 67, 75, 80	0
34	2c	206/239 (86%)	1.72	71 (34%) 1 1	65, 75, 79, 81	0
35	1d	208/209 (99%)	1.15	22 (10%) 11 8	54, 65, 73, 79	0
35	2d	208/209 (99%)	1.32	28 (13%) 7 5	56, 66, 73, 75	0
36	1e	148/162 (91%)	0.79	3 (2%) 65 60	43, 61, 68, 74	0
36	2e	148/162 (91%)	1.07	13 (8%) 15 12	58, 66, 73, 81	0
37	1f	100/101 (99%)	0.72	5 (5%) 34 30	50, 59, 68, 70	0
37	2f	100/101 (99%)	0.73	1 (1%) 79 76	56, 64, 72, 77	0
38	1g	155/156 (99%)	0.93	11 (7%) 22 18	53, 65, 71, 77	0
38	2g	155/156 (99%)	1.61	46 (29%) 1 1	66, 73, 78, 80	0
39	1h	137/138 (99%)	0.86	10 (7%) 21 17	52, 62, 67, 72	0
39	2h	137/138 (99%)	1.09	6 (4%) 39 34	61, 68, 73, 75	0
40	1i	127/128 (99%)	1.53	30 (23%) 2 1	56, 69, 75, 77	0
40	2i	126/128 (98%)	2.31	78 (61%) 0 0	68, 76, 80, 83	0
41	1j	97/105 (92%)	1.48	23 (23%) 2 1	57, 71, 76, 78	0
41	2j	96/105 (91%)	2.51	68 (70%) 0 0	68, 76, 81, 84	0
42	1k	114/129 (88%)	0.69	2 (1%) 67 63	42, 59, 68, 71	0
42	2k	114/129 (88%)	1.11	11 (9%) 13 10	56, 67, 73, 76	0
43	1l	121/132 (91%)	0.72	5 (4%) 41 37	48, 57, 65, 70	0
43	2l	121/132 (91%)	0.91	9 (7%) 20 17	53, 61, 68, 71	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
44	1m	116/126 (92%)	1.23	16 (13%) 6 5	56, 67, 73, 77	0
44	2m	114/126 (90%)	1.87	43 (37%) 1 0	69, 74, 79, 80	0
45	1n	60/61 (98%)	1.23	6 (10%) 12 9	58, 64, 72, 74	0
45	2n	60/61 (98%)	2.48	38 (63%) 0 0	66, 74, 79, 84	0
46	1o	88/89 (98%)	0.89	3 (3%) 48 44	43, 60, 70, 73	0
46	2o	88/89 (98%)	1.02	7 (7%) 18 15	58, 67, 72, 76	0
47	1p	82/88 (93%)	1.51	18 (21%) 2 2	55, 66, 73, 82	0
47	2p	82/88 (93%)	1.30	13 (15%) 5 4	57, 64, 69, 74	0
48	1q	99/105 (94%)	0.99	5 (5%) 33 30	49, 62, 71, 73	0
48	2q	99/105 (94%)	0.82	2 (2%) 65 60	54, 65, 71, 74	0
49	1r	68/88 (77%)	0.75	3 (4%) 39 34	52, 59, 71, 73	0
49	2r	68/88 (77%)	1.17	8 (11%) 9 6	61, 67, 74, 77	0
50	1s	83/93 (89%)	1.29	11 (13%) 7 5	59, 69, 74, 77	0
50	2s	83/93 (89%)	2.10	44 (53%) 0 0	63, 75, 80, 81	0
51	1t	96/106 (90%)	1.34	17 (17%) 4 3	59, 65, 73, 76	0
51	2t	98/106 (92%)	1.00	5 (5%) 33 30	54, 64, 72, 74	0
52	1u	23/27 (85%)	1.56	6 (26%) 1 1	61, 66, 69, 71	0
52	2u	23/27 (85%)	2.65	15 (65%) 0 0	71, 74, 76, 79	0
53	1y	97/113 (85%)	0.90	6 (6%) 26 23	49, 60, 70, 77	0
53	2y	96/113 (84%)	2.59	69 (71%) 0 0	69, 78, 84, 85	0
54	1w	4/5 (80%)	-0.17	0 100 100	28, 31, 44, 61	0
54	2w	4/5 (80%)	0.21	0 100 100	39, 46, 55, 70	0
55	1x	3/4 (75%)	0.38	1 (33%) 1 1	29, 29, 34, 51	0
55	2x	3/4 (75%)	0.53	1 (33%) 1 1	43, 43, 45, 60	0
56	1v	3/3 (100%)	-0.06	0 100 100	23, 23, 29, 38	0
56	2v	3/3 (100%)	0.94	0 100 100	46, 46, 51, 57	0
All	All	20798/21492 (96%)	0.49	1705 (8%) 17 14	18, 59, 79, 95	0

The worst 5 of 1705 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
45	2n	2	ALA	9.3
1	1A	1087	G	7.0

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Mol	Chain	Res	Type	RSRZ
41	2j	37	PRO	6.7
1	1A	2804	C	6.6
45	1n	2	ALA	6.5

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	5MU	2A	1915	21/22	0.82	0.12	71,79,86,100	0
32	2MG	2a	1207	24/25	0.82	0.15	70,77,81,86	0
1	5MU	1A	1915	21/22	0.86	0.13	63,71,76,84	0
32	M2G	2a	966	25/26	0.88	0.16	64,70,83,97	0
1	PSU	2A	1911	20/21	0.89	0.11	66,71,78,83	0
1	PSU	2A	1917	20/21	0.89	0.10	65,74,85,87	0
32	5MC	2a	1400	21/22	0.90	0.18	62,74,78,82	0
43	0TD	1l	92	10/11	0.91	0.12	50,56,60,61	0
43	0TD	2l	92	10/11	0.91	0.13	58,63,69,74	0
32	5MC	1a	967	21/22	0.92	0.13	57,63,72,79	0
1	PSU	1A	1917	20/21	0.92	0.10	55,59,65,69	0
32	5MC	2a	967	21/22	0.92	0.14	65,69,75,77	0
32	PSU	2a	516	20/21	0.93	0.10	65,70,72,79	0
1	OMC	2A	1920	21/22	0.93	0.11	58,64,68,72	0
32	2MG	1a	1207	24/25	0.94	0.10	61,67,72,73	0
32	PSU	1a	516	20/21	0.94	0.09	56,61,65,68	0
32	M2G	1a	966	25/26	0.94	0.11	48,57,63,70	0
32	5MC	2a	1404	21/22	0.94	0.10	51,61,65,69	0
1	PSU	1A	1911	20/21	0.94	0.09	54,60,63,67	0
32	MA6	1a	1519	24/25	0.95	0.10	39,45,50,52	0
32	5MC	1a	1400	21/22	0.95	0.10	49,53,58,60	0
32	4OC	1a	1402	22/23	0.95	0.10	44,50,59,63	0
32	4OC	2a	1402	22/23	0.95	0.10	52,60,68,70	0
32	G7M	2a	527	24/25	0.95	0.09	55,60,64,67	0
32	5MC	2a	1407	21/22	0.95	0.10	52,62,64,65	0
32	UR3	2a	1498	21/22	0.95	0.10	55,61,67,72	0
32	MA6	2a	1518	24/25	0.95	0.11	54,62,66,67	0
32	5MC	1a	1407	21/22	0.95	0.11	42,51,57,59	0
32	5MC	1a	1404	21/22	0.96	0.09	45,48,52,54	0
32	G7M	1a	527	24/25	0.96	0.10	41,53,58,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
32	UR3	1a	1498	21/22	0.96	0.09	46,51,54,62	0
32	MA6	1a	1518	24/25	0.96	0.10	38,47,50,52	0
1	5MC	1A	1942	21/22	0.96	0.08	31,40,45,49	0
32	MA6	2a	1519	24/25	0.96	0.12	52,59,63,67	0
1	5MC	2A	1942	21/22	0.96	0.09	47,50,52,62	0
55	8AN	2x	76	22/23	0.96	0.09	39,45,50,54	0
1	OMG	1A	2251	24/25	0.97	0.08	20,26,31,38	0
1	5MC	2A	1962	21/22	0.97	0.08	39,45,49,56	0
1	OMG	2A	2251	24/25	0.97	0.08	33,40,44,48	0
1	2MA	2A	2503	23/24	0.97	0.07	28,33,38,40	0
1	OMC	1A	1920	21/22	0.97	0.09	42,53,58,60	0
1	5MU	2A	1939	21/22	0.97	0.07	32,38,42,45	0
1	2MA	1A	2503	23/24	0.98	0.06	19,23,25,27	0
1	OMU	1A	2552	21/22	0.98	0.07	22,28,34,35	0
1	PSU	1A	2605	20/21	0.98	0.07	22,27,31,33	0
1	5MC	1A	1962	21/22	0.98	0.07	26,34,38,40	0
1	5MU	1A	1939	21/22	0.98	0.07	23,29,33,36	0
1	OMU	2A	2552	21/22	0.98	0.07	33,38,42,43	0
55	8AN	1x	76	22/23	0.98	0.06	21,30,34,34	0
1	PSU	2A	2605	20/21	0.98	0.07	31,36,43,43	0

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3686	1/1	0.48	0.18	76,76,76,76	0
57	MG	1A	3747	1/1	0.55	0.18	66,66,66,66	0
57	MG	1B	230	1/1	0.63	0.18	74,74,74,74	0
57	MG	2G	203	1/1	0.63	0.28	76,76,76,76	0
57	MG	21	101	1/1	0.63	0.21	69,69,69,69	0
57	MG	2O	202	1/1	0.64	0.23	80,80,80,80	0
57	MG	2A	3340	1/1	0.64	0.19	68,68,68,68	0
57	MG	1A	3414	1/1	0.66	0.20	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3545	1/1	0.66	0.23	73,73,73,73	0
57	MG	2A	3419	1/1	0.70	0.20	54,54,54,54	0
57	MG	1A	3808	1/1	0.70	0.14	79,79,79,79	0
57	MG	2a	3134	1/1	0.70	0.26	82,82,82,82	0
57	MG	2A	3546	1/1	0.71	0.20	79,79,79,79	0
57	MG	1A	3588	1/1	0.72	0.17	51,51,51,51	0
57	MG	1A	3644	1/1	0.72	0.25	73,73,73,73	0
57	MG	1A	3867	1/1	0.72	0.19	67,67,67,67	0
57	MG	2A	3457	1/1	0.72	0.12	78,78,78,78	0
57	MG	2Q	202	1/1	0.72	0.32	56,56,56,56	0
57	MG	2A	3506	1/1	0.72	0.20	69,69,69,69	0
57	MG	1B	229	1/1	0.72	0.16	66,66,66,66	0
57	MG	1a	1774	1/1	0.73	0.27	69,69,69,69	0
57	MG	2A	3456	1/1	0.73	0.24	68,68,68,68	0
57	MG	1A	3651	1/1	0.73	0.16	65,65,65,65	0
57	MG	1A	3438	1/1	0.74	0.25	67,67,67,67	0
57	MG	1A	3519	1/1	0.75	0.14	52,52,52,52	0
57	MG	2A	3588	1/1	0.75	0.17	46,46,46,46	0
57	MG	1A	3638	1/1	0.75	0.29	37,37,37,37	0
57	MG	2A	3254	1/1	0.75	0.29	76,76,76,76	0
57	MG	1A	3978	1/1	0.76	0.16	35,35,35,35	0
57	MG	1t	3102	1/1	0.76	0.21	64,64,64,64	0
57	MG	2A	3234	1/1	0.76	0.16	65,65,65,65	0
57	MG	2A	3246	1/1	0.76	0.21	70,70,70,70	0
57	MG	2A	3592	1/1	0.76	0.17	58,58,58,58	0
57	MG	1A	3988	1/1	0.76	0.19	55,55,55,55	0
57	MG	1A	4011	1/1	0.76	0.15	33,33,33,33	0
57	MG	2A	3418	1/1	0.76	0.18	58,58,58,58	0
57	MG	1B	218	1/1	0.76	0.18	64,64,64,64	0
57	MG	1A	3602	1/1	0.76	0.13	44,44,44,44	0
57	MG	1A	3924	1/1	0.76	0.15	48,48,48,48	0
57	MG	1A	3420	1/1	0.77	0.21	72,72,72,72	0
57	MG	1A	3571	1/1	0.77	0.14	65,65,65,65	0
57	MG	1A	3855	1/1	0.77	0.13	56,56,56,56	0
57	MG	1A	3861	1/1	0.77	0.17	49,49,49,49	0
57	MG	1A	3578	1/1	0.77	0.14	45,45,45,45	0
57	MG	1A	3323	1/1	0.77	0.45	79,79,79,79	0
57	MG	2a	3022	1/1	0.77	0.36	73,73,73,73	0
57	MG	2a	3050	1/1	0.77	0.41	86,86,86,86	0
57	MG	1a	1745	1/1	0.77	0.18	70,70,70,70	0
59	ARG	1A	4018	12/12	0.77	0.20	41,65,74,75	0
57	MG	2B	211	1/1	0.78	0.21	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1a	1700	1/1	0.78	0.22	74,74,74,74	0
57	MG	1A	3624	1/1	0.78	0.15	38,38,38,38	0
57	MG	2A	3330	1/1	0.78	0.14	57,57,57,57	0
57	MG	1A	3709	1/1	0.78	0.17	54,54,54,54	0
57	MG	1d	304	1/1	0.78	0.19	71,71,71,71	0
57	MG	1A	3712	1/1	0.78	0.15	69,69,69,69	0
57	MG	2a	3065	1/1	0.78	0.39	74,74,74,74	0
57	MG	1T	202	1/1	0.78	0.21	67,67,67,67	0
57	MG	2A	3713	1/1	0.78	0.14	61,61,61,61	0
57	MG	2A	3436	1/1	0.79	0.14	70,70,70,70	0
57	MG	2B	207	1/1	0.79	0.22	70,70,70,70	0
57	MG	2A	3200	1/1	0.79	0.29	73,73,73,73	0
57	MG	2G	201	1/1	0.79	0.14	74,74,74,74	0
57	MG	1A	3264	1/1	0.79	0.23	69,69,69,69	0
57	MG	2A	3463	1/1	0.79	0.20	63,63,63,63	0
57	MG	2A	3472	1/1	0.79	0.17	57,57,57,57	0
57	MG	1A	3937	1/1	0.79	0.13	65,65,65,65	0
57	MG	1a	1769	1/1	0.79	0.16	69,69,69,69	0
57	MG	1A	3944	1/1	0.79	0.14	80,80,80,80	0
57	MG	1a	1797	1/1	0.79	0.25	77,77,77,77	0
57	MG	1A	3462	1/1	0.79	0.22	63,63,63,63	0
57	MG	1A	3147	1/1	0.79	0.13	80,80,80,80	0
57	MG	2A	3387	1/1	0.80	0.17	51,51,51,51	0
57	MG	1a	1846	1/1	0.80	0.21	73,73,73,73	0
57	MG	1a	1601	1/1	0.80	0.16	68,68,68,68	0
57	MG	1A	3095	1/1	0.80	0.17	63,63,63,63	0
57	MG	2A	3128	1/1	0.80	0.21	67,67,67,67	0
57	MG	2A	3134	1/1	0.80	0.32	70,70,70,70	0
57	MG	1a	1724	1/1	0.80	0.19	69,69,69,69	0
57	MG	1A	3346	1/1	0.80	0.19	50,50,50,50	0
57	MG	1A	3432	1/1	0.80	0.13	29,29,29,29	0
57	MG	1a	1772	1/1	0.80	0.16	69,69,69,69	0
57	MG	2a	3027	1/1	0.80	0.28	67,67,67,67	0
57	MG	1A	3916	1/1	0.80	0.11	57,57,57,57	0
57	MG	1A	3918	1/1	0.80	0.12	23,23,23,23	0
57	MG	2a	3086	1/1	0.80	0.20	64,64,64,64	0
57	MG	2A	3383	1/1	0.80	0.18	66,66,66,66	0
57	MG	2A	3636	1/1	0.80	0.15	70,70,70,70	0
57	MG	1a	1671	1/1	0.81	0.18	62,62,62,62	0
57	MG	2A	3709	1/1	0.81	0.18	57,57,57,57	0
57	MG	2A	3445	1/1	0.81	0.14	51,51,51,51	0
57	MG	1a	1686	1/1	0.81	0.20	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1a	1789	1/1	0.81	0.19	70,70,70,70	0
57	MG	1A	3790	1/1	0.81	0.14	53,53,53,53	0
57	MG	1a	1813	1/1	0.81	0.23	73,73,73,73	0
57	MG	1a	1841	1/1	0.81	0.12	61,61,61,61	0
57	MG	2A	3525	1/1	0.81	0.13	62,62,62,62	0
57	MG	1a	1709	1/1	0.81	0.31	65,65,65,65	0
57	MG	1A	3536	1/1	0.81	0.17	56,56,56,56	0
57	MG	2a	3026	1/1	0.81	0.29	75,75,75,75	0
57	MG	2A	3581	1/1	0.81	0.15	70,70,70,70	0
57	MG	2a	3048	1/1	0.81	0.36	69,69,69,69	0
57	MG	1A	3522	1/1	0.81	0.15	53,53,53,53	0
57	MG	2A	3053	1/1	0.81	0.20	60,60,60,60	0
57	MG	2A	3594	1/1	0.81	0.15	73,73,73,73	0
57	MG	2a	3129	1/1	0.81	0.15	67,67,67,67	0
57	MG	2a	3132	1/1	0.81	0.17	59,59,59,59	0
57	MG	1a	1622	1/1	0.81	0.18	61,61,61,61	0
57	MG	2A	3658	1/1	0.81	0.18	75,75,75,75	0
57	MG	1a	1697	1/1	0.82	0.26	62,62,62,62	0
57	MG	1a	1823	1/1	0.82	0.17	61,61,61,61	0
57	MG	1a	1828	1/1	0.82	0.28	75,75,75,75	0
57	MG	2A	3732	1/1	0.82	0.16	68,68,68,68	0
57	MG	2A	3740	1/1	0.82	0.17	71,71,71,71	0
57	MG	2A	3430	1/1	0.82	0.18	67,67,67,67	0
57	MG	1a	1699	1/1	0.82	0.42	78,78,78,78	0
57	MG	2B	213	1/1	0.82	0.26	70,70,70,70	0
57	MG	1A	3464	1/1	0.82	0.15	37,37,37,37	0
57	MG	1E	304	1/1	0.82	0.12	29,29,29,29	0
57	MG	1n	102	1/1	0.82	0.11	55,55,55,55	0
57	MG	1A	3502	1/1	0.82	0.15	62,62,62,62	0
57	MG	1W	203	1/1	0.82	0.12	67,67,67,67	0
57	MG	2A	3081	1/1	0.82	0.19	61,61,61,61	0
57	MG	2a	3025	1/1	0.82	0.22	69,69,69,69	0
57	MG	1a	1754	1/1	0.82	0.15	60,60,60,60	0
57	MG	1A	3269	1/1	0.82	0.18	56,56,56,56	0
57	MG	1A	3332	1/1	0.82	0.12	26,26,26,26	0
57	MG	2A	3577	1/1	0.82	0.17	73,73,73,73	0
57	MG	2a	3060	1/1	0.82	0.30	81,81,81,81	0
57	MG	1a	1638	1/1	0.82	0.34	70,70,70,70	0
57	MG	1a	1775	1/1	0.82	0.13	67,67,67,67	0
57	MG	1a	1787	1/1	0.82	0.17	61,61,61,61	0
57	MG	1A	3836	1/1	0.82	0.09	44,44,44,44	0
57	MG	1a	1792	1/1	0.82	0.22	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3535	1/1	0.82	0.16	58,58,58,58	0
57	MG	1A	3559	1/1	0.83	0.15	59,59,59,59	0
57	MG	1A	3852	1/1	0.83	0.11	58,58,58,58	0
57	MG	1A	3952	1/1	0.83	0.18	58,58,58,58	0
57	MG	2A	3173	1/1	0.83	0.29	74,74,74,74	0
57	MG	1A	3708	1/1	0.83	0.36	63,63,63,63	0
57	MG	2A	3541	1/1	0.83	0.18	58,58,58,58	0
57	MG	1A	3619	1/1	0.83	0.20	58,58,58,58	0
57	MG	2P	202	1/1	0.83	0.17	73,73,73,73	0
57	MG	1a	1650	1/1	0.83	0.22	72,72,72,72	0
57	MG	2A	3547	1/1	0.83	0.20	60,60,60,60	0
57	MG	2a	3010	1/1	0.83	0.43	73,73,73,73	0
57	MG	2A	3548	1/1	0.83	0.13	61,61,61,61	0
57	MG	1A	3185	1/1	0.83	0.18	62,62,62,62	0
57	MG	1A	4014	1/1	0.83	0.15	61,61,61,61	0
57	MG	1a	1688	1/1	0.83	0.25	59,59,59,59	0
57	MG	1B	211	1/1	0.83	0.17	68,68,68,68	0
57	MG	1A	3881	1/1	0.83	0.11	66,66,66,66	0
57	MG	1B	225	1/1	0.83	0.20	55,55,55,55	0
57	MG	2a	3063	1/1	0.83	0.27	71,71,71,71	0
57	MG	2A	3643	1/1	0.83	0.16	68,68,68,68	0
57	MG	1A	3625	1/1	0.83	0.16	54,54,54,54	0
57	MG	2a	3112	1/1	0.83	0.24	74,74,74,74	0
57	MG	1A	3513	1/1	0.83	0.10	20,20,20,20	0
57	MG	1a	1730	1/1	0.83	0.18	63,63,63,63	0
57	MG	1A	3085	1/1	0.83	0.16	66,66,66,66	0
57	MG	1N	204	1/1	0.83	0.09	52,52,52,52	0
57	MG	2A	3715	1/1	0.84	0.15	59,59,59,59	0
57	MG	2A	3722	1/1	0.84	0.14	66,66,66,66	0
57	MG	2A	3728	1/1	0.84	0.18	55,55,55,55	0
57	MG	1A	3897	1/1	0.84	0.14	55,55,55,55	0
57	MG	2A	3449	1/1	0.84	0.17	58,58,58,58	0
57	MG	1a	1776	1/1	0.84	0.15	59,59,59,59	0
57	MG	1A	3528	1/1	0.84	0.21	63,63,63,63	0
57	MG	19	102	1/1	0.84	0.15	65,65,65,65	0
57	MG	2B	215	1/1	0.84	0.16	66,66,66,66	0
57	MG	1A	3664	1/1	0.84	0.09	21,21,21,21	0
57	MG	2A	3476	1/1	0.84	0.20	62,62,62,62	0
57	MG	1A	3256	1/1	0.84	0.17	67,67,67,67	0
57	MG	2A	3520	1/1	0.84	0.16	60,60,60,60	0
57	MG	1a	1628	1/1	0.84	0.25	64,64,64,64	0
57	MG	1A	3437	1/1	0.84	0.10	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2a	3002	1/1	0.84	0.17	73,73,73,73	0
57	MG	1A	3431	1/1	0.84	0.16	61,61,61,61	0
57	MG	2A	3264	1/1	0.84	0.15	62,62,62,62	0
57	MG	2A	3271	1/1	0.84	0.40	54,54,54,54	0
57	MG	2A	3318	1/1	0.84	0.16	66,66,66,66	0
57	MG	2A	3560	1/1	0.84	0.12	37,37,37,37	0
57	MG	1a	1832	1/1	0.84	0.20	56,56,56,56	0
57	MG	1a	1839	1/1	0.84	0.14	72,72,72,72	0
57	MG	2a	3051	1/1	0.84	0.34	72,72,72,72	0
57	MG	2A	3373	1/1	0.84	0.20	69,69,69,69	0
57	MG	2a	3061	1/1	0.84	0.20	61,61,61,61	0
57	MG	1a	1756	1/1	0.84	0.15	48,48,48,48	0
57	MG	1a	1757	1/1	0.84	0.12	53,53,53,53	0
57	MG	2a	3073	1/1	0.84	0.30	71,71,71,71	0
57	MG	2a	3077	1/1	0.84	0.16	74,74,74,74	0
57	MG	2A	3403	1/1	0.84	0.12	62,62,62,62	0
57	MG	1a	1866	1/1	0.84	0.18	70,70,70,70	0
57	MG	1A	3737	1/1	0.84	0.12	46,46,46,46	0
57	MG	2A	3423	1/1	0.84	0.12	61,61,61,61	0
57	MG	1A	3746	1/1	0.84	0.17	65,65,65,65	0
57	MG	2j	201	1/1	0.84	0.34	66,66,66,66	0
57	MG	1A	3617	1/1	0.84	0.24	55,55,55,55	0
57	MG	2A	3132	1/1	0.85	0.19	65,65,65,65	0
57	MG	1a	1806	1/1	0.85	0.14	70,70,70,70	0
57	MG	2A	3147	1/1	0.85	0.20	59,59,59,59	0
57	MG	2A	3451	1/1	0.85	0.29	46,46,46,46	0
57	MG	2A	3151	1/1	0.85	0.17	67,67,67,67	0
57	MG	1A	3893	1/1	0.85	0.13	56,56,56,56	0
57	MG	2A	3462	1/1	0.85	0.12	70,70,70,70	0
57	MG	1a	1751	1/1	0.85	0.26	82,82,82,82	0
57	MG	2A	3227	1/1	0.85	0.18	65,65,65,65	0
57	MG	1A	3393	1/1	0.85	0.11	32,32,32,32	0
57	MG	2A	3477	1/1	0.85	0.13	65,65,65,65	0
57	MG	1a	1829	1/1	0.85	0.21	71,71,71,71	0
57	MG	1A	3690	1/1	0.85	0.10	55,55,55,55	0
57	MG	1a	1834	1/1	0.85	0.22	69,69,69,69	0
57	MG	1A	3691	1/1	0.85	0.13	65,65,65,65	0
57	MG	2A	3302	1/1	0.85	0.14	58,58,58,58	0
57	MG	2T	203	1/1	0.85	0.15	74,74,74,74	0
57	MG	2A	3317	1/1	0.85	0.18	64,64,64,64	0
57	MG	1A	3703	1/1	0.85	0.18	64,64,64,64	0
57	MG	1A	3472	1/1	0.85	0.10	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2a	3011	1/1	0.85	0.34	75,75,75,75	0
57	MG	2A	3553	1/1	0.85	0.18	76,76,76,76	0
57	MG	2A	3558	1/1	0.85	0.13	61,61,61,61	0
57	MG	1A	3557	1/1	0.85	0.10	46,46,46,46	0
57	MG	2A	3568	1/1	0.85	0.13	57,57,57,57	0
57	MG	2A	3345	1/1	0.85	0.23	69,69,69,69	0
57	MG	1A	3643	1/1	0.85	0.17	64,64,64,64	0
57	MG	2A	3584	1/1	0.85	0.15	43,43,43,43	0
57	MG	1A	3481	1/1	0.85	0.11	30,30,30,30	0
57	MG	1A	3330	1/1	0.85	0.17	62,62,62,62	0
57	MG	17	104	1/1	0.85	0.23	56,56,56,56	0
57	MG	2A	3600	1/1	0.85	0.15	55,55,55,55	0
57	MG	2A	3618	1/1	0.85	0.13	48,48,48,48	0
57	MG	2A	3626	1/1	0.85	0.12	45,45,45,45	0
57	MG	2A	3629	1/1	0.85	0.16	40,40,40,40	0
57	MG	2A	3634	1/1	0.85	0.16	36,36,36,36	0
57	MG	1A	3993	1/1	0.85	0.14	65,65,65,65	0
57	MG	2A	3089	1/1	0.85	0.19	63,63,63,63	0
57	MG	2A	3100	1/1	0.85	0.17	60,60,60,60	0
57	MG	2a	3179	1/1	0.85	0.11	67,67,67,67	0
57	MG	2a	3181	1/1	0.85	0.21	77,77,77,77	0
57	MG	2a	3189	1/1	0.85	0.28	66,66,66,66	0
57	MG	2A	3662	1/1	0.85	0.10	53,53,53,53	0
57	MG	1A	3886	1/1	0.85	0.23	60,60,60,60	0
57	MG	2A	3730	1/1	0.86	0.13	59,59,59,59	0
57	MG	2A	3494	1/1	0.86	0.10	68,68,68,68	0
57	MG	1A	3486	1/1	0.86	0.09	23,23,23,23	0
57	MG	2A	3742	1/1	0.86	0.17	71,71,71,71	0
57	MG	2A	3743	1/1	0.86	0.23	62,62,62,62	0
57	MG	2B	201	1/1	0.86	0.22	71,71,71,71	0
57	MG	2A	3517	1/1	0.86	0.13	67,67,67,67	0
57	MG	1A	3935	1/1	0.86	0.09	57,57,57,57	0
57	MG	1A	3795	1/1	0.86	0.14	69,69,69,69	0
57	MG	2A	3527	1/1	0.86	0.18	65,65,65,65	0
57	MG	1a	1842	1/1	0.86	0.19	74,74,74,74	0
57	MG	1A	3942	1/1	0.86	0.12	43,43,43,43	0
57	MG	1A	3796	1/1	0.86	0.16	61,61,61,61	0
57	MG	1A	3692	1/1	0.86	0.12	65,65,65,65	0
57	MG	1a	1768	1/1	0.86	0.12	67,67,67,67	0
57	MG	1A	3425	1/1	0.86	0.17	41,41,41,41	0
57	MG	2A	3348	1/1	0.86	0.15	64,64,64,64	0
57	MG	2A	3024	1/1	0.86	0.13	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3706	1/1	0.86	0.26	44,44,44,44	0
57	MG	2A	3572	1/1	0.86	0.28	61,61,61,61	0
57	MG	1A	3507	1/1	0.86	0.17	61,61,61,61	0
57	MG	2A	3391	1/1	0.86	0.16	69,69,69,69	0
57	MG	1A	3653	1/1	0.86	0.17	58,58,58,58	0
57	MG	2A	3404	1/1	0.86	0.17	76,76,76,76	0
57	MG	2A	3092	1/1	0.86	0.23	64,64,64,64	0
57	MG	1A	3656	1/1	0.86	0.19	56,56,56,56	0
57	MG	2A	3422	1/1	0.86	0.21	56,56,56,56	0
57	MG	2A	3616	1/1	0.86	0.10	64,64,64,64	0
57	MG	1A	3721	1/1	0.86	0.10	36,36,36,36	0
57	MG	2a	3062	1/1	0.86	0.26	75,75,75,75	0
57	MG	2A	3131	1/1	0.86	0.17	66,66,66,66	0
57	MG	1A	3381	1/1	0.86	0.13	51,51,51,51	0
57	MG	1a	1694	1/1	0.86	0.31	68,68,68,68	0
57	MG	1A	3681	1/1	0.86	0.19	68,68,68,68	0
57	MG	1B	227	1/1	0.86	0.11	59,59,59,59	0
57	MG	2A	3650	1/1	0.86	0.14	65,65,65,65	0
57	MG	2a	3120	1/1	0.86	0.16	69,69,69,69	0
57	MG	2a	3121	1/1	0.86	0.22	82,82,82,82	0
57	MG	1A	3344	1/1	0.86	0.08	28,28,28,28	0
57	MG	1A	3768	1/1	0.86	0.17	52,52,52,52	0
57	MG	2A	3460	1/1	0.86	0.23	77,77,77,77	0
57	MG	2a	3147	1/1	0.86	0.20	77,77,77,77	0
57	MG	2a	3167	1/1	0.86	0.11	64,64,64,64	0
57	MG	2A	3223	1/1	0.86	0.27	70,70,70,70	0
57	MG	1a	1717	1/1	0.86	0.39	73,73,73,73	0
57	MG	2a	3182	1/1	0.86	0.17	73,73,73,73	0
57	MG	2a	3185	1/1	0.86	0.21	69,69,69,69	0
57	MG	1a	1721	1/1	0.86	0.23	65,65,65,65	0
57	MG	2A	3244	1/1	0.86	0.15	46,46,46,46	0
57	MG	1A	3788	1/1	0.86	0.22	57,57,57,57	0
60	MPD	1T	208	8/8	0.86	0.18	59,64,68,69	0
57	MG	1A	3183	1/1	0.87	0.12	56,56,56,56	0
57	MG	2A	3739	1/1	0.87	0.18	68,68,68,68	0
57	MG	2A	3096	1/1	0.87	0.22	76,76,76,76	0
57	MG	1A	3885	1/1	0.87	0.14	43,43,43,43	0
57	MG	1A	3418	1/1	0.87	0.13	27,27,27,27	0
57	MG	1A	3723	1/1	0.87	0.13	59,59,59,59	0
57	MG	1A	3537	1/1	0.87	0.13	60,60,60,60	0
57	MG	1A	3554	1/1	0.87	0.14	49,49,49,49	0
57	MG	1T	205	1/1	0.87	0.16	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	3419	1/1	0.87	0.13	31,31,31,31	0
57	MG	2B	216	1/1	0.87	0.09	77,77,77,77	0
57	MG	10	106	1/1	0.87	0.15	56,56,56,56	0
57	MG	2A	3514	1/1	0.87	0.15	61,61,61,61	0
57	MG	2A	3193	1/1	0.87	0.20	66,66,66,66	0
57	MG	2A	3197	1/1	0.87	0.28	49,49,49,49	0
57	MG	15	105	1/1	0.87	0.11	48,48,48,48	0
57	MG	2T	201	1/1	0.87	0.17	64,64,64,64	0
57	MG	2A	3210	1/1	0.87	0.11	60,60,60,60	0
57	MG	2T	204	1/1	0.87	0.17	56,56,56,56	0
57	MG	2A	3214	1/1	0.87	0.14	61,61,61,61	0
57	MG	1a	1781	1/1	0.87	0.25	71,71,71,71	0
57	MG	1a	1782	1/1	0.87	0.20	71,71,71,71	0
57	MG	1A	3751	1/1	0.87	0.10	26,26,26,26	0
57	MG	1A	3762	1/1	0.87	0.22	62,62,62,62	0
57	MG	2A	3550	1/1	0.87	0.15	62,62,62,62	0
57	MG	1A	3144	1/1	0.87	0.20	60,60,60,60	0
57	MG	1a	1616	1/1	0.87	0.19	59,59,59,59	0
57	MG	1A	3659	1/1	0.87	0.10	47,47,47,47	0
57	MG	1A	3367	1/1	0.87	0.19	72,72,72,72	0
57	MG	1a	1821	1/1	0.87	0.21	67,67,67,67	0
57	MG	1A	3948	1/1	0.87	0.09	24,24,24,24	0
57	MG	1A	3951	1/1	0.87	0.13	49,49,49,49	0
57	MG	1A	3088	1/1	0.87	0.16	53,53,53,53	0
57	MG	1a	1672	1/1	0.87	0.13	53,53,53,53	0
57	MG	1A	3974	1/1	0.87	0.11	50,50,50,50	0
57	MG	1A	3160	1/1	0.87	0.23	62,62,62,62	0
57	MG	2A	3366	1/1	0.87	0.13	58,58,58,58	0
57	MG	1A	3982	1/1	0.87	0.22	74,74,74,74	0
57	MG	2a	3110	1/1	0.87	0.29	77,77,77,77	0
57	MG	1A	3598	1/1	0.87	0.18	63,63,63,63	0
57	MG	1A	3397	1/1	0.87	0.10	44,44,44,44	0
57	MG	1a	1858	1/1	0.87	0.19	67,67,67,67	0
57	MG	2a	3127	1/1	0.87	0.12	62,62,62,62	0
57	MG	1A	3994	1/1	0.87	0.19	62,62,62,62	0
57	MG	1a	1704	1/1	0.87	0.24	62,62,62,62	0
57	MG	2a	3133	1/1	0.87	0.19	64,64,64,64	0
57	MG	2A	3415	1/1	0.87	0.12	37,37,37,37	0
57	MG	2a	3138	1/1	0.87	0.20	52,52,52,52	0
57	MG	2a	3144	1/1	0.87	0.14	65,65,65,65	0
57	MG	1e	202	1/1	0.87	0.15	65,65,65,65	0
57	MG	1A	3409	1/1	0.87	0.11	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	3447	1/1	0.87	0.12	64,64,64,64	0
57	MG	2A	3016	1/1	0.87	0.20	73,73,73,73	0
57	MG	1B	203	1/1	0.87	0.14	59,59,59,59	0
57	MG	1A	3456	1/1	0.87	0.13	55,55,55,55	0
57	MG	2A	3065	1/1	0.87	0.29	63,63,63,63	0
57	MG	2A	3446	1/1	0.87	0.12	57,57,57,57	0
57	MG	2j	202	1/1	0.87	0.10	80,80,80,80	0
57	MG	1A	3533	1/1	0.87	0.12	48,48,48,48	0
60	MPD	1A	4019	8/8	0.87	0.22	50,54,62,65	0
57	MG	1A	3870	1/1	0.87	0.16	58,58,58,58	0
60	MPD	2A	3748	8/8	0.87	0.22	56,60,66,66	0
60	MPD	2B	220	8/8	0.87	0.19	59,60,67,75	0
57	MG	2A	3664	1/1	0.88	0.10	57,57,57,57	0
57	MG	2A	3676	1/1	0.88	0.10	64,64,64,64	0
57	MG	2A	3678	1/1	0.88	0.10	68,68,68,68	0
57	MG	1a	1734	1/1	0.88	0.10	66,66,66,66	0
57	MG	2A	3390	1/1	0.88	0.14	48,48,48,48	0
57	MG	1y	202	1/1	0.88	0.38	71,71,71,71	0
57	MG	2A	3400	1/1	0.88	0.15	63,63,63,63	0
57	MG	2A	3716	1/1	0.88	0.17	69,69,69,69	0
57	MG	1A	3616	1/1	0.88	0.22	58,58,58,58	0
57	MG	1A	3459	1/1	0.88	0.21	45,45,45,45	0
57	MG	2A	3413	1/1	0.88	0.12	53,53,53,53	0
57	MG	1A	3825	1/1	0.88	0.27	35,35,35,35	0
57	MG	2A	3055	1/1	0.88	0.21	63,63,63,63	0
57	MG	2A	3060	1/1	0.88	0.12	51,51,51,51	0
57	MG	1A	3377	1/1	0.88	0.12	54,54,54,54	0
57	MG	2A	3067	1/1	0.88	0.13	57,57,57,57	0
57	MG	1A	3851	1/1	0.88	0.10	52,52,52,52	0
57	MG	2A	3435	1/1	0.88	0.13	35,35,35,35	0
57	MG	1a	1759	1/1	0.88	0.22	64,64,64,64	0
57	MG	2A	3091	1/1	0.88	0.19	63,63,63,63	0
57	MG	1a	1767	1/1	0.88	0.17	63,63,63,63	0
57	MG	18	101	1/1	0.88	0.36	57,57,57,57	0
57	MG	1A	3199	1/1	0.88	0.30	51,51,51,51	0
57	MG	2G	202	1/1	0.88	0.18	66,66,66,66	0
57	MG	2A	3127	1/1	0.88	0.16	55,55,55,55	0
57	MG	1A	3466	1/1	0.88	0.11	63,63,63,63	0
57	MG	1a	1603	1/1	0.88	0.15	64,64,64,64	0
57	MG	1A	3422	1/1	0.88	0.10	61,61,61,61	0
57	MG	1A	3477	1/1	0.88	0.10	21,21,21,21	0
57	MG	1a	1780	1/1	0.88	0.23	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3387	1/1	0.88	0.09	24,24,24,24	0
57	MG	2A	3165	1/1	0.88	0.18	58,58,58,58	0
57	MG	2A	3479	1/1	0.88	0.13	65,65,65,65	0
57	MG	2a	3005	1/1	0.88	0.17	62,62,62,62	0
57	MG	2A	3480	1/1	0.88	0.12	62,62,62,62	0
57	MG	2A	3490	1/1	0.88	0.09	61,61,61,61	0
57	MG	2a	3016	1/1	0.88	0.15	59,59,59,59	0
57	MG	1a	1637	1/1	0.88	0.20	73,73,73,73	0
57	MG	2A	3186	1/1	0.88	0.20	61,61,61,61	0
57	MG	2A	3192	1/1	0.88	0.12	58,58,58,58	0
57	MG	1A	3880	1/1	0.88	0.09	25,25,25,25	0
57	MG	2a	3035	1/1	0.88	0.37	72,72,72,72	0
57	MG	2a	3037	1/1	0.88	0.16	71,71,71,71	0
57	MG	2a	3041	1/1	0.88	0.21	65,65,65,65	0
57	MG	1A	3200	1/1	0.88	0.17	65,65,65,65	0
57	MG	2A	3523	1/1	0.88	0.15	63,63,63,63	0
57	MG	1A	3343	1/1	0.88	0.12	41,41,41,41	0
57	MG	2A	3209	1/1	0.88	0.20	63,63,63,63	0
57	MG	1A	3286	1/1	0.88	0.12	72,72,72,72	0
57	MG	1a	1675	1/1	0.88	0.16	80,80,80,80	0
57	MG	1a	1679	1/1	0.88	0.11	59,59,59,59	0
57	MG	1B	207	1/1	0.88	0.17	55,55,55,55	0
57	MG	2a	3067	1/1	0.88	0.29	69,69,69,69	0
57	MG	2A	3228	1/1	0.88	0.13	62,62,62,62	0
57	MG	2A	3549	1/1	0.88	0.12	67,67,67,67	0
57	MG	2a	3084	1/1	0.88	0.22	75,75,75,75	0
57	MG	1A	3412	1/1	0.88	0.21	51,51,51,51	0
57	MG	2a	3090	1/1	0.88	0.14	68,68,68,68	0
57	MG	2a	3104	1/1	0.88	0.43	71,71,71,71	0
57	MG	2A	3551	1/1	0.88	0.15	68,68,68,68	0
57	MG	2A	3552	1/1	0.88	0.14	58,58,58,58	0
57	MG	2A	3240	1/1	0.88	0.22	58,58,58,58	0
57	MG	2A	3241	1/1	0.88	0.18	70,70,70,70	0
57	MG	2a	3122	1/1	0.88	0.18	75,75,75,75	0
57	MG	1a	1693	1/1	0.88	0.35	73,73,73,73	0
57	MG	1A	3758	1/1	0.88	0.15	54,54,54,54	0
57	MG	2A	3248	1/1	0.88	0.23	52,52,52,52	0
57	MG	1A	3903	1/1	0.88	0.11	25,25,25,25	0
57	MG	1A	3591	1/1	0.88	0.19	63,63,63,63	0
57	MG	2a	3137	1/1	0.88	0.15	65,65,65,65	0
57	MG	1A	3672	1/1	0.88	0.14	51,51,51,51	0
57	MG	2A	3296	1/1	0.88	0.34	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3919	1/1	0.88	0.12	45,45,45,45	0
57	MG	2a	3162	1/1	0.88	0.15	59,59,59,59	0
57	MG	2A	3306	1/1	0.88	0.32	62,62,62,62	0
57	MG	1a	1708	1/1	0.88	0.26	45,45,45,45	0
57	MG	2a	3180	1/1	0.88	0.16	64,64,64,64	0
57	MG	1A	3303	1/1	0.88	0.17	66,66,66,66	0
57	MG	2A	3617	1/1	0.88	0.08	40,40,40,40	0
57	MG	2A	3319	1/1	0.88	0.12	34,34,34,34	0
57	MG	1A	3035	1/1	0.88	0.20	50,50,50,50	0
57	MG	1R	205	1/1	0.88	0.17	44,44,44,44	0
57	MG	1T	201	1/1	0.88	0.17	67,67,67,67	0
57	MG	1e	201	1/1	0.88	0.18	60,60,60,60	0
57	MG	1a	1726	1/1	0.88	0.14	60,60,60,60	0
57	MG	1h	202	1/1	0.88	0.15	63,63,63,63	0
57	MG	1A	3608	1/1	0.88	0.10	60,60,60,60	0
57	MG	2A	3385	1/1	0.88	0.12	75,75,75,75	0
57	MG	1A	3342	1/1	0.89	0.11	51,51,51,51	0
57	MG	2A	3143	1/1	0.89	0.18	63,63,63,63	0
57	MG	1a	1793	1/1	0.89	0.11	61,61,61,61	0
57	MG	2A	3717	1/1	0.89	0.24	44,44,44,44	0
57	MG	2A	3718	1/1	0.89	0.08	76,76,76,76	0
57	MG	2A	3425	1/1	0.89	0.12	45,45,45,45	0
57	MG	1a	1795	1/1	0.89	0.23	68,68,68,68	0
57	MG	2A	3159	1/1	0.89	0.08	44,44,44,44	0
57	MG	1A	3435	1/1	0.89	0.13	66,66,66,66	0
57	MG	2A	3734	1/1	0.89	0.16	63,63,63,63	0
57	MG	2A	3172	1/1	0.89	0.16	64,64,64,64	0
57	MG	1a	1800	1/1	0.89	0.11	76,76,76,76	0
57	MG	2A	3447	1/1	0.89	0.15	54,54,54,54	0
57	MG	2A	3181	1/1	0.89	0.22	64,64,64,64	0
57	MG	2A	3185	1/1	0.89	0.25	51,51,51,51	0
57	MG	2A	3452	1/1	0.89	0.15	61,61,61,61	0
57	MG	1A	3817	1/1	0.89	0.16	62,62,62,62	0
57	MG	1A	3663	1/1	0.89	0.13	41,41,41,41	0
57	MG	2A	3458	1/1	0.89	0.13	51,51,51,51	0
57	MG	1A	3301	1/1	0.89	0.21	51,51,51,51	0
57	MG	2E	305	1/1	0.89	0.16	63,63,63,63	0
57	MG	2A	3194	1/1	0.89	0.16	64,64,64,64	0
57	MG	2A	3195	1/1	0.89	0.18	60,60,60,60	0
57	MG	1A	3735	1/1	0.89	0.14	54,54,54,54	0
57	MG	1a	1698	1/1	0.89	0.27	59,59,59,59	0
57	MG	1A	3670	1/1	0.89	0.09	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3032	1/1	0.89	0.18	53,53,53,53	0
57	MG	1A	3311	1/1	0.89	0.30	49,49,49,49	0
57	MG	2A	3221	1/1	0.89	0.18	54,54,54,54	0
57	MG	1A	3684	1/1	0.89	0.14	71,71,71,71	0
57	MG	2Y	201	1/1	0.89	0.22	61,61,61,61	0
57	MG	2A	3501	1/1	0.89	0.11	55,55,55,55	0
57	MG	1A	3354	1/1	0.89	0.17	57,57,57,57	0
57	MG	2A	3508	1/1	0.89	0.14	53,53,53,53	0
57	MG	1A	3595	1/1	0.89	0.14	67,67,67,67	0
57	MG	1T	206	1/1	0.89	0.13	70,70,70,70	0
57	MG	2a	3014	1/1	0.89	0.17	69,69,69,69	0
57	MG	2A	3239	1/1	0.89	0.21	59,59,59,59	0
57	MG	1A	3976	1/1	0.89	0.13	53,53,53,53	0
57	MG	1a	1859	1/1	0.89	0.19	73,73,73,73	0
57	MG	2A	3242	1/1	0.89	0.25	62,62,62,62	0
57	MG	2A	3530	1/1	0.89	0.13	69,69,69,69	0
57	MG	2a	3034	1/1	0.89	0.24	63,63,63,63	0
57	MG	1A	3767	1/1	0.89	0.07	33,33,33,33	0
57	MG	1A	3883	1/1	0.89	0.10	47,47,47,47	0
57	MG	2A	3247	1/1	0.89	0.11	59,59,59,59	0
57	MG	2a	3043	1/1	0.89	0.30	59,59,59,59	0
57	MG	2a	3047	1/1	0.89	0.14	60,60,60,60	0
57	MG	1a	1731	1/1	0.89	0.11	48,48,48,48	0
57	MG	1A	3884	1/1	0.89	0.08	44,44,44,44	0
57	MG	2A	3257	1/1	0.89	0.14	63,63,63,63	0
57	MG	2A	3260	1/1	0.89	0.14	57,57,57,57	0
57	MG	1g	202	1/1	0.89	0.14	61,61,61,61	0
57	MG	1A	3989	1/1	0.89	0.23	49,49,49,49	0
57	MG	2A	3273	1/1	0.89	0.17	57,57,57,57	0
57	MG	2A	3292	1/1	0.89	0.12	45,45,45,45	0
57	MG	1m	201	1/1	0.89	0.09	72,72,72,72	0
57	MG	2a	3071	1/1	0.89	0.13	59,59,59,59	0
57	MG	1a	1747	1/1	0.89	0.22	64,64,64,64	0
57	MG	1a	1749	1/1	0.89	0.11	60,60,60,60	0
57	MG	2a	3080	1/1	0.89	0.17	61,61,61,61	0
57	MG	2A	3574	1/1	0.89	0.10	52,52,52,52	0
57	MG	1A	3990	1/1	0.89	0.09	53,53,53,53	0
57	MG	1A	3487	1/1	0.89	0.11	54,54,54,54	0
57	MG	1A	3362	1/1	0.89	0.10	39,39,39,39	0
57	MG	1a	1611	1/1	0.89	0.29	66,66,66,66	0
57	MG	1A	4005	1/1	0.89	0.13	56,56,56,56	0
57	MG	1A	4010	1/1	0.89	0.19	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	2A	3062	1/1	0.89	0.13	57,57,57,57	0
57	MG	1A	3887	1/1	0.89	0.14	53,53,53,53	0
57	MG	1A	3652	1/1	0.89	0.12	30,30,30,30	0
57	MG	1B	201	1/1	0.89	0.16	60,60,60,60	0
57	MG	2A	3621	1/1	0.89	0.10	53,53,53,53	0
57	MG	2A	3624	1/1	0.89	0.14	40,40,40,40	0
57	MG	2A	3082	1/1	0.89	0.10	69,69,69,69	0
57	MG	1a	1639	1/1	0.89	0.28	69,69,69,69	0
57	MG	1a	1642	1/1	0.89	0.24	63,63,63,63	0
57	MG	1B	202	1/1	0.89	0.13	49,49,49,49	0
57	MG	2A	3641	1/1	0.89	0.18	58,58,58,58	0
57	MG	2A	3393	1/1	0.89	0.14	62,62,62,62	0
57	MG	1a	1778	1/1	0.89	0.22	62,62,62,62	0
57	MG	1a	1660	1/1	0.89	0.18	62,62,62,62	0
57	MG	1A	3793	1/1	0.89	0.15	55,55,55,55	0
57	MG	2A	3408	1/1	0.89	0.12	61,61,61,61	0
57	MG	2A	3666	1/1	0.89	0.09	50,50,50,50	0
57	MG	2A	3670	1/1	0.89	0.13	37,37,37,37	0
57	MG	1B	206	1/1	0.89	0.11	47,47,47,47	0
57	MG	2A	3677	1/1	0.89	0.09	72,72,72,72	0
57	MG	2A	3414	1/1	0.89	0.10	34,34,34,34	0
57	MG	1A	3340	1/1	0.89	0.10	49,49,49,49	0
57	MG	2A	3695	1/1	0.89	0.12	41,41,41,41	0
57	MG	2A	3697	1/1	0.89	0.12	58,58,58,58	0
60	MPD	1a	1867	8/8	0.89	0.15	52,59,62,64	0
57	MG	2A	3708	1/1	0.89	0.11	51,51,51,51	0
57	MG	1a	1677	1/1	0.89	0.09	51,51,51,51	0
57	MG	2A	3731	1/1	0.90	0.25	51,51,51,51	0
57	MG	1A	3779	1/1	0.90	0.07	30,30,30,30	0
57	MG	2A	3467	1/1	0.90	0.14	45,45,45,45	0
57	MG	2A	3735	1/1	0.90	0.16	52,52,52,52	0
57	MG	2A	3738	1/1	0.90	0.15	64,64,64,64	0
57	MG	1A	3468	1/1	0.90	0.10	43,43,43,43	0
57	MG	1d	302	1/1	0.90	0.17	57,57,57,57	0
57	MG	1A	3943	1/1	0.90	0.14	62,62,62,62	0
57	MG	1A	3683	1/1	0.90	0.09	69,69,69,69	0
57	MG	1a	1733	1/1	0.90	0.12	41,41,41,41	0
57	MG	2B	202	1/1	0.90	0.09	71,71,71,71	0
57	MG	2B	206	1/1	0.90	0.13	61,61,61,61	0
57	MG	1A	3011	1/1	0.90	0.10	56,56,56,56	0
57	MG	2B	208	1/1	0.90	0.19	57,57,57,57	0
57	MG	2A	3243	1/1	0.90	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	2A	3498	1/1	0.90	0.14	54,54,54,54	0
57	MG	2A	3500	1/1	0.90	0.17	68,68,68,68	0
57	MG	1A	3304	1/1	0.90	0.25	70,70,70,70	0
57	MG	2B	218	1/1	0.90	0.15	74,74,74,74	0
57	MG	13	102	1/1	0.90	0.11	59,59,59,59	0
57	MG	1A	3063	1/1	0.90	0.13	55,55,55,55	0
57	MG	2A	3511	1/1	0.90	0.12	61,61,61,61	0
57	MG	15	106	1/1	0.90	0.09	57,57,57,57	0
57	MG	2I	201	1/1	0.90	0.17	65,65,65,65	0
57	MG	1A	3969	1/1	0.90	0.15	47,47,47,47	0
57	MG	2A	3005	1/1	0.90	0.12	63,63,63,63	0
57	MG	1A	3973	1/1	0.90	0.10	52,52,52,52	0
57	MG	2A	3261	1/1	0.90	0.11	51,51,51,51	0
57	MG	1A	3552	1/1	0.90	0.09	37,37,37,37	0
57	MG	2A	3529	1/1	0.90	0.10	51,51,51,51	0
57	MG	2A	3265	1/1	0.90	0.17	55,55,55,55	0
57	MG	2A	3539	1/1	0.90	0.16	39,39,39,39	0
57	MG	2A	3032	1/1	0.90	0.34	59,59,59,59	0
57	MG	2A	3043	1/1	0.90	0.27	68,68,68,68	0
57	MG	2A	3279	1/1	0.90	0.13	50,50,50,50	0
57	MG	2A	3285	1/1	0.90	0.25	55,55,55,55	0
57	MG	2A	3047	1/1	0.90	0.10	68,68,68,68	0
57	MG	1A	3697	1/1	0.90	0.19	63,63,63,63	0
57	MG	2A	3299	1/1	0.90	0.27	61,61,61,61	0
57	MG	1A	3698	1/1	0.90	0.11	53,53,53,53	0
57	MG	1a	1607	1/1	0.90	0.11	67,67,67,67	0
57	MG	2A	3308	1/1	0.90	0.26	65,65,65,65	0
57	MG	2a	3028	1/1	0.90	0.14	74,74,74,74	0
57	MG	2a	3029	1/1	0.90	0.17	62,62,62,62	0
57	MG	2a	3032	1/1	0.90	0.18	72,72,72,72	0
57	MG	1A	3833	1/1	0.90	0.11	40,40,40,40	0
57	MG	1A	3701	1/1	0.90	0.12	42,42,42,42	0
57	MG	1A	3077	1/1	0.90	0.13	62,62,62,62	0
57	MG	2a	3040	1/1	0.90	0.13	64,64,64,64	0
57	MG	2A	3078	1/1	0.90	0.17	55,55,55,55	0
57	MG	1A	3449	1/1	0.90	0.07	38,38,38,38	0
57	MG	2a	3044	1/1	0.90	0.14	71,71,71,71	0
57	MG	1A	3494	1/1	0.90	0.11	32,32,32,32	0
57	MG	1A	3645	1/1	0.90	0.15	59,59,59,59	0
57	MG	2A	3357	1/1	0.90	0.11	48,48,48,48	0
57	MG	2A	3587	1/1	0.90	0.11	43,43,43,43	0
57	MG	2a	3059	1/1	0.90	0.14	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3863	1/1	0.90	0.07	62,62,62,62	0
57	MG	1A	3648	1/1	0.90	0.12	36,36,36,36	0
57	MG	1A	3715	1/1	0.90	0.10	38,38,38,38	0
57	MG	1A	3396	1/1	0.90	0.08	28,28,28,28	0
57	MG	2A	3120	1/1	0.90	0.20	72,72,72,72	0
57	MG	1A	3275	1/1	0.90	0.10	37,37,37,37	0
57	MG	1a	1791	1/1	0.90	0.14	61,61,61,61	0
57	MG	1A	3582	1/1	0.90	0.26	42,42,42,42	0
57	MG	1a	1674	1/1	0.90	0.10	55,55,55,55	0
57	MG	2A	3625	1/1	0.90	0.08	52,52,52,52	0
57	MG	1A	3461	1/1	0.90	0.07	31,31,31,31	0
57	MG	1B	204	1/1	0.90	0.08	48,48,48,48	0
57	MG	2A	3631	1/1	0.90	0.15	51,51,51,51	0
57	MG	1a	1798	1/1	0.90	0.13	62,62,62,62	0
57	MG	2a	3107	1/1	0.90	0.27	54,54,54,54	0
57	MG	2A	3635	1/1	0.90	0.14	49,49,49,49	0
57	MG	1A	3517	1/1	0.90	0.11	42,42,42,42	0
57	MG	2a	3113	1/1	0.90	0.11	73,73,73,73	0
57	MG	2a	3119	1/1	0.90	0.16	59,59,59,59	0
57	MG	2A	3640	1/1	0.90	0.14	54,54,54,54	0
57	MG	1a	1804	1/1	0.90	0.23	67,67,67,67	0
57	MG	2A	3642	1/1	0.90	0.19	54,54,54,54	0
57	MG	2a	3126	1/1	0.90	0.21	62,62,62,62	0
57	MG	1A	3165	1/1	0.90	0.10	41,41,41,41	0
57	MG	2A	3416	1/1	0.90	0.12	50,50,50,50	0
57	MG	1a	1809	1/1	0.90	0.13	65,65,65,65	0
57	MG	1a	1812	1/1	0.90	0.21	56,56,56,56	0
57	MG	1A	3216	1/1	0.90	0.07	57,57,57,57	0
57	MG	1A	3754	1/1	0.90	0.23	57,57,57,57	0
57	MG	2A	3424	1/1	0.90	0.16	61,61,61,61	0
57	MG	1A	3434	1/1	0.90	0.11	38,38,38,38	0
57	MG	2A	3427	1/1	0.90	0.22	68,68,68,68	0
57	MG	2a	3150	1/1	0.90	0.09	55,55,55,55	0
57	MG	1A	3759	1/1	0.90	0.08	34,34,34,34	0
57	MG	1A	3531	1/1	0.90	0.09	56,56,56,56	0
57	MG	2a	3168	1/1	0.90	0.15	55,55,55,55	0
57	MG	1A	3763	1/1	0.90	0.14	42,42,42,42	0
57	MG	1D	301	1/1	0.90	0.17	59,59,59,59	0
57	MG	2A	3699	1/1	0.90	0.19	46,46,46,46	0
57	MG	2A	3196	1/1	0.90	0.18	71,71,71,71	0
57	MG	2a	3183	1/1	0.90	0.22	75,75,75,75	0
57	MG	1A	3673	1/1	0.90	0.08	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	2a	3188	1/1	0.90	0.16	57,57,57,57	0
57	MG	1E	307	1/1	0.90	0.12	54,54,54,54	0
57	MG	2A	3201	1/1	0.90	0.27	59,59,59,59	0
57	MG	1A	3674	1/1	0.90	0.16	60,60,60,60	0
57	MG	2x	101	1/1	0.90	0.10	57,57,57,57	0
57	MG	1P	205	1/1	0.90	0.14	67,67,67,67	0
57	MG	1a	1856	1/1	0.90	0.23	68,68,68,68	0
57	MG	2A	3720	1/1	0.90	0.09	65,65,65,65	0
57	MG	1a	1857	1/1	0.90	0.08	65,65,65,65	0
57	MG	1A	3776	1/1	0.90	0.08	25,25,25,25	0
57	MG	2A	3225	1/1	0.90	0.18	65,65,65,65	0
57	MG	1V	205	1/1	0.91	0.13	57,57,57,57	0
57	MG	2A	3481	1/1	0.91	0.13	59,59,59,59	0
57	MG	2A	3486	1/1	0.91	0.20	47,47,47,47	0
57	MG	1A	3306	1/1	0.91	0.17	32,32,32,32	0
57	MG	1a	1719	1/1	0.91	0.11	57,57,57,57	0
57	MG	1a	1863	1/1	0.91	0.12	63,63,63,63	0
57	MG	1a	1864	1/1	0.91	0.20	62,62,62,62	0
57	MG	1Y	201	1/1	0.91	0.12	59,59,59,59	0
57	MG	1b	301	1/1	0.91	0.23	66,66,66,66	0
57	MG	10	101	1/1	0.91	0.16	39,39,39,39	0
57	MG	1A	3987	1/1	0.91	0.19	39,39,39,39	0
57	MG	1a	1729	1/1	0.91	0.10	54,54,54,54	0
57	MG	10	107	1/1	0.91	0.10	50,50,50,50	0
57	MG	2E	304	1/1	0.91	0.10	36,36,36,36	0
57	MG	2A	3518	1/1	0.91	0.15	44,44,44,44	0
57	MG	1f	202	1/1	0.91	0.14	49,49,49,49	0
57	MG	1g	201	1/1	0.91	0.12	47,47,47,47	0
57	MG	11	104	1/1	0.91	0.13	48,48,48,48	0
57	MG	1A	3475	1/1	0.91	0.08	20,20,20,20	0
57	MG	1A	3773	1/1	0.91	0.06	23,23,23,23	0
57	MG	1a	1742	1/1	0.91	0.13	61,61,61,61	0
57	MG	2Q	201	1/1	0.91	0.11	56,56,56,56	0
57	MG	1A	3205	1/1	0.91	0.07	52,52,52,52	0
57	MG	1A	3480	1/1	0.91	0.08	24,24,24,24	0
57	MG	1A	3390	1/1	0.91	0.08	40,40,40,40	0
57	MG	1A	3789	1/1	0.91	0.09	25,25,25,25	0
57	MG	1A	4007	1/1	0.91	0.10	59,59,59,59	0
57	MG	1A	4009	1/1	0.91	0.11	35,35,35,35	0
57	MG	2A	3034	1/1	0.91	0.19	65,65,65,65	0
57	MG	1A	3483	1/1	0.91	0.08	26,26,26,26	0
57	MG	1a	1608	1/1	0.91	0.12	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	1a	1761	1/1	0.91	0.18	62,62,62,62	0
57	MG	1A	3610	1/1	0.91	0.19	42,42,42,42	0
57	MG	2A	3555	1/1	0.91	0.16	55,55,55,55	0
57	MG	2A	3556	1/1	0.91	0.15	65,65,65,65	0
57	MG	2a	3024	1/1	0.91	0.26	68,68,68,68	0
57	MG	1A	3668	1/1	0.91	0.10	50,50,50,50	0
57	MG	1a	1619	1/1	0.91	0.21	57,57,57,57	0
57	MG	2A	3563	1/1	0.91	0.13	32,32,32,32	0
57	MG	1A	3911	1/1	0.91	0.17	55,55,55,55	0
57	MG	2A	3322	1/1	0.91	0.08	48,48,48,48	0
57	MG	1a	1626	1/1	0.91	0.28	65,65,65,65	0
57	MG	1a	1627	1/1	0.91	0.33	67,67,67,67	0
57	MG	1A	3122	1/1	0.91	0.19	55,55,55,55	0
57	MG	1a	1631	1/1	0.91	0.15	63,63,63,63	0
57	MG	2A	3585	1/1	0.91	0.15	49,49,49,49	0
57	MG	1A	3801	1/1	0.91	0.09	48,48,48,48	0
57	MG	2a	3042	1/1	0.91	0.24	68,68,68,68	0
57	MG	1A	3217	1/1	0.91	0.09	54,54,54,54	0
57	MG	2A	3368	1/1	0.91	0.09	48,48,48,48	0
57	MG	1A	3809	1/1	0.91	0.12	23,23,23,23	0
57	MG	1A	3813	1/1	0.91	0.10	46,46,46,46	0
57	MG	2A	3604	1/1	0.91	0.12	55,55,55,55	0
57	MG	2A	3606	1/1	0.91	0.09	50,50,50,50	0
57	MG	2a	3054	1/1	0.91	0.26	62,62,62,62	0
57	MG	2a	3055	1/1	0.91	0.33	59,59,59,59	0
57	MG	2A	3607	1/1	0.91	0.09	48,48,48,48	0
57	MG	2A	3611	1/1	0.91	0.10	67,67,67,67	0
57	MG	2A	3612	1/1	0.91	0.09	63,63,63,63	0
57	MG	2A	3384	1/1	0.91	0.08	41,41,41,41	0
57	MG	2A	3098	1/1	0.91	0.17	57,57,57,57	0
57	MG	1B	208	1/1	0.91	0.33	66,66,66,66	0
57	MG	2a	3066	1/1	0.91	0.19	68,68,68,68	0
57	MG	2A	3116	1/1	0.91	0.17	72,72,72,72	0
57	MG	2a	3070	1/1	0.91	0.17	60,60,60,60	0
57	MG	1A	3729	1/1	0.91	0.14	58,58,58,58	0
57	MG	1a	1661	1/1	0.91	0.17	64,64,64,64	0
57	MG	1a	1662	1/1	0.91	0.29	59,59,59,59	0
57	MG	2a	3078	1/1	0.91	0.23	74,74,74,74	0
57	MG	1a	1794	1/1	0.91	0.14	59,59,59,59	0
57	MG	1A	3251	1/1	0.91	0.15	58,58,58,58	0
57	MG	2a	3085	1/1	0.91	0.11	60,60,60,60	0
57	MG	1A	3498	1/1	0.91	0.07	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2a	3089	1/1	0.91	0.24	63,63,63,63	0
57	MG	2A	3410	1/1	0.91	0.11	66,66,66,66	0
57	MG	2a	3091	1/1	0.91	0.12	66,66,66,66	0
57	MG	2a	3094	1/1	0.91	0.25	55,55,55,55	0
57	MG	2a	3097	1/1	0.91	0.42	71,71,71,71	0
57	MG	2a	3098	1/1	0.91	0.16	54,54,54,54	0
57	MG	1A	3676	1/1	0.91	0.07	61,61,61,61	0
57	MG	2A	3146	1/1	0.91	0.21	57,57,57,57	0
57	MG	1A	3842	1/1	0.91	0.09	54,54,54,54	0
57	MG	1A	3402	1/1	0.91	0.11	21,21,21,21	0
57	MG	2A	3153	1/1	0.91	0.13	47,47,47,47	0
57	MG	1A	3505	1/1	0.91	0.08	44,44,44,44	0
57	MG	2A	3420	1/1	0.91	0.10	40,40,40,40	0
57	MG	2A	3164	1/1	0.91	0.11	60,60,60,60	0
57	MG	2A	3663	1/1	0.91	0.08	66,66,66,66	0
57	MG	2a	3125	1/1	0.91	0.18	73,73,73,73	0
57	MG	1a	1683	1/1	0.91	0.18	63,63,63,63	0
57	MG	2A	3171	1/1	0.91	0.12	53,53,53,53	0
57	MG	1D	315	1/1	0.91	0.20	39,39,39,39	0
57	MG	2A	3674	1/1	0.91	0.07	75,75,75,75	0
57	MG	1A	3954	1/1	0.91	0.11	64,64,64,64	0
57	MG	1a	1689	1/1	0.91	0.21	64,64,64,64	0
57	MG	2A	3433	1/1	0.91	0.17	55,55,55,55	0
57	MG	2A	3682	1/1	0.91	0.10	64,64,64,64	0
57	MG	1A	3958	1/1	0.91	0.11	49,49,49,49	0
57	MG	2A	3694	1/1	0.91	0.08	67,67,67,67	0
57	MG	1a	1825	1/1	0.91	0.13	74,74,74,74	0
57	MG	2a	3153	1/1	0.91	0.13	69,69,69,69	0
57	MG	2a	3160	1/1	0.91	0.12	68,68,68,68	0
57	MG	2A	3188	1/1	0.91	0.11	61,61,61,61	0
57	MG	1a	1827	1/1	0.91	0.13	59,59,59,59	0
57	MG	1A	3639	1/1	0.91	0.09	34,34,34,34	0
57	MG	1A	3972	1/1	0.91	0.10	46,46,46,46	0
57	MG	1A	3364	1/1	0.91	0.09	53,53,53,53	0
57	MG	1A	3572	1/1	0.91	0.14	45,45,45,45	0
57	MG	2A	3454	1/1	0.91	0.12	79,79,79,79	0
57	MG	1a	1838	1/1	0.91	0.09	49,49,49,49	0
57	MG	1A	3193	1/1	0.91	0.22	60,60,60,60	0
57	MG	1a	1702	1/1	0.91	0.18	63,63,63,63	0
57	MG	2A	3202	1/1	0.91	0.32	64,64,64,64	0
57	MG	2e	201	1/1	0.91	0.26	68,68,68,68	0
57	MG	2A	3725	1/1	0.91	0.18	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	3202	1/1	0.91	0.30	59,59,59,59	0
57	MG	1a	1705	1/1	0.91	0.21	57,57,57,57	0
57	MG	2A	3466	1/1	0.91	0.14	67,67,67,67	0
57	MG	1a	1851	1/1	0.91	0.16	55,55,55,55	0
57	MG	1a	1852	1/1	0.91	0.10	60,60,60,60	0
57	MG	2A	3222	1/1	0.91	0.11	56,56,56,56	0
57	MG	1a	1855	1/1	0.91	0.14	58,58,58,58	0
57	MG	1A	3980	1/1	0.91	0.06	65,65,65,65	0
57	MG	1A	3704	1/1	0.92	0.16	34,34,34,34	0
57	MG	1B	216	1/1	0.92	0.14	48,48,48,48	0
57	MG	1A	3606	1/1	0.92	0.13	37,37,37,37	0
57	MG	2A	3359	1/1	0.92	0.08	38,38,38,38	0
57	MG	2A	3689	1/1	0.92	0.14	73,73,73,73	0
57	MG	2A	3691	1/1	0.92	0.08	53,53,53,53	0
57	MG	2A	3363	1/1	0.92	0.11	39,39,39,39	0
57	MG	1a	1707	1/1	0.92	0.35	67,67,67,67	0
57	MG	2A	3367	1/1	0.92	0.08	33,33,33,33	0
57	MG	1y	201	1/1	0.92	0.12	57,57,57,57	0
57	MG	2A	3700	1/1	0.92	0.07	54,54,54,54	0
57	MG	2A	3702	1/1	0.92	0.10	51,51,51,51	0
57	MG	1A	3500	1/1	0.92	0.10	53,53,53,53	0
57	MG	2A	3374	1/1	0.92	0.07	33,33,33,33	0
57	MG	2A	3001	1/1	0.92	0.29	61,61,61,61	0
57	MG	1A	3872	1/1	0.92	0.09	49,49,49,49	0
57	MG	1a	1710	1/1	0.92	0.11	56,56,56,56	0
57	MG	1a	1715	1/1	0.92	0.16	72,72,72,72	0
57	MG	1A	3283	1/1	0.92	0.19	54,54,54,54	0
57	MG	2A	3719	1/1	0.92	0.14	67,67,67,67	0
57	MG	1A	3615	1/1	0.92	0.18	34,34,34,34	0
57	MG	2A	3039	1/1	0.92	0.14	60,60,60,60	0
57	MG	2A	3395	1/1	0.92	0.12	62,62,62,62	0
57	MG	2A	3727	1/1	0.92	0.10	64,64,64,64	0
57	MG	1A	3882	1/1	0.92	0.06	32,32,32,32	0
57	MG	1D	312	1/1	0.92	0.24	44,44,44,44	0
57	MG	2A	3048	1/1	0.92	0.13	62,62,62,62	0
57	MG	2A	3050	1/1	0.92	0.19	59,59,59,59	0
57	MG	2A	3733	1/1	0.92	0.10	51,51,51,51	0
57	MG	1A	3713	1/1	0.92	0.10	56,56,56,56	0
57	MG	1a	1727	1/1	0.92	0.23	57,57,57,57	0
57	MG	2A	3056	1/1	0.92	0.20	62,62,62,62	0
57	MG	1A	3285	1/1	0.92	0.08	63,63,63,63	0
57	MG	1E	306	1/1	0.92	0.10	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3741	1/1	0.92	0.17	56,56,56,56	0
57	MG	2A	3064	1/1	0.92	0.14	51,51,51,51	0
57	MG	1A	3718	1/1	0.92	0.08	66,66,66,66	0
57	MG	2A	3744	1/1	0.92	0.25	69,69,69,69	0
57	MG	2A	3746	1/1	0.92	0.08	52,52,52,52	0
57	MG	1G	202	1/1	0.92	0.12	51,51,51,51	0
57	MG	2A	3075	1/1	0.92	0.12	63,63,63,63	0
57	MG	2B	204	1/1	0.92	0.18	70,70,70,70	0
57	MG	2B	205	1/1	0.92	0.24	68,68,68,68	0
57	MG	2A	3077	1/1	0.92	0.12	66,66,66,66	0
57	MG	1A	3155	1/1	0.92	0.19	46,46,46,46	0
57	MG	1a	1738	1/1	0.92	0.10	62,62,62,62	0
57	MG	2B	209	1/1	0.92	0.14	57,57,57,57	0
57	MG	1A	3512	1/1	0.92	0.12	28,28,28,28	0
57	MG	1A	3158	1/1	0.92	0.32	41,41,41,41	0
57	MG	2B	214	1/1	0.92	0.08	82,82,82,82	0
57	MG	1a	1746	1/1	0.92	0.11	61,61,61,61	0
57	MG	1A	3372	1/1	0.92	0.12	63,63,63,63	0
57	MG	1a	1748	1/1	0.92	0.07	62,62,62,62	0
57	MG	2D	304	1/1	0.92	0.15	51,51,51,51	0
57	MG	1A	3901	1/1	0.92	0.12	33,33,33,33	0
57	MG	1A	3629	1/1	0.92	0.10	43,43,43,43	0
57	MG	2A	3115	1/1	0.92	0.11	60,60,60,60	0
57	MG	2A	3448	1/1	0.92	0.08	53,53,53,53	0
57	MG	1A	3906	1/1	0.92	0.10	27,27,27,27	0
57	MG	1T	207	1/1	0.92	0.19	60,60,60,60	0
57	MG	1U	203	1/1	0.92	0.16	60,60,60,60	0
57	MG	1A	3302	1/1	0.92	0.16	61,61,61,61	0
57	MG	1W	201	1/1	0.92	0.12	42,42,42,42	0
57	MG	1a	1763	1/1	0.92	0.23	71,71,71,71	0
57	MG	2R	201	1/1	0.92	0.12	40,40,40,40	0
57	MG	1A	3443	1/1	0.92	0.11	43,43,43,43	0
57	MG	2A	3139	1/1	0.92	0.14	63,63,63,63	0
57	MG	2A	3141	1/1	0.92	0.11	49,49,49,49	0
57	MG	2V	201	1/1	0.92	0.15	66,66,66,66	0
57	MG	1A	3748	1/1	0.92	0.18	57,57,57,57	0
57	MG	2A	3464	1/1	0.92	0.20	61,61,61,61	0
57	MG	1A	3379	1/1	0.92	0.09	39,39,39,39	0
57	MG	10	103	1/1	0.92	0.10	45,45,45,45	0
57	MG	1A	3031	1/1	0.92	0.13	50,50,50,50	0
57	MG	1A	3926	1/1	0.92	0.10	57,57,57,57	0
57	MG	2a	3012	1/1	0.92	0.30	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3934	1/1	0.92	0.16	53,53,53,53	0
57	MG	1A	3106	1/1	0.92	0.08	42,42,42,42	0
57	MG	1a	1779	1/1	0.92	0.15	56,56,56,56	0
57	MG	2A	3169	1/1	0.92	0.20	69,69,69,69	0
57	MG	2A	3170	1/1	0.92	0.27	62,62,62,62	0
57	MG	2A	3488	1/1	0.92	0.11	59,59,59,59	0
57	MG	1A	3388	1/1	0.92	0.08	21,21,21,21	0
57	MG	2A	3491	1/1	0.92	0.08	57,57,57,57	0
57	MG	1A	3389	1/1	0.92	0.05	28,28,28,28	0
57	MG	2A	3495	1/1	0.92	0.10	67,67,67,67	0
57	MG	1A	3014	1/1	0.92	0.11	49,49,49,49	0
57	MG	2A	3177	1/1	0.92	0.18	56,56,56,56	0
57	MG	2A	3179	1/1	0.92	0.19	57,57,57,57	0
57	MG	2a	3039	1/1	0.92	0.13	72,72,72,72	0
57	MG	1a	1784	1/1	0.92	0.11	60,60,60,60	0
57	MG	2A	3184	1/1	0.92	0.10	52,52,52,52	0
57	MG	1A	3544	1/1	0.92	0.08	35,35,35,35	0
57	MG	1a	1788	1/1	0.92	0.14	70,70,70,70	0
57	MG	1A	3547	1/1	0.92	0.09	44,44,44,44	0
57	MG	2a	3045	1/1	0.92	0.14	64,64,64,64	0
57	MG	2a	3046	1/1	0.92	0.20	55,55,55,55	0
57	MG	1A	3229	1/1	0.92	0.22	42,42,42,42	0
57	MG	1A	3662	1/1	0.92	0.06	14,14,14,14	0
57	MG	2a	3049	1/1	0.92	0.20	65,65,65,65	0
57	MG	2A	3521	1/1	0.92	0.10	62,62,62,62	0
57	MG	1A	3777	1/1	0.92	0.12	43,43,43,43	0
57	MG	2a	3052	1/1	0.92	0.33	59,59,59,59	0
57	MG	1A	3322	1/1	0.92	0.12	46,46,46,46	0
57	MG	1A	3960	1/1	0.92	0.18	72,72,72,72	0
57	MG	1A	3962	1/1	0.92	0.09	44,44,44,44	0
57	MG	2A	3198	1/1	0.92	0.18	57,57,57,57	0
57	MG	1a	1617	1/1	0.92	0.14	55,55,55,55	0
57	MG	1a	1799	1/1	0.92	0.16	65,65,65,65	0
57	MG	2A	3544	1/1	0.92	0.13	67,67,67,67	0
57	MG	1a	1618	1/1	0.92	0.13	56,56,56,56	0
57	MG	2A	3203	1/1	0.92	0.27	67,67,67,67	0
57	MG	1a	1803	1/1	0.92	0.13	54,54,54,54	0
57	MG	1A	3967	1/1	0.92	0.13	60,60,60,60	0
57	MG	2A	3213	1/1	0.92	0.23	65,65,65,65	0
57	MG	2a	3072	1/1	0.92	0.14	71,71,71,71	0
57	MG	1a	1805	1/1	0.92	0.15	59,59,59,59	0
57	MG	1A	3785	1/1	0.92	0.09	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	1a	1808	1/1	0.92	0.13	59,59,59,59	0
57	MG	1A	3239	1/1	0.92	0.29	60,60,60,60	0
57	MG	1A	3558	1/1	0.92	0.12	46,46,46,46	0
57	MG	1A	3327	1/1	0.92	0.14	56,56,56,56	0
57	MG	1a	1817	1/1	0.92	0.08	56,56,56,56	0
57	MG	1A	3792	1/1	0.92	0.07	52,52,52,52	0
57	MG	2A	3235	1/1	0.92	0.26	54,54,54,54	0
57	MG	2A	3237	1/1	0.92	0.15	58,58,58,58	0
57	MG	2a	3092	1/1	0.92	0.31	69,69,69,69	0
57	MG	2A	3569	1/1	0.92	0.07	58,58,58,58	0
57	MG	2a	3096	1/1	0.92	0.28	68,68,68,68	0
57	MG	1A	3136	1/1	0.92	0.11	46,46,46,46	0
57	MG	1A	3979	1/1	0.92	0.08	33,33,33,33	0
57	MG	2A	3575	1/1	0.92	0.08	35,35,35,35	0
57	MG	1A	3189	1/1	0.92	0.12	49,49,49,49	0
57	MG	1a	1641	1/1	0.92	0.14	54,54,54,54	0
57	MG	1A	3258	1/1	0.92	0.08	41,41,41,41	0
57	MG	1a	1643	1/1	0.92	0.19	59,59,59,59	0
57	MG	2a	3115	1/1	0.92	0.12	63,63,63,63	0
57	MG	2a	3118	1/1	0.92	0.13	63,63,63,63	0
57	MG	1a	1648	1/1	0.92	0.25	68,68,68,68	0
57	MG	1A	3581	1/1	0.92	0.13	55,55,55,55	0
57	MG	1a	1655	1/1	0.92	0.09	61,61,61,61	0
57	MG	2A	3253	1/1	0.92	0.13	57,57,57,57	0
57	MG	2A	3599	1/1	0.92	0.08	43,43,43,43	0
57	MG	1A	3806	1/1	0.92	0.09	50,50,50,50	0
57	MG	1A	3191	1/1	0.92	0.16	59,59,59,59	0
57	MG	1A	3682	1/1	0.92	0.08	60,60,60,60	0
57	MG	1a	1669	1/1	0.92	0.14	61,61,61,61	0
57	MG	1A	3587	1/1	0.92	0.07	38,38,38,38	0
57	MG	1A	3027	1/1	0.92	0.13	64,64,64,64	0
57	MG	2a	3136	1/1	0.92	0.22	61,61,61,61	0
57	MG	2A	3615	1/1	0.92	0.07	32,32,32,32	0
57	MG	1A	4004	1/1	0.92	0.16	50,50,50,50	0
57	MG	1A	3823	1/1	0.92	0.13	65,65,65,65	0
57	MG	1A	3040	1/1	0.92	0.13	56,56,56,56	0
57	MG	2a	3149	1/1	0.92	0.09	60,60,60,60	0
57	MG	2A	3280	1/1	0.92	0.13	49,49,49,49	0
57	MG	1A	3345	1/1	0.92	0.10	43,43,43,43	0
57	MG	2A	3287	1/1	0.92	0.18	58,58,58,58	0
57	MG	1a	1860	1/1	0.92	0.12	62,62,62,62	0
57	MG	2A	3627	1/1	0.92	0.10	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3294	1/1	0.92	0.41	65,65,65,65	0
57	MG	2a	3172	1/1	0.92	0.15	68,68,68,68	0
57	MG	2A	3295	1/1	0.92	0.22	59,59,59,59	0
57	MG	1A	3834	1/1	0.92	0.07	41,41,41,41	0
57	MG	2A	3298	1/1	0.92	0.31	56,56,56,56	0
57	MG	1A	3835	1/1	0.92	0.09	25,25,25,25	0
57	MG	2A	3639	1/1	0.92	0.06	78,78,78,78	0
57	MG	1A	3278	1/1	0.92	0.13	57,57,57,57	0
57	MG	1A	3599	1/1	0.92	0.11	59,59,59,59	0
57	MG	2A	3307	1/1	0.92	0.18	55,55,55,55	0
57	MG	1a	1690	1/1	0.92	0.24	70,70,70,70	0
57	MG	1A	3848	1/1	0.92	0.11	27,27,27,27	0
57	MG	1A	3600	1/1	0.92	0.08	31,31,31,31	0
57	MG	1A	3700	1/1	0.92	0.11	40,40,40,40	0
57	MG	1A	3426	1/1	0.92	0.07	22,22,22,22	0
57	MG	1A	3859	1/1	0.92	0.10	46,46,46,46	0
57	MG	2A	3331	1/1	0.92	0.19	66,66,66,66	0
57	MG	1A	3603	1/1	0.92	0.11	37,37,37,37	0
57	MG	2A	3341	1/1	0.92	0.15	47,47,47,47	0
57	MG	2A	3344	1/1	0.92	0.14	59,59,59,59	0
57	MG	1A	3515	1/1	0.93	0.07	59,59,59,59	0
57	MG	1A	3213	1/1	0.93	0.09	54,54,54,54	0
57	MG	1A	3455	1/1	0.93	0.11	56,56,56,56	0
57	MG	2A	3453	1/1	0.93	0.21	51,51,51,51	0
57	MG	1a	1822	1/1	0.93	0.09	53,53,53,53	0
57	MG	2A	3737	1/1	0.93	0.12	67,67,67,67	0
57	MG	1A	3921	1/1	0.93	0.11	61,61,61,61	0
57	MG	1a	1681	1/1	0.93	0.10	59,59,59,59	0
57	MG	1A	3034	1/1	0.93	0.17	53,53,53,53	0
57	MG	1a	1685	1/1	0.93	0.10	53,53,53,53	0
57	MG	1A	3086	1/1	0.93	0.07	35,35,35,35	0
57	MG	1A	3529	1/1	0.93	0.07	37,37,37,37	0
57	MG	1A	3609	1/1	0.93	0.11	50,50,50,50	0
57	MG	1A	3695	1/1	0.93	0.09	54,54,54,54	0
57	MG	1a	1691	1/1	0.93	0.16	64,64,64,64	0
57	MG	1a	1840	1/1	0.93	0.07	58,58,58,58	0
57	MG	2A	3474	1/1	0.93	0.06	61,61,61,61	0
57	MG	1A	3404	1/1	0.93	0.07	25,25,25,25	0
57	MG	1F	315	1/1	0.93	0.08	33,33,33,33	0
57	MG	1a	1695	1/1	0.93	0.13	55,55,55,55	0
57	MG	2A	3207	1/1	0.93	0.13	53,53,53,53	0
57	MG	1A	3614	1/1	0.93	0.12	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2B	210	1/1	0.93	0.23	66,66,66,66	0
57	MG	1G	203	1/1	0.93	0.08	51,51,51,51	0
57	MG	2B	212	1/1	0.93	0.17	64,64,64,64	0
57	MG	1H	202	1/1	0.93	0.07	41,41,41,41	0
57	MG	1A	3407	1/1	0.93	0.09	45,45,45,45	0
57	MG	2A	3217	1/1	0.93	0.10	60,60,60,60	0
57	MG	2A	3492	1/1	0.93	0.12	48,48,48,48	0
57	MG	2A	3493	1/1	0.93	0.10	62,62,62,62	0
57	MG	2D	303	1/1	0.93	0.16	52,52,52,52	0
57	MG	1a	1701	1/1	0.93	0.18	59,59,59,59	0
57	MG	2D	307	1/1	0.93	0.08	35,35,35,35	0
57	MG	1O	201	1/1	0.93	0.09	54,54,54,54	0
57	MG	1P	204	1/1	0.93	0.12	39,39,39,39	0
57	MG	1A	3811	1/1	0.93	0.09	29,29,29,29	0
57	MG	1a	1862	1/1	0.93	0.12	60,60,60,60	0
57	MG	2A	3504	1/1	0.93	0.10	64,64,64,64	0
57	MG	1a	1706	1/1	0.93	0.12	56,56,56,56	0
57	MG	2N	201	1/1	0.93	0.11	70,70,70,70	0
57	MG	2O	201	1/1	0.93	0.10	62,62,62,62	0
57	MG	1Q	205	1/1	0.93	0.11	54,54,54,54	0
57	MG	1a	1865	1/1	0.93	0.12	60,60,60,60	0
57	MG	1R	204	1/1	0.93	0.11	48,48,48,48	0
57	MG	1A	3045	1/1	0.93	0.17	55,55,55,55	0
57	MG	2Q	203	1/1	0.93	0.10	57,57,57,57	0
57	MG	1A	3465	1/1	0.93	0.10	49,49,49,49	0
57	MG	2R	202	1/1	0.93	0.13	55,55,55,55	0
57	MG	1d	303	1/1	0.93	0.32	55,55,55,55	0
57	MG	1a	1711	1/1	0.93	0.14	59,59,59,59	0
57	MG	1a	1714	1/1	0.93	0.44	63,63,63,63	0
57	MG	2U	201	1/1	0.93	0.24	68,68,68,68	0
57	MG	1A	3154	1/1	0.93	0.10	38,38,38,38	0
57	MG	1a	1716	1/1	0.93	0.24	63,63,63,63	0
57	MG	20	102	1/1	0.93	0.16	69,69,69,69	0
57	MG	2A	3528	1/1	0.93	0.17	67,67,67,67	0
57	MG	23	101	1/1	0.93	0.13	59,59,59,59	0
57	MG	25	101	1/1	0.93	0.38	52,52,52,52	0
57	MG	1A	3621	1/1	0.93	0.12	18,18,18,18	0
57	MG	2a	3003	1/1	0.93	0.18	64,64,64,64	0
57	MG	1A	3240	1/1	0.93	0.21	53,53,53,53	0
57	MG	2a	3006	1/1	0.93	0.17	63,63,63,63	0
57	MG	2a	3009	1/1	0.93	0.07	66,66,66,66	0
57	MG	2A	3533	1/1	0.93	0.09	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3534	1/1	0.93	0.09	60,60,60,60	0
57	MG	2A	3535	1/1	0.93	0.08	69,69,69,69	0
57	MG	2A	3250	1/1	0.93	0.10	59,59,59,59	0
57	MG	2a	3015	1/1	0.93	0.16	51,51,51,51	0
57	MG	2A	3251	1/1	0.93	0.22	48,48,48,48	0
57	MG	2a	3019	1/1	0.93	0.19	57,57,57,57	0
57	MG	1A	3010	1/1	0.93	0.13	51,51,51,51	0
57	MG	1l	201	1/1	0.93	0.13	54,54,54,54	0
57	MG	2A	3256	1/1	0.93	0.11	53,53,53,53	0
57	MG	1a	1723	1/1	0.93	0.21	64,64,64,64	0
57	MG	1A	3963	1/1	0.93	0.08	51,51,51,51	0
57	MG	1A	3966	1/1	0.93	0.09	37,37,37,37	0
57	MG	2A	3262	1/1	0.93	0.11	52,52,52,52	0
57	MG	1A	3626	1/1	0.93	0.12	53,53,53,53	0
57	MG	2a	3033	1/1	0.93	0.20	68,68,68,68	0
57	MG	1A	3627	1/1	0.93	0.06	26,26,26,26	0
57	MG	1A	3551	1/1	0.93	0.15	33,33,33,33	0
57	MG	1A	3365	1/1	0.93	0.08	21,21,21,21	0
57	MG	1A	3197	1/1	0.93	0.12	53,53,53,53	0
57	MG	10	105	1/1	0.93	0.07	39,39,39,39	0
57	MG	2A	3025	1/1	0.93	0.11	52,52,52,52	0
57	MG	1A	3641	1/1	0.93	0.10	33,33,33,33	0
57	MG	1a	1739	1/1	0.93	0.08	58,58,58,58	0
57	MG	1A	3257	1/1	0.93	0.11	63,63,63,63	0
57	MG	1A	3423	1/1	0.93	0.11	27,27,27,27	0
57	MG	2A	3573	1/1	0.93	0.09	59,59,59,59	0
57	MG	1A	3373	1/1	0.93	0.14	52,52,52,52	0
57	MG	1A	3862	1/1	0.93	0.10	48,48,48,48	0
57	MG	1A	3984	1/1	0.93	0.07	24,24,24,24	0
57	MG	2A	3580	1/1	0.93	0.07	54,54,54,54	0
57	MG	2A	3301	1/1	0.93	0.19	53,53,53,53	0
57	MG	1A	3985	1/1	0.93	0.20	48,48,48,48	0
57	MG	2A	3305	1/1	0.93	0.31	63,63,63,63	0
57	MG	2A	3586	1/1	0.93	0.10	71,71,71,71	0
57	MG	1A	3738	1/1	0.93	0.08	30,30,30,30	0
57	MG	18	103	1/1	0.93	0.18	39,39,39,39	0
57	MG	1a	1755	1/1	0.93	0.19	61,61,61,61	0
57	MG	2A	3315	1/1	0.93	0.13	58,58,58,58	0
57	MG	2A	3598	1/1	0.93	0.10	58,58,58,58	0
57	MG	2a	3064	1/1	0.93	0.24	66,66,66,66	0
57	MG	1A	3742	1/1	0.93	0.14	49,49,49,49	0
57	MG	1A	3868	1/1	0.93	0.07	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	1602	1/1	0.93	0.15	70,70,70,70	0
57	MG	2a	3069	1/1	0.93	0.08	61,61,61,61	0
57	MG	1A	3869	1/1	0.93	0.08	38,38,38,38	0
57	MG	2A	3070	1/1	0.93	0.15	56,56,56,56	0
57	MG	2A	3072	1/1	0.93	0.13	51,51,51,51	0
57	MG	2A	3334	1/1	0.93	0.09	41,41,41,41	0
57	MG	2a	3075	1/1	0.93	0.13	59,59,59,59	0
57	MG	1A	3560	1/1	0.93	0.17	71,71,71,71	0
57	MG	1A	3562	1/1	0.93	0.10	53,53,53,53	0
57	MG	1A	3996	1/1	0.93	0.09	15,15,15,15	0
57	MG	2A	3079	1/1	0.93	0.08	49,49,49,49	0
57	MG	2A	3620	1/1	0.93	0.12	70,70,70,70	0
57	MG	2A	3080	1/1	0.93	0.14	54,54,54,54	0
57	MG	2A	3350	1/1	0.93	0.13	43,43,43,43	0
57	MG	1a	1614	1/1	0.93	0.10	65,65,65,65	0
57	MG	1A	3998	1/1	0.93	0.10	43,43,43,43	0
57	MG	2A	3083	1/1	0.93	0.16	61,61,61,61	0
57	MG	1A	4003	1/1	0.93	0.07	48,48,48,48	0
57	MG	1A	3879	1/1	0.93	0.09	44,44,44,44	0
57	MG	1A	3564	1/1	0.93	0.08	49,49,49,49	0
57	MG	1A	3374	1/1	0.93	0.12	45,45,45,45	0
57	MG	2a	3100	1/1	0.93	0.30	60,60,60,60	0
57	MG	1A	3319	1/1	0.93	0.14	52,52,52,52	0
57	MG	2a	3105	1/1	0.93	0.09	76,76,76,76	0
57	MG	2A	3637	1/1	0.93	0.10	59,59,59,59	0
57	MG	2A	3379	1/1	0.93	0.11	41,41,41,41	0
57	MG	2a	3111	1/1	0.93	0.09	51,51,51,51	0
57	MG	2A	3382	1/1	0.93	0.07	43,43,43,43	0
57	MG	1A	3576	1/1	0.93	0.07	50,50,50,50	0
57	MG	2a	3114	1/1	0.93	0.11	68,68,68,68	0
57	MG	2A	3101	1/1	0.93	0.12	51,51,51,51	0
57	MG	1A	3661	1/1	0.93	0.09	46,46,46,46	0
57	MG	2A	3649	1/1	0.93	0.12	71,71,71,71	0
57	MG	1A	3101	1/1	0.93	0.15	37,37,37,37	0
57	MG	2A	3653	1/1	0.93	0.07	52,52,52,52	0
57	MG	2A	3657	1/1	0.93	0.11	55,55,55,55	0
57	MG	2a	3123	1/1	0.93	0.10	64,64,64,64	0
57	MG	2A	3388	1/1	0.93	0.07	43,43,43,43	0
57	MG	2A	3118	1/1	0.93	0.12	48,48,48,48	0
57	MG	2A	3119	1/1	0.93	0.14	55,55,55,55	0
57	MG	1a	1783	1/1	0.93	0.10	45,45,45,45	0
57	MG	2A	3122	1/1	0.93	0.12	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3123	1/1	0.93	0.11	83,83,83,83	0
57	MG	2A	3402	1/1	0.93	0.09	50,50,50,50	0
57	MG	2a	3135	1/1	0.93	0.21	66,66,66,66	0
57	MG	1a	1634	1/1	0.93	0.17	58,58,58,58	0
57	MG	1a	1635	1/1	0.93	0.29	56,56,56,56	0
57	MG	2A	3406	1/1	0.93	0.07	32,32,32,32	0
57	MG	2a	3142	1/1	0.93	0.07	62,62,62,62	0
57	MG	2A	3681	1/1	0.93	0.10	56,56,56,56	0
57	MG	2A	3129	1/1	0.93	0.21	41,41,41,41	0
57	MG	1A	4016	1/1	0.93	0.10	42,42,42,42	0
57	MG	1A	3070	1/1	0.93	0.06	37,37,37,37	0
57	MG	2A	3690	1/1	0.93	0.09	65,65,65,65	0
57	MG	2a	3158	1/1	0.93	0.11	62,62,62,62	0
57	MG	1a	1790	1/1	0.93	0.15	67,67,67,67	0
57	MG	2a	3161	1/1	0.93	0.09	66,66,66,66	0
57	MG	1A	3268	1/1	0.93	0.11	45,45,45,45	0
57	MG	1a	1640	1/1	0.93	0.17	68,68,68,68	0
57	MG	1A	3038	1/1	0.93	0.07	37,37,37,37	0
57	MG	2a	3171	1/1	0.93	0.16	66,66,66,66	0
57	MG	1A	3273	1/1	0.93	0.07	55,55,55,55	0
57	MG	1B	205	1/1	0.93	0.07	47,47,47,47	0
57	MG	2A	3421	1/1	0.93	0.10	42,42,42,42	0
57	MG	2A	3704	1/1	0.93	0.10	34,34,34,34	0
57	MG	2A	3705	1/1	0.93	0.11	48,48,48,48	0
57	MG	1A	3898	1/1	0.93	0.10	64,64,64,64	0
57	MG	1A	3180	1/1	0.93	0.22	49,49,49,49	0
57	MG	2a	3187	1/1	0.93	0.20	55,55,55,55	0
57	MG	2A	3154	1/1	0.93	0.13	56,56,56,56	0
57	MG	1A	3902	1/1	0.93	0.07	18,18,18,18	0
57	MG	2a	3190	1/1	0.93	0.14	67,67,67,67	0
57	MG	1a	1657	1/1	0.93	0.14	57,57,57,57	0
57	MG	2f	201	1/1	0.93	0.17	60,60,60,60	0
57	MG	1B	210	1/1	0.93	0.10	53,53,53,53	0
57	MG	1A	3211	1/1	0.93	0.28	68,68,68,68	0
57	MG	1B	215	1/1	0.93	0.11	54,54,54,54	0
57	MG	1a	1667	1/1	0.93	0.29	62,62,62,62	0
57	MG	2A	3442	1/1	0.93	0.06	38,38,38,38	0
57	MG	1A	3597	1/1	0.93	0.10	33,33,33,33	0
57	MG	1A	3448	1/1	0.93	0.14	54,54,54,54	0
57	MG	2A	3175	1/1	0.93	0.21	49,49,49,49	0
57	MG	1B	219	1/1	0.93	0.08	44,44,44,44	0
57	MG	2A	3167	1/1	0.94	0.25	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	1810	1/1	0.94	0.10	54,54,54,54	0
57	MG	2A	3450	1/1	0.94	0.12	61,61,61,61	0
57	MG	1A	3376	1/1	0.94	0.09	38,38,38,38	0
57	MG	1a	1670	1/1	0.94	0.19	53,53,53,53	0
57	MG	1a	1815	1/1	0.94	0.08	54,54,54,54	0
57	MG	1a	1816	1/1	0.94	0.09	64,64,64,64	0
57	MG	2A	3174	1/1	0.94	0.07	59,59,59,59	0
57	MG	1A	3501	1/1	0.94	0.08	55,55,55,55	0
57	MG	1B	220	1/1	0.94	0.07	30,30,30,30	0
57	MG	1A	3030	1/1	0.94	0.06	34,34,34,34	0
57	MG	2A	3461	1/1	0.94	0.11	62,62,62,62	0
57	MG	1A	3765	1/1	0.94	0.10	56,56,56,56	0
57	MG	1a	1824	1/1	0.94	0.10	67,67,67,67	0
57	MG	1B	228	1/1	0.94	0.16	70,70,70,70	0
57	MG	2A	3465	1/1	0.94	0.07	37,37,37,37	0
57	MG	1a	1826	1/1	0.94	0.12	52,52,52,52	0
57	MG	1A	3586	1/1	0.94	0.15	56,56,56,56	0
57	MG	2A	3469	1/1	0.94	0.06	58,58,58,58	0
57	MG	1a	1680	1/1	0.94	0.10	56,56,56,56	0
57	MG	2A	3473	1/1	0.94	0.15	59,59,59,59	0
57	MG	1A	3904	1/1	0.94	0.06	28,28,28,28	0
57	MG	1a	1830	1/1	0.94	0.15	62,62,62,62	0
57	MG	1a	1831	1/1	0.94	0.09	57,57,57,57	0
57	MG	2A	3478	1/1	0.94	0.15	53,53,53,53	0
57	MG	1A	3108	1/1	0.94	0.06	58,58,58,58	0
57	MG	1a	1833	1/1	0.94	0.09	59,59,59,59	0
57	MG	1A	3909	1/1	0.94	0.15	44,44,44,44	0
57	MG	2D	306	1/1	0.94	0.20	44,44,44,44	0
57	MG	2A	3483	1/1	0.94	0.17	53,53,53,53	0
57	MG	2A	3484	1/1	0.94	0.07	39,39,39,39	0
57	MG	1A	3770	1/1	0.94	0.06	25,25,25,25	0
57	MG	2F	301	1/1	0.94	0.21	41,41,41,41	0
57	MG	1A	3121	1/1	0.94	0.09	39,39,39,39	0
57	MG	1A	3774	1/1	0.94	0.08	43,43,43,43	0
57	MG	1A	3590	1/1	0.94	0.06	53,53,53,53	0
57	MG	2A	3206	1/1	0.94	0.09	46,46,46,46	0
57	MG	1A	3442	1/1	0.94	0.10	50,50,50,50	0
57	MG	1a	1844	1/1	0.94	0.08	57,57,57,57	0
57	MG	1F	317	1/1	0.94	0.18	47,47,47,47	0
57	MG	2P	201	1/1	0.94	0.11	57,57,57,57	0
57	MG	1A	3923	1/1	0.94	0.06	59,59,59,59	0
57	MG	1A	3384	1/1	0.94	0.12	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	1G	204	1/1	0.94	0.10	41,41,41,41	0
57	MG	2A	3503	1/1	0.94	0.08	31,31,31,31	0
57	MG	2A	3220	1/1	0.94	0.07	46,46,46,46	0
57	MG	1A	3329	1/1	0.94	0.13	37,37,37,37	0
57	MG	1A	3064	1/1	0.94	0.09	45,45,45,45	0
57	MG	1A	3272	1/1	0.94	0.08	53,53,53,53	0
57	MG	2A	3512	1/1	0.94	0.12	25,25,25,25	0
57	MG	1A	3520	1/1	0.94	0.07	23,23,23,23	0
57	MG	2A	3516	1/1	0.94	0.14	56,56,56,56	0
57	MG	1A	3939	1/1	0.94	0.09	42,42,42,42	0
57	MG	1Q	202	1/1	0.94	0.08	31,31,31,31	0
57	MG	2A	3230	1/1	0.94	0.16	43,43,43,43	0
57	MG	2A	3232	1/1	0.94	0.07	48,48,48,48	0
57	MG	1Q	204	1/1	0.94	0.07	35,35,35,35	0
57	MG	25	102	1/1	0.94	0.15	45,45,45,45	0
57	MG	28	3800	1/1	0.94	0.09	55,55,55,55	0
57	MG	1A	3941	1/1	0.94	0.11	45,45,45,45	0
57	MG	1A	3791	1/1	0.94	0.07	29,29,29,29	0
57	MG	1A	3680	1/1	0.94	0.15	62,62,62,62	0
57	MG	1A	3601	1/1	0.94	0.08	40,40,40,40	0
57	MG	2a	3007	1/1	0.94	0.10	53,53,53,53	0
57	MG	2a	3008	1/1	0.94	0.15	53,53,53,53	0
57	MG	1d	301	1/1	0.94	0.11	65,65,65,65	0
57	MG	1A	3521	1/1	0.94	0.19	37,37,37,37	0
57	MG	1A	3333	1/1	0.94	0.12	45,45,45,45	0
57	MG	1a	1712	1/1	0.94	0.36	55,55,55,55	0
57	MG	1a	1713	1/1	0.94	0.28	54,54,54,54	0
57	MG	1A	3799	1/1	0.94	0.07	31,31,31,31	0
57	MG	1f	201	1/1	0.94	0.33	74,74,74,74	0
57	MG	1A	3953	1/1	0.94	0.08	56,56,56,56	0
57	MG	2a	3020	1/1	0.94	0.23	67,67,67,67	0
57	MG	1U	201	1/1	0.94	0.20	47,47,47,47	0
57	MG	1A	3337	1/1	0.94	0.10	13,13,13,13	0
57	MG	1a	1718	1/1	0.94	0.34	62,62,62,62	0
57	MG	1V	204	1/1	0.94	0.09	47,47,47,47	0
57	MG	1l	202	1/1	0.94	0.10	67,67,67,67	0
57	MG	1A	3688	1/1	0.94	0.08	46,46,46,46	0
57	MG	1A	3168	1/1	0.94	0.10	47,47,47,47	0
57	MG	2a	3030	1/1	0.94	0.13	58,58,58,58	0
57	MG	1n	103	1/1	0.94	0.18	62,62,62,62	0
57	MG	1t	3101	1/1	0.94	0.10	50,50,50,50	0
57	MG	1A	3460	1/1	0.94	0.06	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	2A	3557	1/1	0.94	0.09	62,62,62,62	0
57	MG	2A	3268	1/1	0.94	0.14	54,54,54,54	0
57	MG	1A	3174	1/1	0.94	0.13	50,50,50,50	0
57	MG	1A	3693	1/1	0.94	0.09	37,37,37,37	0
57	MG	2A	3566	1/1	0.94	0.07	61,61,61,61	0
57	MG	2A	3278	1/1	0.94	0.29	50,50,50,50	0
57	MG	1A	3534	1/1	0.94	0.11	48,48,48,48	0
57	MG	2A	3002	1/1	0.94	0.10	50,50,50,50	0
57	MG	1A	3818	1/1	0.94	0.08	23,23,23,23	0
57	MG	1A	3123	1/1	0.94	0.27	59,59,59,59	0
57	MG	2A	3291	1/1	0.94	0.11	51,51,51,51	0
57	MG	2A	3022	1/1	0.94	0.26	49,49,49,49	0
57	MG	2A	3023	1/1	0.94	0.20	58,58,58,58	0
57	MG	1A	3824	1/1	0.94	0.06	12,12,12,12	0
57	MG	2A	3582	1/1	0.94	0.11	57,57,57,57	0
57	MG	1A	3182	1/1	0.94	0.20	39,39,39,39	0
57	MG	2A	3027	1/1	0.94	0.11	60,60,60,60	0
57	MG	1a	1737	1/1	0.94	0.14	57,57,57,57	0
57	MG	1A	3830	1/1	0.94	0.13	47,47,47,47	0
57	MG	2A	3037	1/1	0.94	0.24	66,66,66,66	0
57	MG	2A	3591	1/1	0.94	0.07	50,50,50,50	0
57	MG	1A	3831	1/1	0.94	0.12	48,48,48,48	0
57	MG	1a	1740	1/1	0.94	0.12	62,62,62,62	0
57	MG	1A	3227	1/1	0.94	0.12	38,38,38,38	0
57	MG	1A	3618	1/1	0.94	0.07	26,26,26,26	0
57	MG	1A	3125	1/1	0.94	0.14	51,51,51,51	0
57	MG	2A	3052	1/1	0.94	0.08	41,41,41,41	0
57	MG	1A	3620	1/1	0.94	0.06	41,41,41,41	0
57	MG	1A	3841	1/1	0.94	0.15	55,55,55,55	0
57	MG	19	103	1/1	0.94	0.08	54,54,54,54	0
57	MG	2A	3327	1/1	0.94	0.12	58,58,58,58	0
57	MG	2A	3059	1/1	0.94	0.22	50,50,50,50	0
57	MG	1A	3238	1/1	0.94	0.11	63,63,63,63	0
57	MG	1A	3844	1/1	0.94	0.11	42,42,42,42	0
57	MG	2A	3063	1/1	0.94	0.13	47,47,47,47	0
57	MG	2a	3079	1/1	0.94	0.12	47,47,47,47	0
57	MG	1A	3622	1/1	0.94	0.08	26,26,26,26	0
57	MG	2a	3081	1/1	0.94	0.34	56,56,56,56	0
57	MG	1a	1605	1/1	0.94	0.10	52,52,52,52	0
57	MG	2A	3623	1/1	0.94	0.07	39,39,39,39	0
57	MG	2A	3066	1/1	0.94	0.10	50,50,50,50	0
57	MG	2a	3087	1/1	0.94	0.23	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	3347	1/1	0.94	0.10	35,35,35,35	0
57	MG	1A	3850	1/1	0.94	0.12	51,51,51,51	0
57	MG	2A	3068	1/1	0.94	0.10	48,48,48,48	0
57	MG	2A	3355	1/1	0.94	0.07	52,52,52,52	0
57	MG	2A	3630	1/1	0.94	0.10	61,61,61,61	0
57	MG	2A	3356	1/1	0.94	0.11	38,38,38,38	0
57	MG	2A	3632	1/1	0.94	0.12	57,57,57,57	0
57	MG	1A	3357	1/1	0.94	0.07	26,26,26,26	0
57	MG	2a	3099	1/1	0.94	0.32	51,51,51,51	0
57	MG	1A	3710	1/1	0.94	0.07	49,49,49,49	0
57	MG	2A	3360	1/1	0.94	0.11	55,55,55,55	0
57	MG	2A	3361	1/1	0.94	0.08	45,45,45,45	0
57	MG	2A	3362	1/1	0.94	0.07	46,46,46,46	0
57	MG	2a	3108	1/1	0.94	0.41	63,63,63,63	0
57	MG	1A	3473	1/1	0.94	0.08	39,39,39,39	0
57	MG	1a	1764	1/1	0.94	0.07	49,49,49,49	0
57	MG	1a	1766	1/1	0.94	0.07	55,55,55,55	0
57	MG	1a	1615	1/1	0.94	0.14	61,61,61,61	0
57	MG	2A	3647	1/1	0.94	0.09	54,54,54,54	0
57	MG	2A	3370	1/1	0.94	0.09	33,33,33,33	0
57	MG	1A	3997	1/1	0.94	0.09	50,50,50,50	0
57	MG	1A	3358	1/1	0.94	0.06	20,20,20,20	0
57	MG	1a	1771	1/1	0.94	0.11	55,55,55,55	0
57	MG	2A	3380	1/1	0.94	0.12	73,73,73,73	0
57	MG	1A	3999	1/1	0.94	0.10	63,63,63,63	0
57	MG	1a	1773	1/1	0.94	0.18	58,58,58,58	0
57	MG	1A	4002	1/1	0.94	0.07	24,24,24,24	0
57	MG	1A	3128	1/1	0.94	0.09	36,36,36,36	0
57	MG	2A	3668	1/1	0.94	0.08	54,54,54,54	0
57	MG	1A	3479	1/1	0.94	0.08	27,27,27,27	0
57	MG	1a	1777	1/1	0.94	0.20	55,55,55,55	0
57	MG	1A	3719	1/1	0.94	0.26	33,33,33,33	0
57	MG	1A	3865	1/1	0.94	0.09	35,35,35,35	0
57	MG	2A	3104	1/1	0.94	0.17	53,53,53,53	0
57	MG	2A	3111	1/1	0.94	0.15	53,53,53,53	0
57	MG	2A	3397	1/1	0.94	0.19	66,66,66,66	0
57	MG	1A	3632	1/1	0.94	0.08	21,21,21,21	0
57	MG	2a	3139	1/1	0.94	0.08	56,56,56,56	0
57	MG	2a	3141	1/1	0.94	0.13	63,63,63,63	0
57	MG	2A	3688	1/1	0.94	0.08	50,50,50,50	0
57	MG	1a	1632	1/1	0.94	0.08	42,42,42,42	0
57	MG	1a	1633	1/1	0.94	0.14	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	3047	1/1	0.94	0.15	43,43,43,43	0
57	MG	2A	3405	1/1	0.94	0.09	58,58,58,58	0
57	MG	1A	3728	1/1	0.94	0.09	43,43,43,43	0
57	MG	2a	3157	1/1	0.94	0.10	50,50,50,50	0
57	MG	1A	3094	1/1	0.94	0.11	44,44,44,44	0
57	MG	1A	3871	1/1	0.94	0.08	26,26,26,26	0
57	MG	1A	3640	1/1	0.94	0.09	29,29,29,29	0
57	MG	1A	3875	1/1	0.94	0.08	51,51,51,51	0
57	MG	1A	3255	1/1	0.94	0.08	43,43,43,43	0
57	MG	1A	3563	1/1	0.94	0.08	60,60,60,60	0
57	MG	2A	3706	1/1	0.94	0.09	56,56,56,56	0
57	MG	2A	3707	1/1	0.94	0.08	51,51,51,51	0
57	MG	2a	3174	1/1	0.94	0.09	64,64,64,64	0
57	MG	2a	3176	1/1	0.94	0.10	73,73,73,73	0
57	MG	1A	3370	1/1	0.94	0.07	24,24,24,24	0
57	MG	1A	3566	1/1	0.94	0.16	47,47,47,47	0
57	MG	2A	3711	1/1	0.94	0.09	46,46,46,46	0
57	MG	2A	3135	1/1	0.94	0.14	54,54,54,54	0
57	MG	2A	3137	1/1	0.94	0.10	51,51,51,51	0
57	MG	1A	3646	1/1	0.94	0.13	34,34,34,34	0
57	MG	1a	1654	1/1	0.94	0.09	56,56,56,56	0
57	MG	1A	3071	1/1	0.94	0.08	32,32,32,32	0
57	MG	2A	3144	1/1	0.94	0.11	51,51,51,51	0
57	MG	2A	3145	1/1	0.94	0.10	62,62,62,62	0
57	MG	2A	3721	1/1	0.94	0.14	57,57,57,57	0
57	MG	1a	1656	1/1	0.94	0.23	51,51,51,51	0
57	MG	1A	3650	1/1	0.94	0.08	47,47,47,47	0
57	MG	1A	3752	1/1	0.94	0.17	42,42,42,42	0
57	MG	2r	101	1/1	0.94	0.13	74,74,74,74	0
57	MG	1B	212	1/1	0.94	0.06	51,51,51,51	0
57	MG	2A	3729	1/1	0.94	0.10	52,52,52,52	0
59	ARG	1B	231	12/12	0.94	0.10	29,39,47,50	0
57	MG	2A	3437	1/1	0.94	0.07	43,43,43,43	0
57	MG	1A	3316	1/1	0.94	0.10	45,45,45,45	0
60	MPD	18	104	8/8	0.94	0.13	30,35,42,46	0
57	MG	1a	1663	1/1	0.94	0.21	53,53,53,53	0
57	MG	1a	1665	1/1	0.94	0.14	50,50,50,50	0
57	MG	1A	3056	1/1	0.94	0.11	48,48,48,48	0
61	ZN	24	501	1/1	0.94	0.14	120,120,120,120	0
57	MG	1A	3368	1/1	0.95	0.10	37,37,37,37	0
57	MG	1A	3082	1/1	0.95	0.24	35,35,35,35	0
57	MG	2A	3389	1/1	0.95	0.11	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	3228	1/1	0.95	0.07	39,39,39,39	0
57	MG	1U	206	1/1	0.95	0.21	36,36,36,36	0
57	MG	2A	3712	1/1	0.95	0.07	51,51,51,51	0
57	MG	1A	3450	1/1	0.95	0.11	45,45,45,45	0
57	MG	1A	3927	1/1	0.95	0.08	35,35,35,35	0
57	MG	1A	3928	1/1	0.95	0.07	56,56,56,56	0
57	MG	2A	3084	1/1	0.95	0.08	46,46,46,46	0
57	MG	1W	202	1/1	0.95	0.07	41,41,41,41	0
57	MG	1A	3929	1/1	0.95	0.08	54,54,54,54	0
57	MG	1A	3931	1/1	0.95	0.10	45,45,45,45	0
57	MG	2A	3093	1/1	0.95	0.10	45,45,45,45	0
57	MG	1a	1758	1/1	0.95	0.18	59,59,59,59	0
57	MG	2A	3097	1/1	0.95	0.15	47,47,47,47	0
57	MG	2A	3409	1/1	0.95	0.07	48,48,48,48	0
57	MG	1A	3649	1/1	0.95	0.06	35,35,35,35	0
57	MG	10	102	1/1	0.95	0.15	36,36,36,36	0
57	MG	1A	3452	1/1	0.95	0.06	25,25,25,25	0
57	MG	1A	3454	1/1	0.95	0.08	51,51,51,51	0
57	MG	2A	3106	1/1	0.95	0.26	57,57,57,57	0
57	MG	2A	3417	1/1	0.95	0.07	50,50,50,50	0
57	MG	2A	3107	1/1	0.95	0.09	64,64,64,64	0
57	MG	1A	3305	1/1	0.95	0.32	40,40,40,40	0
57	MG	1A	3002	1/1	0.95	0.13	57,57,57,57	0
57	MG	10	108	1/1	0.95	0.08	54,54,54,54	0
57	MG	2A	3117	1/1	0.95	0.18	49,49,49,49	0
57	MG	11	101	1/1	0.95	0.11	39,39,39,39	0
57	MG	1A	3308	1/1	0.95	0.07	38,38,38,38	0
57	MG	1A	3786	1/1	0.95	0.08	45,45,45,45	0
57	MG	1A	3657	1/1	0.95	0.20	47,47,47,47	0
57	MG	2A	3428	1/1	0.95	0.06	41,41,41,41	0
57	MG	2A	3745	1/1	0.95	0.30	59,59,59,59	0
57	MG	2A	3429	1/1	0.95	0.06	34,34,34,34	0
57	MG	1A	3176	1/1	0.95	0.10	52,52,52,52	0
57	MG	15	107	1/1	0.95	0.10	66,66,66,66	0
57	MG	1A	3315	1/1	0.95	0.17	36,36,36,36	0
57	MG	1A	3380	1/1	0.95	0.07	47,47,47,47	0
57	MG	1A	3567	1/1	0.95	0.06	46,46,46,46	0
57	MG	2A	3438	1/1	0.95	0.18	64,64,64,64	0
57	MG	2A	3440	1/1	0.95	0.14	66,66,66,66	0
57	MG	1A	3041	1/1	0.95	0.12	47,47,47,47	0
57	MG	2A	3443	1/1	0.95	0.11	48,48,48,48	0
57	MG	2A	3133	1/1	0.95	0.13	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3957	1/1	0.95	0.11	51,51,51,51	0
57	MG	1A	3794	1/1	0.95	0.07	58,58,58,58	0
57	MG	1A	3666	1/1	0.95	0.07	48,48,48,48	0
57	MG	1A	3065	1/1	0.95	0.17	52,52,52,52	0
57	MG	2A	3140	1/1	0.95	0.28	61,61,61,61	0
57	MG	1a	1604	1/1	0.95	0.15	55,55,55,55	0
57	MG	1A	3797	1/1	0.95	0.07	74,74,74,74	0
57	MG	1A	3798	1/1	0.95	0.07	42,42,42,42	0
57	MG	1A	3669	1/1	0.95	0.06	50,50,50,50	0
57	MG	2A	3455	1/1	0.95	0.07	41,41,41,41	0
57	MG	2D	308	1/1	0.95	0.20	54,54,54,54	0
57	MG	1a	1610	1/1	0.95	0.22	52,52,52,52	0
57	MG	1A	3968	1/1	0.95	0.09	52,52,52,52	0
57	MG	1A	3573	1/1	0.95	0.11	46,46,46,46	0
57	MG	2F	303	1/1	0.95	0.12	52,52,52,52	0
57	MG	2A	3459	1/1	0.95	0.08	36,36,36,36	0
57	MG	1A	3970	1/1	0.95	0.07	22,22,22,22	0
57	MG	1A	3802	1/1	0.95	0.08	33,33,33,33	0
57	MG	2A	3156	1/1	0.95	0.08	69,69,69,69	0
57	MG	2A	3157	1/1	0.95	0.13	44,44,44,44	0
57	MG	1A	3805	1/1	0.95	0.06	44,44,44,44	0
57	MG	2A	3162	1/1	0.95	0.09	50,50,50,50	0
57	MG	1a	1796	1/1	0.95	0.13	58,58,58,58	0
57	MG	1A	3127	1/1	0.95	0.07	49,49,49,49	0
57	MG	1A	3807	1/1	0.95	0.24	47,47,47,47	0
57	MG	1A	3577	1/1	0.95	0.09	22,22,22,22	0
57	MG	1a	1624	1/1	0.95	0.21	58,58,58,58	0
57	MG	1a	1801	1/1	0.95	0.09	55,55,55,55	0
57	MG	1a	1802	1/1	0.95	0.07	57,57,57,57	0
57	MG	1A	3066	1/1	0.95	0.09	33,33,33,33	0
57	MG	2T	202	1/1	0.95	0.09	60,60,60,60	0
57	MG	1A	3325	1/1	0.95	0.08	30,30,30,30	0
57	MG	1A	3981	1/1	0.95	0.10	43,43,43,43	0
57	MG	1a	1630	1/1	0.95	0.08	41,41,41,41	0
57	MG	2A	3178	1/1	0.95	0.09	52,52,52,52	0
57	MG	2V	203	1/1	0.95	0.15	62,62,62,62	0
57	MG	2W	201	1/1	0.95	0.24	49,49,49,49	0
57	MG	1A	3677	1/1	0.95	0.09	62,62,62,62	0
57	MG	1A	3678	1/1	0.95	0.07	37,37,37,37	0
57	MG	1A	3326	1/1	0.95	0.11	34,34,34,34	0
57	MG	2A	3487	1/1	0.95	0.07	66,66,66,66	0
57	MG	1a	1811	1/1	0.95	0.13	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	3820	1/1	0.95	0.09	36,36,36,36	0
57	MG	1A	3822	1/1	0.95	0.17	29,29,29,29	0
57	MG	2A	3191	1/1	0.95	0.13	44,44,44,44	0
57	MG	1A	3583	1/1	0.95	0.15	45,45,45,45	0
57	MG	1A	3584	1/1	0.95	0.12	51,51,51,51	0
57	MG	1A	3391	1/1	0.95	0.07	43,43,43,43	0
57	MG	2A	3496	1/1	0.95	0.11	53,53,53,53	0
57	MG	1A	3828	1/1	0.95	0.08	47,47,47,47	0
57	MG	1A	3392	1/1	0.95	0.06	30,30,30,30	0
57	MG	1A	3685	1/1	0.95	0.13	20,20,20,20	0
57	MG	1A	3478	1/1	0.95	0.07	28,28,28,28	0
57	MG	2A	3199	1/1	0.95	0.17	50,50,50,50	0
57	MG	2a	3013	1/1	0.95	0.09	50,50,50,50	0
57	MG	1a	1644	1/1	0.95	0.24	56,56,56,56	0
57	MG	1a	1646	1/1	0.95	0.14	41,41,41,41	0
57	MG	1A	3129	1/1	0.95	0.15	41,41,41,41	0
57	MG	1a	1649	1/1	0.95	0.14	63,63,63,63	0
57	MG	2A	3513	1/1	0.95	0.07	35,35,35,35	0
57	MG	2a	3021	1/1	0.95	0.10	53,53,53,53	0
57	MG	2A	3204	1/1	0.95	0.11	52,52,52,52	0
57	MG	1A	3395	1/1	0.95	0.10	24,24,24,24	0
57	MG	1a	1652	1/1	0.95	0.15	51,51,51,51	0
57	MG	1a	1653	1/1	0.95	0.11	36,36,36,36	0
57	MG	1A	3593	1/1	0.95	0.07	19,19,19,19	0
57	MG	2A	3211	1/1	0.95	0.09	42,42,42,42	0
57	MG	2A	3212	1/1	0.95	0.09	57,57,57,57	0
57	MG	1A	3594	1/1	0.95	0.09	48,48,48,48	0
57	MG	2a	3031	1/1	0.95	0.13	55,55,55,55	0
57	MG	1A	3328	1/1	0.95	0.10	47,47,47,47	0
57	MG	2A	3215	1/1	0.95	0.22	57,57,57,57	0
57	MG	2A	3216	1/1	0.95	0.14	55,55,55,55	0
57	MG	1A	3190	1/1	0.95	0.10	43,43,43,43	0
57	MG	2A	3532	1/1	0.95	0.10	62,62,62,62	0
57	MG	2a	3038	1/1	0.95	0.08	63,63,63,63	0
57	MG	2A	3219	1/1	0.95	0.14	62,62,62,62	0
57	MG	1a	1658	1/1	0.95	0.09	60,60,60,60	0
57	MG	1a	1659	1/1	0.95	0.12	54,54,54,54	0
57	MG	2A	3536	1/1	0.95	0.07	52,52,52,52	0
57	MG	1A	3847	1/1	0.95	0.10	46,46,46,46	0
57	MG	1A	3398	1/1	0.95	0.06	33,33,33,33	0
57	MG	2A	3224	1/1	0.95	0.13	44,44,44,44	0
57	MG	1a	1843	1/1	0.95	0.15	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	3849	1/1	0.95	0.10	53,53,53,53	0
57	MG	1a	1845	1/1	0.95	0.14	62,62,62,62	0
57	MG	1A	3130	1/1	0.95	0.28	37,37,37,37	0
57	MG	1a	1848	1/1	0.95	0.07	35,35,35,35	0
57	MG	1A	3488	1/1	0.95	0.09	25,25,25,25	0
57	MG	1A	3702	1/1	0.95	0.14	43,43,43,43	0
57	MG	1a	1854	1/1	0.95	0.16	60,60,60,60	0
57	MG	1a	1668	1/1	0.95	0.13	52,52,52,52	0
57	MG	2a	3057	1/1	0.95	0.20	63,63,63,63	0
57	MG	2A	3554	1/1	0.95	0.08	51,51,51,51	0
57	MG	1A	3854	1/1	0.95	0.09	24,24,24,24	0
57	MG	1A	3491	1/1	0.95	0.07	63,63,63,63	0
57	MG	1A	3858	1/1	0.95	0.06	53,53,53,53	0
57	MG	1A	3331	1/1	0.95	0.07	23,23,23,23	0
57	MG	1A	3497	1/1	0.95	0.10	26,26,26,26	0
57	MG	2A	3561	1/1	0.95	0.07	44,44,44,44	0
57	MG	1A	3707	1/1	0.95	0.05	44,44,44,44	0
57	MG	1a	1676	1/1	0.95	0.11	46,46,46,46	0
57	MG	1A	3406	1/1	0.95	0.17	58,58,58,58	0
57	MG	1A	3864	1/1	0.95	0.07	28,28,28,28	0
57	MG	2A	3571	1/1	0.95	0.07	76,76,76,76	0
57	MG	1A	3192	1/1	0.95	0.09	59,59,59,59	0
57	MG	1A	3028	1/1	0.95	0.22	28,28,28,28	0
57	MG	1A	3711	1/1	0.95	0.08	27,27,27,27	0
57	MG	1A	3096	1/1	0.95	0.11	33,33,33,33	0
57	MG	2A	3576	1/1	0.95	0.07	24,24,24,24	0
57	MG	1A	3270	1/1	0.95	0.09	44,44,44,44	0
57	MG	1A	3097	1/1	0.95	0.13	53,53,53,53	0
57	MG	1A	3148	1/1	0.95	0.12	47,47,47,47	0
57	MG	1A	3873	1/1	0.95	0.11	29,29,29,29	0
57	MG	2A	3263	1/1	0.95	0.24	58,58,58,58	0
57	MG	1B	226	1/1	0.95	0.08	32,32,32,32	0
57	MG	1a	1692	1/1	0.95	0.22	55,55,55,55	0
57	MG	1A	3020	1/1	0.95	0.26	30,30,30,30	0
57	MG	1A	3876	1/1	0.95	0.10	40,40,40,40	0
57	MG	2A	3272	1/1	0.95	0.15	30,30,30,30	0
57	MG	1A	3421	1/1	0.95	0.04	29,29,29,29	0
57	MG	1i	201	1/1	0.95	0.11	54,54,54,54	0
57	MG	2a	3095	1/1	0.95	0.07	53,53,53,53	0
57	MG	2A	3596	1/1	0.95	0.12	50,50,50,50	0
57	MG	1a	1696	1/1	0.95	0.37	57,57,57,57	0
57	MG	1A	3074	1/1	0.95	0.13	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3022	1/1	0.95	0.10	38,38,38,38	0
57	MG	2A	3286	1/1	0.95	0.14	53,53,53,53	0
57	MG	2a	3101	1/1	0.95	0.42	62,62,62,62	0
57	MG	2a	3103	1/1	0.95	0.19	54,54,54,54	0
57	MG	1A	3349	1/1	0.95	0.10	25,25,25,25	0
57	MG	1A	3350	1/1	0.95	0.09	53,53,53,53	0
57	MG	2a	3106	1/1	0.95	0.17	64,64,64,64	0
57	MG	2A	3609	1/1	0.95	0.07	46,46,46,46	0
57	MG	1o	102	1/1	0.95	0.17	54,54,54,54	0
57	MG	2A	3293	1/1	0.95	0.25	52,52,52,52	0
57	MG	1D	319	1/1	0.95	0.07	61,61,61,61	0
57	MG	1A	3429	1/1	0.95	0.05	13,13,13,13	0
57	MG	1a	1703	1/1	0.95	0.38	62,62,62,62	0
57	MG	1A	3353	1/1	0.95	0.06	30,30,30,30	0
57	MG	1x	101	1/1	0.95	0.09	33,33,33,33	0
57	MG	2a	3116	1/1	0.95	0.07	49,49,49,49	0
57	MG	2a	3117	1/1	0.95	0.10	55,55,55,55	0
57	MG	1A	3740	1/1	0.95	0.06	24,24,24,24	0
57	MG	2A	3622	1/1	0.95	0.07	52,52,52,52	0
57	MG	1E	308	1/1	0.95	0.08	36,36,36,36	0
57	MG	1F	311	1/1	0.95	0.20	38,38,38,38	0
57	MG	2A	3008	1/1	0.95	0.07	37,37,37,37	0
57	MG	2A	3010	1/1	0.95	0.14	58,58,58,58	0
57	MG	1F	312	1/1	0.95	0.10	49,49,49,49	0
57	MG	2A	3309	1/1	0.95	0.25	58,58,58,58	0
57	MG	2A	3017	1/1	0.95	0.12	56,56,56,56	0
57	MG	2a	3128	1/1	0.95	0.10	48,48,48,48	0
57	MG	2A	3019	1/1	0.95	0.28	49,49,49,49	0
57	MG	2a	3130	1/1	0.95	0.13	61,61,61,61	0
57	MG	1F	314	1/1	0.95	0.32	42,42,42,42	0
57	MG	1A	3113	1/1	0.95	0.14	37,37,37,37	0
57	MG	2A	3320	1/1	0.95	0.15	50,50,50,50	0
57	MG	1A	3114	1/1	0.95	0.19	31,31,31,31	0
57	MG	2A	3326	1/1	0.95	0.05	36,36,36,36	0
57	MG	1G	201	1/1	0.95	0.09	58,58,58,58	0
57	MG	1A	3896	1/1	0.95	0.06	43,43,43,43	0
57	MG	1A	3288	1/1	0.95	0.07	51,51,51,51	0
57	MG	1A	3289	1/1	0.95	0.10	52,52,52,52	0
57	MG	2A	3338	1/1	0.95	0.13	64,64,64,64	0
57	MG	1A	3900	1/1	0.95	0.08	54,54,54,54	0
57	MG	2a	3145	1/1	0.95	0.07	57,57,57,57	0
57	MG	2A	3648	1/1	0.95	0.06	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	1N	202	1/1	0.95	0.11	36,36,36,36	0
57	MG	2A	3041	1/1	0.95	0.16	46,46,46,46	0
57	MG	2A	3651	1/1	0.95	0.08	60,60,60,60	0
57	MG	2A	3652	1/1	0.95	0.07	63,63,63,63	0
57	MG	2A	3042	1/1	0.95	0.05	25,25,25,25	0
57	MG	1N	203	1/1	0.95	0.06	48,48,48,48	0
57	MG	2A	3046	1/1	0.95	0.15	60,60,60,60	0
57	MG	1A	3750	1/1	0.95	0.10	28,28,28,28	0
57	MG	1a	1720	1/1	0.95	0.15	60,60,60,60	0
57	MG	1A	3635	1/1	0.95	0.10	45,45,45,45	0
57	MG	2a	3170	1/1	0.95	0.12	54,54,54,54	0
57	MG	1P	202	1/1	0.95	0.19	48,48,48,48	0
57	MG	2A	3667	1/1	0.95	0.10	47,47,47,47	0
57	MG	1A	3637	1/1	0.95	0.08	37,37,37,37	0
57	MG	2A	3669	1/1	0.95	0.12	36,36,36,36	0
57	MG	2a	3177	1/1	0.95	0.08	54,54,54,54	0
57	MG	1a	1725	1/1	0.95	0.18	54,54,54,54	0
57	MG	1A	3298	1/1	0.95	0.07	48,48,48,48	0
57	MG	2A	3057	1/1	0.95	0.14	50,50,50,50	0
57	MG	1A	3755	1/1	0.95	0.10	44,44,44,44	0
57	MG	1A	3907	1/1	0.95	0.05	26,26,26,26	0
57	MG	1A	3440	1/1	0.95	0.11	54,54,54,54	0
57	MG	1R	203	1/1	0.95	0.09	32,32,32,32	0
57	MG	2A	3684	1/1	0.95	0.07	40,40,40,40	0
57	MG	2A	3369	1/1	0.95	0.10	38,38,38,38	0
57	MG	1A	3910	1/1	0.95	0.12	25,25,25,25	0
57	MG	2A	3372	1/1	0.95	0.11	50,50,50,50	0
57	MG	1A	3167	1/1	0.95	0.12	45,45,45,45	0
57	MG	1A	3219	1/1	0.95	0.12	46,46,46,46	0
57	MG	2A	3692	1/1	0.95	0.07	33,33,33,33	0
57	MG	2A	3377	1/1	0.95	0.14	63,63,63,63	0
57	MG	1A	3545	1/1	0.95	0.10	47,47,47,47	0
58	CLM	2A	3747	20/20	0.95	0.10	33,38,53,58	0
57	MG	1T	203	1/1	0.95	0.07	48,48,48,48	0
57	MG	2A	3698	1/1	0.95	0.07	62,62,62,62	0
57	MG	2A	3381	1/1	0.95	0.11	44,44,44,44	0
57	MG	2A	3069	1/1	0.95	0.30	57,57,57,57	0
57	MG	2A	3701	1/1	0.95	0.08	60,60,60,60	0
57	MG	1A	3764	1/1	0.95	0.06	27,27,27,27	0
57	MG	2A	3703	1/1	0.95	0.06	49,49,49,49	0
57	MG	1A	3920	1/1	0.95	0.06	54,54,54,54	0
57	MG	1a	1744	1/1	0.95	0.08	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	3723	1/1	0.96	0.23	51,51,51,51	0
57	MG	1A	3845	1/1	0.96	0.07	55,55,55,55	0
57	MG	2A	3726	1/1	0.96	0.07	38,38,38,38	0
57	MG	1a	1645	1/1	0.96	0.18	54,54,54,54	0
57	MG	2A	3434	1/1	0.96	0.07	56,56,56,56	0
57	MG	1A	3846	1/1	0.96	0.07	41,41,41,41	0
57	MG	2A	3158	1/1	0.96	0.28	55,55,55,55	0
57	MG	1A	4013	1/1	0.96	0.09	40,40,40,40	0
57	MG	1A	3401	1/1	0.96	0.05	17,17,17,17	0
57	MG	2A	3439	1/1	0.96	0.08	42,42,42,42	0
57	MG	2A	3163	1/1	0.96	0.05	62,62,62,62	0
57	MG	2A	3441	1/1	0.96	0.08	50,50,50,50	0
57	MG	1A	4015	1/1	0.96	0.07	50,50,50,50	0
57	MG	1a	1651	1/1	0.96	0.06	39,39,39,39	0
57	MG	2A	3444	1/1	0.96	0.07	46,46,46,46	0
57	MG	1A	3112	1/1	0.96	0.16	34,34,34,34	0
57	MG	1A	3589	1/1	0.96	0.07	44,44,44,44	0
57	MG	1A	3699	1/1	0.96	0.17	39,39,39,39	0
57	MG	1A	3089	1/1	0.96	0.10	32,32,32,32	0
57	MG	1A	3280	1/1	0.96	0.12	33,33,33,33	0
57	MG	1A	3482	1/1	0.96	0.08	44,44,44,44	0
57	MG	1A	3281	1/1	0.96	0.12	25,25,25,25	0
57	MG	1A	3484	1/1	0.96	0.09	26,26,26,26	0
57	MG	1A	3408	1/1	0.96	0.08	25,25,25,25	0
57	MG	2B	203	1/1	0.96	0.24	65,65,65,65	0
57	MG	1B	209	1/1	0.96	0.07	38,38,38,38	0
57	MG	1a	1835	1/1	0.96	0.09	55,55,55,55	0
57	MG	1a	1837	1/1	0.96	0.14	55,55,55,55	0
57	MG	1A	3132	1/1	0.96	0.27	40,40,40,40	0
57	MG	1A	3410	1/1	0.96	0.07	19,19,19,19	0
57	MG	1a	1664	1/1	0.96	0.24	55,55,55,55	0
57	MG	1A	3050	1/1	0.96	0.23	43,43,43,43	0
57	MG	2A	3189	1/1	0.96	0.13	59,59,59,59	0
57	MG	1a	1666	1/1	0.96	0.09	64,64,64,64	0
57	MG	1A	3347	1/1	0.96	0.05	38,38,38,38	0
57	MG	1A	3495	1/1	0.96	0.07	46,46,46,46	0
57	MG	1B	217	1/1	0.96	0.11	61,61,61,61	0
57	MG	1A	3866	1/1	0.96	0.10	40,40,40,40	0
57	MG	1A	3415	1/1	0.96	0.05	32,32,32,32	0
57	MG	1a	1849	1/1	0.96	0.07	55,55,55,55	0
57	MG	2A	3470	1/1	0.96	0.06	50,50,50,50	0
57	MG	1A	3604	1/1	0.96	0.17	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1B	222	1/1	0.96	0.09	42,42,42,42	0
57	MG	1A	3605	1/1	0.96	0.07	46,46,46,46	0
57	MG	2E	301	1/1	0.96	0.13	38,38,38,38	0
57	MG	1A	3716	1/1	0.96	0.20	27,27,27,27	0
57	MG	1A	3717	1/1	0.96	0.08	37,37,37,37	0
57	MG	1a	1678	1/1	0.96	0.20	55,55,55,55	0
57	MG	1A	3416	1/1	0.96	0.10	48,48,48,48	0
57	MG	1A	3607	1/1	0.96	0.15	31,31,31,31	0
57	MG	1A	3417	1/1	0.96	0.07	24,24,24,24	0
57	MG	2A	3482	1/1	0.96	0.06	51,51,51,51	0
57	MG	1A	3181	1/1	0.96	0.16	38,38,38,38	0
57	MG	1D	306	1/1	0.96	0.08	52,52,52,52	0
57	MG	1A	3726	1/1	0.96	0.06	71,71,71,71	0
57	MG	1a	1687	1/1	0.96	0.11	54,54,54,54	0
57	MG	1D	314	1/1	0.96	0.08	50,50,50,50	0
57	MG	1A	3727	1/1	0.96	0.07	35,35,35,35	0
57	MG	1D	316	1/1	0.96	0.13	49,49,49,49	0
57	MG	1A	3221	1/1	0.96	0.07	39,39,39,39	0
57	MG	1D	321	1/1	0.96	0.12	51,51,51,51	0
57	MG	1A	3611	1/1	0.96	0.17	27,27,27,27	0
57	MG	1A	3733	1/1	0.96	0.06	35,35,35,35	0
57	MG	1A	3734	1/1	0.96	0.08	50,50,50,50	0
57	MG	2A	3497	1/1	0.96	0.09	68,68,68,68	0
57	MG	1A	3613	1/1	0.96	0.10	26,26,26,26	0
57	MG	2A	3499	1/1	0.96	0.11	58,58,58,58	0
57	MG	1F	308	1/1	0.96	0.12	34,34,34,34	0
57	MG	1F	309	1/1	0.96	0.07	36,36,36,36	0
57	MG	1A	3139	1/1	0.96	0.07	37,37,37,37	0
57	MG	2A	3226	1/1	0.96	0.06	46,46,46,46	0
57	MG	2W	202	1/1	0.96	0.17	50,50,50,50	0
57	MG	2X	101	1/1	0.96	0.08	47,47,47,47	0
57	MG	1h	201	1/1	0.96	0.20	49,49,49,49	0
57	MG	20	101	1/1	0.96	0.08	60,60,60,60	0
57	MG	2A	3507	1/1	0.96	0.12	66,66,66,66	0
57	MG	1A	3292	1/1	0.96	0.05	34,34,34,34	0
57	MG	1F	313	1/1	0.96	0.10	32,32,32,32	0
57	MG	1A	3739	1/1	0.96	0.07	45,45,45,45	0
57	MG	2A	3233	1/1	0.96	0.08	55,55,55,55	0
57	MG	25	103	1/1	0.96	0.09	55,55,55,55	0
57	MG	1A	3894	1/1	0.96	0.07	50,50,50,50	0
57	MG	28	3801	1/1	0.96	0.09	48,48,48,48	0
57	MG	1F	316	1/1	0.96	0.10	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3236	1/1	0.96	0.09	39,39,39,39	0
57	MG	2a	3004	1/1	0.96	0.10	61,61,61,61	0
57	MG	1A	3509	1/1	0.96	0.08	57,57,57,57	0
57	MG	1F	318	1/1	0.96	0.12	46,46,46,46	0
57	MG	1o	101	1/1	0.96	0.10	49,49,49,49	0
57	MG	1A	3741	1/1	0.96	0.09	48,48,48,48	0
57	MG	1A	3356	1/1	0.96	0.05	22,22,22,22	0
57	MG	2A	3526	1/1	0.96	0.07	47,47,47,47	0
57	MG	1A	3899	1/1	0.96	0.09	54,54,54,54	0
57	MG	1A	3743	1/1	0.96	0.07	38,38,38,38	0
57	MG	1A	3744	1/1	0.96	0.17	54,54,54,54	0
57	MG	1A	3294	1/1	0.96	0.08	42,42,42,42	0
57	MG	1A	3514	1/1	0.96	0.05	34,34,34,34	0
57	MG	1A	3296	1/1	0.96	0.07	38,38,38,38	0
57	MG	2a	3017	1/1	0.96	0.07	58,58,58,58	0
57	MG	1A	3359	1/1	0.96	0.08	31,31,31,31	0
57	MG	2A	3252	1/1	0.96	0.31	44,44,44,44	0
57	MG	1A	3428	1/1	0.96	0.11	24,24,24,24	0
57	MG	2A	3537	1/1	0.96	0.11	53,53,53,53	0
57	MG	2A	3538	1/1	0.96	0.07	48,48,48,48	0
57	MG	1A	3908	1/1	0.96	0.06	19,19,19,19	0
57	MG	2A	3540	1/1	0.96	0.05	48,48,48,48	0
57	MG	2A	3255	1/1	0.96	0.13	39,39,39,39	0
57	MG	2A	3542	1/1	0.96	0.06	34,34,34,34	0
57	MG	2A	3014	1/1	0.96	0.08	59,59,59,59	0
57	MG	1A	3361	1/1	0.96	0.09	46,46,46,46	0
57	MG	1A	3115	1/1	0.96	0.07	33,33,33,33	0
57	MG	2A	3018	1/1	0.96	0.19	36,36,36,36	0
57	MG	1A	3117	1/1	0.96	0.18	30,30,30,30	0
57	MG	2A	3021	1/1	0.96	0.05	34,34,34,34	0
57	MG	1A	3914	1/1	0.96	0.12	35,35,35,35	0
57	MG	1A	3757	1/1	0.96	0.06	37,37,37,37	0
57	MG	1A	3524	1/1	0.96	0.10	58,58,58,58	0
57	MG	1A	3628	1/1	0.96	0.08	53,53,53,53	0
57	MG	1A	3526	1/1	0.96	0.04	22,22,22,22	0
57	MG	1A	3231	1/1	0.96	0.16	38,38,38,38	0
57	MG	2A	3275	1/1	0.96	0.12	58,58,58,58	0
57	MG	1A	3232	1/1	0.96	0.12	27,27,27,27	0
57	MG	2A	3035	1/1	0.96	0.20	52,52,52,52	0
57	MG	2A	3559	1/1	0.96	0.06	54,54,54,54	0
57	MG	2A	3036	1/1	0.96	0.08	50,50,50,50	0
57	MG	2A	3281	1/1	0.96	0.12	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3282	1/1	0.96	0.31	68,68,68,68	0
57	MG	1A	3436	1/1	0.96	0.08	48,48,48,48	0
57	MG	1A	3120	1/1	0.96	0.08	35,35,35,35	0
57	MG	1A	3369	1/1	0.96	0.05	26,26,26,26	0
57	MG	2A	3288	1/1	0.96	0.21	66,66,66,66	0
57	MG	2A	3289	1/1	0.96	0.15	54,54,54,54	0
57	MG	1A	3769	1/1	0.96	0.09	55,55,55,55	0
57	MG	2a	3056	1/1	0.96	0.13	58,58,58,58	0
57	MG	1A	3151	1/1	0.96	0.07	44,44,44,44	0
57	MG	2A	3045	1/1	0.96	0.09	59,59,59,59	0
57	MG	1A	3081	1/1	0.96	0.10	46,46,46,46	0
57	MG	1A	3642	1/1	0.96	0.16	34,34,34,34	0
57	MG	2A	3578	1/1	0.96	0.07	52,52,52,52	0
57	MG	2A	3579	1/1	0.96	0.07	61,61,61,61	0
57	MG	1A	3775	1/1	0.96	0.05	37,37,37,37	0
57	MG	2A	3049	1/1	0.96	0.12	55,55,55,55	0
57	MG	1A	3936	1/1	0.96	0.06	41,41,41,41	0
57	MG	2A	3300	1/1	0.96	0.10	51,51,51,51	0
57	MG	2a	3068	1/1	0.96	0.20	67,67,67,67	0
57	MG	2A	3051	1/1	0.96	0.11	48,48,48,48	0
57	MG	1A	3250	1/1	0.96	0.07	42,42,42,42	0
57	MG	2A	3303	1/1	0.96	0.14	43,43,43,43	0
57	MG	2A	3304	1/1	0.96	0.26	58,58,58,58	0
57	MG	1A	3539	1/1	0.96	0.08	51,51,51,51	0
57	MG	2a	3074	1/1	0.96	0.24	51,51,51,51	0
57	MG	2A	3054	1/1	0.96	0.15	57,57,57,57	0
57	MG	2a	3076	1/1	0.96	0.07	54,54,54,54	0
57	MG	1A	3540	1/1	0.96	0.05	23,23,23,23	0
57	MG	1A	3782	1/1	0.96	0.11	38,38,38,38	0
57	MG	2A	3597	1/1	0.96	0.09	39,39,39,39	0
57	MG	1A	3542	1/1	0.96	0.07	37,37,37,37	0
57	MG	2A	3311	1/1	0.96	0.09	51,51,51,51	0
57	MG	2a	3083	1/1	0.96	0.28	60,60,60,60	0
57	MG	1A	3647	1/1	0.96	0.12	65,65,65,65	0
57	MG	2A	3601	1/1	0.96	0.09	58,58,58,58	0
57	MG	1A	3947	1/1	0.96	0.11	25,25,25,25	0
57	MG	2A	3061	1/1	0.96	0.08	47,47,47,47	0
57	MG	2a	3088	1/1	0.96	0.10	55,55,55,55	0
57	MG	1a	1753	1/1	0.96	0.08	53,53,53,53	0
57	MG	1A	3543	1/1	0.96	0.06	32,32,32,32	0
57	MG	1A	3949	1/1	0.96	0.06	44,44,44,44	0
57	MG	2A	3324	1/1	0.96	0.07	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	2a	3093	1/1	0.96	0.26	52,52,52,52	0
57	MG	1A	3445	1/1	0.96	0.15	40,40,40,40	0
57	MG	1A	3446	1/1	0.96	0.11	44,44,44,44	0
57	MG	1A	3546	1/1	0.96	0.08	31,31,31,31	0
57	MG	1A	3008	1/1	0.96	0.06	36,36,36,36	0
57	MG	2A	3332	1/1	0.96	0.07	54,54,54,54	0
57	MG	15	101	1/1	0.96	0.15	43,43,43,43	0
57	MG	2A	3335	1/1	0.96	0.06	41,41,41,41	0
57	MG	2A	3337	1/1	0.96	0.06	35,35,35,35	0
57	MG	2a	3102	1/1	0.96	0.08	55,55,55,55	0
57	MG	15	104	1/1	0.96	0.14	26,26,26,26	0
57	MG	2A	3339	1/1	0.96	0.09	49,49,49,49	0
57	MG	1A	3549	1/1	0.96	0.09	44,44,44,44	0
57	MG	2A	3073	1/1	0.96	0.07	32,32,32,32	0
57	MG	2A	3342	1/1	0.96	0.09	42,42,42,42	0
57	MG	1a	1765	1/1	0.96	0.10	52,52,52,52	0
57	MG	1A	3550	1/1	0.96	0.11	42,42,42,42	0
57	MG	2A	3346	1/1	0.96	0.16	52,52,52,52	0
57	MG	2A	3633	1/1	0.96	0.09	49,49,49,49	0
57	MG	1A	3312	1/1	0.96	0.17	30,30,30,30	0
57	MG	1A	3252	1/1	0.96	0.10	44,44,44,44	0
57	MG	1A	3553	1/1	0.96	0.06	49,49,49,49	0
57	MG	2A	3353	1/1	0.96	0.08	52,52,52,52	0
57	MG	2A	3638	1/1	0.96	0.07	50,50,50,50	0
57	MG	1a	1770	1/1	0.96	0.09	59,59,59,59	0
57	MG	1A	3378	1/1	0.96	0.09	48,48,48,48	0
57	MG	19	101	1/1	0.96	0.10	58,58,58,58	0
57	MG	1A	3556	1/1	0.96	0.12	53,53,53,53	0
57	MG	2A	3085	1/1	0.96	0.17	58,58,58,58	0
57	MG	2A	3645	1/1	0.96	0.08	67,67,67,67	0
57	MG	2a	3124	1/1	0.96	0.14	59,59,59,59	0
57	MG	2A	3087	1/1	0.96	0.36	47,47,47,47	0
57	MG	2A	3088	1/1	0.96	0.10	41,41,41,41	0
57	MG	1A	3253	1/1	0.96	0.06	45,45,45,45	0
57	MG	2A	3364	1/1	0.96	0.11	34,34,34,34	0
57	MG	1A	3453	1/1	0.96	0.09	58,58,58,58	0
57	MG	1A	3060	1/1	0.96	0.17	37,37,37,37	0
57	MG	1A	3194	1/1	0.96	0.10	34,34,34,34	0
57	MG	2A	3094	1/1	0.96	0.10	48,48,48,48	0
57	MG	2A	3095	1/1	0.96	0.18	65,65,65,65	0
57	MG	1A	3382	1/1	0.96	0.07	45,45,45,45	0
57	MG	1A	3196	1/1	0.96	0.13	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	3975	1/1	0.96	0.05	42,42,42,42	0
57	MG	2A	3099	1/1	0.96	0.06	53,53,53,53	0
57	MG	1A	3033	1/1	0.96	0.07	34,34,34,34	0
57	MG	1A	3977	1/1	0.96	0.05	48,48,48,48	0
57	MG	1A	3810	1/1	0.96	0.08	42,42,42,42	0
57	MG	1a	1613	1/1	0.96	0.10	49,49,49,49	0
57	MG	2A	3673	1/1	0.96	0.06	19,19,19,19	0
57	MG	2a	3146	1/1	0.96	0.09	71,71,71,71	0
57	MG	1a	1786	1/1	0.96	0.08	61,61,61,61	0
57	MG	2A	3108	1/1	0.96	0.08	52,52,52,52	0
57	MG	2A	3110	1/1	0.96	0.12	57,57,57,57	0
57	MG	2a	3152	1/1	0.96	0.06	56,56,56,56	0
57	MG	2A	3386	1/1	0.96	0.11	43,43,43,43	0
57	MG	2a	3154	1/1	0.96	0.05	65,65,65,65	0
57	MG	2a	3156	1/1	0.96	0.06	53,53,53,53	0
57	MG	1A	3565	1/1	0.96	0.09	56,56,56,56	0
57	MG	2A	3113	1/1	0.96	0.07	46,46,46,46	0
57	MG	2A	3683	1/1	0.96	0.08	58,58,58,58	0
57	MG	2A	3114	1/1	0.96	0.13	63,63,63,63	0
57	MG	1A	3675	1/1	0.96	0.17	38,38,38,38	0
57	MG	2a	3164	1/1	0.96	0.12	63,63,63,63	0
57	MG	1A	3260	1/1	0.96	0.21	33,33,33,33	0
57	MG	2A	3392	1/1	0.96	0.16	59,59,59,59	0
57	MG	1A	3262	1/1	0.96	0.13	25,25,25,25	0
57	MG	1A	3983	1/1	0.96	0.06	55,55,55,55	0
57	MG	1A	3819	1/1	0.96	0.10	37,37,37,37	0
57	MG	2a	3173	1/1	0.96	0.07	64,64,64,64	0
57	MG	1a	1621	1/1	0.96	0.17	58,58,58,58	0
57	MG	1A	3569	1/1	0.96	0.07	14,14,14,14	0
57	MG	2A	3696	1/1	0.96	0.06	37,37,37,37	0
57	MG	1A	3679	1/1	0.96	0.07	55,55,55,55	0
57	MG	2A	3125	1/1	0.96	0.07	36,36,36,36	0
57	MG	1A	3463	1/1	0.96	0.12	54,54,54,54	0
57	MG	1A	3198	1/1	0.96	0.09	41,41,41,41	0
57	MG	1A	3265	1/1	0.96	0.10	39,39,39,39	0
57	MG	2a	3184	1/1	0.96	0.16	72,72,72,72	0
57	MG	1a	1629	1/1	0.96	0.13	47,47,47,47	0
57	MG	1A	3827	1/1	0.96	0.05	18,18,18,18	0
57	MG	2A	3411	1/1	0.96	0.11	61,61,61,61	0
57	MG	1A	3161	1/1	0.96	0.08	46,46,46,46	0
57	MG	1A	3829	1/1	0.96	0.07	38,38,38,38	0
57	MG	1A	3164	1/1	0.96	0.05	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3136	1/1	0.96	0.14	58,58,58,58	0
57	MG	1A	3471	1/1	0.96	0.08	39,39,39,39	0
57	MG	2A	3710	1/1	0.96	0.06	64,64,64,64	0
57	MG	1A	3687	1/1	0.96	0.11	32,32,32,32	0
57	MG	2t	201	1/1	0.96	0.13	40,40,40,40	0
57	MG	1A	3087	1/1	0.96	0.11	37,37,37,37	0
57	MG	1a	1807	1/1	0.96	0.07	45,45,45,45	0
57	MG	2A	3714	1/1	0.96	0.08	47,47,47,47	0
57	MG	1A	3004	1/1	0.96	0.10	45,45,45,45	0
57	MG	1A	3474	1/1	0.96	0.07	52,52,52,52	0
57	MG	1A	3336	1/1	0.96	0.04	32,32,32,32	0
57	MG	1A	4006	1/1	0.96	0.17	32,32,32,32	0
57	MG	1A	3206	1/1	0.96	0.24	43,43,43,43	0
57	MG	2A	3150	1/1	0.96	0.10	50,50,50,50	0
57	MG	1A	3694	1/1	0.96	0.08	54,54,54,54	0
57	MG	1a	1814	1/1	0.96	0.15	58,58,58,58	0
57	MG	1A	3837	1/1	0.97	0.05	37,37,37,37	0
57	MG	2A	3044	1/1	0.97	0.14	44,44,44,44	0
57	MG	1a	1752	1/1	0.97	0.11	37,37,37,37	0
57	MG	1A	3839	1/1	0.97	0.06	43,43,43,43	0
57	MG	1A	3508	1/1	0.97	0.06	46,46,46,46	0
57	MG	1A	3204	1/1	0.97	0.09	36,36,36,36	0
57	MG	2A	3502	1/1	0.97	0.05	62,62,62,62	0
57	MG	2B	217	1/1	0.97	0.08	57,57,57,57	0
57	MG	2A	3259	1/1	0.97	0.06	51,51,51,51	0
57	MG	2B	219	1/1	0.97	0.08	61,61,61,61	0
57	MG	2D	302	1/1	0.97	0.41	44,44,44,44	0
57	MG	17	102	1/1	0.97	0.05	31,31,31,31	0
57	MG	2A	3505	1/1	0.97	0.06	61,61,61,61	0
57	MG	2D	305	1/1	0.97	0.05	34,34,34,34	0
57	MG	1A	3714	1/1	0.97	0.05	30,30,30,30	0
57	MG	17	105	1/1	0.97	0.08	50,50,50,50	0
57	MG	1A	3039	1/1	0.97	0.09	37,37,37,37	0
57	MG	2A	3510	1/1	0.97	0.06	51,51,51,51	0
57	MG	2E	302	1/1	0.97	0.05	37,37,37,37	0
57	MG	2E	303	1/1	0.97	0.15	45,45,45,45	0
57	MG	1a	1760	1/1	0.97	0.11	60,60,60,60	0
57	MG	18	102	1/1	0.97	0.05	35,35,35,35	0
57	MG	2E	306	1/1	0.97	0.06	42,42,42,42	0
57	MG	2E	308	1/1	0.97	0.08	54,54,54,54	0
57	MG	2A	3266	1/1	0.97	0.15	39,39,39,39	0
57	MG	1A	3062	1/1	0.97	0.06	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3270	1/1	0.97	0.16	44,44,44,44	0
57	MG	1A	3274	1/1	0.97	0.05	54,54,54,54	0
57	MG	1A	3348	1/1	0.97	0.08	50,50,50,50	0
57	MG	2A	3519	1/1	0.97	0.05	38,38,38,38	0
57	MG	2A	3058	1/1	0.97	0.10	38,38,38,38	0
57	MG	2A	3274	1/1	0.97	0.23	50,50,50,50	0
57	MG	2A	3522	1/1	0.97	0.04	59,59,59,59	0
57	MG	1A	3991	1/1	0.97	0.08	35,35,35,35	0
57	MG	2A	3276	1/1	0.97	0.14	40,40,40,40	0
57	MG	1A	3516	1/1	0.97	0.07	19,19,19,19	0
57	MG	1A	3720	1/1	0.97	0.17	47,47,47,47	0
57	MG	1A	3995	1/1	0.97	0.09	44,44,44,44	0
57	MG	1A	3208	1/1	0.97	0.07	33,33,33,33	0
57	MG	1A	3424	1/1	0.97	0.11	42,42,42,42	0
57	MG	2A	3531	1/1	0.97	0.10	44,44,44,44	0
57	MG	1a	1606	1/1	0.97	0.11	48,48,48,48	0
57	MG	1A	3853	1/1	0.97	0.06	28,28,28,28	0
57	MG	1A	3007	1/1	0.97	0.07	29,29,29,29	0
57	MG	1a	1609	1/1	0.97	0.10	55,55,55,55	0
57	MG	1A	3352	1/1	0.97	0.03	18,18,18,18	0
57	MG	2V	202	1/1	0.97	0.14	49,49,49,49	0
57	MG	1A	3856	1/1	0.97	0.13	35,35,35,35	0
57	MG	2A	3071	1/1	0.97	0.22	46,46,46,46	0
57	MG	1a	1612	1/1	0.97	0.12	28,28,28,28	0
57	MG	1A	3427	1/1	0.97	0.07	26,26,26,26	0
57	MG	2A	3074	1/1	0.97	0.08	42,42,42,42	0
57	MG	1A	3001	1/1	0.97	0.06	29,29,29,29	0
57	MG	2A	3543	1/1	0.97	0.06	49,49,49,49	0
57	MG	2A	3297	1/1	0.97	0.12	40,40,40,40	0
57	MG	1A	3214	1/1	0.97	0.07	18,18,18,18	0
57	MG	1A	3355	1/1	0.97	0.07	31,31,31,31	0
57	MG	1A	3016	1/1	0.97	0.12	36,36,36,36	0
57	MG	1A	3284	1/1	0.97	0.10	49,49,49,49	0
57	MG	27	101	1/1	0.97	0.13	41,41,41,41	0
57	MG	1a	1785	1/1	0.97	0.05	64,64,64,64	0
57	MG	1A	3532	1/1	0.97	0.11	26,26,26,26	0
57	MG	2a	3001	1/1	0.97	0.06	40,40,40,40	0
57	MG	1A	3124	1/1	0.97	0.07	34,34,34,34	0
57	MG	1A	3630	1/1	0.97	0.07	29,29,29,29	0
57	MG	1a	1623	1/1	0.97	0.05	47,47,47,47	0
57	MG	1A	3090	1/1	0.97	0.15	25,25,25,25	0
57	MG	1a	1625	1/1	0.97	0.06	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	1A	3287	1/1	0.97	0.11	31,31,31,31	0
57	MG	2A	3310	1/1	0.97	0.07	51,51,51,51	0
57	MG	2A	3090	1/1	0.97	0.04	38,38,38,38	0
57	MG	2A	3312	1/1	0.97	0.09	46,46,46,46	0
57	MG	2A	3313	1/1	0.97	0.06	52,52,52,52	0
57	MG	2A	3314	1/1	0.97	0.09	51,51,51,51	0
57	MG	2A	3562	1/1	0.97	0.08	37,37,37,37	0
57	MG	1A	3636	1/1	0.97	0.07	46,46,46,46	0
57	MG	2A	3564	1/1	0.97	0.09	58,58,58,58	0
57	MG	1A	3220	1/1	0.97	0.11	30,30,30,30	0
57	MG	1A	3745	1/1	0.97	0.07	50,50,50,50	0
57	MG	2a	3018	1/1	0.97	0.10	46,46,46,46	0
57	MG	1A	3170	1/1	0.97	0.11	34,34,34,34	0
57	MG	2A	3570	1/1	0.97	0.07	47,47,47,47	0
57	MG	1A	3222	1/1	0.97	0.15	40,40,40,40	0
57	MG	2A	3321	1/1	0.97	0.08	37,37,37,37	0
57	MG	2a	3023	1/1	0.97	0.10	50,50,50,50	0
57	MG	1A	3366	1/1	0.97	0.06	18,18,18,18	0
57	MG	1A	3878	1/1	0.97	0.10	59,59,59,59	0
57	MG	1A	3444	1/1	0.97	0.03	26,26,26,26	0
57	MG	1A	3293	1/1	0.97	0.08	53,53,53,53	0
57	MG	2A	3328	1/1	0.97	0.12	42,42,42,42	0
57	MG	1a	1636	1/1	0.97	0.06	38,38,38,38	0
57	MG	1A	3224	1/1	0.97	0.15	33,33,33,33	0
57	MG	2A	3103	1/1	0.97	0.13	51,51,51,51	0
57	MG	1A	3126	1/1	0.97	0.06	66,66,66,66	0
57	MG	2A	3105	1/1	0.97	0.19	53,53,53,53	0
57	MG	2A	3336	1/1	0.97	0.05	33,33,33,33	0
57	MG	1A	3297	1/1	0.97	0.10	42,42,42,42	0
57	MG	2a	3036	1/1	0.97	0.07	43,43,43,43	0
57	MG	1A	3371	1/1	0.97	0.05	29,29,29,29	0
57	MG	1A	3005	1/1	0.97	0.09	26,26,26,26	0
57	MG	1A	3179	1/1	0.97	0.26	38,38,38,38	0
57	MG	1A	3761	1/1	0.97	0.10	47,47,47,47	0
57	MG	1A	3888	1/1	0.97	0.11	31,31,31,31	0
57	MG	2A	3593	1/1	0.97	0.05	60,60,60,60	0
57	MG	1A	3890	1/1	0.97	0.03	34,34,34,34	0
57	MG	2A	3595	1/1	0.97	0.03	44,44,44,44	0
57	MG	1A	3230	1/1	0.97	0.18	28,28,28,28	0
57	MG	1a	1647	1/1	0.97	0.12	54,54,54,54	0
57	MG	1A	3069	1/1	0.97	0.10	24,24,24,24	0
57	MG	1A	3036	1/1	0.97	0.07	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3349	1/1	0.97	0.06	47,47,47,47	0
57	MG	1A	3235	1/1	0.97	0.17	34,34,34,34	0
57	MG	2A	3603	1/1	0.97	0.04	45,45,45,45	0
57	MG	1A	3766	1/1	0.97	0.10	34,34,34,34	0
57	MG	2a	3053	1/1	0.97	0.15	55,55,55,55	0
57	MG	2A	3121	1/1	0.97	0.06	45,45,45,45	0
57	MG	1a	1819	1/1	0.97	0.10	54,54,54,54	0
57	MG	1A	3053	1/1	0.97	0.17	30,30,30,30	0
57	MG	1A	3655	1/1	0.97	0.07	46,46,46,46	0
57	MG	2A	3126	1/1	0.97	0.10	40,40,40,40	0
57	MG	2A	3613	1/1	0.97	0.05	65,65,65,65	0
57	MG	1A	3307	1/1	0.97	0.13	26,26,26,26	0
57	MG	1D	303	1/1	0.97	0.14	35,35,35,35	0
57	MG	1A	3072	1/1	0.97	0.12	37,37,37,37	0
57	MG	1A	3184	1/1	0.97	0.10	54,54,54,54	0
57	MG	2A	3619	1/1	0.97	0.08	42,42,42,42	0
57	MG	1D	313	1/1	0.97	0.13	29,29,29,29	0
57	MG	1A	3660	1/1	0.97	0.04	20,20,20,20	0
57	MG	1A	3383	1/1	0.97	0.07	48,48,48,48	0
57	MG	1A	3241	1/1	0.97	0.15	33,33,33,33	0
57	MG	1D	317	1/1	0.97	0.16	32,32,32,32	0
57	MG	1D	318	1/1	0.97	0.06	53,53,53,53	0
57	MG	2A	3138	1/1	0.97	0.10	24,24,24,24	0
57	MG	1A	3385	1/1	0.97	0.10	35,35,35,35	0
57	MG	1D	320	1/1	0.97	0.07	47,47,47,47	0
57	MG	2A	3378	1/1	0.97	0.06	40,40,40,40	0
57	MG	1A	3244	1/1	0.97	0.14	46,46,46,46	0
57	MG	1E	302	1/1	0.97	0.18	39,39,39,39	0
57	MG	1A	3780	1/1	0.97	0.11	43,43,43,43	0
57	MG	1A	3781	1/1	0.97	0.16	33,33,33,33	0
57	MG	1A	3912	1/1	0.97	0.04	18,18,18,18	0
57	MG	1A	3467	1/1	0.97	0.06	45,45,45,45	0
57	MG	2a	3082	1/1	0.97	0.27	61,61,61,61	0
57	MG	2A	3149	1/1	0.97	0.19	46,46,46,46	0
57	MG	1F	305	1/1	0.97	0.10	35,35,35,35	0
57	MG	1a	1673	1/1	0.97	0.09	44,44,44,44	0
57	MG	2A	3152	1/1	0.97	0.14	41,41,41,41	0
57	MG	1A	3915	1/1	0.97	0.12	35,35,35,35	0
57	MG	1A	3784	1/1	0.97	0.11	42,42,42,42	0
57	MG	2A	3155	1/1	0.97	0.05	44,44,44,44	0
57	MG	1A	3667	1/1	0.97	0.10	24,24,24,24	0
57	MG	2A	3646	1/1	0.97	0.06	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3246	1/1	0.97	0.16	34,34,34,34	0
57	MG	1A	3787	1/1	0.97	0.04	21,21,21,21	0
57	MG	2A	3396	1/1	0.97	0.06	49,49,49,49	0
57	MG	1A	3317	1/1	0.97	0.09	34,34,34,34	0
57	MG	2A	3160	1/1	0.97	0.10	49,49,49,49	0
57	MG	2A	3401	1/1	0.97	0.14	56,56,56,56	0
57	MG	2A	3161	1/1	0.97	0.13	46,46,46,46	0
57	MG	2A	3656	1/1	0.97	0.05	68,68,68,68	0
57	MG	1A	3249	1/1	0.97	0.09	42,42,42,42	0
57	MG	1A	3570	1/1	0.97	0.08	33,33,33,33	0
57	MG	2A	3659	1/1	0.97	0.10	45,45,45,45	0
57	MG	1A	3320	1/1	0.97	0.07	34,34,34,34	0
57	MG	1A	3321	1/1	0.97	0.08	26,26,26,26	0
57	MG	1A	3133	1/1	0.97	0.07	51,51,51,51	0
57	MG	2A	3665	1/1	0.97	0.06	56,56,56,56	0
57	MG	2A	3168	1/1	0.97	0.07	45,45,45,45	0
57	MG	1A	3574	1/1	0.97	0.15	33,33,33,33	0
57	MG	1A	3930	1/1	0.97	0.13	35,35,35,35	0
57	MG	1A	3575	1/1	0.97	0.12	53,53,53,53	0
57	MG	1H	201	1/1	0.97	0.08	53,53,53,53	0
57	MG	2A	3671	1/1	0.97	0.05	37,37,37,37	0
57	MG	2A	3672	1/1	0.97	0.06	33,33,33,33	0
57	MG	1A	3394	1/1	0.97	0.06	18,18,18,18	0
57	MG	1N	201	1/1	0.97	0.06	36,36,36,36	0
57	MG	1A	3186	1/1	0.97	0.10	32,32,32,32	0
57	MG	1A	3104	1/1	0.97	0.09	34,34,34,34	0
57	MG	1A	3579	1/1	0.97	0.08	25,25,25,25	0
57	MG	1A	3105	1/1	0.97	0.13	30,30,30,30	0
57	MG	2A	3180	1/1	0.97	0.05	47,47,47,47	0
57	MG	1A	3141	1/1	0.97	0.07	36,36,36,36	0
57	MG	2A	3183	1/1	0.97	0.07	41,41,41,41	0
57	MG	1A	3803	1/1	0.97	0.14	31,31,31,31	0
57	MG	2A	3687	1/1	0.97	0.09	58,58,58,58	0
57	MG	1A	3804	1/1	0.97	0.07	51,51,51,51	0
57	MG	2A	3426	1/1	0.97	0.13	55,55,55,55	0
57	MG	1A	3399	1/1	0.97	0.07	18,18,18,18	0
57	MG	1A	3945	1/1	0.97	0.06	21,21,21,21	0
57	MG	1A	3400	1/1	0.97	0.08	25,25,25,25	0
57	MG	2a	3131	1/1	0.97	0.07	63,63,63,63	0
57	MG	2A	3693	1/1	0.97	0.07	64,64,64,64	0
57	MG	2A	3190	1/1	0.97	0.07	51,51,51,51	0
57	MG	1A	3585	1/1	0.97	0.12	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3073	1/1	0.97	0.05	37,37,37,37	0
57	MG	1A	3145	1/1	0.97	0.06	38,38,38,38	0
57	MG	1A	3403	1/1	0.97	0.04	19,19,19,19	0
57	MG	1A	3054	1/1	0.97	0.08	34,34,34,34	0
57	MG	1A	3489	1/1	0.97	0.06	24,24,24,24	0
57	MG	1A	3955	1/1	0.97	0.12	42,42,42,42	0
57	MG	1A	3816	1/1	0.97	0.06	39,39,39,39	0
57	MG	1A	3490	1/1	0.97	0.06	31,31,31,31	0
57	MG	1n	101	1/1	0.97	0.29	56,56,56,56	0
57	MG	1A	3259	1/1	0.97	0.07	49,49,49,49	0
57	MG	1U	202	1/1	0.97	0.22	33,33,33,33	0
57	MG	2a	3148	1/1	0.97	0.08	62,62,62,62	0
57	MG	1A	3961	1/1	0.97	0.13	44,44,44,44	0
57	MG	1U	204	1/1	0.97	0.16	33,33,33,33	0
57	MG	2a	3151	1/1	0.97	0.07	53,53,53,53	0
57	MG	1A	3492	1/1	0.97	0.04	27,27,27,27	0
57	MG	1A	3493	1/1	0.97	0.06	22,22,22,22	0
57	MG	2A	3208	1/1	0.97	0.07	52,52,52,52	0
57	MG	2a	3155	1/1	0.97	0.06	60,60,60,60	0
57	MG	1A	3964	1/1	0.97	0.08	46,46,46,46	0
57	MG	1V	206	1/1	0.97	0.08	53,53,53,53	0
57	MG	1A	3821	1/1	0.97	0.12	36,36,36,36	0
57	MG	2a	3159	1/1	0.97	0.08	60,60,60,60	0
57	MG	1x	102	1/1	0.97	0.04	38,38,38,38	0
57	MG	1A	3055	1/1	0.97	0.12	43,43,43,43	0
57	MG	1A	3150	1/1	0.97	0.06	40,40,40,40	0
57	MG	2A	3003	1/1	0.97	0.06	52,52,52,52	0
57	MG	2a	3166	1/1	0.97	0.05	69,69,69,69	0
57	MG	1X	101	1/1	0.97	0.10	33,33,33,33	0
57	MG	2A	3006	1/1	0.97	0.07	48,48,48,48	0
57	MG	2a	3169	1/1	0.97	0.05	51,51,51,51	0
57	MG	1A	3335	1/1	0.97	0.06	23,23,23,23	0
57	MG	1A	3263	1/1	0.97	0.07	47,47,47,47	0
57	MG	2A	3012	1/1	0.97	0.21	58,58,58,58	0
57	MG	2A	3724	1/1	0.97	0.08	38,38,38,38	0
57	MG	2A	3013	1/1	0.97	0.06	23,23,23,23	0
57	MG	2a	3175	1/1	0.97	0.07	71,71,71,71	0
57	MG	1A	3971	1/1	0.97	0.05	26,26,26,26	0
57	MG	1a	1728	1/1	0.97	0.15	52,52,52,52	0
57	MG	1A	3499	1/1	0.97	0.06	39,39,39,39	0
57	MG	10	104	1/1	0.97	0.08	57,57,57,57	0
57	MG	1A	3021	1/1	0.97	0.06	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3705	1/1	0.97	0.08	55,55,55,55	0
57	MG	2A	3229	1/1	0.97	0.07	47,47,47,47	0
57	MG	2A	3471	1/1	0.97	0.07	61,61,61,61	0
57	MG	1A	3339	1/1	0.97	0.06	31,31,31,31	0
57	MG	2A	3231	1/1	0.97	0.07	54,54,54,54	0
57	MG	2A	3736	1/1	0.97	0.15	46,46,46,46	0
57	MG	1a	1735	1/1	0.97	0.06	56,56,56,56	0
57	MG	1A	3058	1/1	0.97	0.12	46,46,46,46	0
57	MG	1A	3503	1/1	0.97	0.06	44,44,44,44	0
57	MG	11	102	1/1	0.97	0.06	34,34,34,34	0
57	MG	2A	3030	1/1	0.97	0.05	18,18,18,18	0
57	MG	2A	3031	1/1	0.97	0.12	55,55,55,55	0
57	MG	11	103	1/1	0.97	0.08	43,43,43,43	0
57	MG	2A	3033	1/1	0.97	0.14	47,47,47,47	0
57	MG	1A	3084	1/1	0.97	0.33	38,38,38,38	0
57	MG	11	105	1/1	0.97	0.06	36,36,36,36	0
57	MG	13	101	1/1	0.97	0.11	31,31,31,31	0
57	MG	1A	3506	1/1	0.97	0.04	22,22,22,22	0
57	MG	2A	3245	1/1	0.97	0.06	51,51,51,51	0
57	MG	2A	3038	1/1	0.97	0.09	48,48,48,48	0
57	MG	13	103	1/1	0.97	0.06	40,40,40,40	0
57	MG	2A	3040	1/1	0.97	0.16	50,50,50,50	0
57	MG	2A	3249	1/1	0.97	0.21	59,59,59,59	0
57	MG	1A	3157	1/1	0.97	0.11	29,29,29,29	0
61	ZN	14	501	1/1	0.97	0.07	108,108,108,108	0
61	ZN	2Y	202	1/1	0.97	0.05	88,88,88,88	0
57	MG	15	103	1/1	0.97	0.13	30,30,30,30	0
57	MG	1A	3135	1/1	0.98	0.20	31,31,31,31	0
57	MG	2F	304	1/1	0.98	0.20	45,45,45,45	0
57	MG	1A	3555	1/1	0.98	0.07	41,41,41,41	0
57	MG	1A	3242	1/1	0.98	0.14	35,35,35,35	0
57	MG	1A	3080	1/1	0.98	0.09	26,26,26,26	0
57	MG	1A	3245	1/1	0.98	0.35	40,40,40,40	0
57	MG	1A	3654	1/1	0.98	0.10	38,38,38,38	0
57	MG	1B	213	1/1	0.98	0.04	36,36,36,36	0
57	MG	2A	3102	1/1	0.98	0.07	39,39,39,39	0
57	MG	1B	214	1/1	0.98	0.06	43,43,43,43	0
57	MG	1A	3137	1/1	0.98	0.07	45,45,45,45	0
57	MG	1A	3247	1/1	0.98	0.14	40,40,40,40	0
57	MG	1A	3889	1/1	0.98	0.04	33,33,33,33	0
57	MG	2A	3316	1/1	0.98	0.08	42,42,42,42	0
57	MG	1A	3138	1/1	0.98	0.20	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	3892	1/1	0.98	0.06	42,42,42,42	0
57	MG	1A	3658	1/1	0.98	0.04	34,34,34,34	0
57	MG	1B	221	1/1	0.98	0.06	35,35,35,35	0
57	MG	2A	3112	1/1	0.98	0.08	47,47,47,47	0
57	MG	1A	3107	1/1	0.98	0.14	35,35,35,35	0
57	MG	2A	3323	1/1	0.98	0.12	18,18,18,18	0
57	MG	1B	223	1/1	0.98	0.07	44,44,44,44	0
57	MG	1B	224	1/1	0.98	0.04	42,42,42,42	0
57	MG	1A	3188	1/1	0.98	0.07	41,41,41,41	0
57	MG	1A	3771	1/1	0.98	0.04	37,37,37,37	0
57	MG	1A	3049	1/1	0.98	0.28	44,44,44,44	0
57	MG	2W	203	1/1	0.98	0.05	54,54,54,54	0
57	MG	1a	1818	1/1	0.98	0.04	67,67,67,67	0
57	MG	1A	3142	1/1	0.98	0.05	28,28,28,28	0
57	MG	2A	3333	1/1	0.98	0.04	36,36,36,36	0
57	MG	2A	3565	1/1	0.98	0.06	47,47,47,47	0
57	MG	1a	1820	1/1	0.98	0.09	57,57,57,57	0
57	MG	2A	3567	1/1	0.98	0.07	56,56,56,56	0
57	MG	1A	3110	1/1	0.98	0.14	21,21,21,21	0
57	MG	1A	3568	1/1	0.98	0.16	38,38,38,38	0
57	MG	1A	3665	1/1	0.98	0.04	52,52,52,52	0
57	MG	1A	3778	1/1	0.98	0.05	26,26,26,26	0
57	MG	1D	305	1/1	0.98	0.06	39,39,39,39	0
57	MG	1A	3029	1/1	0.98	0.08	35,35,35,35	0
57	MG	1D	307	1/1	0.98	0.07	34,34,34,34	0
57	MG	2A	3130	1/1	0.98	0.12	46,46,46,46	0
57	MG	2A	3343	1/1	0.98	0.03	21,21,21,21	0
57	MG	1D	308	1/1	0.98	0.16	48,48,48,48	0
57	MG	1D	310	1/1	0.98	0.05	41,41,41,41	0
57	MG	1A	3037	1/1	0.98	0.10	45,45,45,45	0
57	MG	1A	3019	1/1	0.98	0.14	28,28,28,28	0
57	MG	1A	3195	1/1	0.98	0.12	33,33,33,33	0
57	MG	1A	3783	1/1	0.98	0.09	40,40,40,40	0
57	MG	2A	3583	1/1	0.98	0.06	54,54,54,54	0
57	MG	1A	3334	1/1	0.98	0.06	24,24,24,24	0
57	MG	2A	3351	1/1	0.98	0.10	49,49,49,49	0
57	MG	2A	3352	1/1	0.98	0.06	43,43,43,43	0
57	MG	1A	3671	1/1	0.98	0.04	43,43,43,43	0
57	MG	1a	1836	1/1	0.98	0.06	39,39,39,39	0
57	MG	2A	3589	1/1	0.98	0.04	47,47,47,47	0
57	MG	2A	3590	1/1	0.98	0.08	31,31,31,31	0
57	MG	1A	3149	1/1	0.98	0.16	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	3913	1/1	0.98	0.06	41,41,41,41	0
57	MG	2A	3142	1/1	0.98	0.08	39,39,39,39	0
57	MG	1A	3485	1/1	0.98	0.07	25,25,25,25	0
57	MG	1A	3261	1/1	0.98	0.20	36,36,36,36	0
57	MG	1A	3067	1/1	0.98	0.18	32,32,32,32	0
57	MG	1E	303	1/1	0.98	0.05	31,31,31,31	0
57	MG	1A	3917	1/1	0.98	0.05	51,51,51,51	0
57	MG	2A	3365	1/1	0.98	0.07	30,30,30,30	0
57	MG	2A	3148	1/1	0.98	0.08	36,36,36,36	0
57	MG	1A	3068	1/1	0.98	0.23	30,30,30,30	0
57	MG	2A	3602	1/1	0.98	0.04	46,46,46,46	0
57	MG	1A	3152	1/1	0.98	0.18	42,42,42,42	0
57	MG	1A	3411	1/1	0.98	0.03	35,35,35,35	0
57	MG	2A	3605	1/1	0.98	0.09	44,44,44,44	0
57	MG	1a	1847	1/1	0.98	0.07	59,59,59,59	0
57	MG	2A	3371	1/1	0.98	0.09	34,34,34,34	0
57	MG	1F	302	1/1	0.98	0.09	29,29,29,29	0
57	MG	2A	3610	1/1	0.98	0.07	67,67,67,67	0
57	MG	1F	303	1/1	0.98	0.14	25,25,25,25	0
57	MG	1F	304	1/1	0.98	0.10	35,35,35,35	0
57	MG	2A	3375	1/1	0.98	0.04	35,35,35,35	0
57	MG	2A	3376	1/1	0.98	0.04	36,36,36,36	0
57	MG	1A	3341	1/1	0.98	0.05	22,22,22,22	0
57	MG	1a	1853	1/1	0.98	0.04	58,58,58,58	0
57	MG	1F	306	1/1	0.98	0.09	35,35,35,35	0
57	MG	1F	307	1/1	0.98	0.12	27,27,27,27	0
57	MG	1A	3922	1/1	0.98	0.06	52,52,52,52	0
57	MG	1A	3153	1/1	0.98	0.26	36,36,36,36	0
57	MG	1F	310	1/1	0.98	0.06	31,31,31,31	0
57	MG	1A	3201	1/1	0.98	0.14	40,40,40,40	0
57	MG	1A	3119	1/1	0.98	0.07	29,29,29,29	0
57	MG	1a	1861	1/1	0.98	0.12	52,52,52,52	0
57	MG	2A	3166	1/1	0.98	0.13	49,49,49,49	0
57	MG	1A	3013	1/1	0.98	0.07	16,16,16,16	0
57	MG	1A	3496	1/1	0.98	0.07	53,53,53,53	0
57	MG	1A	3156	1/1	0.98	0.11	25,25,25,25	0
57	MG	1a	1682	1/1	0.98	0.13	42,42,42,42	0
57	MG	1A	3800	1/1	0.98	0.13	46,46,46,46	0
57	MG	1a	1684	1/1	0.98	0.10	44,44,44,44	0
57	MG	2a	3058	1/1	0.98	0.14	45,45,45,45	0
57	MG	1A	3009	1/1	0.98	0.06	30,30,30,30	0
57	MG	1A	3932	1/1	0.98	0.06	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3933	1/1	0.98	0.10	58,58,58,58	0
57	MG	2A	3398	1/1	0.98	0.04	32,32,32,32	0
57	MG	1A	3207	1/1	0.98	0.13	37,37,37,37	0
57	MG	1A	3015	1/1	0.98	0.05	37,37,37,37	0
57	MG	1A	3592	1/1	0.98	0.15	49,49,49,49	0
57	MG	1A	3210	1/1	0.98	0.23	32,32,32,32	0
57	MG	1A	3938	1/1	0.98	0.04	61,61,61,61	0
57	MG	2A	3182	1/1	0.98	0.06	45,45,45,45	0
57	MG	2A	3644	1/1	0.98	0.05	53,53,53,53	0
57	MG	1A	3351	1/1	0.98	0.05	51,51,51,51	0
57	MG	1A	3940	1/1	0.98	0.10	41,41,41,41	0
57	MG	1A	3279	1/1	0.98	0.03	23,23,23,23	0
57	MG	1A	3596	1/1	0.98	0.04	34,34,34,34	0
57	MG	2A	3187	1/1	0.98	0.14	56,56,56,56	0
57	MG	2A	3412	1/1	0.98	0.04	52,52,52,52	0
57	MG	1A	3696	1/1	0.98	0.12	43,43,43,43	0
57	MG	1P	201	1/1	0.98	0.20	31,31,31,31	0
57	MG	1A	3504	1/1	0.98	0.05	43,43,43,43	0
57	MG	1A	3159	1/1	0.98	0.06	32,32,32,32	0
57	MG	1A	3946	1/1	0.98	0.03	27,27,27,27	0
57	MG	1A	3812	1/1	0.98	0.09	45,45,45,45	0
57	MG	1Q	203	1/1	0.98	0.08	46,46,46,46	0
57	MG	2A	3660	1/1	0.98	0.06	43,43,43,43	0
57	MG	2A	3661	1/1	0.98	0.10	58,58,58,58	0
57	MG	1A	3212	1/1	0.98	0.20	28,28,28,28	0
57	MG	1A	3814	1/1	0.98	0.05	42,42,42,42	0
57	MG	1R	201	1/1	0.98	0.09	32,32,32,32	0
57	MG	1A	3950	1/1	0.98	0.07	35,35,35,35	0
57	MG	1A	3815	1/1	0.98	0.06	37,37,37,37	0
57	MG	1A	3282	1/1	0.98	0.21	41,41,41,41	0
57	MG	1A	3093	1/1	0.98	0.04	13,13,13,13	0
57	MG	1A	3059	1/1	0.98	0.08	37,37,37,37	0
57	MG	1A	3510	1/1	0.98	0.07	16,16,16,16	0
57	MG	1T	204	1/1	0.98	0.12	53,53,53,53	0
57	MG	2A	3205	1/1	0.98	0.06	46,46,46,46	0
57	MG	2A	3431	1/1	0.98	0.10	45,45,45,45	0
57	MG	2A	3432	1/1	0.98	0.05	35,35,35,35	0
57	MG	1A	3956	1/1	0.98	0.07	53,53,53,53	0
57	MG	2A	3004	1/1	0.98	0.06	38,38,38,38	0
57	MG	1A	3511	1/1	0.98	0.04	20,20,20,20	0
57	MG	2A	3679	1/1	0.98	0.05	55,55,55,55	0
57	MG	1A	3430	1/1	0.98	0.07	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3007	1/1	0.98	0.06	40,40,40,40	0
57	MG	1A	3959	1/1	0.98	0.06	41,41,41,41	0
57	MG	1A	3215	1/1	0.98	0.06	25,25,25,25	0
57	MG	2A	3011	1/1	0.98	0.05	36,36,36,36	0
57	MG	1A	3162	1/1	0.98	0.07	27,27,27,27	0
57	MG	1A	3433	1/1	0.98	0.04	26,26,26,26	0
57	MG	2a	3109	1/1	0.98	0.04	64,64,64,64	0
57	MG	1A	3163	1/1	0.98	0.11	40,40,40,40	0
57	MG	1a	1722	1/1	0.98	0.12	47,47,47,47	0
57	MG	2A	3218	1/1	0.98	0.17	47,47,47,47	0
57	MG	1V	201	1/1	0.98	0.15	25,25,25,25	0
57	MG	1V	202	1/1	0.98	0.17	26,26,26,26	0
57	MG	1V	203	1/1	0.98	0.06	42,42,42,42	0
57	MG	2A	3020	1/1	0.98	0.17	39,39,39,39	0
57	MG	1A	3826	1/1	0.98	0.06	25,25,25,25	0
57	MG	1A	3965	1/1	0.98	0.04	27,27,27,27	0
57	MG	1A	3218	1/1	0.98	0.12	28,28,28,28	0
57	MG	1V	207	1/1	0.98	0.04	52,52,52,52	0
57	MG	1A	3518	1/1	0.98	0.04	51,51,51,51	0
57	MG	2A	3026	1/1	0.98	0.06	42,42,42,42	0
57	MG	1A	3612	1/1	0.98	0.13	32,32,32,32	0
57	MG	2A	3029	1/1	0.98	0.03	29,29,29,29	0
57	MG	1a	1732	1/1	0.98	0.06	33,33,33,33	0
57	MG	1A	3363	1/1	0.98	0.04	13,13,13,13	0
57	MG	1A	3012	1/1	0.98	0.05	35,35,35,35	0
57	MG	1A	3291	1/1	0.98	0.07	16,16,16,16	0
57	MG	1Y	202	1/1	0.98	0.04	63,63,63,63	0
57	MG	1Z	301	1/1	0.98	0.11	60,60,60,60	0
57	MG	1A	3439	1/1	0.98	0.04	12,12,12,12	0
57	MG	2A	3238	1/1	0.98	0.20	44,44,44,44	0
57	MG	1A	3523	1/1	0.98	0.05	20,20,20,20	0
57	MG	1A	3061	1/1	0.98	0.04	36,36,36,36	0
57	MG	1a	1743	1/1	0.98	0.04	40,40,40,40	0
57	MG	1A	3525	1/1	0.98	0.06	42,42,42,42	0
57	MG	1A	3441	1/1	0.98	0.09	30,30,30,30	0
57	MG	1A	3840	1/1	0.98	0.04	41,41,41,41	0
57	MG	1A	3166	1/1	0.98	0.20	27,27,27,27	0
57	MG	2a	3140	1/1	0.98	0.08	51,51,51,51	0
57	MG	1A	3722	1/1	0.98	0.04	24,24,24,24	0
57	MG	2A	3475	1/1	0.98	0.04	53,53,53,53	0
57	MG	2a	3143	1/1	0.98	0.10	61,61,61,61	0
57	MG	1A	3843	1/1	0.98	0.04	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	1a	1750	1/1	0.98	0.05	49,49,49,49	0
57	MG	1A	3075	1/1	0.98	0.20	29,29,29,29	0
57	MG	1A	3724	1/1	0.98	0.10	31,31,31,31	0
57	MG	1A	3725	1/1	0.98	0.05	39,39,39,39	0
57	MG	1A	3295	1/1	0.98	0.07	31,31,31,31	0
57	MG	1A	3223	1/1	0.98	0.08	33,33,33,33	0
57	MG	1A	3986	1/1	0.98	0.07	38,38,38,38	0
57	MG	1A	3098	1/1	0.98	0.26	37,37,37,37	0
57	MG	2A	3485	1/1	0.98	0.09	48,48,48,48	0
57	MG	1A	3225	1/1	0.98	0.23	37,37,37,37	0
57	MG	15	102	1/1	0.98	0.15	27,27,27,27	0
57	MG	2A	3258	1/1	0.98	0.12	45,45,45,45	0
57	MG	2A	3489	1/1	0.98	0.06	28,28,28,28	0
57	MG	1A	3731	1/1	0.98	0.07	49,49,49,49	0
57	MG	1A	3732	1/1	0.98	0.05	20,20,20,20	0
57	MG	1a	1762	1/1	0.98	0.06	52,52,52,52	0
57	MG	1A	3300	1/1	0.98	0.11	30,30,30,30	0
57	MG	1A	3992	1/1	0.98	0.05	47,47,47,47	0
57	MG	2a	3163	1/1	0.98	0.05	64,64,64,64	0
57	MG	1A	3226	1/1	0.98	0.05	29,29,29,29	0
57	MG	2a	3165	1/1	0.98	0.05	60,60,60,60	0
57	MG	17	101	1/1	0.98	0.07	34,34,34,34	0
57	MG	1A	3169	1/1	0.98	0.08	43,43,43,43	0
57	MG	2A	3267	1/1	0.98	0.04	37,37,37,37	0
57	MG	17	103	1/1	0.98	0.12	38,38,38,38	0
57	MG	2A	3269	1/1	0.98	0.14	27,27,27,27	0
57	MG	1A	3736	1/1	0.98	0.10	37,37,37,37	0
57	MG	1A	3857	1/1	0.98	0.05	34,34,34,34	0
57	MG	1A	3631	1/1	0.98	0.07	33,33,33,33	0
57	MG	1A	3538	1/1	0.98	0.20	27,27,27,27	0
57	MG	1A	3860	1/1	0.98	0.11	41,41,41,41	0
57	MG	1A	4000	1/1	0.98	0.04	44,44,44,44	0
57	MG	1A	3633	1/1	0.98	0.08	45,45,45,45	0
57	MG	2a	3178	1/1	0.98	0.04	50,50,50,50	0
57	MG	2A	3277	1/1	0.98	0.04	29,29,29,29	0
57	MG	2A	3509	1/1	0.98	0.04	32,32,32,32	0
57	MG	1A	3634	1/1	0.98	0.05	37,37,37,37	0
57	MG	1A	3451	1/1	0.98	0.04	23,23,23,23	0
57	MG	1A	3100	1/1	0.98	0.04	46,46,46,46	0
57	MG	1A	3172	1/1	0.98	0.12	23,23,23,23	0
57	MG	2A	3076	1/1	0.98	0.09	46,46,46,46	0
57	MG	2a	3186	1/1	0.98	0.11	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3284	1/1	0.98	0.13	53,53,53,53	0
57	MG	1A	3076	1/1	0.98	0.10	29,29,29,29	0
57	MG	1A	4008	1/1	0.98	0.14	34,34,34,34	0
57	MG	1A	3175	1/1	0.98	0.13	28,28,28,28	0
57	MG	1A	3131	1/1	0.98	0.12	25,25,25,25	0
57	MG	1A	3457	1/1	0.98	0.05	43,43,43,43	0
57	MG	2D	301	1/1	0.98	0.13	38,38,38,38	0
57	MG	2A	3290	1/1	0.98	0.06	44,44,44,44	0
57	MG	1A	4012	1/1	0.98	0.17	42,42,42,42	0
57	MG	2A	3524	1/1	0.98	0.05	30,30,30,30	0
57	MG	1A	3458	1/1	0.98	0.06	51,51,51,51	0
58	CLM	1A	4017	20/20	0.98	0.06	18,23,33,39	0
57	MG	1A	3548	1/1	0.98	0.12	34,34,34,34	0
57	MG	1A	3178	1/1	0.98	0.13	29,29,29,29	0
57	MG	2A	3086	1/1	0.98	0.05	39,39,39,39	0
57	MG	1A	3017	1/1	0.98	0.13	31,31,31,31	0
57	MG	1A	3753	1/1	0.98	0.10	39,39,39,39	0
57	MG	1A	3079	1/1	0.98	0.06	41,41,41,41	0
57	MG	1A	3877	1/1	0.98	0.04	25,25,25,25	0
57	MG	1A	3314	1/1	0.98	0.04	16,16,16,16	0
57	MG	1A	3756	1/1	0.98	0.04	39,39,39,39	0
57	MG	1A	3134	1/1	0.98	0.14	26,26,26,26	0
61	ZN	15	108	1/1	0.98	0.04	43,43,43,43	0
57	MG	1a	1620	1/1	0.98	0.05	39,39,39,39	0
57	MG	2F	302	1/1	0.98	0.05	40,40,40,40	0
61	ZN	29	501	1/1	0.98	0.05	65,65,65,65	0
61	ZN	2n	501	1/1	0.98	0.05	86,86,86,86	0
62	SF4	1d	305	8/8	0.98	0.05	59,64,67,72	0
62	SF4	2d	501	8/8	0.98	0.04	63,75,82,85	0
57	MG	1A	3530	1/1	0.99	0.04	25,25,25,25	0
57	MG	1a	1741	1/1	0.99	0.04	36,36,36,36	0
57	MG	1A	3209	1/1	0.99	0.12	36,36,36,36	0
57	MG	1A	3146	1/1	0.99	0.06	29,29,29,29	0
57	MG	2A	3685	1/1	0.99	0.04	34,34,34,34	0
57	MG	1A	3469	1/1	0.99	0.06	42,42,42,42	0
57	MG	1A	3470	1/1	0.99	0.03	31,31,31,31	0
57	MG	1D	302	1/1	0.99	0.18	33,33,33,33	0
57	MG	1A	3177	1/1	0.99	0.09	30,30,30,30	0
57	MG	1D	304	1/1	0.99	0.09	38,38,38,38	0
57	MG	1A	3299	1/1	0.99	0.14	31,31,31,31	0
57	MG	1A	3118	1/1	0.99	0.04	19,19,19,19	0
57	MG	2A	3354	1/1	0.99	0.04	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3413	1/1	0.99	0.02	28,28,28,28	0
57	MG	1A	3891	1/1	0.99	0.03	40,40,40,40	0
57	MG	1D	309	1/1	0.99	0.04	16,16,16,16	0
57	MG	2A	3358	1/1	0.99	0.06	39,39,39,39	0
57	MG	2A	3468	1/1	0.99	0.05	32,32,32,32	0
57	MG	1A	3044	1/1	0.99	0.06	20,20,20,20	0
57	MG	1D	311	1/1	0.99	0.08	32,32,32,32	0
57	MG	1a	1850	1/1	0.99	0.07	51,51,51,51	0
57	MG	1A	3254	1/1	0.99	0.16	25,25,25,25	0
57	MG	1A	3541	1/1	0.99	0.03	28,28,28,28	0
57	MG	1A	3895	1/1	0.99	0.03	27,27,27,27	0
57	MG	1A	3018	1/1	0.99	0.07	27,27,27,27	0
57	MG	1A	3046	1/1	0.99	0.02	19,19,19,19	0
57	MG	1A	3006	1/1	0.99	0.02	21,21,21,21	0
57	MG	1A	3360	1/1	0.99	0.03	20,20,20,20	0
57	MG	1A	3749	1/1	0.99	0.05	23,23,23,23	0
57	MG	1A	3078	1/1	0.99	0.24	32,32,32,32	0
57	MG	1A	3048	1/1	0.99	0.09	41,41,41,41	0
57	MG	1E	301	1/1	0.99	0.09	25,25,25,25	0
57	MG	1A	3099	1/1	0.99	0.18	28,28,28,28	0
57	MG	1A	3309	1/1	0.99	0.07	19,19,19,19	0
57	MG	1A	3905	1/1	0.99	0.04	49,49,49,49	0
57	MG	1E	305	1/1	0.99	0.10	39,39,39,39	0
57	MG	1A	3310	1/1	0.99	0.06	35,35,35,35	0
57	MG	1A	3023	1/1	0.99	0.18	32,32,32,32	0
57	MG	1A	3187	1/1	0.99	0.10	27,27,27,27	0
57	MG	1F	301	1/1	0.99	0.15	23,23,23,23	0
57	MG	1A	3686	1/1	0.99	0.03	33,33,33,33	0
57	MG	1A	3313	1/1	0.99	0.13	34,34,34,34	0
57	MG	2A	3176	1/1	0.99	0.09	42,42,42,42	0
57	MG	1A	3832	1/1	0.99	0.07	49,49,49,49	0
57	MG	1A	3024	1/1	0.99	0.06	15,15,15,15	0
57	MG	1A	3760	1/1	0.99	0.07	33,33,33,33	0
57	MG	2A	3608	1/1	0.99	0.06	34,34,34,34	0
57	MG	1A	3689	1/1	0.99	0.03	37,37,37,37	0
57	MG	1A	3102	1/1	0.99	0.09	29,29,29,29	0
57	MG	2A	3283	1/1	0.99	0.06	37,37,37,37	0
57	MG	1A	3103	1/1	0.99	0.20	26,26,26,26	0
57	MG	1A	3838	1/1	0.99	0.05	33,33,33,33	0
57	MG	2A	3614	1/1	0.99	0.04	50,50,50,50	0
57	MG	1A	3623	1/1	0.99	0.07	29,29,29,29	0
57	MG	1A	3266	1/1	0.99	0.14	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	2A	3394	1/1	0.99	0.08	39,39,39,39	0
57	MG	1A	3318	1/1	0.99	0.04	36,36,36,36	0
57	MG	1A	4001	1/1	0.99	0.06	40,40,40,40	0
57	MG	1A	3267	1/1	0.99	0.17	30,30,30,30	0
57	MG	1A	3375	1/1	0.99	0.05	27,27,27,27	0
57	MG	2A	3399	1/1	0.99	0.04	36,36,36,36	0
57	MG	1A	3561	1/1	0.99	0.09	33,33,33,33	0
57	MG	1A	3051	1/1	0.99	0.13	30,30,30,30	0
57	MG	1A	3925	1/1	0.99	0.06	49,49,49,49	0
57	MG	1A	3083	1/1	0.99	0.19	34,34,34,34	0
57	MG	1A	3772	1/1	0.99	0.03	41,41,41,41	0
57	MG	2A	3628	1/1	0.99	0.03	21,21,21,21	0
57	MG	2A	3515	1/1	0.99	0.07	46,46,46,46	0
57	MG	1A	3052	1/1	0.99	0.14	30,30,30,30	0
57	MG	1A	3271	1/1	0.99	0.07	34,34,34,34	0
57	MG	2A	3407	1/1	0.99	0.06	49,49,49,49	0
57	MG	1A	3324	1/1	0.99	0.07	22,22,22,22	0
57	MG	1A	3025	1/1	0.99	0.14	33,33,33,33	0
57	MG	1A	3026	1/1	0.99	0.12	30,30,30,30	0
57	MG	1A	3109	1/1	0.99	0.14	31,31,31,31	0
57	MG	1A	3003	1/1	0.99	0.05	21,21,21,21	0
57	MG	1A	3276	1/1	0.99	0.20	40,40,40,40	0
57	MG	1A	3386	1/1	0.99	0.03	32,32,32,32	0
57	MG	1A	3277	1/1	0.99	0.03	27,27,27,27	0
57	MG	1P	203	1/1	0.99	0.17	23,23,23,23	0
57	MG	1A	3111	1/1	0.99	0.06	34,34,34,34	0
57	MG	1A	3233	1/1	0.99	0.03	32,32,32,32	0
57	MG	2A	3009	1/1	0.99	0.03	34,34,34,34	0
57	MG	1Q	201	1/1	0.99	0.03	36,36,36,36	0
57	MG	2A	3109	1/1	0.99	0.05	33,33,33,33	0
57	MG	1A	3234	1/1	0.99	0.05	33,33,33,33	0
57	MG	1A	3042	1/1	0.99	0.07	17,17,17,17	0
57	MG	1A	3236	1/1	0.99	0.20	27,27,27,27	0
57	MG	1A	3237	1/1	0.99	0.13	28,28,28,28	0
57	MG	2A	3015	1/1	0.99	0.14	33,33,33,33	0
57	MG	1A	3580	1/1	0.99	0.08	26,26,26,26	0
57	MG	1R	202	1/1	0.99	0.09	34,34,34,34	0
57	MG	2A	3655	1/1	0.99	0.08	35,35,35,35	0
57	MG	1A	3057	1/1	0.99	0.07	19,19,19,19	0
57	MG	1A	3338	1/1	0.99	0.09	37,37,37,37	0
57	MG	1A	3043	1/1	0.99	0.05	24,24,24,24	0
57	MG	1A	3091	1/1	0.99	0.04	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	3203	1/1	0.99	0.19	42,42,42,42	0
57	MG	2A	3325	1/1	0.99	0.04	40,40,40,40	0
57	MG	2E	307	1/1	0.99	0.08	33,33,33,33	0
57	MG	1A	3171	1/1	0.99	0.16	35,35,35,35	0
57	MG	1A	3243	1/1	0.99	0.15	28,28,28,28	0
57	MG	2A	3124	1/1	0.99	0.07	42,42,42,42	0
57	MG	2A	3329	1/1	0.99	0.18	47,47,47,47	0
57	MG	1A	3290	1/1	0.99	0.10	20,20,20,20	0
57	MG	1A	3143	1/1	0.99	0.03	22,22,22,22	0
57	MG	1A	3874	1/1	0.99	0.06	31,31,31,31	0
57	MG	2A	3028	1/1	0.99	0.03	27,27,27,27	0
57	MG	1A	3173	1/1	0.99	0.12	23,23,23,23	0
57	MG	1A	3116	1/1	0.99	0.11	31,31,31,31	0
57	MG	1A	3405	1/1	0.99	0.04	24,24,24,24	0
57	MG	1A	3527	1/1	0.99	0.21	20,20,20,20	0
57	MG	1U	205	1/1	0.99	0.12	26,26,26,26	0
61	ZN	16	501	1/1	0.99	0.05	39,39,39,39	0
61	ZN	19	104	1/1	0.99	0.04	40,40,40,40	0
61	ZN	1n	104	1/1	0.99	0.03	63,63,63,63	0
57	MG	2A	3675	1/1	0.99	0.06	50,50,50,50	0
57	MG	1a	1736	1/1	0.99	0.07	39,39,39,39	0
61	ZN	25	104	1/1	0.99	0.05	56,56,56,56	0
61	ZN	26	501	1/1	0.99	0.04	57,57,57,57	0
57	MG	1A	3730	1/1	0.99	0.07	24,24,24,24	0
57	MG	1A	3092	1/1	0.99	0.08	28,28,28,28	0
57	MG	1A	3248	1/1	0.99	0.09	28,28,28,28	0
57	MG	2A	3680	1/1	0.99	0.03	35,35,35,35	0
57	MG	1A	3140	1/1	1.00	0.07	23,23,23,23	0
57	MG	2A	3654	1/1	1.00	0.05	37,37,37,37	0
61	ZN	1Y	203	1/1	1.00	0.03	56,56,56,56	0
57	MG	1A	3476	1/1	1.00	0.06	41,41,41,41	0

6.5 Other polymers (i)

There are no such residues in this entry.