wwPDB X-ray Structure Validation Summary Report (i)

Aug 4, 2026 – 09:21 PM EDT

PDB ID	:	7U2I / pdb_00007u2i
Title	:	Crystal structure of the Thermus thermophilus 70S ribosome in complex with mRNA, aminoacylated A-site Gly-NH-tRNAgly, aminoacylated P-site fMet-NH-tRNAmet, deacylated E-site tRNAgly, and chloramphenicol at 2.55A resolution
Authors	:	Syroegin, E.A.; Aleksandrova, E.V.; Polikanov, Y.S.
Deposited on	:	2022-02-24
Resolution	:	2.55 Å(reported)

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

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

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

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

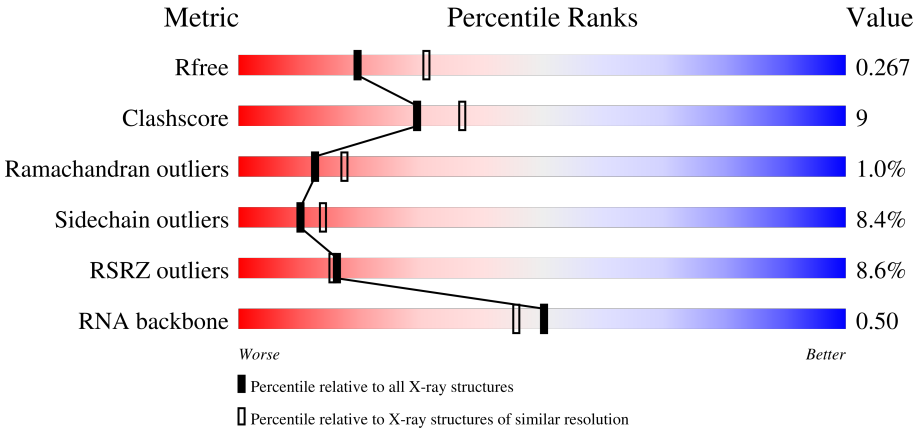
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.55 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	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)
RNA backbone	3983	1112 (2.80-2.28)

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

Mol	Chain	Length	Quality of chain
1	1A	2915	4% 67% 25% 6%
1	2A	2915	4% 60% 29% 7%
2	1B	121	79% 19%
2	2B	121	55% 32% 12%

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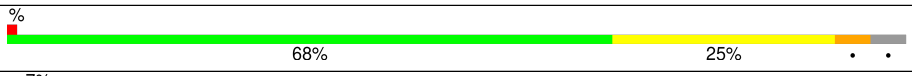
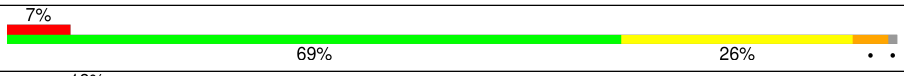
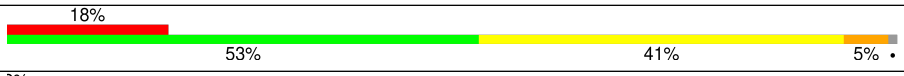
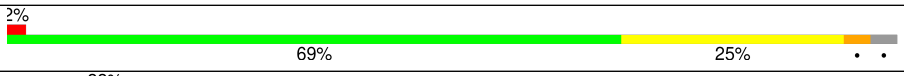
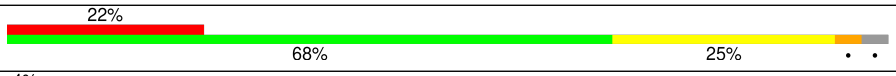
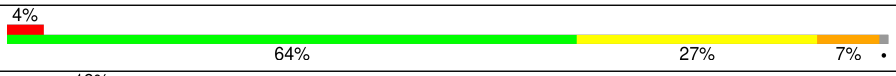
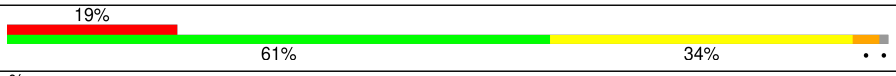
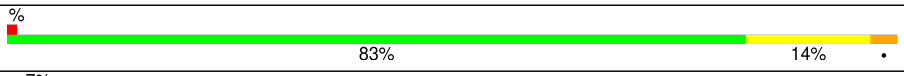
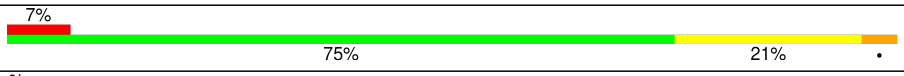
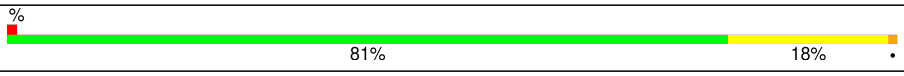
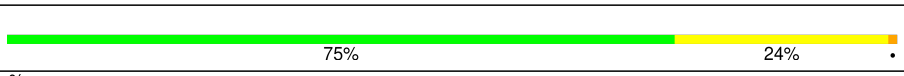
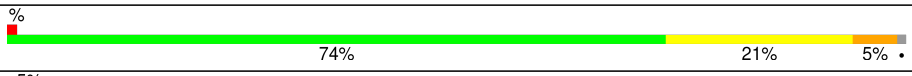
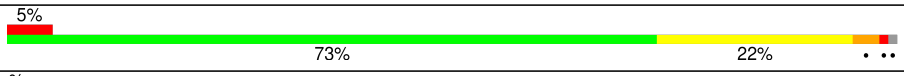
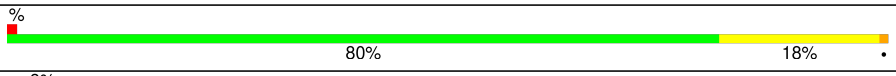
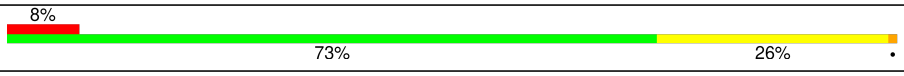
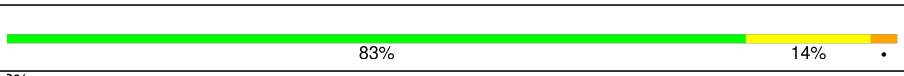
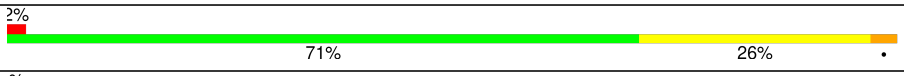
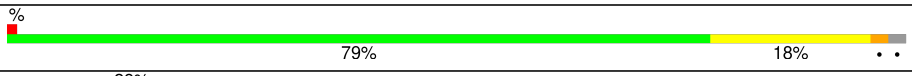
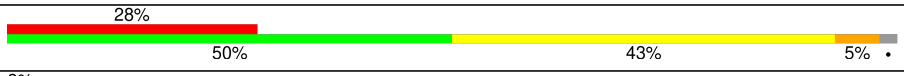
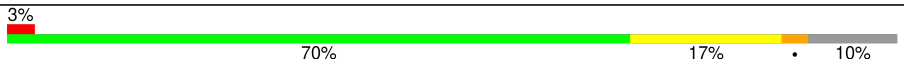
Mol	Chain	Length	Quality of chain
3	1D	276	
3	2D	276	
4	1E	206	
4	2E	206	
5	1F	210	
5	2F	210	
6	1G	182	
6	2G	182	
7	1H	180	
7	2H	180	
8	1I	148	
8	2I	148	
9	1N	140	
9	2N	140	
10	1O	122	
10	2O	122	
11	1P	150	
11	2P	150	
12	1Q	141	
12	2Q	141	
13	1R	118	
13	2R	118	
14	1S	112	
14	2S	112	
15	1T	146	

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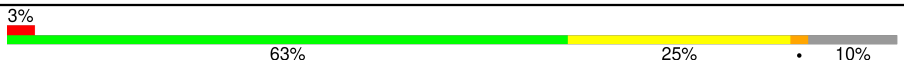
Mol	Chain	Length	Quality of chain
15	2T	146	
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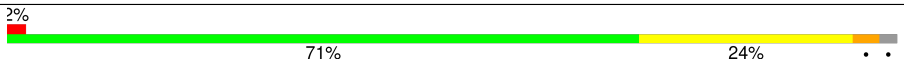
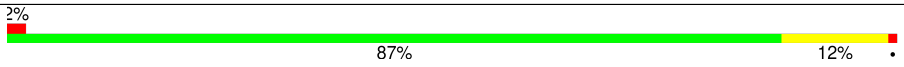
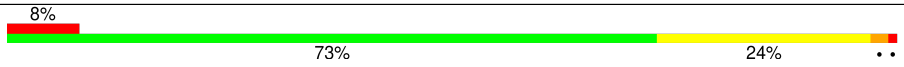
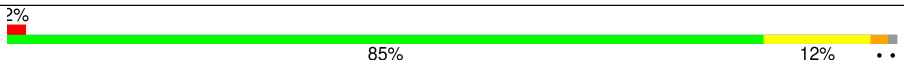
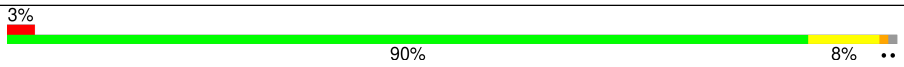
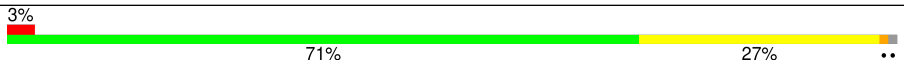
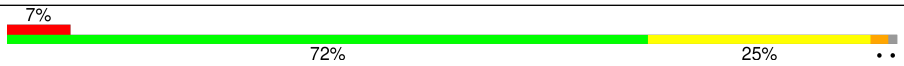
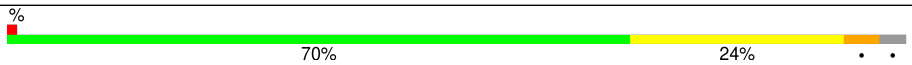
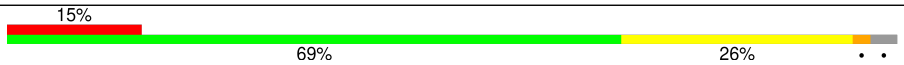
16	2U	118	
17	1V	101	
17	2V	101	
18	1W	113	
18	2W	113	
19	1X	96	
19	2X	96	
20	1Y	110	
20	2Y	110	
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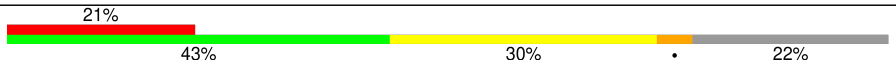
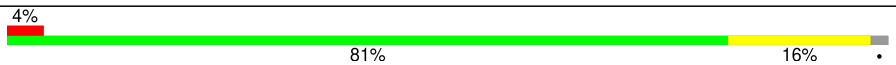
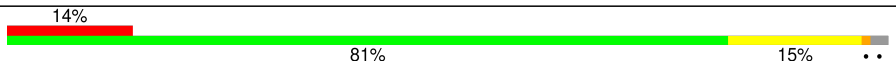
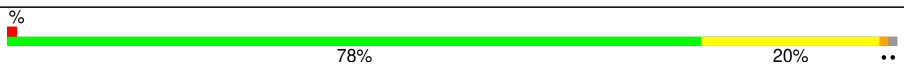
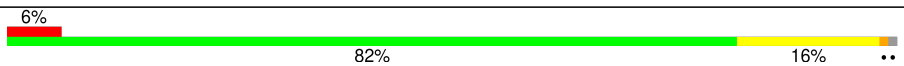
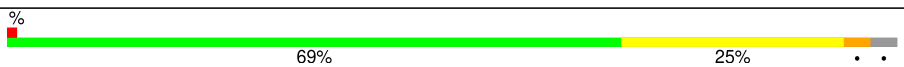
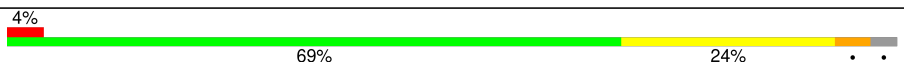
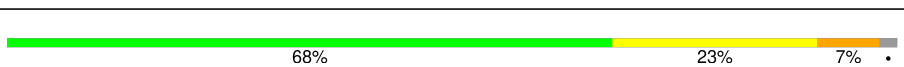
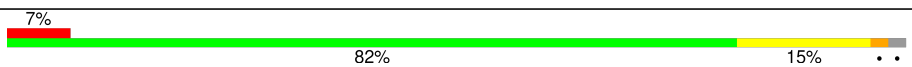
21	2Z	206	
22	10	85	
22	20	85	
23	11	98	
23	21	98	
24	12	72	
24	22	72	
25	13	60	
25	23	60	
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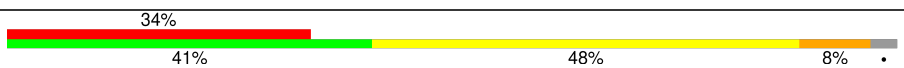
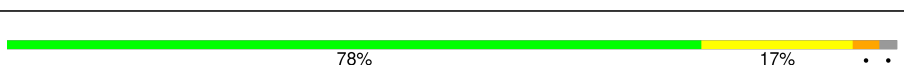
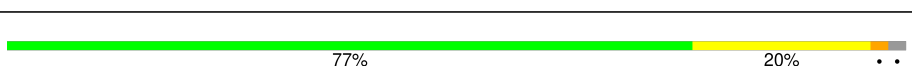
26	24	71	
27	15	60	
27	25	60	

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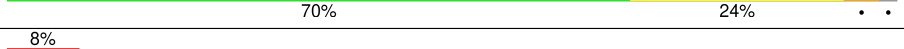
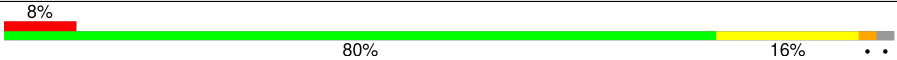
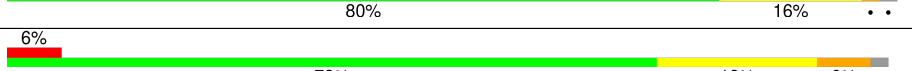
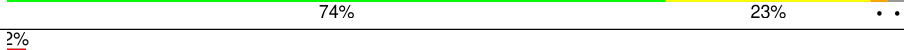
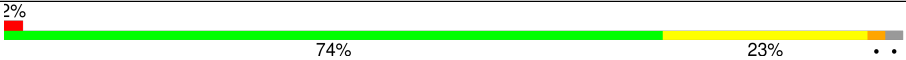
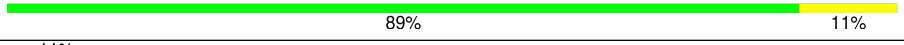
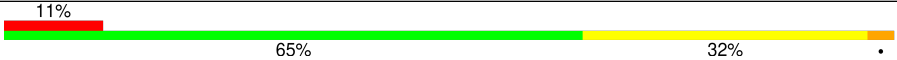
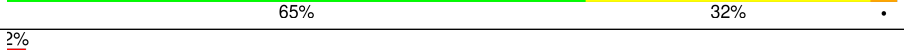
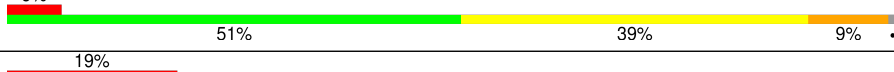
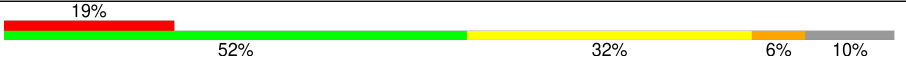
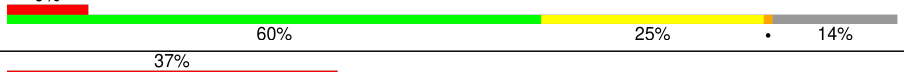
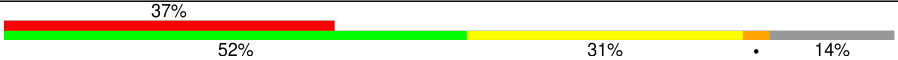
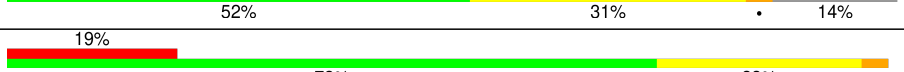
28	26	54	
29	17	49	
29	27	49	
30	18	65	
30	28	65	
31	19	37	
31	29	37	
32	1a	1521	
32	2a	1521	
33	1b	256	
33	2b	256	
34	1c	239	
34	2c	239	
35	1d	209	
35	2d	209	
36	1e	162	
36	2e	162	
37	1f	101	
37	2f	101	
38	1g	156	
38	2g	156	
39	1h	138	
39	2h	138	
40	1i	128	

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Mol	Chain	Length	Quality of chain
40	2i	128	60% 55% 37% 7%
41	1j	105	31% 56% 30% 6% 8%
41	2j	105	50% 47% 37% 8% 9%
42	1k	129	5% 67% 17% 12%
42	2k	129	12% 62% 23% 12%
43	1l	132	5% 79% 14% 8%
43	2l	132	21% 64% 26% 8%
44	1m	126	10% 60% 31% 6%
44	2m	126	26% 52% 41%
45	1n	61	11% 74% 23%
45	2n	61	61% 54% 39% 5%
46	1o	89	7% 67% 27%
46	2o	89	9% 65% 30%
47	1p	88	18% 57% 35% 7%
47	2p	88	8% 59% 31% 7%
48	1q	105	15% 74% 18% 6%
48	2q	105	7% 70% 23% 6%
49	1r	88	% 57% 18% 23%
49	2r	88	7% 48% 28% 23%
50	1s	93	12% 61% 24% 11%
50	2s	93	58% 42% 40% 8% 11%
51	1t	106	16% 62% 24% 5% 9%
51	2t	106	6% 67% 20% 9%
52	1u	27	15% 52% 33% 15%
52	2u	27	41% 44% 41% 15%

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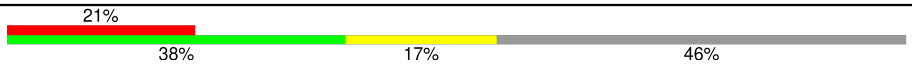
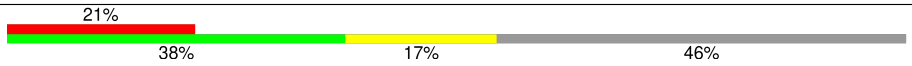
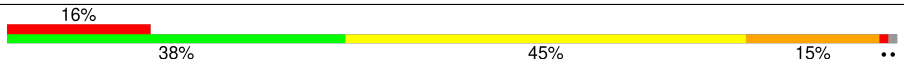
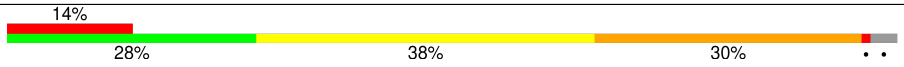
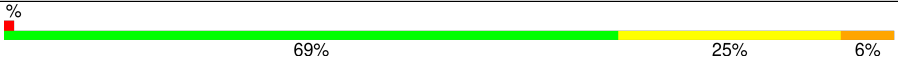
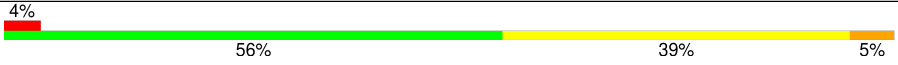
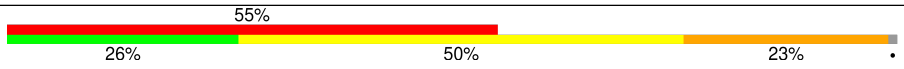
Mol	Chain	Length	Quality of chain
53	1v	24	
53	2v	24	
54	1w	74	
54	2w	74	
55	1x	77	
55	2x	77	
56	1y	74	
56	2y	74	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
54	4SU	2w	8	-	-	X	-
57	MG	1U	210	-	-	-	X
57	MG	1a	1636	-	-	-	X
57	MG	1a	1722	-	-	-	X
57	MG	2A	3218	-	-	-	X
57	MG	2A	3325	-	-	-	X
57	MG	2A	3424	-	-	-	X
57	MG	2v	103	-	-	-	X

2 Entry composition (i)

There are 62 unique types of molecules in this entry. The entry contains 300046 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	2871	Total	C	N	O	P	0	0	0
			61852	27531	11572	19878	2871			
1	2A	2800	Total	C	N	O	P	0	0	0
			60322	26848	11284	19390	2800			

- 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
			2577	1146	476	835	120			
2	2B	120	Total	C	N	O	P	0	0	0
			2575	1146	476	833	120			

- 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
			2136	1349	423	361	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	202	Total	C	N	O	S	0	0	0
			1583	1009	297	275	2			
5	2F	202	Total	C	N	O	S	0	0	0
			1579	1007	296	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
			1423	913	253	253	4			
6	2G	181	Total	C	N	O	S	0	0	0
			1428	913	258	253	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	174	Total	C	N	O	S	0	0	0
			1330	845	248	236	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	1I	146	Total	C	N	O	S	0	0	0
			1097	701	191	204	1			
8	2I	146	Total	C	N	O	S	0	0	0
			1064	681	186	196	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
			1117	719	207	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
			873	550	174	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
			771	495	140	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
			806	517	152	131	6			
20	2Y	107	Total	C	N	O	S	0	0	0
			806	517	152	131	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	1Z	154	Total	C	N	O	S	0	0	0
			1240	795	222	220	3			
21	2Z	160	Total	C	N	O	S	0	0	0
			1271	814	228	227	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
			653	404	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
			755	475	148	131	1			
23	21	97	Total	C	N	O	S	0	0	0
			755	475	148	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
			588	365	118	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
			552	349	99	99	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	24	69	Total	C	N	O	S	0	0	0
			532	339	97	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
			455	285	89	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	1503	Total	C	N	O	P	0	0	0
			32327	14396	5990	10438	1503			

- 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
			1846	1179	331	331	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
			1548	973	301	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
			1655	1038	326	284	7			
35	2d	208	Total	C	N	O	S	0	0	0
			1674	1050	333	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
			1129	714	213	198	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
			810	514	144	149	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
			1231	766	243	216	6			
38	2g	155	Total	C	N	O	S	0	0	0
			1235	769	244	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
			1088	689	206	191	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
			983	623	193	167			
40	2i	127	Total	C	N	O	0	0	0
			978	619	190	169			

- 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
			709	440	138	131			
41	2j	96	Total	C	N	O	0	0	0
			714	445	138	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
			829	516	155	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	123	Total	C	N	O	S	0	0	0
			958	592	198	166	2			
44	2m	122	Total	C	N	O	S	0	0	0
			950	586	197	165	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
			652	417	120	113	2			
50	2s	83	Total	C	N	O	S	0	0	0
			646	412	119	113	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
			728	446	156	124	2			
51	2t	96	Total	C	N	O	S	0	0	0
			727	446	155	124	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 RNA chain called MG-mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	1v	13	Total	C	N	O	P	0	0	0
			286	128	59	86	13			
53	2v	13	Total	C	N	O	P	0	0	0
			286	128	59	86	13			

- Molecule 54 is a RNA chain called A-site Aminoacyl-tRNA Gly-NH-tRNAgly.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
54	1w	73	Total	C	N	O	P	S	0	0	0
			1556	695	275	512	73	1			
54	2w	72	Total	C	N	O	P	S	0	0	0
			1536	686	273	504	72	1			

- Molecule 55 is a RNA chain called P-site Aminoacyl-tRNA fMet-NH-tRNAmet.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
55	1x	77	Total	C	N	O	P	S	0	0	0
			1656	740	299	538	77	2			
55	2x	77	Total	C	N	O	P	S	0	0	0
			1656	740	299	538	77	2			

- Molecule 56 is a RNA chain called E-site Deacylated tRNAgly.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
56	1y	73	Total	C	N	O	P	S	0	0	0
			1552	693	273	512	73	1			
56	2y	73	Total	C	N	O	P	S	0	0	0
			1552	693	273	512	73	1			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	1A	1095	Total	Mg	0	0
			1095	1095		
57	1B	36	Total	Mg	0	0
			36	36		
57	1D	13	Total	Mg	0	0
			13	13		
57	1E	12	Total	Mg	0	0
			12	12		
57	1F	15	Total	Mg	0	0
			15	15		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	1G	4	Total Mg 4 4	0	0
57	1I	1	Total Mg 1 1	0	0
57	1N	5	Total Mg 5 5	0	0
57	1O	5	Total Mg 5 5	0	0
57	1P	5	Total Mg 5 5	0	0
57	1Q	7	Total Mg 7 7	0	0
57	1R	7	Total Mg 7 7	0	0
57	1S	3	Total Mg 3 3	0	0
57	1T	3	Total Mg 3 3	0	0
57	1U	10	Total Mg 10 10	0	0
57	1V	7	Total Mg 7 7	0	0
57	1W	7	Total Mg 7 7	0	0
57	1X	7	Total Mg 7 7	0	0
57	1Y	3	Total Mg 3 3	0	0
57	1Z	3	Total Mg 3 3	0	0
57	10	9	Total Mg 9 9	0	0
57	11	3	Total Mg 3 3	0	0
57	12	2	Total Mg 2 2	0	0
57	13	5	Total Mg 5 5	0	0
57	15	6	Total Mg 6 6	0	0
57	16	2	Total Mg 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	17	5	Total Mg 5 5	0	0
57	18	6	Total Mg 6 6	0	0
57	19	1	Total Mg 1 1	0	0
57	1a	226	Total Mg 226 226	0	0
57	1b	2	Total Mg 2 2	0	0
57	1e	2	Total Mg 2 2	0	0
57	1f	2	Total Mg 2 2	0	0
57	1h	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	2	Total Mg 2 2	0	0
57	1s	1	Total Mg 1 1	0	0
57	1t	1	Total Mg 1 1	0	0
57	1v	1	Total Mg 1 1	0	0
57	1w	7	Total Mg 7 7	0	0
57	1x	12	Total Mg 12 12	0	0
57	2A	861	Total Mg 861 861	0	0
57	2B	20	Total Mg 20 20	0	0
57	2D	5	Total Mg 5 5	0	0
57	2E	8	Total Mg 8 8	0	0
57	2F	7	Total Mg 7 7	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	2G	1	Total Mg 1 1	0	0
57	2N	1	Total Mg 1 1	0	0
57	2O	1	Total Mg 1 1	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	2	Total Mg 2 2	0	0
57	2V	3	Total Mg 3 3	0	0
57	2W	2	Total Mg 2 2	0	0
57	2X	1	Total Mg 1 1	0	0
57	2Y	1	Total Mg 1 1	0	0
57	2Z	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	4	Total Mg 4 4	0	0
57	25	5	Total Mg 5 5	0	0
57	26	1	Total Mg 1 1	0	0
57	27	3	Total Mg 3 3	0	0
57	28	2	Total Mg 2 2	0	0
57	2a	225	Total Mg 225 225	0	0

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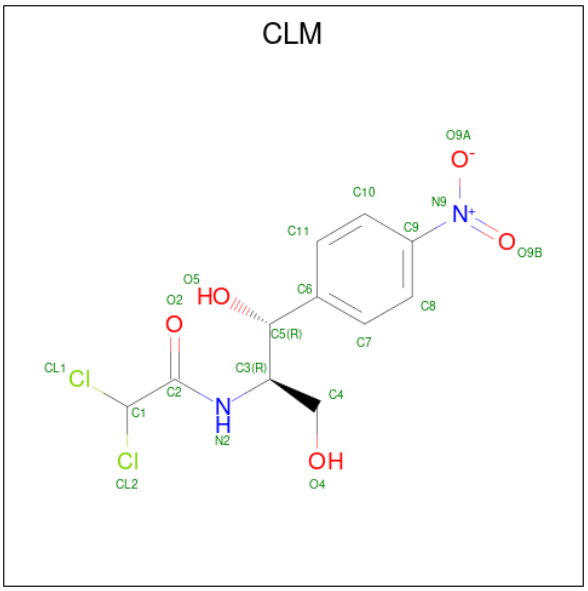
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	2d	2	Total Mg 2 2	0	0
57	2e	1	Total Mg 1 1	0	0
57	2f	2	Total Mg 2 2	0	0
57	2i	1	Total Mg 1 1	0	0
57	2j	1	Total Mg 1 1	0	0
57	2k	1	Total Mg 1 1	0	0
57	2l	3	Total Mg 3 3	0	0
57	2q	2	Total Mg 2 2	0	0
57	2r	1	Total Mg 1 1	0	0
57	2t	1	Total Mg 1 1	0	0
57	2v	4	Total Mg 4 4	0	0
57	2w	4	Total Mg 4 4	0	0
57	2x	4	Total Mg 4 4	0	0
57	2y	1	Total Mg 1 1	0	0

- Molecule 58 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	1A	1	Total K 1 1	0	0
58	2A	1	Total K 1 1	0	0

- Molecule 59 is CHLORAMPHENICOL (CCD ID: CLM) (formula: $C_{11}H_{12}Cl_2N_2O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
59	1A	1	Total	C	Cl	N	O	0	0
			20	11	2	2	5		
59	2A	1	Total	C	Cl	N	O	0	0
			20	11	2	2	5		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1Y	1	Total	Zn	0	0
			1	1		
60	14	1	Total	Zn	0	0
			1	1		
60	15	1	Total	Zn	0	0
			1	1		
60	16	1	Total	Zn	0	0
			1	1		
60	19	1	Total	Zn	0	0
			1	1		
60	1n	1	Total	Zn	0	0
			1	1		
60	2Y	1	Total	Zn	0	0
			1	1		
60	24	1	Total	Zn	0	0
			1	1		
60	25	1	Total	Zn	0	0
			1	1		
60	26	1	Total	Zn	0	0
			1	1		

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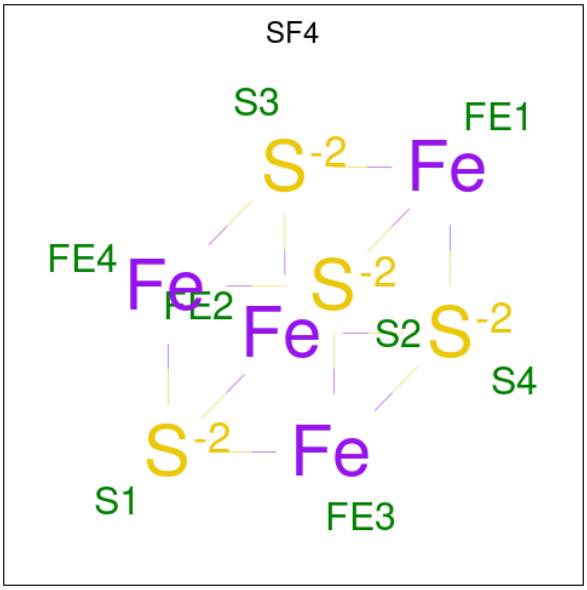
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	29	1	Total Zn 1 1	0	0
60	2n	1	Total Zn 1 1	0	0

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



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

- Molecule 62 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
62	1A	2086	Total O 2086 2086	0	0
62	1B	65	Total O 65 65	0	0
62	1D	28	Total O 28 28	0	0
62	1E	28	Total O 28 28	0	0
62	1F	17	Total O 17 17	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
62	1G	7	Total O 7 7	0	0
62	1H	2	Total O 2 2	0	0
62	1N	5	Total O 5 5	0	0
62	1O	6	Total O 6 6	0	0
62	1P	21	Total O 21 21	0	0
62	1Q	7	Total O 7 7	0	0
62	1R	7	Total O 7 7	0	0
62	1S	3	Total O 3 3	0	0
62	1T	9	Total O 9 9	0	0
62	1U	13	Total O 13 13	0	0
62	1V	9	Total O 9 9	0	0
62	1W	5	Total O 5 5	0	0
62	1X	6	Total O 6 6	0	0
62	1Y	3	Total O 3 3	0	0
62	1Z	1	Total O 1 1	0	0
62	10	12	Total O 12 12	0	0
62	11	10	Total O 10 10	0	0
62	12	3	Total O 3 3	0	0
62	13	6	Total O 6 6	0	0
62	14	1	Total O 1 1	0	0
62	15	6	Total O 6 6	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
62	16	5	Total O 5 5	0	0
62	17	9	Total O 9 9	0	0
62	18	10	Total O 10 10	0	0
62	1a	331	Total O 331 331	0	0
62	1b	1	Total O 1 1	0	0
62	1d	1	Total O 1 1	0	0
62	1e	1	Total O 1 1	0	0
62	1l	3	Total O 3 3	0	0
62	1m	2	Total O 2 2	0	0
62	1q	3	Total O 3 3	0	0
62	1u	1	Total O 1 1	0	0
62	1v	6	Total O 6 6	0	0
62	1w	9	Total O 9 9	0	0
62	1x	11	Total O 11 11	0	0
62	1y	1	Total O 1 1	0	0
62	2A	1147	Total O 1147 1147	0	0
62	2B	21	Total O 21 21	0	0
62	2D	18	Total O 18 18	0	0
62	2E	14	Total O 14 14	0	0
62	2F	12	Total O 12 12	0	0
62	2I	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
62	2N	2	Total O 2 2	0	0
62	2O	2	Total O 2 2	0	0
62	2P	10	Total O 10 10	0	0
62	2Q	1	Total O 1 1	0	0
62	2R	5	Total O 5 5	0	0
62	2T	3	Total O 3 3	0	0
62	2U	3	Total O 3 3	0	0
62	2W	4	Total O 4 4	0	0
62	2X	5	Total O 5 5	0	0
62	2Z	2	Total O 2 2	0	0
62	20	1	Total O 1 1	0	0
62	21	8	Total O 8 8	0	0
62	23	2	Total O 2 2	0	0
62	25	3	Total O 3 3	0	0
62	27	5	Total O 5 5	0	0
62	28	3	Total O 3 3	0	0
62	29	1	Total O 1 1	0	0
62	2a	205	Total O 205 205	0	0
62	2c	1	Total O 1 1	0	0
62	2i	1	Total O 1 1	0	0
62	2j	3	Total O 3 3	0	0

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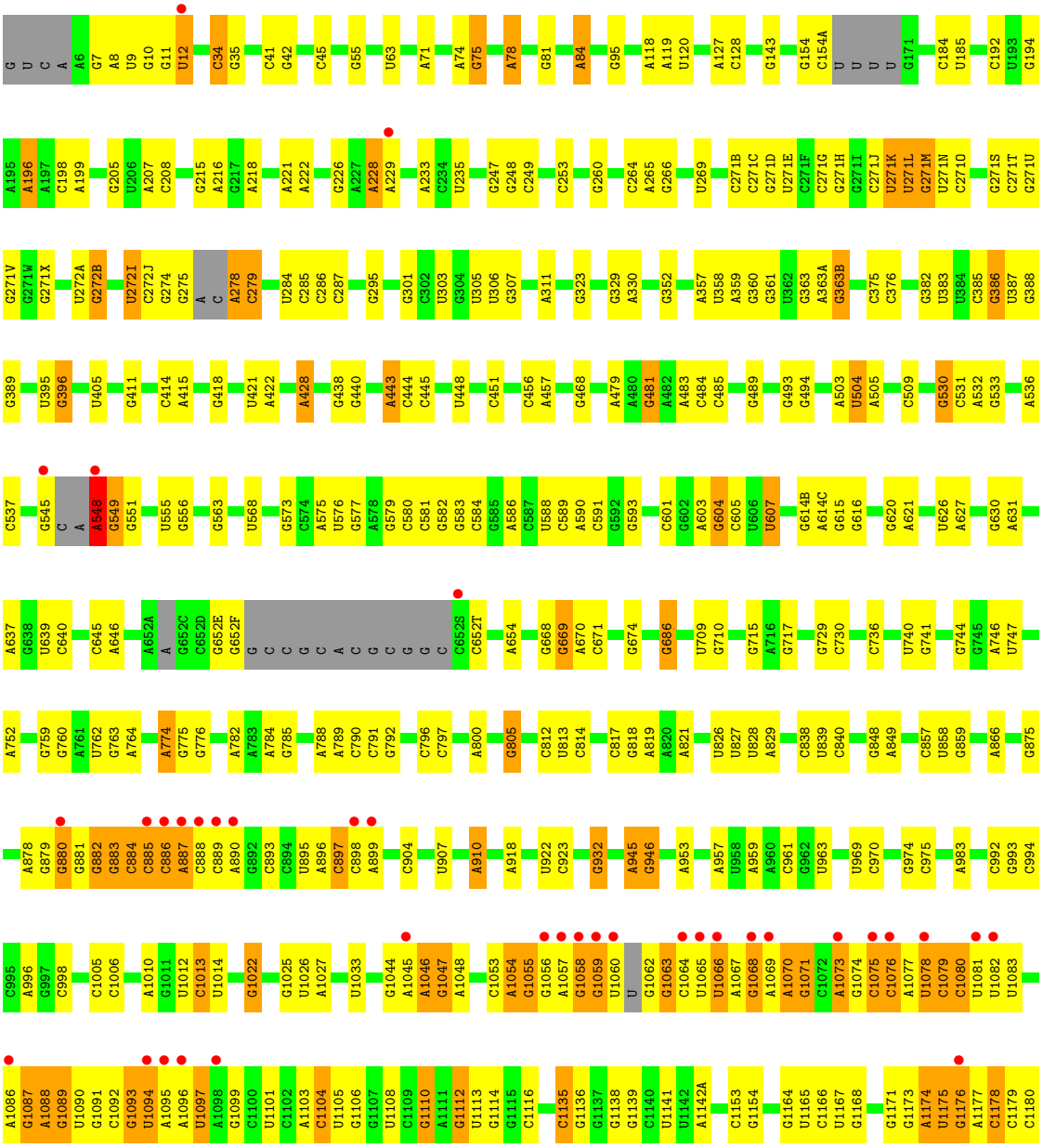
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
62	2l	4	Total O 4 4	0	0
62	2r	1	Total O 1 1	0	0
62	2t	2	Total O 2 2	0	0
62	2v	2	Total O 2 2	0	0
62	2w	1	Total O 1 1	0	0
62	2x	7	Total O 7 7	0	0

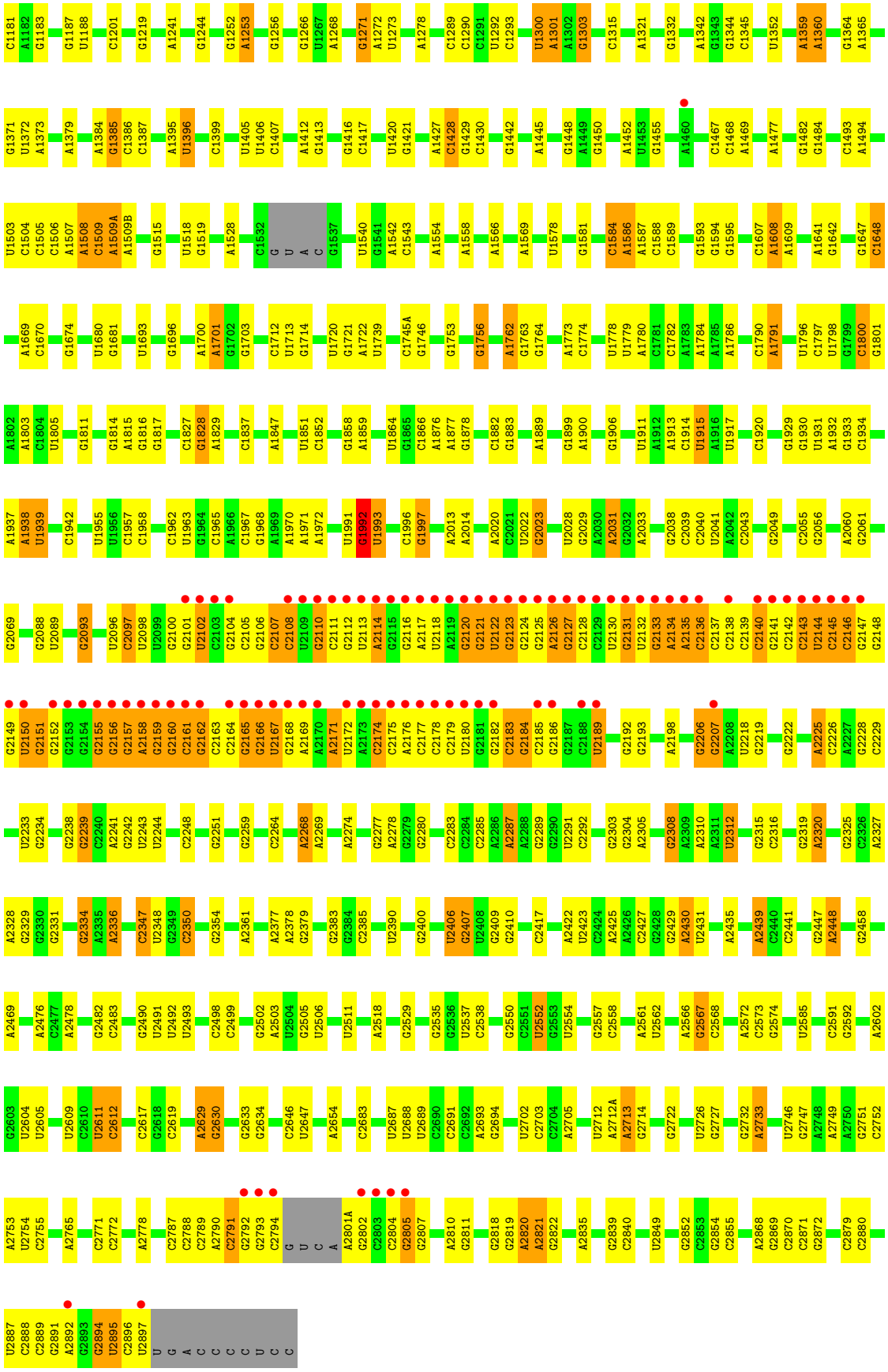
3 Residue-property plots (i)

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

- Molecule 1: 23S Ribosomal RNA

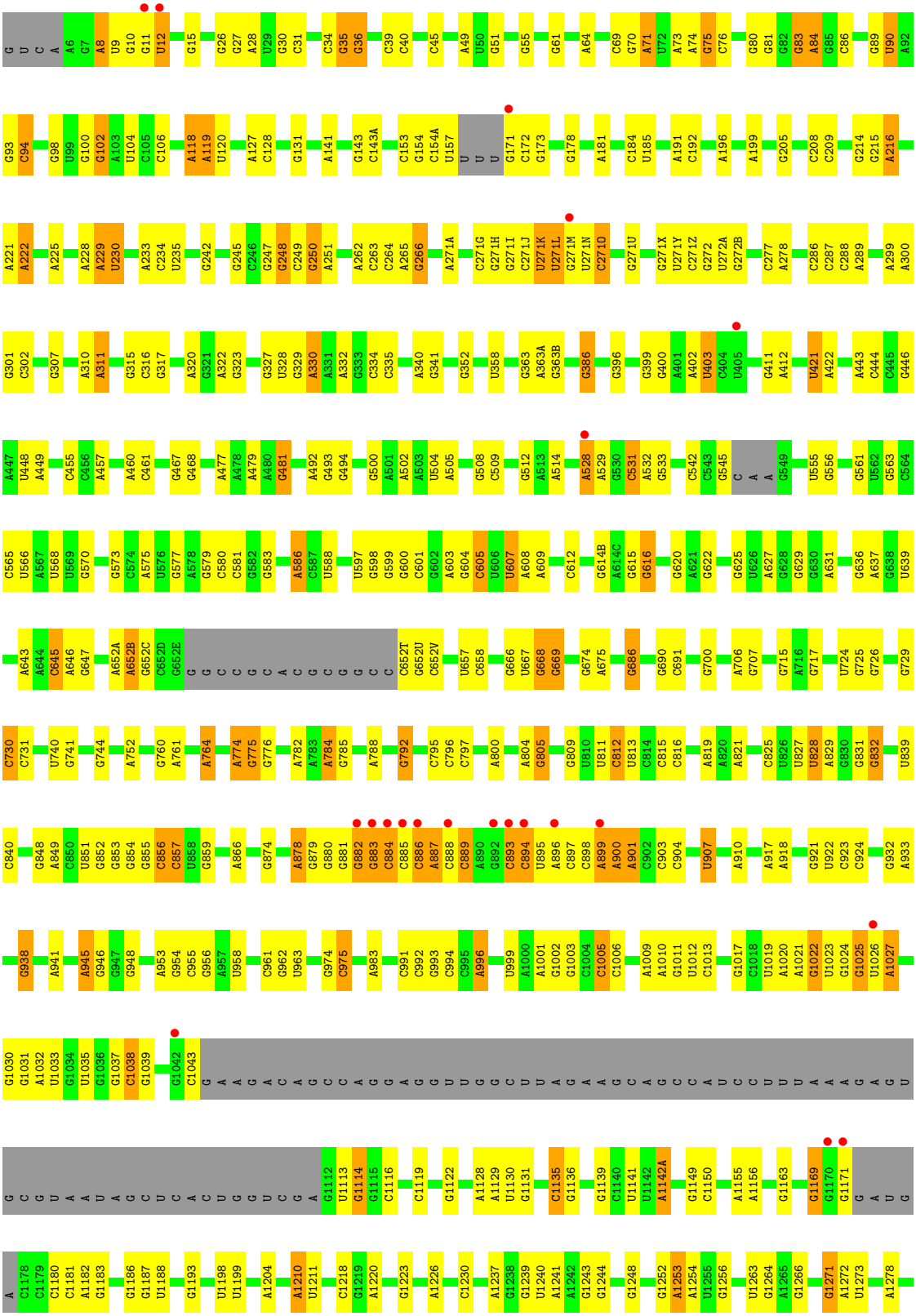
Chain 1A:

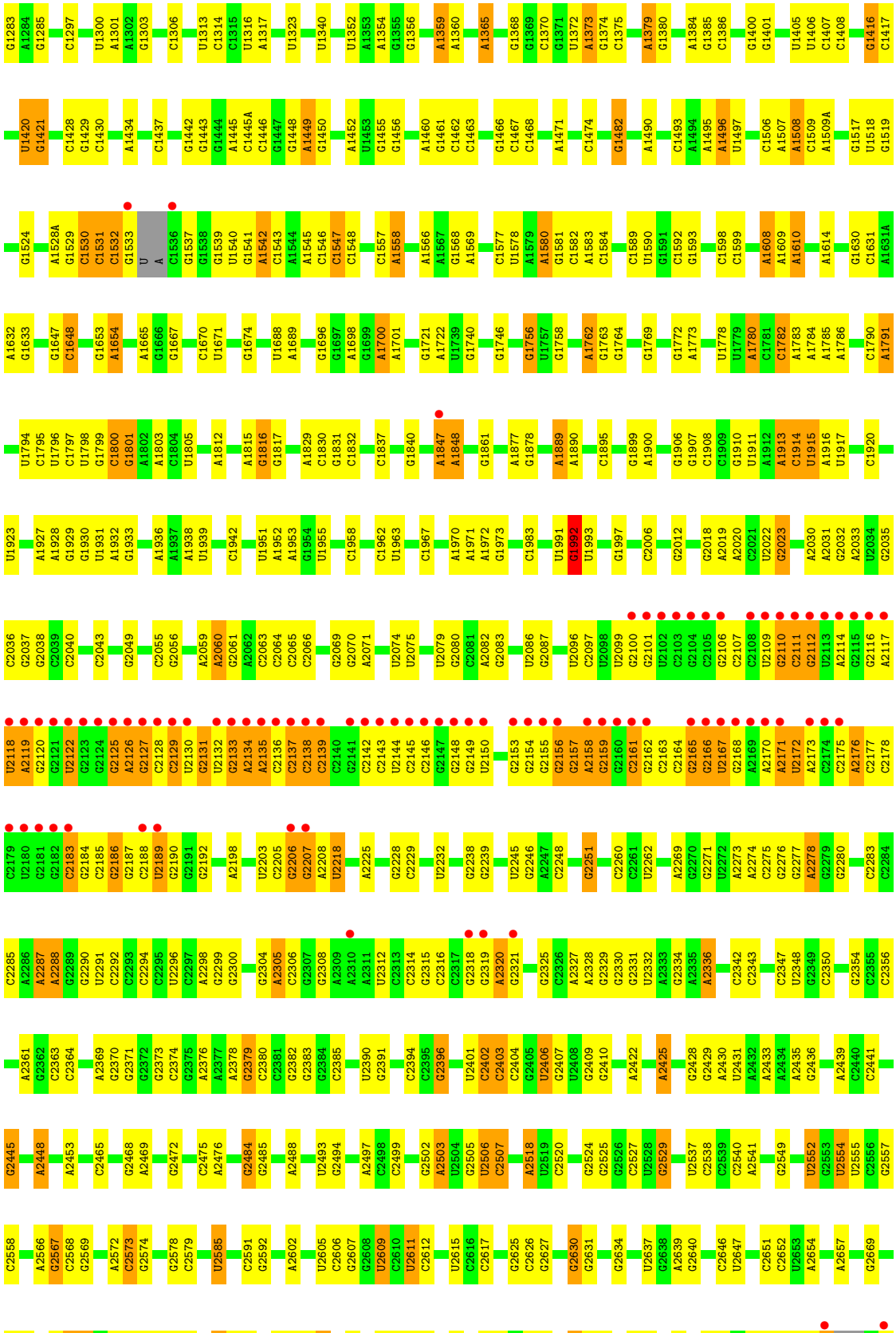


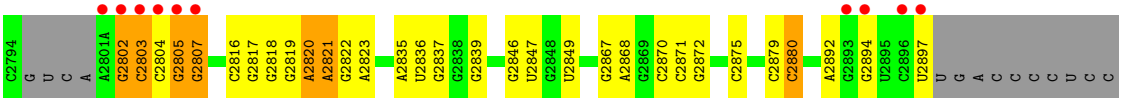


• Molecule 1: 23S Ribosomal RNA

Chain 2A:

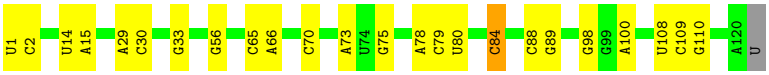






• Molecule 2: 5S Ribosomal RNA

Chain 1B:

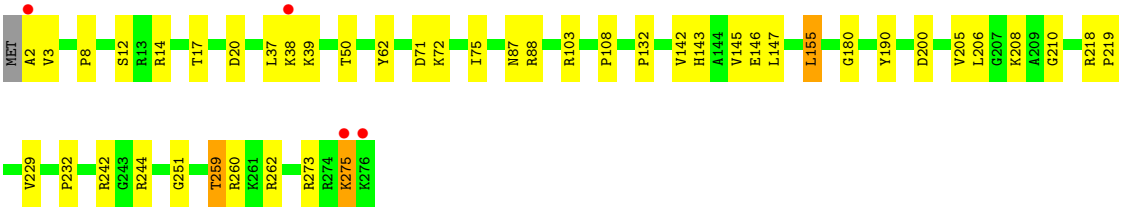


• Molecule 2: 5S Ribosomal RNA

Chain 2B:

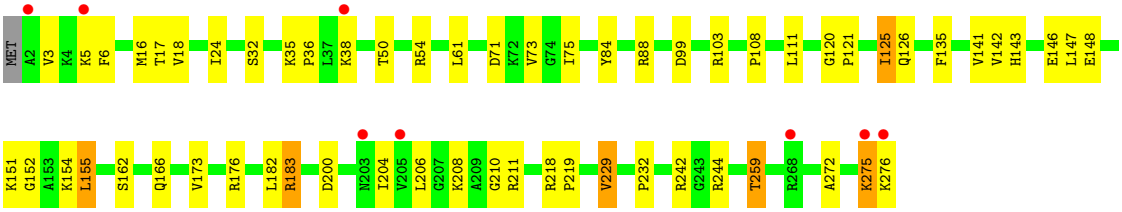
• Molecule 3: 50S ribosomal protein L2

Chain 1D:



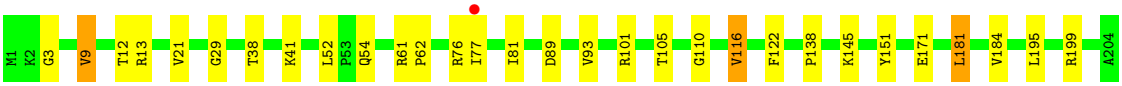
• Molecule 3: 50S ribosomal protein L2

Chain 2D:



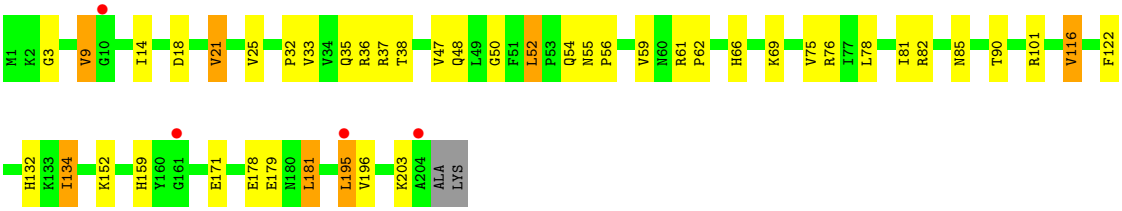
• Molecule 4: 50S ribosomal protein L3

Chain 1E:



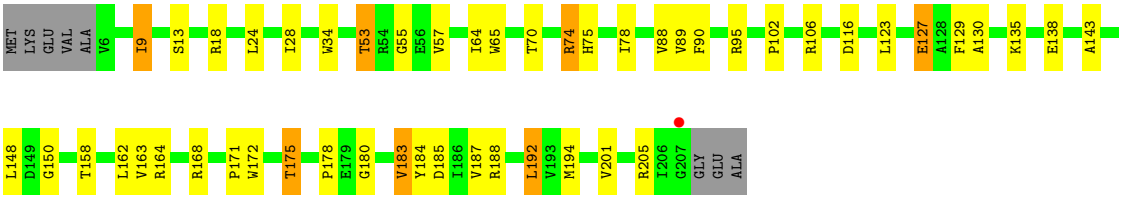
• Molecule 4: 50S ribosomal protein L3

Chain 2E:



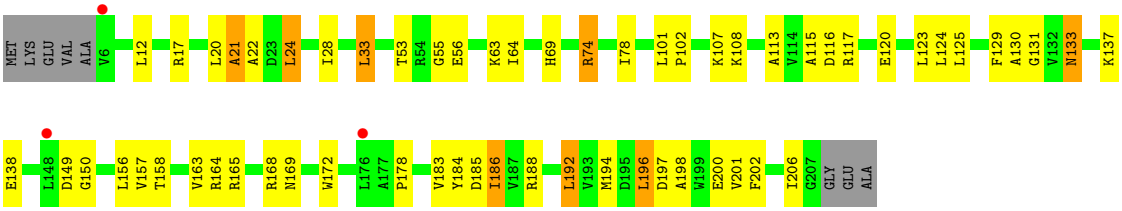
• Molecule 5: 50S ribosomal protein L4

Chain 1F:



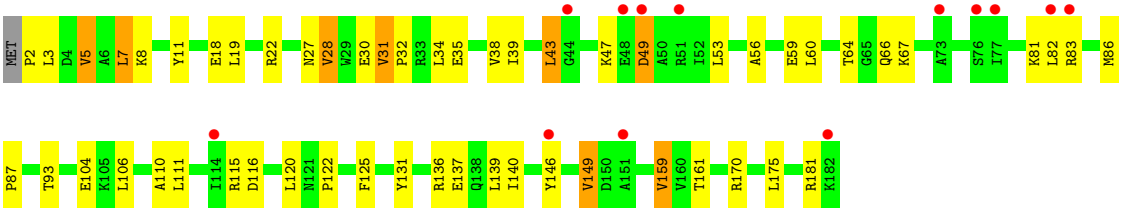
• Molecule 5: 50S ribosomal protein L4

Chain 2F:



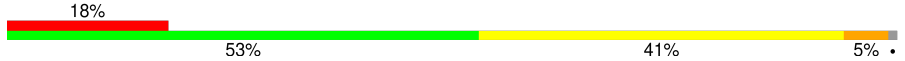
• Molecule 6: 50S ribosomal protein L5

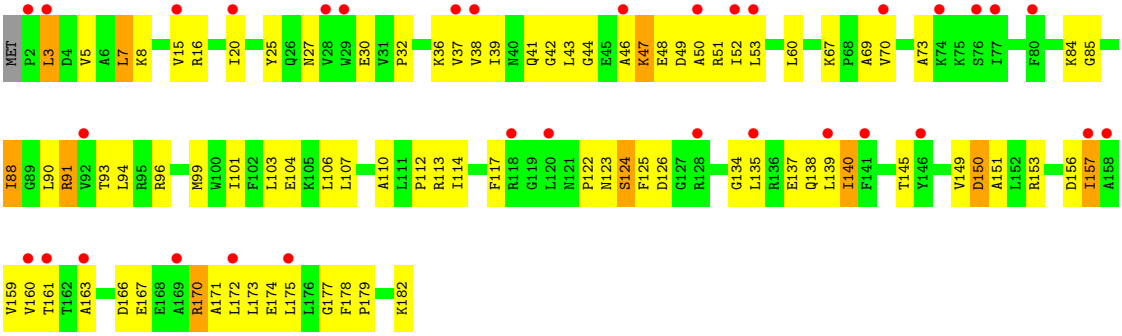
Chain 1G:



• Molecule 6: 50S ribosomal protein L5

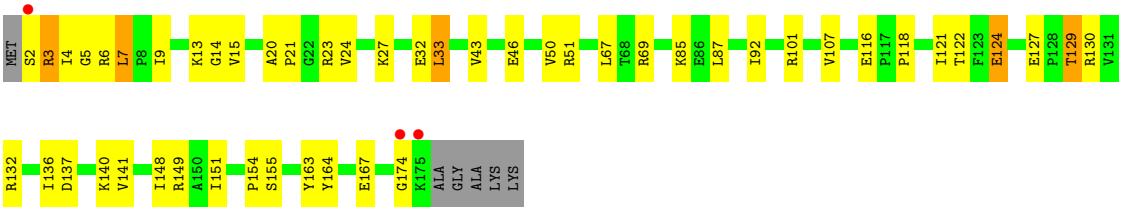
Chain 2G:





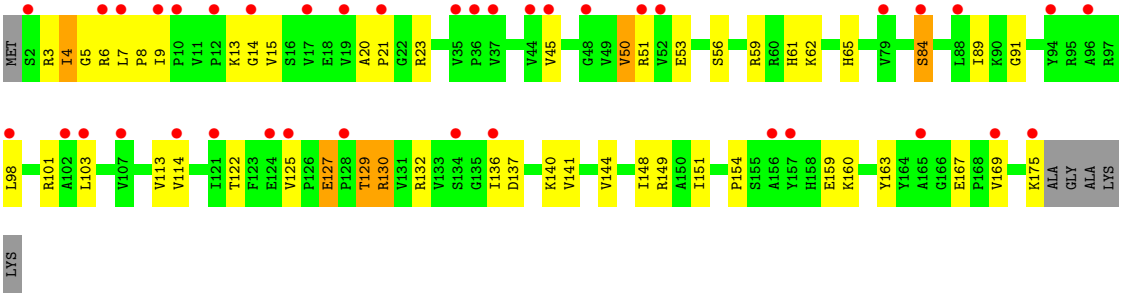
• Molecule 7: 50S ribosomal protein L6

Chain 1H:



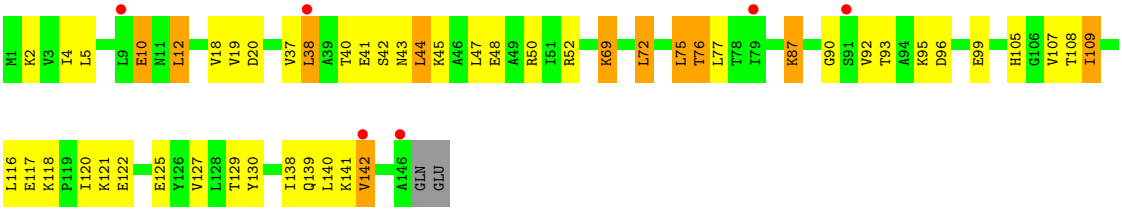
• Molecule 7: 50S ribosomal protein L6

Chain 2H:



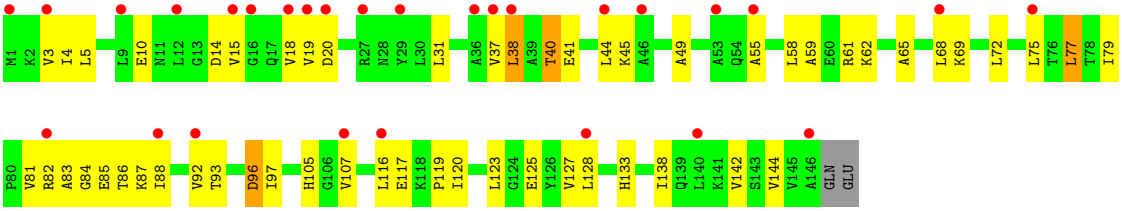
• Molecule 8: 50S ribosomal protein L9

Chain 1I:



• Molecule 8: 50S ribosomal protein L9

Chain 2I:

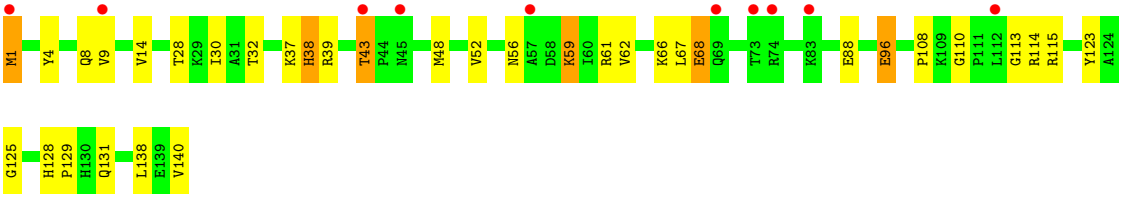


• Molecule 9: 50S ribosomal protein L13

Chain 1N:

• Molecule 9: 50S ribosomal protein L13

Chain 2N:



• Molecule 10: 50S ribosomal protein L14

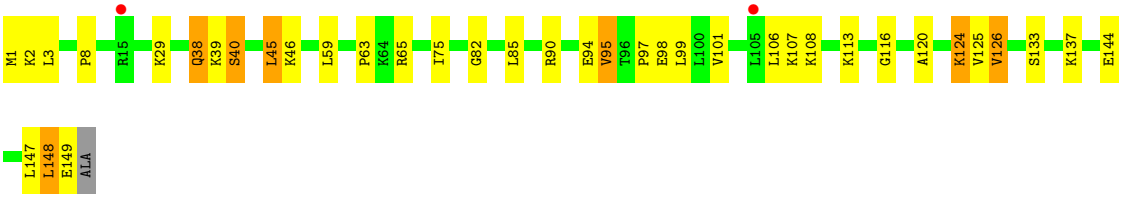
Chain 1O:

• Molecule 10: 50S ribosomal protein L14

Chain 2O:

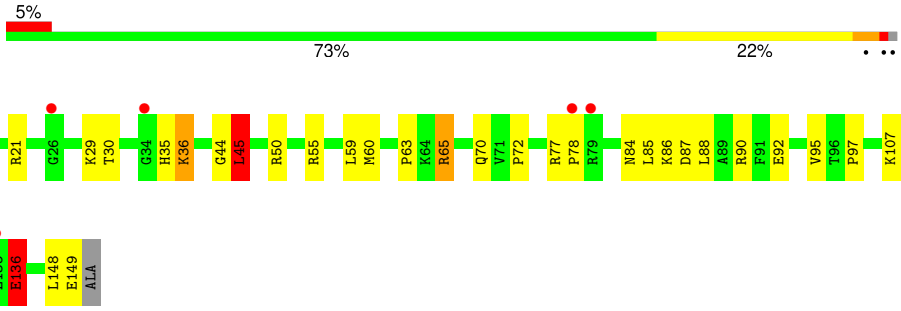
• Molecule 11: 50S ribosomal protein L15

Chain 1P:



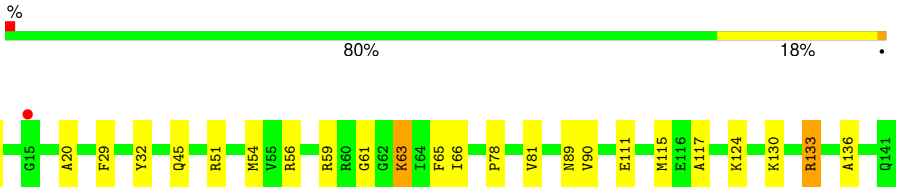
• Molecule 11: 50S ribosomal protein L15

Chain 2P:



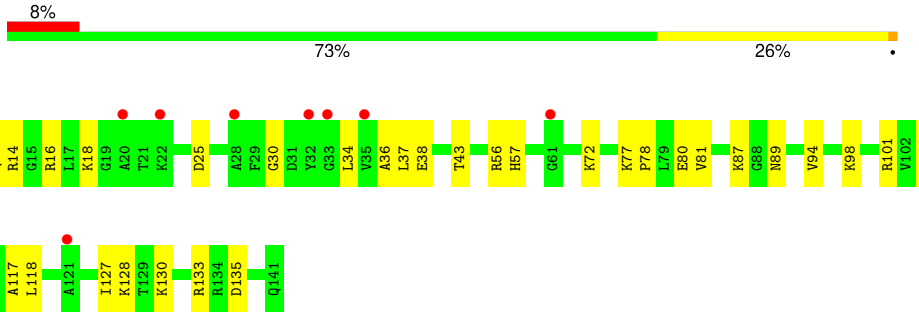
• Molecule 12: 50S ribosomal protein L16

Chain 1Q:



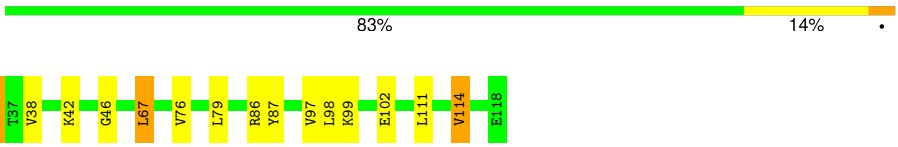
• Molecule 12: 50S ribosomal protein L16

Chain 2Q:



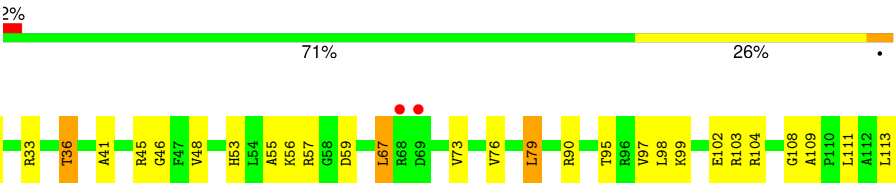
• Molecule 13: 50S ribosomal protein L17

Chain 1R:



• Molecule 13: 50S ribosomal protein L17

Chain 2R:

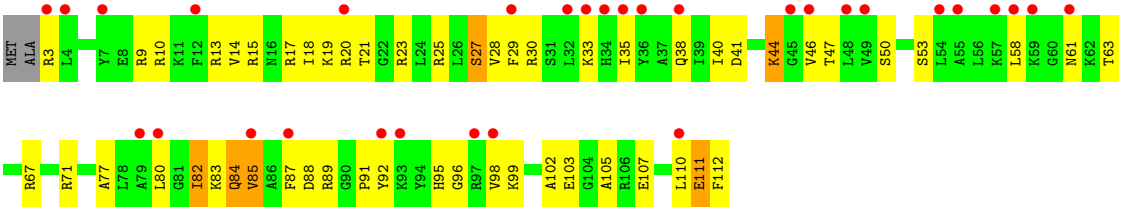


• Molecule 14: 50S ribosomal protein L18

Chain 1S:

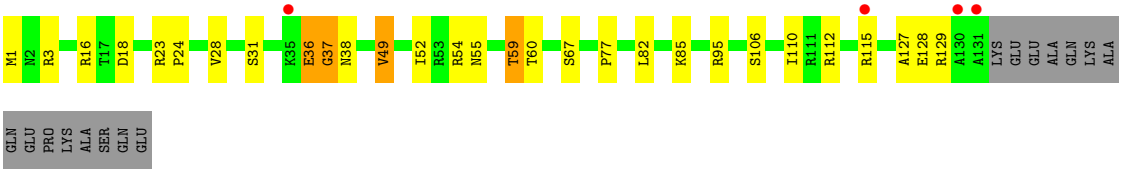
• Molecule 14: 50S ribosomal protein L18

Chain 2S:



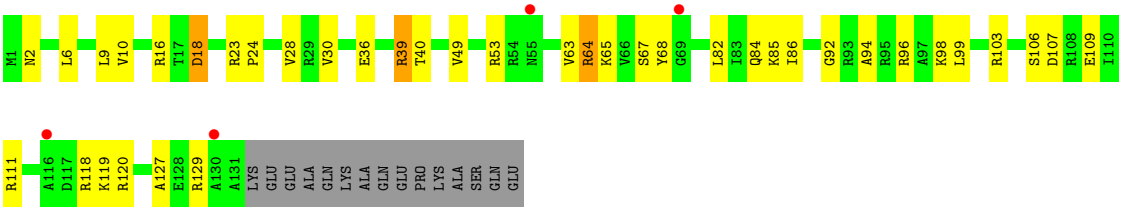
• Molecule 15: 50S ribosomal protein L19

Chain 1T:



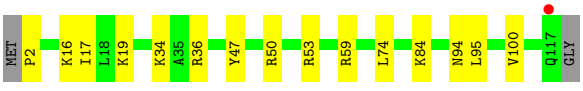
• Molecule 15: 50S ribosomal protein L19

Chain 2T:



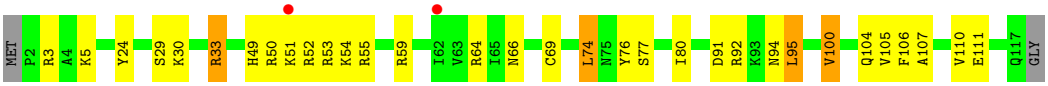
• Molecule 16: 50S ribosomal protein L20

Chain 1U:



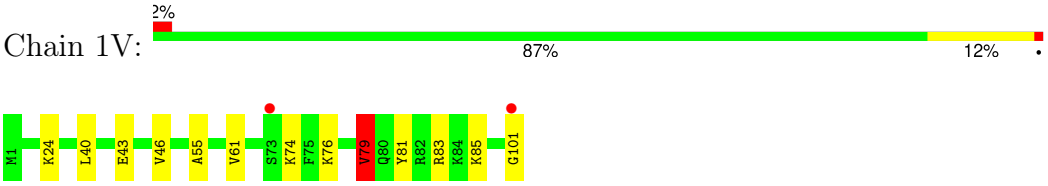
• Molecule 16: 50S ribosomal protein L20

Chain 2U:



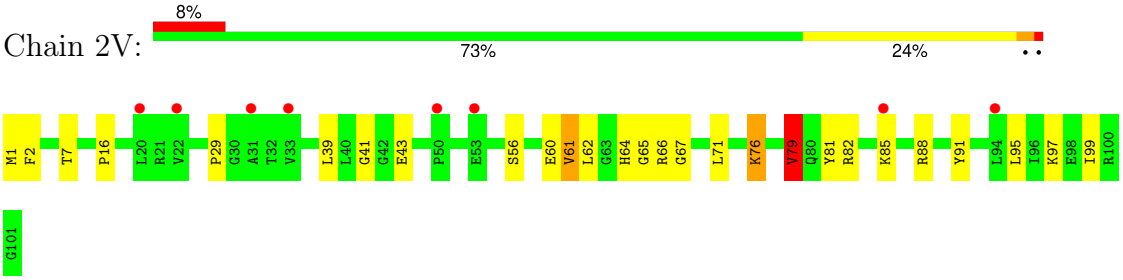
• Molecule 17: 50S ribosomal protein L21

Chain 1V:



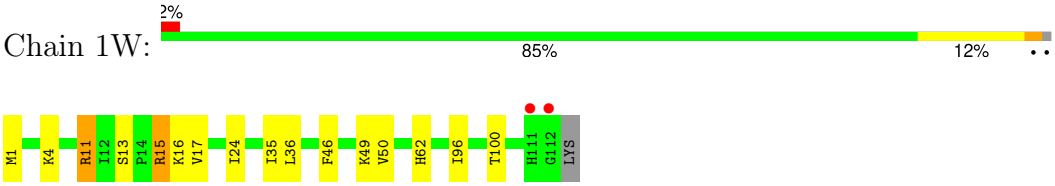
• Molecule 17: 50S ribosomal protein L21

Chain 2V:



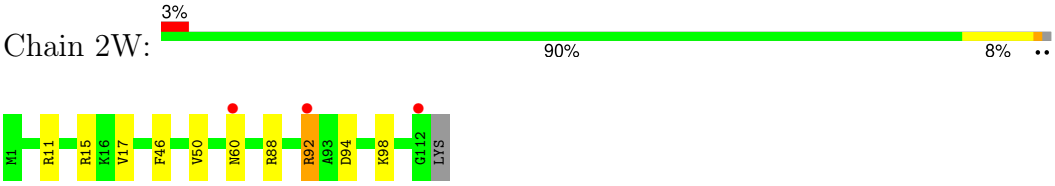
• Molecule 18: 50S ribosomal protein L22

Chain 1W:



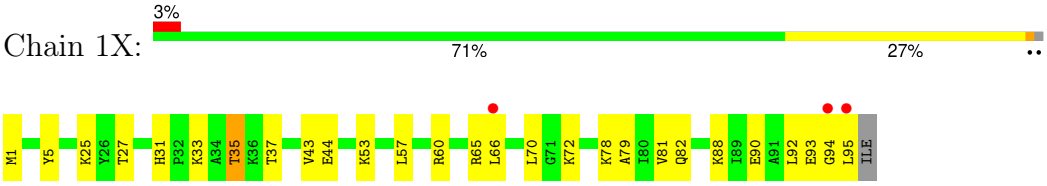
• Molecule 18: 50S ribosomal protein L22

Chain 2W:



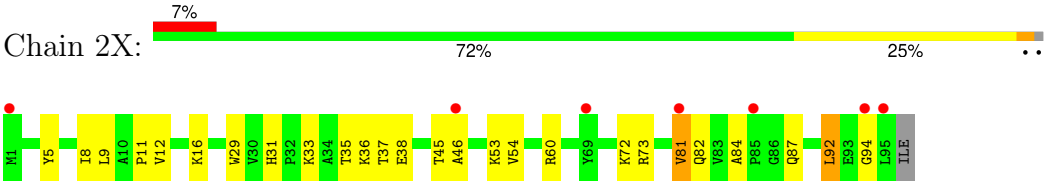
• Molecule 19: 50S ribosomal protein L23

Chain 1X:



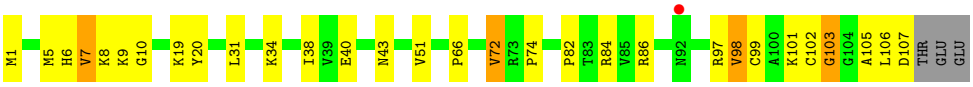
• Molecule 19: 50S ribosomal protein L23

Chain 2X:



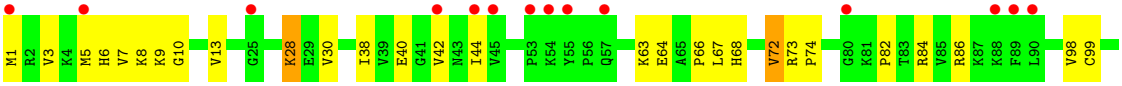
• Molecule 20: 50S ribosomal protein L24

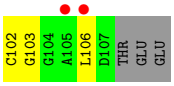
Chain 1Y:



• Molecule 20: 50S ribosomal protein L24

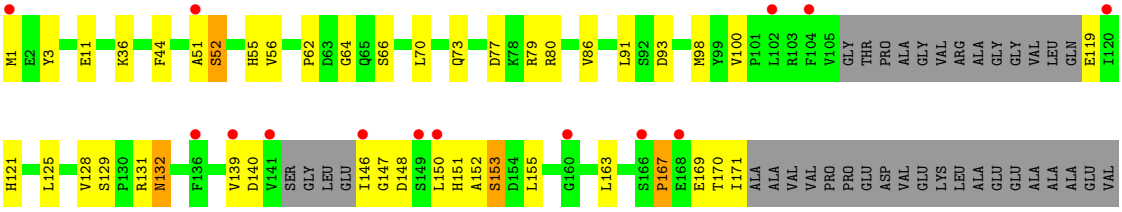
Chain 2Y:





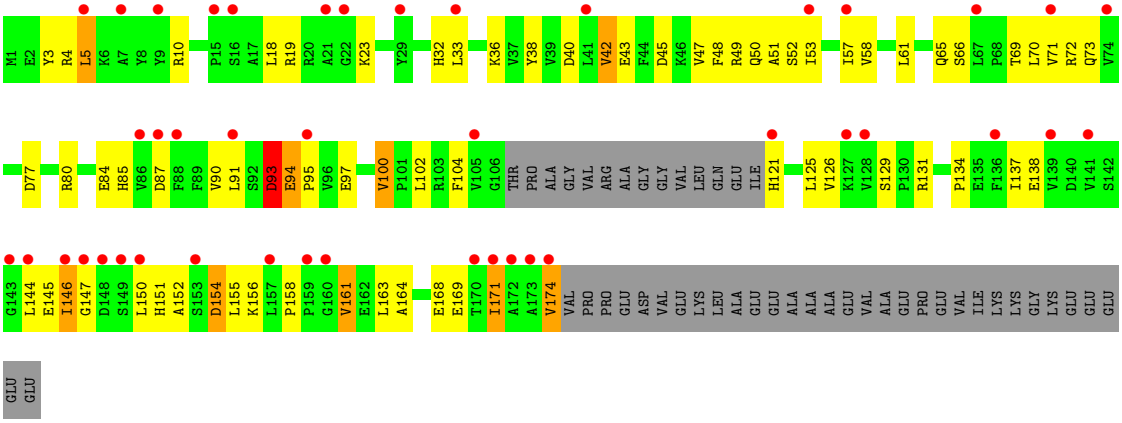
• Molecule 21: 50S ribosomal protein L25

Chain 1Z:



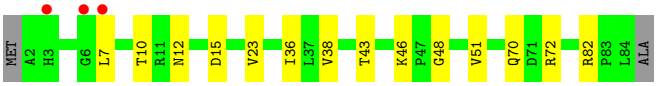
• Molecule 21: 50S ribosomal protein L25

Chain 2Z:

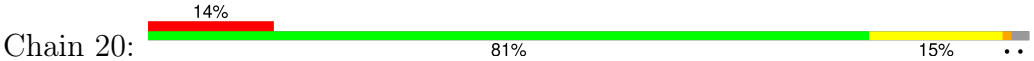


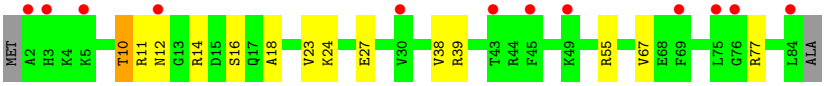
• Molecule 22: 50S ribosomal protein L27

Chain 10:

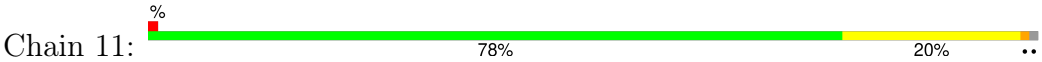


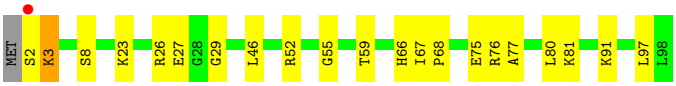
• Molecule 22: 50S ribosomal protein L27



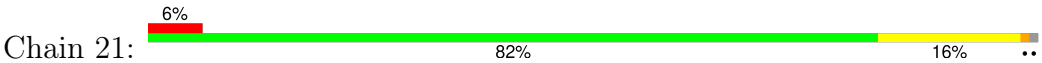


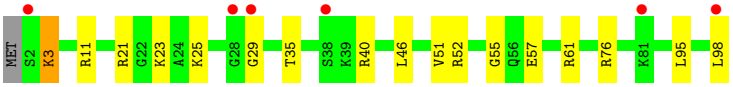
• Molecule 23: 50S ribosomal protein L28



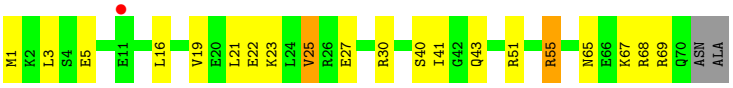


• Molecule 23: 50S ribosomal protein L28

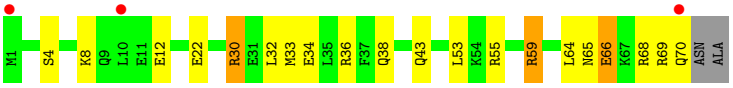




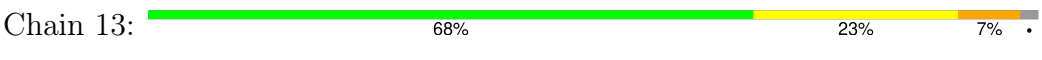
• Molecule 24: 50S ribosomal protein L29

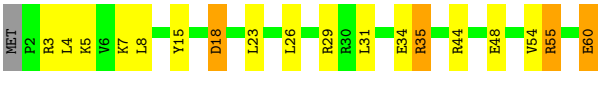


• Molecule 24: 50S ribosomal protein L29



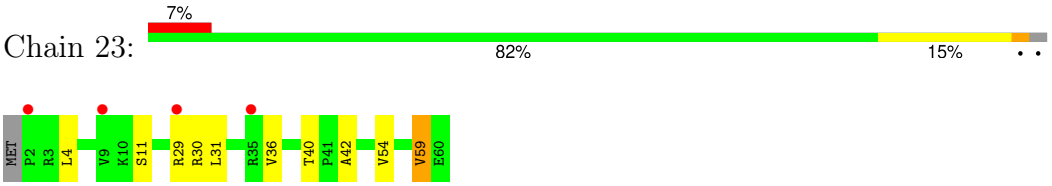
• Molecule 25: 50S ribosomal protein L30





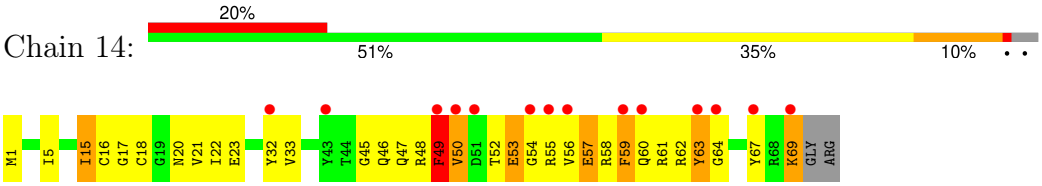
• Molecule 25: 50S ribosomal protein L30

Chain 23:



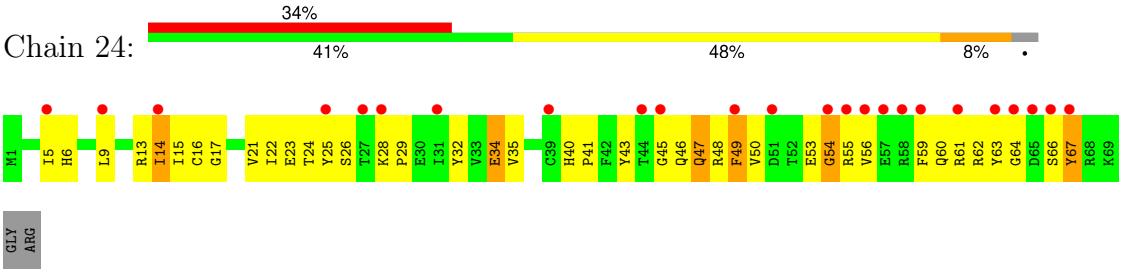
• Molecule 26: 50S ribosomal protein L31

Chain 14:



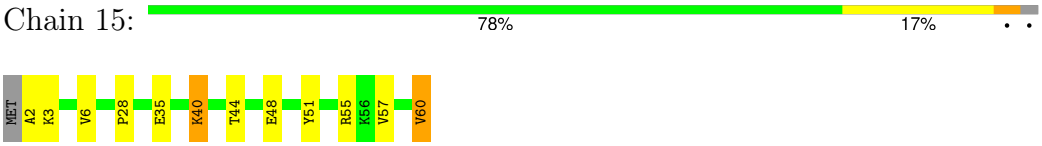
• Molecule 26: 50S ribosomal protein L31

Chain 24:



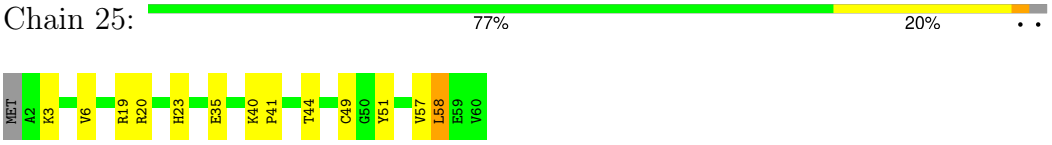
• Molecule 27: 50S ribosomal protein L32

Chain 15:



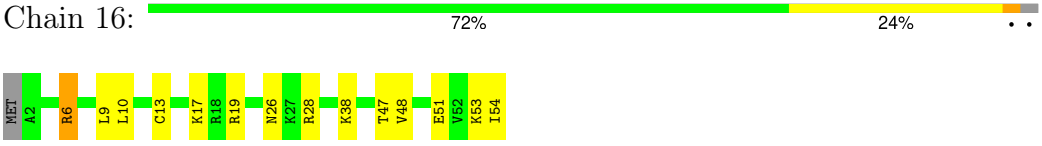
• Molecule 27: 50S ribosomal protein L32

Chain 25:



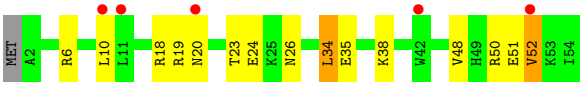
• Molecule 28: 50S ribosomal protein L33

Chain 16:



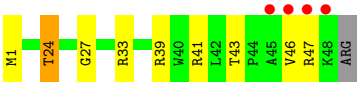
• Molecule 28: 50S ribosomal protein L33

Chain 26:



• Molecule 29: 50S ribosomal protein L34

Chain 17:

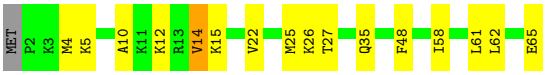


• Molecule 29: 50S ribosomal protein L34

Chain 27:

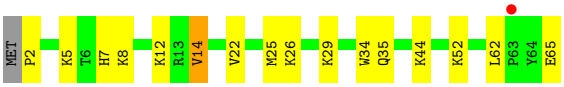
• Molecule 30: 50S ribosomal protein L35

Chain 18:



• Molecule 30: 50S ribosomal protein L35

Chain 28:

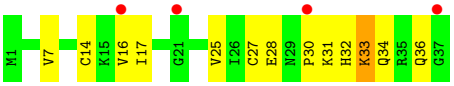


• Molecule 31: 50S ribosomal protein L36

Chain 19:

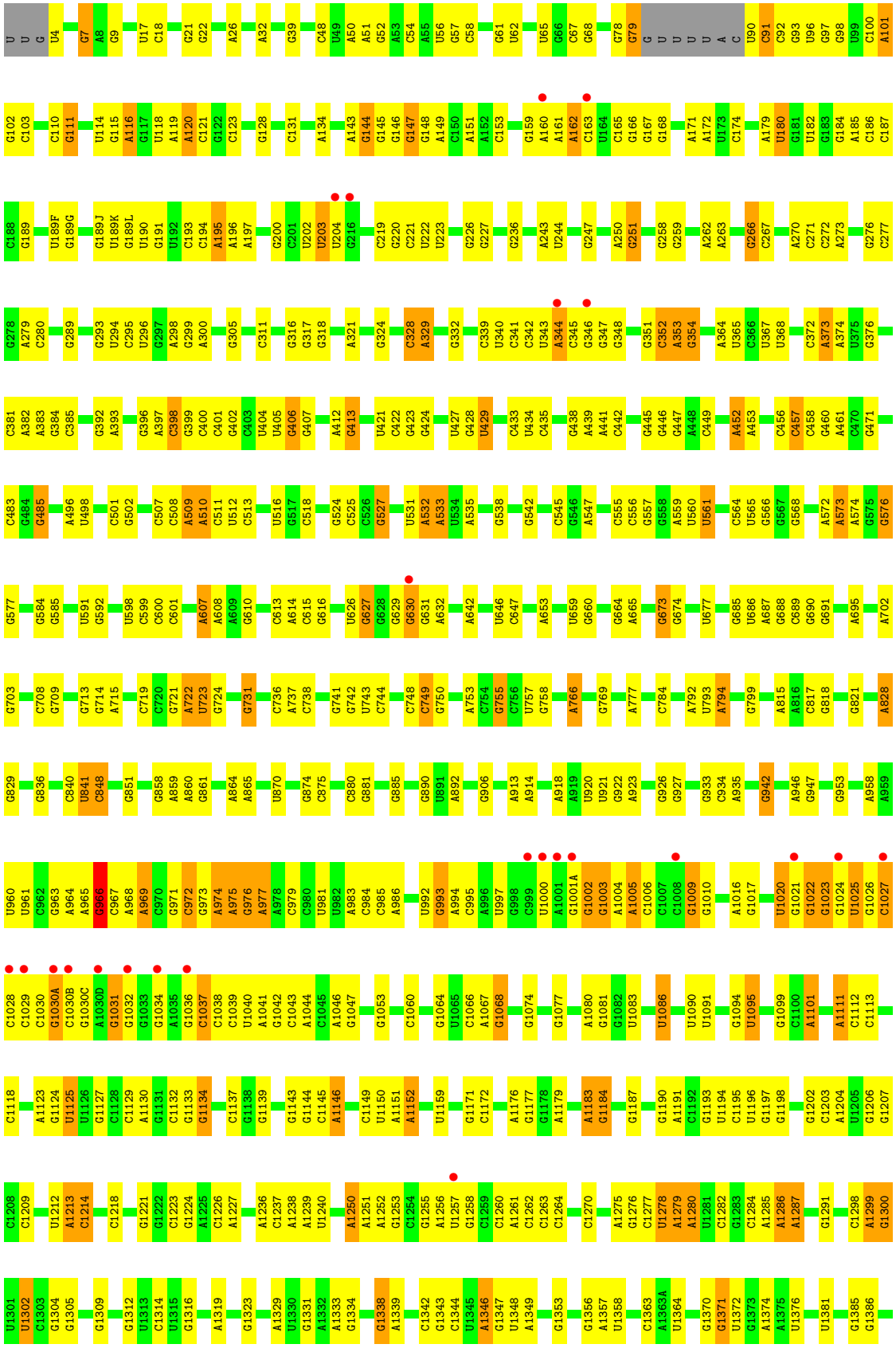
• Molecule 31: 50S ribosomal protein L36

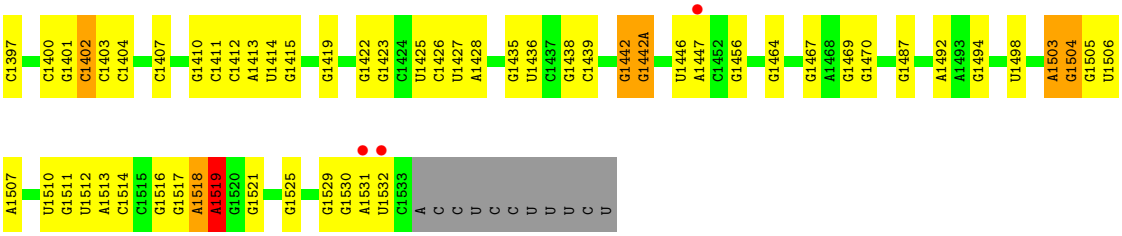
Chain 29:



• Molecule 32: 16S Ribosomal RNA

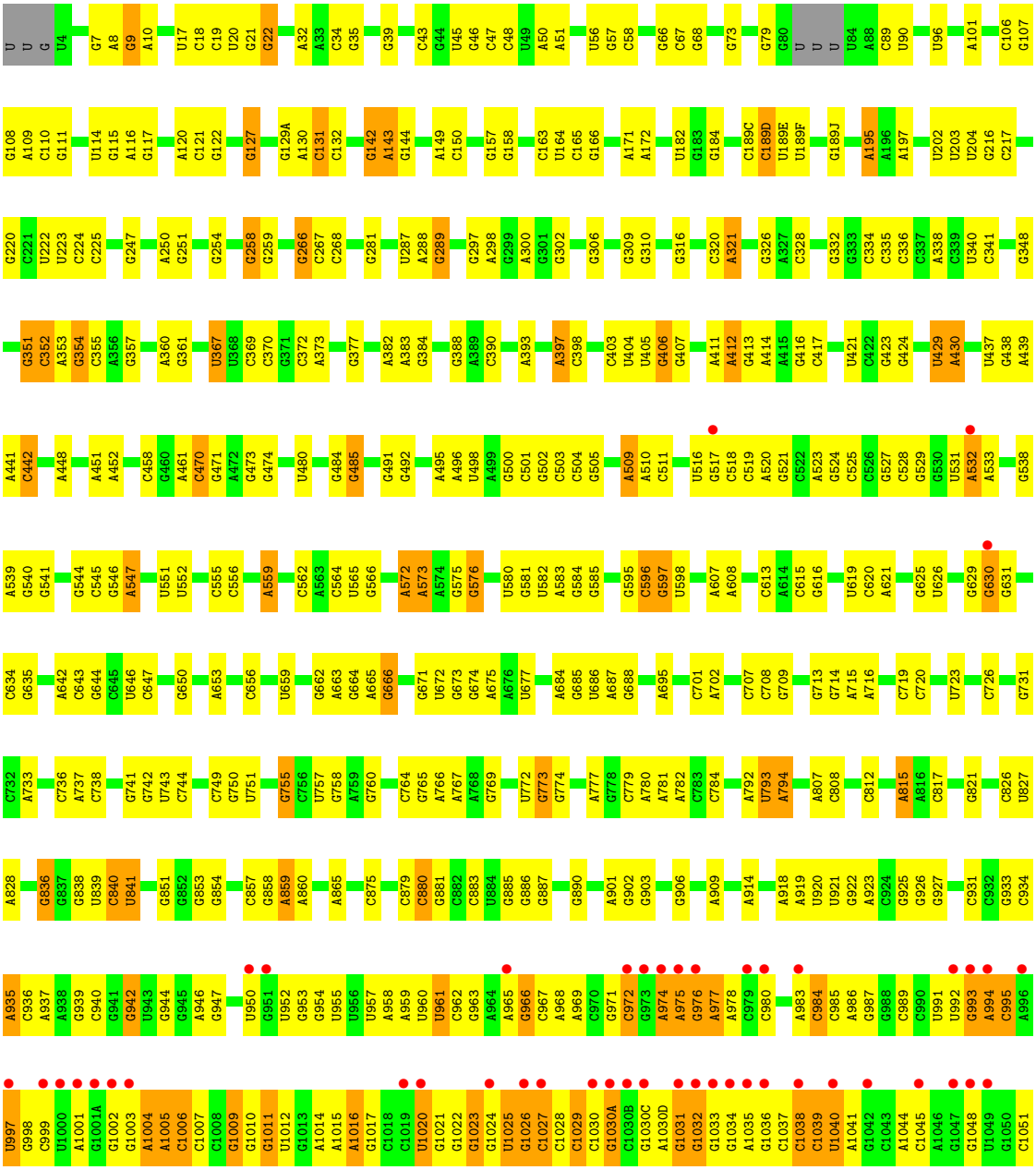
Chain 1a:

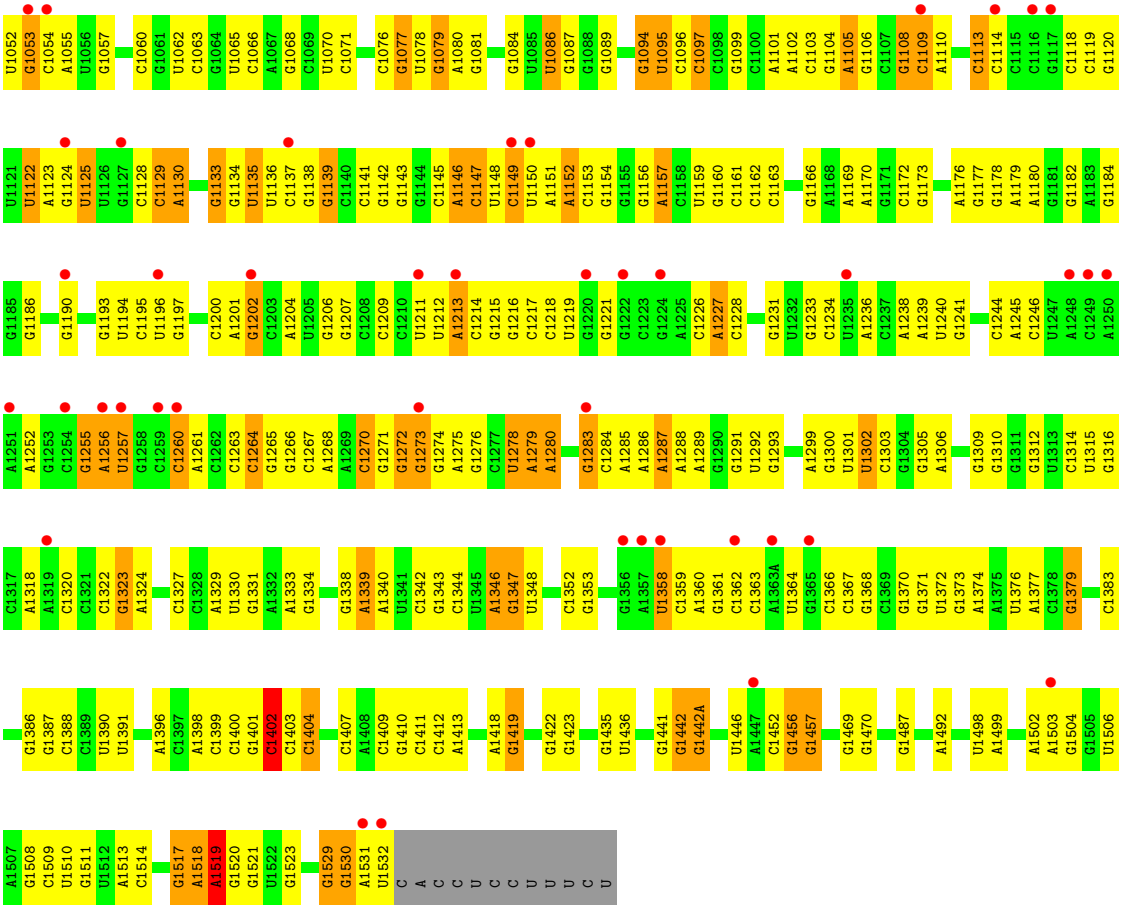




• Molecule 32: 16S Ribosomal RNA

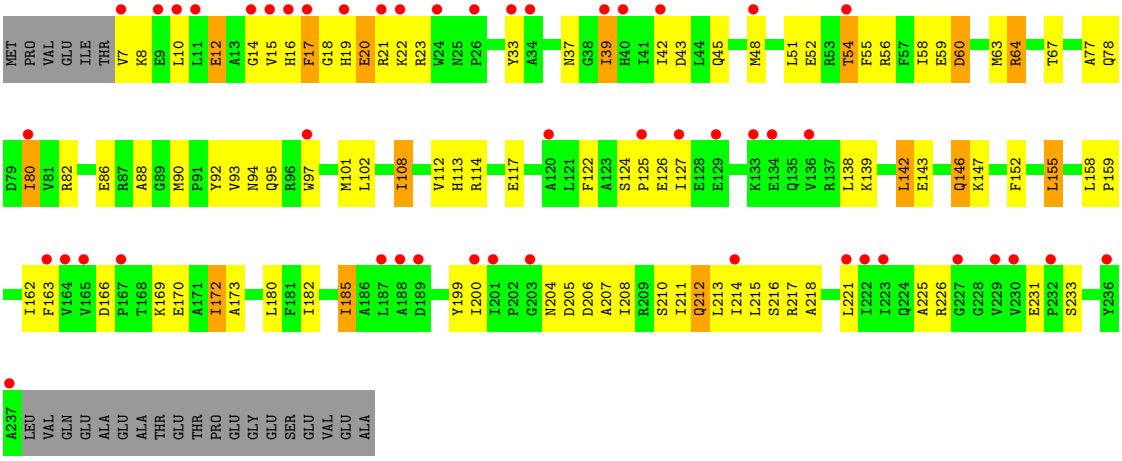
Chain 2a:





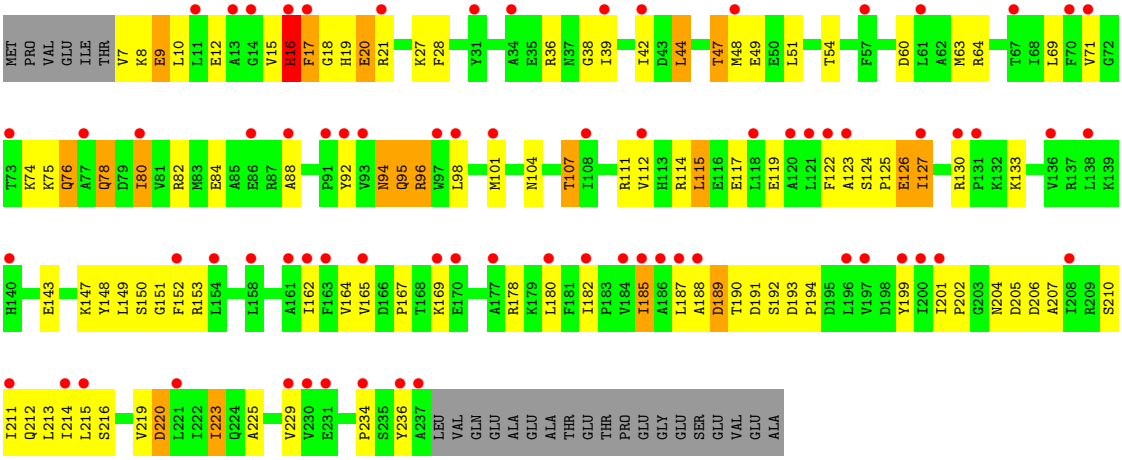
• Molecule 33: 30S ribosomal protein S2

Chain 1b:



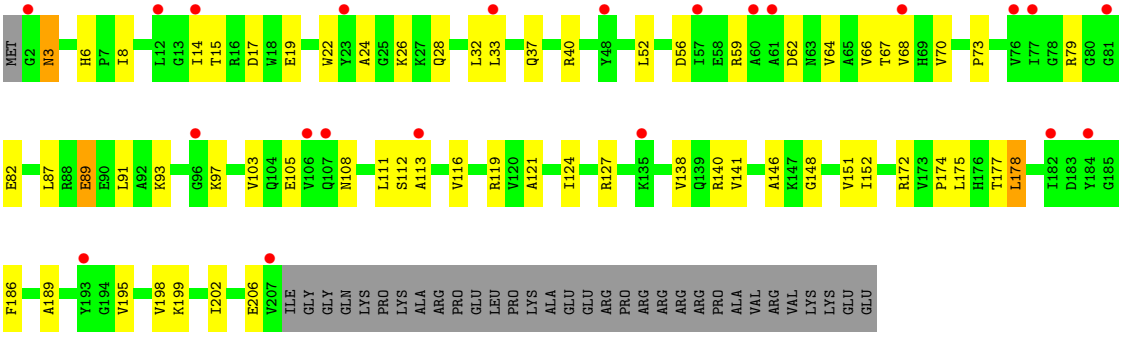
• Molecule 33: 30S ribosomal protein S2

Chain 2b:



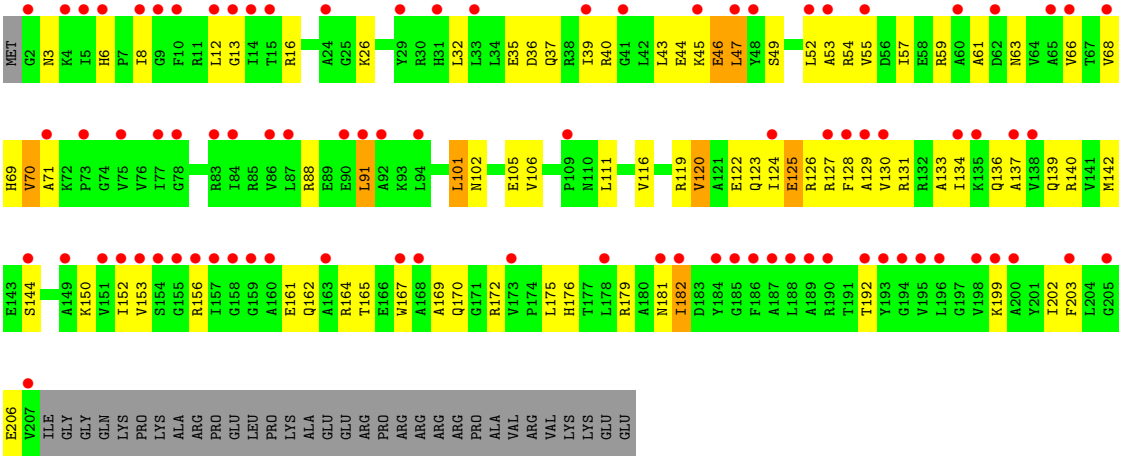
• Molecule 34: 30S ribosomal protein S3

Chain 1c:



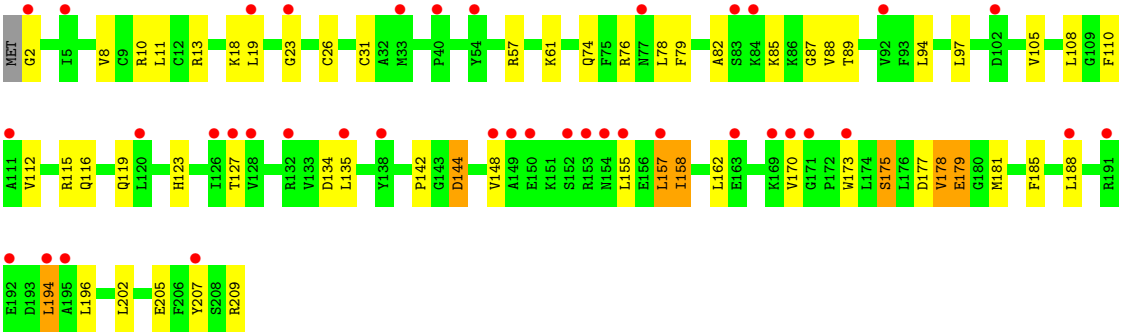
• Molecule 34: 30S ribosomal protein S3

Chain 2c:



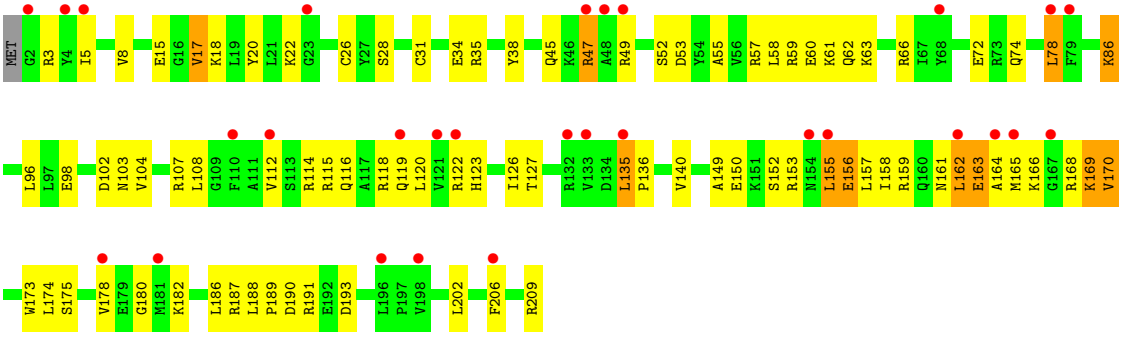
• Molecule 35: 30S ribosomal protein S4

Chain 1d:



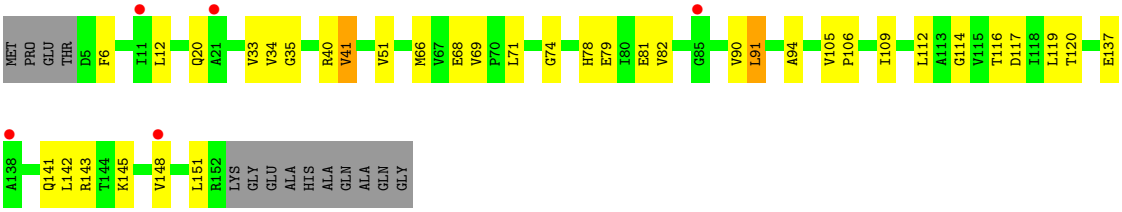
• Molecule 35: 30S ribosomal protein S4

Chain 2d:



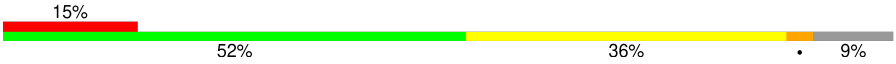
• Molecule 36: 30S ribosomal protein S5

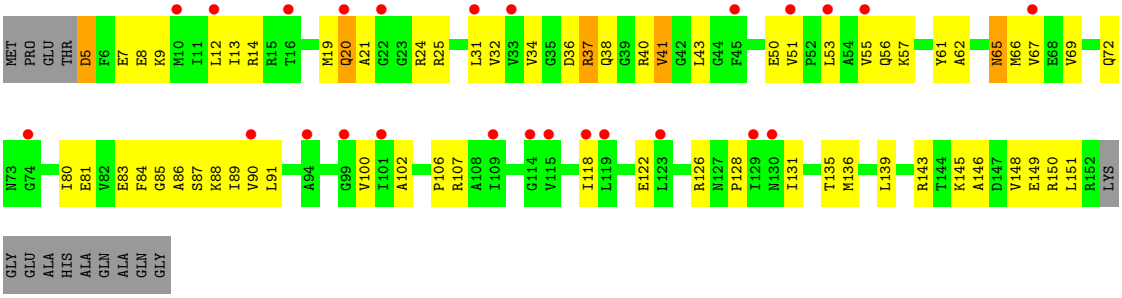
Chain 1e:



• Molecule 36: 30S ribosomal protein S5

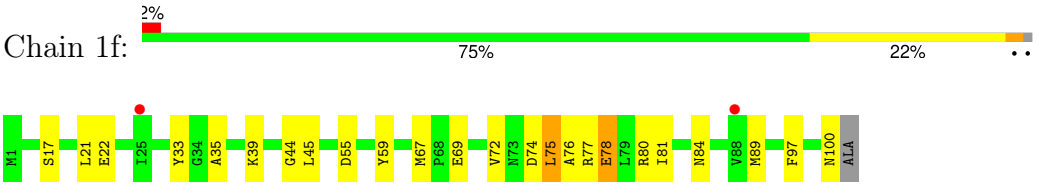
Chain 2e:





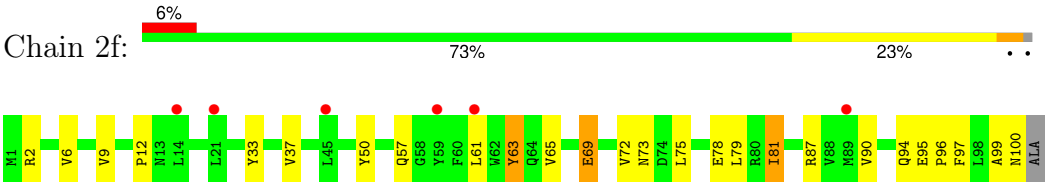
• Molecule 37: 30S ribosomal protein S6

Chain 1f:



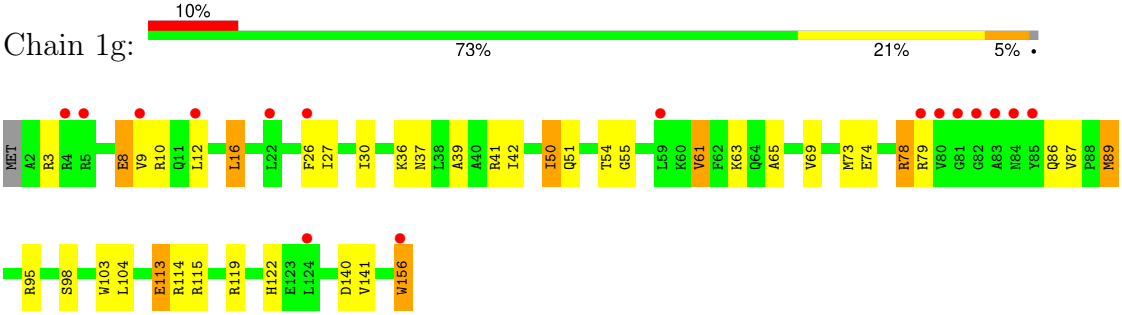
• Molecule 37: 30S ribosomal protein S6

Chain 2f:



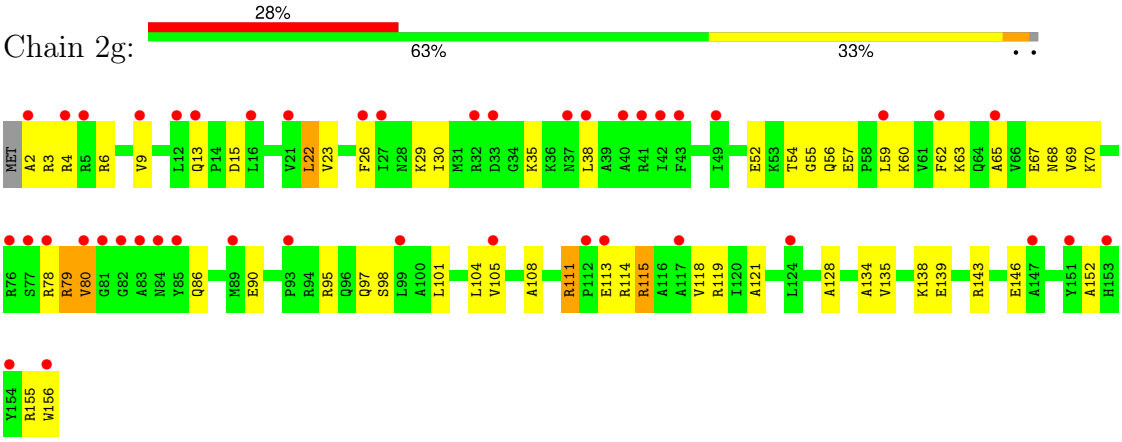
• Molecule 38: 30S ribosomal protein S7

Chain 1g:



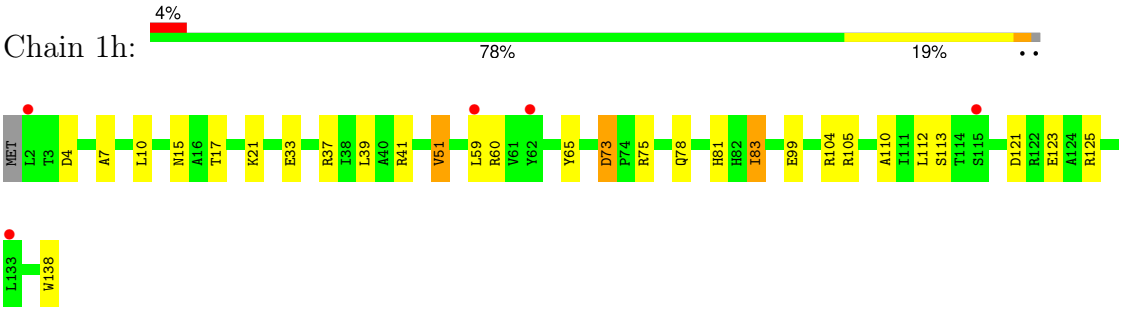
• Molecule 38: 30S ribosomal protein S7

Chain 2g:



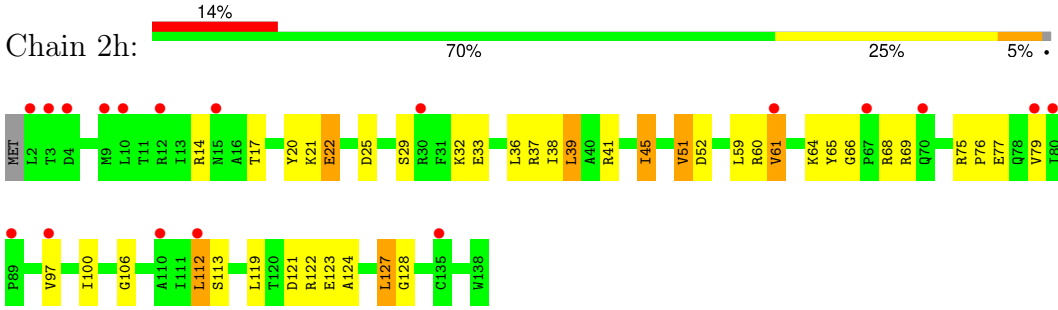
• Molecule 39: 30S ribosomal protein S8

Chain 1h:



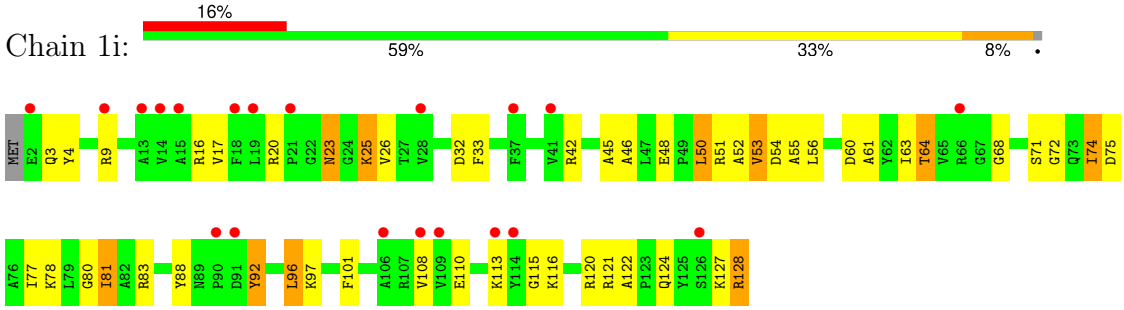
• Molecule 39: 30S ribosomal protein S8

Chain 2h:



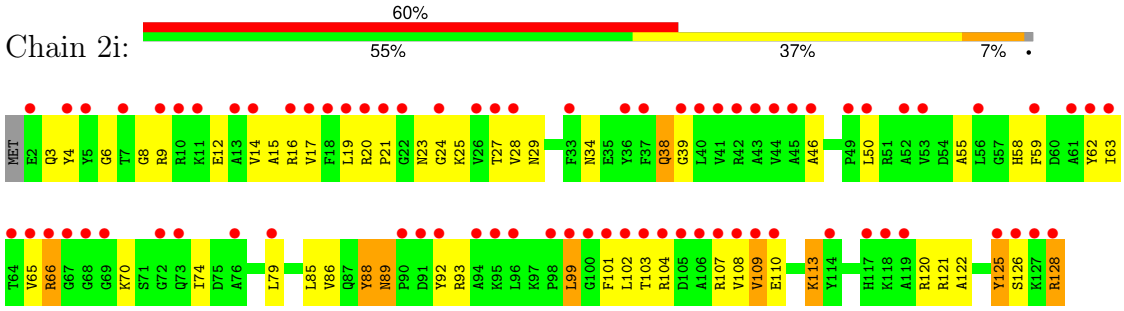
• Molecule 40: 30S ribosomal protein S9

Chain 1i:



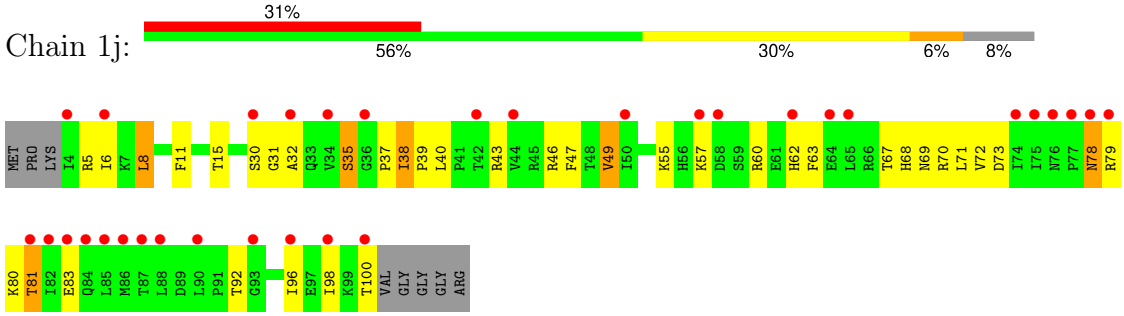
• Molecule 40: 30S ribosomal protein S9

Chain 2i:



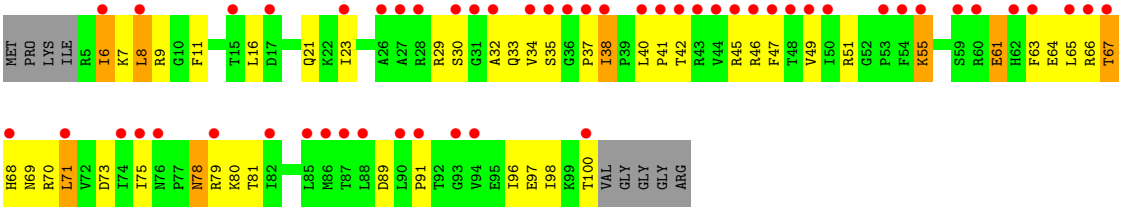
• Molecule 41: 30S ribosomal protein S10

Chain 1j:



• Molecule 41: 30S ribosomal protein S10

Chain 2j:

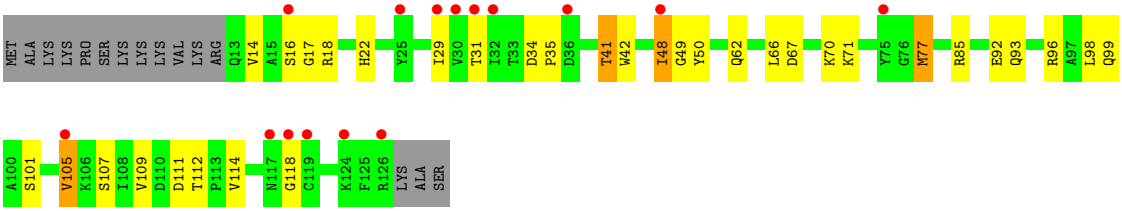


• Molecule 42: 30S ribosomal protein S11

Chain 1k:

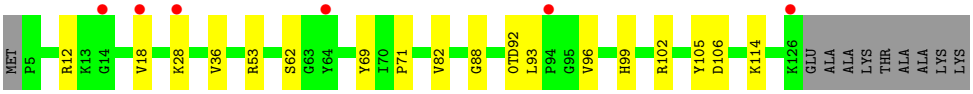
• Molecule 42: 30S ribosomal protein S11

Chain 2k:



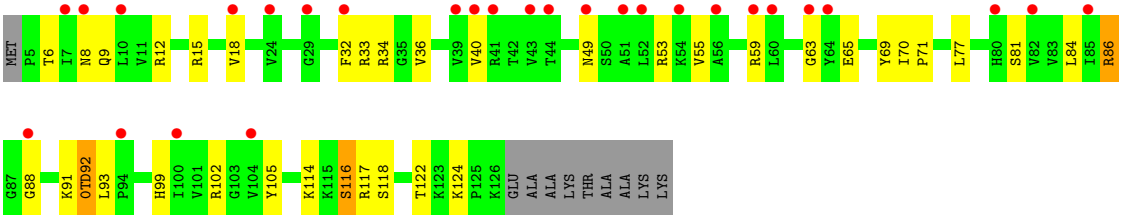
• Molecule 43: 30S ribosomal protein S12

Chain 1l:



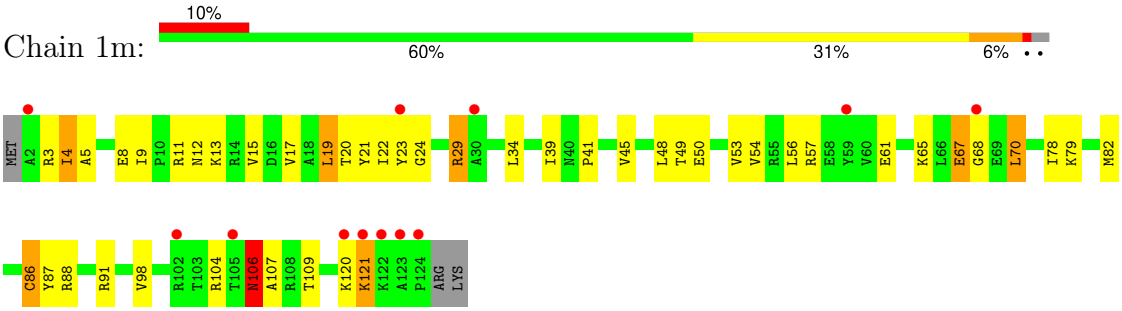
• Molecule 43: 30S ribosomal protein S12

Chain 2l:



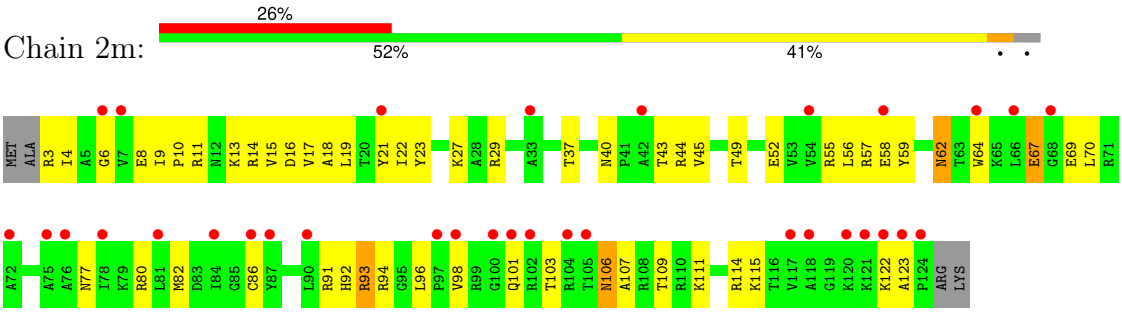
• Molecule 44: 30S ribosomal protein S13

Chain 1m:



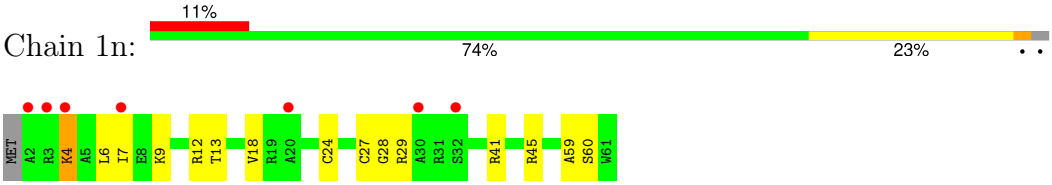
• Molecule 44: 30S ribosomal protein S13

Chain 2m:



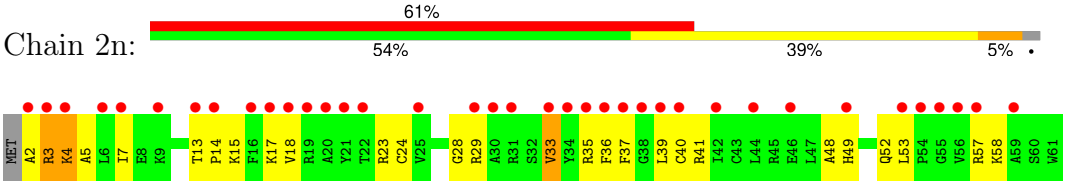
• Molecule 45: 30S ribosomal protein S14 type Z

Chain 1n:



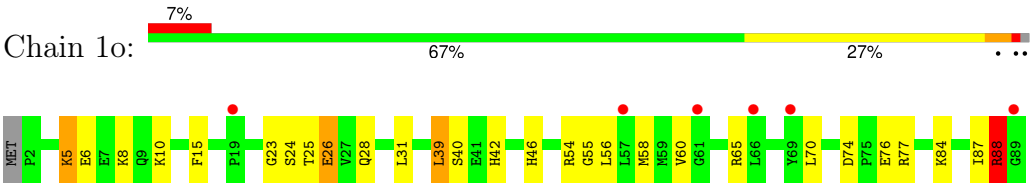
• Molecule 45: 30S ribosomal protein S14 type Z

Chain 2n:



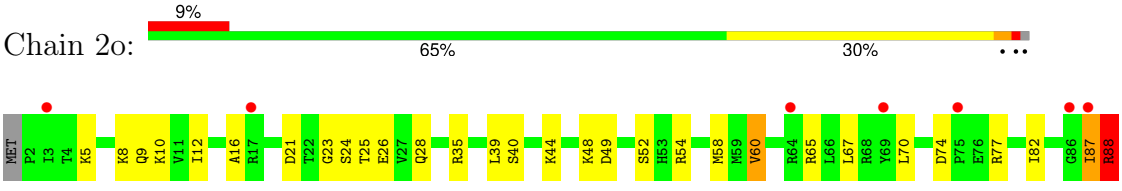
• Molecule 46: 30S ribosomal protein S15

Chain 1o:



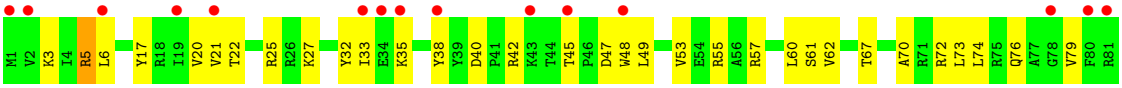
• Molecule 46: 30S ribosomal protein S15

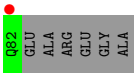
Chain 2o:



• Molecule 47: 30S ribosomal protein S16

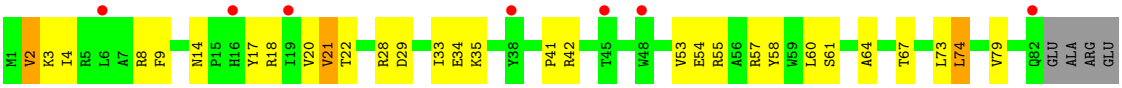
Chain 1p:





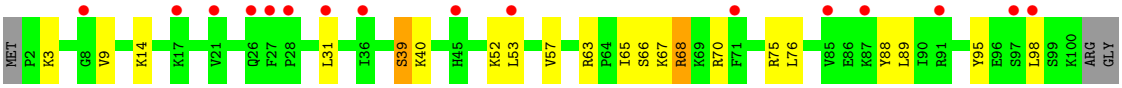
• Molecule 47: 30S ribosomal protein S16

Chain 2p:



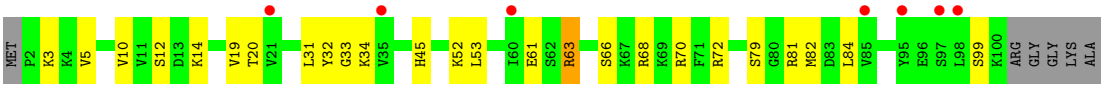
• Molecule 48: 30S ribosomal protein S17

Chain 1q:



• Molecule 48: 30S ribosomal protein S17

Chain 2q:

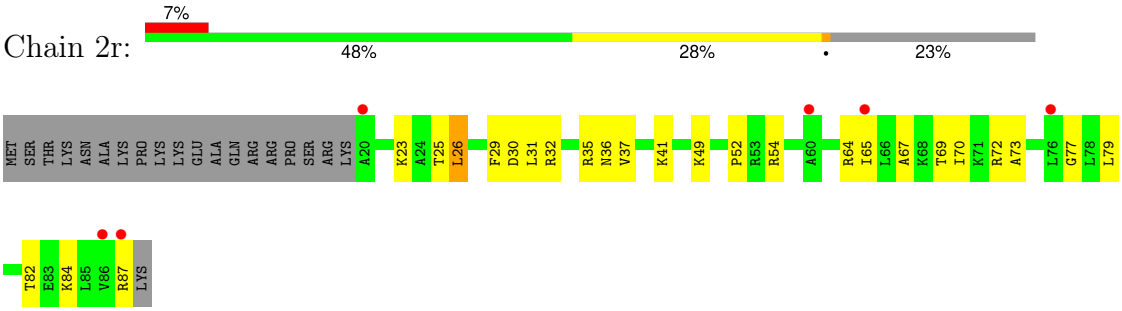


• Molecule 49: 30S ribosomal protein S18

Chain 1r:

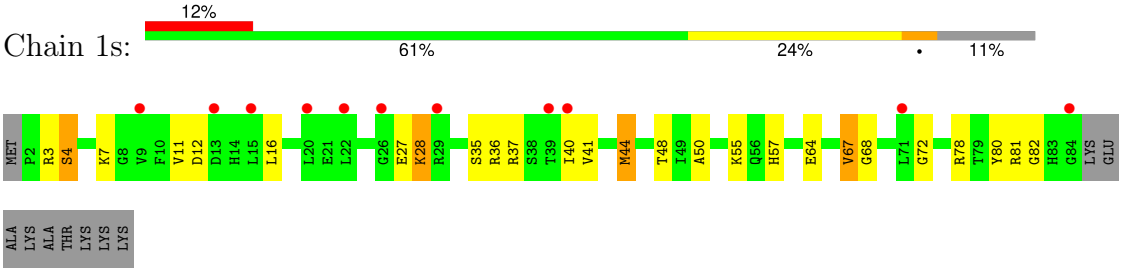
• Molecule 49: 30S ribosomal protein S18

Chain 2r:



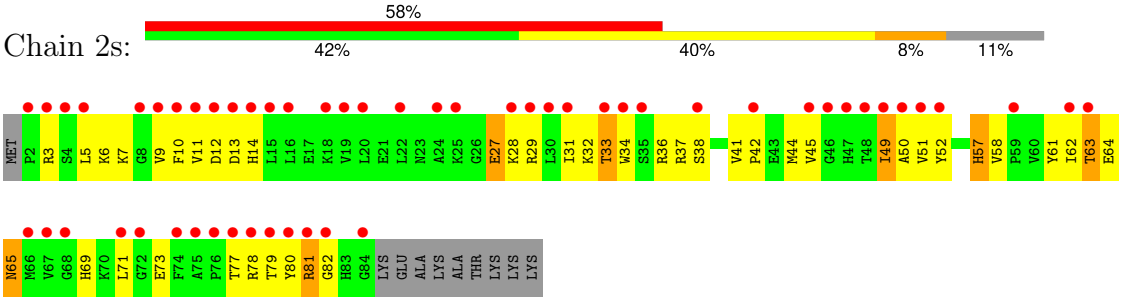
• Molecule 50: 30S ribosomal protein S19

Chain 1s:



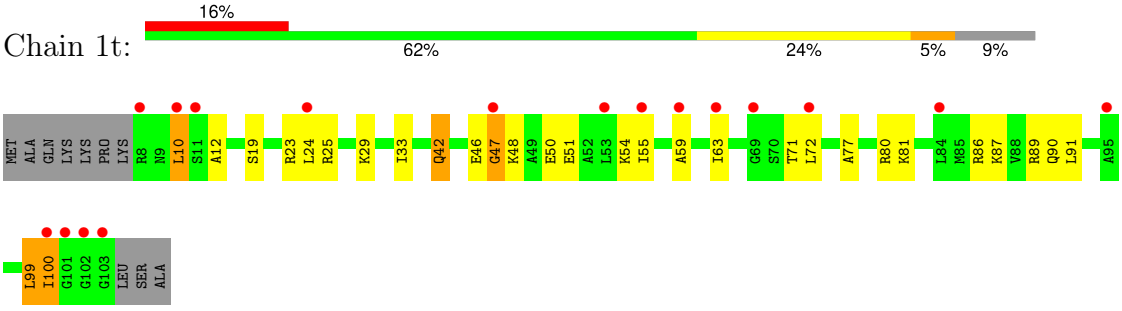
• Molecule 50: 30S ribosomal protein S19

Chain 2s:



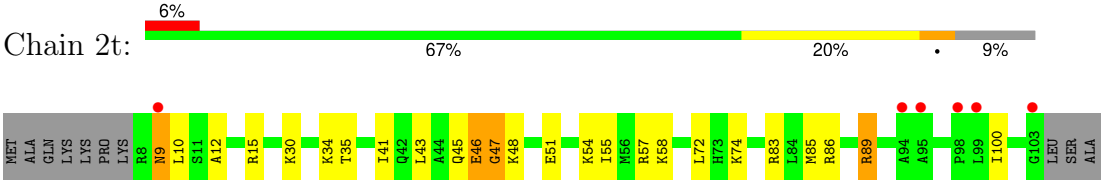
• Molecule 51: 30S ribosomal protein S20

Chain 1t:



• Molecule 51: 30S ribosomal protein S20

Chain 2t:

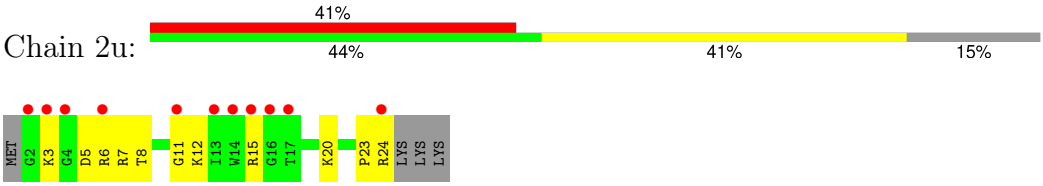


• Molecule 52: 30S ribosomal protein Thx

Chain 1u:

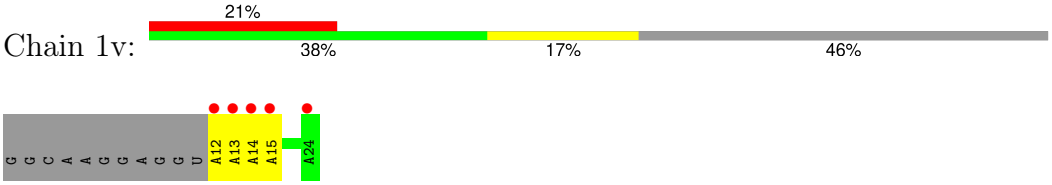
• Molecule 52: 30S ribosomal protein Thx

Chain 2u:



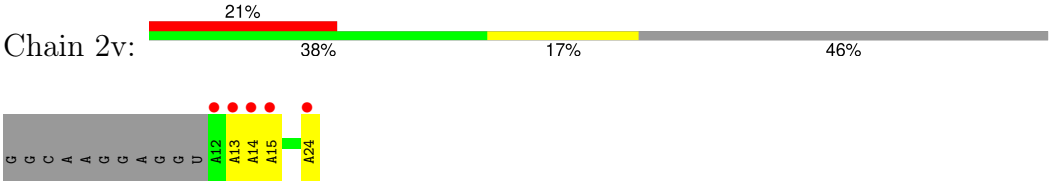
• Molecule 53: MG-mRNA

Chain 1v:



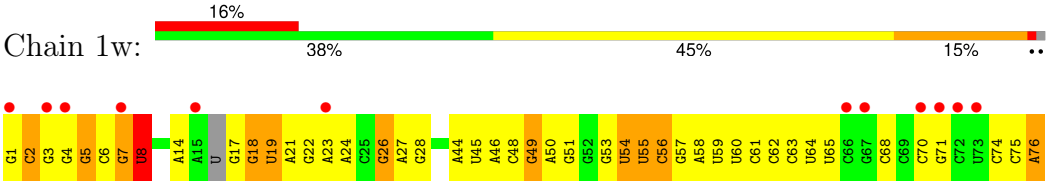
• Molecule 53: MG-mRNA

Chain 2v:



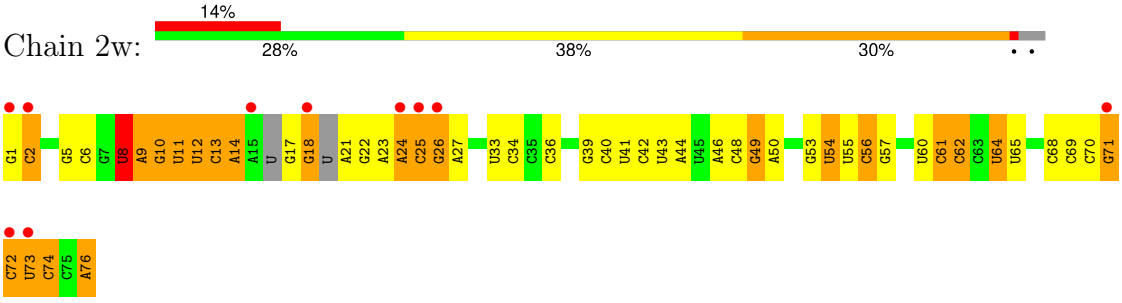
• Molecule 54: A-site Aminoacyl-tRNA Gly-NH-tRNAgly

Chain 1w:



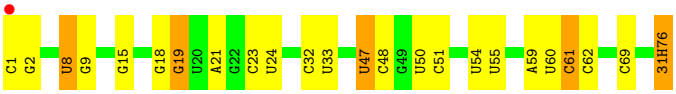
• Molecule 54: A-site Aminoacyl-tRNA Gly-NH-tRNAgly

Chain 2w:

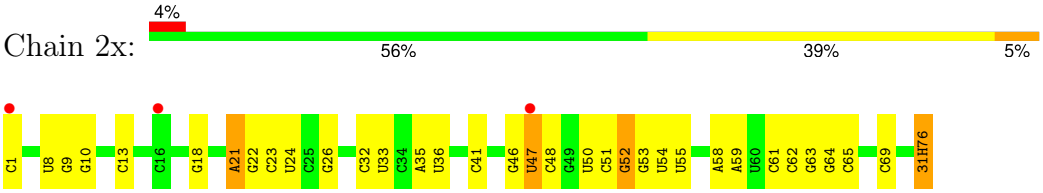


• Molecule 55: P-site Aminoacyl-tRNA fMet-NH-tRNAmet

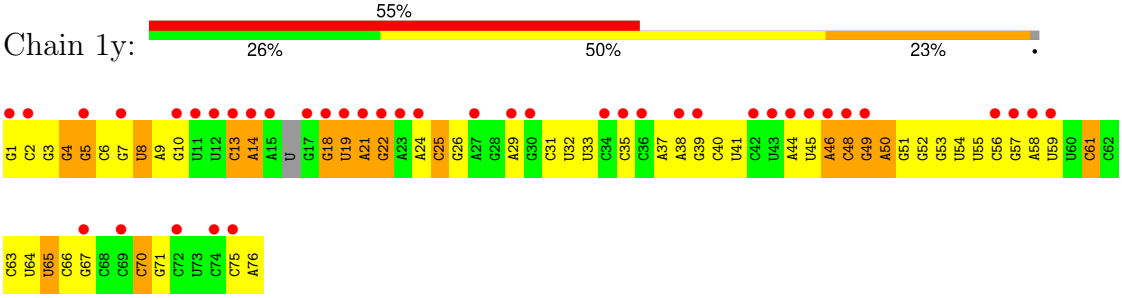
Chain 1x:



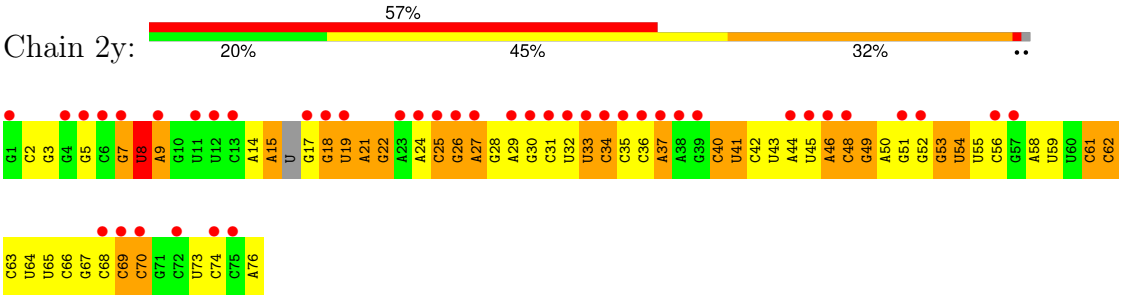
• Molecule 55: P-site Aminoacyl-tRNA fMet-NH-tRNAmet



• Molecule 56: E-site Deacylated tRNAgly



• Molecule 56: E-site Deacylated tRNAgly



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	210.17Å 450.98Å 624.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	153.74 – 2.55 153.74 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.4 (153.74-2.55) 99.4 (153.74-2.55)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.23 (at 2.55Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.223 , 0.268 0.223 , 0.267	Depositor DCC
R_{free} test set	94751 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	57.3	Xtriage
Anisotropy	0.141	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 63.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	300046	wwPDB-VP
Average B, all atoms (Å^2)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.74% 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, 4SU, PSU, M2G, 5MC, K, OMG, SF4, 5MU, CLM, UR3, 31H, MG, 4OC, L3X, 2MG, MA6, 2MA, OMC, ZN, OMU, G7M

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	0.27	0/69011	0.47	2/107720 (0.0%)
1	2A	0.21	1/67295 (0.0%)	0.41	2/105042 (0.0%)
2	1B	0.21	0/2882	0.40	0/4494
2	2B	0.18	0/2879	0.35	0/4487
3	1D	0.26	0/2186	0.49	0/2944
3	2D	0.21	0/2186	0.47	0/2944
4	1E	0.26	0/1592	0.51	0/2149
4	2E	0.21	0/1592	0.43	0/2149
5	1F	0.26	0/1618	0.46	0/2191
5	2F	0.19	0/1614	0.45	2/2186 (0.1%)
6	1G	0.20	0/1448	0.43	0/1957
6	2G	0.20	0/1453	0.43	0/1963
7	1H	0.21	0/1356	0.42	0/1834
7	2H	0.18	0/1356	0.40	0/1834
8	1I	0.19	0/1112	0.43	0/1514
8	2I	0.19	0/1079	0.41	0/1475
9	1N	0.26	0/1144	0.47	0/1543
9	2N	0.18	0/1144	0.41	0/1543
10	1O	0.25	0/943	0.44	0/1269
10	2O	0.19	0/943	0.44	0/1269
11	1P	0.26	0/1152	0.55	0/1533
11	2P	0.21	0/1152	0.51	0/1533
12	1Q	0.25	0/1143	0.47	0/1527
12	2Q	0.22	0/1143	0.46	0/1527
13	1R	0.28	0/982	0.49	0/1312
13	2R	0.20	0/982	0.44	0/1312
14	1S	0.21	0/883	0.47	0/1176
14	2S	0.21	0/880	0.45	0/1172
15	1T	0.26	0/1105	0.50	0/1477
15	2T	0.21	0/1097	0.43	0/1468
16	1U	0.28	0/977	0.46	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	0.25	0/782	0.48	0/1049
17	2V	0.18	0/782	0.41	0/1049
18	1W	0.27	0/897	0.45	0/1205
18	2W	0.21	0/897	0.43	0/1205
19	1X	0.26	0/764	0.53	0/1025
19	2X	0.21	0/764	0.49	2/1025 (0.2%)
20	1Y	0.22	0/819	0.49	0/1095
20	2Y	0.20	0/819	0.46	0/1095
21	1Z	0.21	0/1267	0.46	0/1717
21	2Z	0.22	0/1299	0.47	0/1763
22	10	0.27	0/662	0.49	0/881
22	20	0.19	0/662	0.44	0/881
23	11	0.22	0/762	0.43	0/1014
23	21	0.21	0/762	0.41	0/1014
24	12	0.24	0/590	0.44	0/781
24	22	0.17	0/590	0.35	0/781
25	13	0.26	0/474	0.47	0/635
25	23	0.17	0/469	0.39	0/630
26	14	0.25	0/565	0.60	0/761
26	24	0.24	0/545	0.58	2/737 (0.3%)
27	15	0.26	0/469	0.52	0/635
27	25	0.23	0/469	0.41	0/635
28	16	0.25	0/460	0.46	0/613
28	26	0.20	0/456	0.43	0/608
29	17	0.30	0/426	0.52	0/561
29	27	0.25	0/426	0.47	0/561
30	18	0.25	0/525	0.46	0/691
30	28	0.19	0/525	0.39	0/691
31	19	0.25	0/310	0.45	0/407
31	29	0.19	0/310	0.44	0/407
32	1a	0.19	0/35795	0.39	1/55864 (0.0%)
32	2a	0.19	0/35886	0.38	0/56005
33	1b	0.20	0/1881	0.47	0/2542
33	2b	0.23	0/1860	0.51	0/2518
34	1c	0.20	0/1572	0.39	0/2126
34	2c	0.22	0/1566	0.44	0/2119
35	1d	0.18	0/1685	0.42	0/2262
35	2d	0.19	0/1704	0.44	0/2284
36	1e	0.20	0/1145	0.47	0/1543
36	2e	0.19	0/1149	0.46	0/1548
37	1f	0.18	0/823	0.37	0/1115
37	2f	0.19	0/829	0.42	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
38	1g	0.18	0/1250	0.38	0/1679
38	2g	0.19	0/1254	0.40	0/1683
39	1h	0.18	0/1108	0.40	0/1494
39	2h	0.18	0/1108	0.40	0/1494
40	1i	0.19	0/1002	0.47	0/1346
40	2i	0.21	0/997	0.47	0/1343
41	1j	0.18	0/722	0.45	0/982
41	2j	0.22	0/727	0.47	0/988
42	1k	0.21	0/844	0.48	0/1145
42	2k	0.17	0/848	0.39	0/1149
43	1l	0.21	0/937	0.40	0/1260
43	2l	0.21	0/937	0.48	1/1260 (0.1%)
44	1m	0.19	0/969	0.46	0/1302
44	2m	0.20	0/961	0.48	0/1291
45	1n	0.20	0/501	0.42	0/664
45	2n	0.21	0/501	0.45	0/664
46	1o	0.19	0/739	0.37	0/985
46	2o	0.17	0/739	0.42	0/985
47	1p	0.20	0/697	0.47	0/939
47	2p	0.18	0/693	0.45	0/935
48	1q	0.18	0/836	0.44	0/1117
48	2q	0.17	0/836	0.44	0/1117
49	1r	0.19	0/560	0.46	0/746
49	2r	0.20	0/560	0.40	0/746
50	1s	0.20	0/667	0.49	0/900
50	2s	0.24	0/661	0.58	0/893
51	1t	0.20	0/730	0.49	0/965
51	2t	0.20	0/729	0.43	0/965
52	1u	0.19	0/203	0.43	0/266
52	2u	0.20	0/203	0.47	0/266
53	1v	0.20	0/322	0.33	0/501
53	2v	0.20	0/322	0.33	0/501
54	1w	0.27	1/1639 (0.1%)	0.41	0/2548
54	2w	0.27	0/1616	0.43	0/2510
55	1x	0.26	0/1723	0.41	0/2684
55	2x	0.24	0/1723	0.39	0/2684
56	1y	0.29	1/1664 (0.1%)	0.43	0/2587
56	2y	0.30	1/1664 (0.1%)	0.43	0/2587
All	All	0.22	4/316940 (0.0%)	0.43	12/474518 (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
51	1t	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	2y	8	4SU	O3'-P	5.50	1.61	1.56
54	1w	8	4SU	O3'-P	5.22	1.61	1.56
56	1y	8	4SU	O3'-P	5.18	1.61	1.56
1	2A	2552	OMU	O3'-P	5.05	1.61	1.56

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2A	1992	G	C2'-C3'-O3'	6.55	119.33	109.50
1	1A	1992	G	C2'-C3'-O3'	6.27	118.91	109.50
26	24	56	VAL	N-CA-C	-5.96	106.69	112.29
26	24	54	GLY	N-CA-C	-5.82	106.93	115.30
43	2l	63	GLY	N-CA-C	-5.40	108.65	115.08

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
51	1t	99	LEU	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1A	61852	0	31195	563	0
1	2A	60322	0	30428	638	0
2	1B	2577	0	1305	16	0
2	2B	2575	0	1303	36	0
3	1D	2136	0	2218	33	0
3	2D	2136	0	2218	44	0
4	1E	1559	0	1618	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	2E	1559	0	1618	30	0
5	1F	1583	0	1625	28	0
5	2F	1579	0	1619	43	0
6	1G	1423	0	1436	31	0
6	2G	1428	0	1438	55	0
7	1H	1330	0	1407	30	0
7	2H	1330	0	1407	27	0
8	1I	1097	0	1140	35	0
8	2I	1064	0	1082	34	1
9	1N	1117	0	1184	12	0
9	2N	1117	0	1184	21	0
10	1O	933	0	996	14	0
10	2O	933	0	996	20	0
11	1P	1135	0	1212	29	0
11	2P	1135	0	1212	33	0
12	1Q	1122	0	1179	22	0
12	2Q	1122	0	1179	26	0
13	1R	968	0	1033	12	0
13	2R	968	0	1033	20	0
14	1S	873	0	927	16	0
14	2S	870	0	923	39	0
15	1T	1091	0	1151	16	0
15	2T	1083	0	1136	26	0
16	1U	959	0	1019	10	0
16	2U	959	0	1019	24	0
17	1V	771	0	830	8	0
17	2V	771	0	830	19	0
18	1W	886	0	940	8	0
18	2W	886	0	940	6	0
19	1X	750	0	814	19	0
19	2X	750	0	814	20	0
20	1Y	806	0	881	19	0
20	2Y	806	0	881	18	0
21	1Z	1240	0	1240	29	0
21	2Z	1271	0	1273	45	0
22	10	653	0	674	16	0
22	20	653	0	674	12	0
23	11	755	0	826	15	0
23	21	755	0	826	11	0
24	12	588	0	643	13	0
24	22	588	0	643	14	0
25	13	469	0	518	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	23	464	0	514	6	0
26	14	552	0	533	23	0
26	24	532	0	503	38	0
27	15	455	0	465	8	0
27	25	455	0	465	8	0
28	16	453	0	473	10	0
28	26	449	0	469	10	0
29	17	418	0	467	8	0
29	27	418	0	467	9	0
30	18	517	0	582	14	0
30	28	517	0	582	14	0
31	19	307	0	335	2	0
31	29	307	0	335	9	0
32	1a	32246	0	16293	394	1
32	2a	32327	0	16338	528	0
33	1b	1846	0	1867	64	0
33	2b	1825	0	1828	77	0
34	1c	1548	0	1535	39	0
34	2c	1542	0	1517	59	0
35	1d	1655	0	1672	39	0
35	2d	1674	0	1714	60	0
36	1e	1129	0	1185	20	0
36	2e	1133	0	1191	45	0
37	1f	810	0	804	15	0
37	2f	816	0	808	21	0
38	1g	1231	0	1238	25	0
38	2g	1235	0	1249	38	0
39	1h	1088	0	1126	17	0
39	2h	1088	0	1126	27	0
40	1i	983	0	986	34	0
40	2i	978	0	966	44	0
41	1j	709	0	650	21	0
41	2j	714	0	672	30	0
42	1k	829	0	825	15	0
42	2k	833	0	836	18	0
43	1l	932	0	980	9	0
43	2l	932	0	980	21	0
44	1m	958	0	1002	34	0
44	2m	950	0	988	45	0
45	1n	492	0	529	9	0
45	2n	492	0	529	25	0
46	1o	728	0	760	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
46	2o	728	0	760	19	0
47	1p	681	0	697	25	0
47	2p	677	0	686	19	0
48	1q	823	0	891	13	0
48	2q	823	0	891	10	0
49	1r	555	0	618	14	0
49	2r	555	0	618	19	0
50	1s	652	0	662	21	0
50	2s	646	0	644	41	0
51	1t	728	0	798	20	0
51	2t	727	0	796	17	0
52	1u	199	0	208	6	0
52	2u	199	0	208	8	0
53	1v	286	0	142	1	0
53	2v	286	0	142	1	0
54	1w	1556	0	778	30	0
54	2w	1536	0	770	46	0
55	1x	1656	0	849	15	0
55	2x	1656	0	849	23	0
56	1y	1552	0	791	33	0
56	2y	1552	0	791	51	0
57	10	9	0	0	0	0
57	11	3	0	0	0	0
57	12	2	0	0	0	0
57	13	5	0	0	0	0
57	15	6	0	0	0	0
57	16	2	0	0	0	0
57	17	5	0	0	0	0
57	18	6	0	0	0	0
57	19	1	0	0	0	0
57	1A	1095	0	0	0	0
57	1B	36	0	0	0	0
57	1D	13	0	0	0	0
57	1E	12	0	0	0	0
57	1F	15	0	0	0	0
57	1G	4	0	0	0	0
57	1I	1	0	0	0	0
57	1N	5	0	0	0	0
57	1O	5	0	0	0	0
57	1P	5	0	0	0	0
57	1Q	7	0	0	0	0
57	1R	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	1S	3	0	0	0	0
57	1T	3	0	0	0	0
57	1U	10	0	0	0	0
57	1V	7	0	0	0	0
57	1W	7	0	0	0	0
57	1X	7	0	0	0	0
57	1Y	3	0	0	0	0
57	1Z	3	0	0	0	0
57	1a	226	0	0	0	0
57	1b	2	0	0	0	0
57	1e	2	0	0	0	0
57	1f	2	0	0	0	0
57	1h	1	0	0	0	0
57	1l	2	0	0	0	0
57	1m	1	0	0	0	0
57	1n	2	0	0	0	0
57	1s	1	0	0	0	0
57	1t	1	0	0	0	0
57	1v	1	0	0	0	0
57	1w	7	0	0	0	0
57	1x	12	0	0	0	0
57	20	2	0	0	0	0
57	21	1	0	0	0	0
57	23	4	0	0	0	0
57	25	5	0	0	0	0
57	26	1	0	0	0	0
57	27	3	0	0	0	0
57	28	2	0	0	0	0
57	2A	861	0	0	0	0
57	2B	20	0	0	0	0
57	2D	5	0	0	0	0
57	2E	8	0	0	0	0
57	2F	7	0	0	0	0
57	2G	1	0	0	0	0
57	2N	1	0	0	0	0
57	2O	1	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	2	0	0	0	0
57	2V	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	2W	2	0	0	0	0
57	2X	1	0	0	0	0
57	2Y	1	0	0	0	0
57	2Z	1	0	0	0	0
57	2a	225	0	0	0	0
57	2d	2	0	0	0	0
57	2e	1	0	0	0	0
57	2f	2	0	0	0	0
57	2i	1	0	0	0	0
57	2j	1	0	0	0	0
57	2k	1	0	0	0	0
57	2l	3	0	0	0	0
57	2q	2	0	0	0	0
57	2r	1	0	0	0	0
57	2t	1	0	0	0	0
57	2v	4	0	0	0	0
57	2w	4	0	0	0	0
57	2x	4	0	0	0	0
57	2y	1	0	0	0	0
58	1A	1	0	0	0	0
58	2A	1	0	0	0	0
59	1A	20	0	11	1	0
59	2A	20	0	11	0	0
60	14	1	0	0	0	0
60	15	1	0	0	0	0
60	16	1	0	0	0	0
60	19	1	0	0	0	0
60	1Y	1	0	0	0	0
60	1n	1	0	0	0	0
60	24	1	0	0	0	0
60	25	1	0	0	0	0
60	26	1	0	0	0	0
60	29	1	0	0	0	0
60	2Y	1	0	0	0	0
60	2n	1	0	0	0	0
61	1d	8	0	0	0	0
61	2d	8	0	0	1	0
62	10	12	0	0	1	0
62	11	10	0	0	1	0
62	12	3	0	0	1	0
62	13	6	0	0	0	0
62	14	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
62	15	6	0	0	0	0
62	16	5	0	0	0	0
62	17	9	0	0	1	0
62	18	10	0	0	0	0
62	1A	2086	0	0	75	0
62	1B	65	0	0	0	0
62	1D	28	0	0	0	0
62	1E	28	0	0	1	0
62	1F	17	0	0	1	0
62	1G	7	0	0	1	0
62	1H	2	0	0	0	0
62	1N	5	0	0	0	0
62	1O	6	0	0	0	0
62	1P	21	0	0	0	0
62	1Q	7	0	0	0	0
62	1R	7	0	0	0	0
62	1S	3	0	0	0	0
62	1T	9	0	0	0	0
62	1U	13	0	0	1	0
62	1V	9	0	0	0	0
62	1W	5	0	0	0	0
62	1X	6	0	0	1	0
62	1Y	3	0	0	1	0
62	1Z	1	0	0	0	0
62	1a	331	0	0	28	0
62	1b	1	0	0	0	0
62	1d	1	0	0	0	0
62	1e	1	0	0	0	0
62	1l	3	0	0	0	0
62	1m	2	0	0	1	0
62	1q	3	0	0	0	0
62	1u	1	0	0	1	0
62	1v	6	0	0	0	0
62	1w	9	0	0	2	0
62	1x	11	0	0	0	0
62	1y	1	0	0	0	0
62	20	1	0	0	0	0
62	21	8	0	0	0	0
62	23	2	0	0	0	0
62	25	3	0	0	0	0
62	27	5	0	0	0	0
62	28	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
62	29	1	0	0	0	0
62	2A	1147	0	0	73	0
62	2B	21	0	0	0	0
62	2D	18	0	0	0	0
62	2E	14	0	0	0	0
62	2F	12	0	0	0	0
62	2I	1	0	0	0	0
62	2N	2	0	0	0	0
62	2O	2	0	0	0	0
62	2P	10	0	0	1	0
62	2Q	1	0	0	0	0
62	2R	5	0	0	0	0
62	2T	3	0	0	0	0
62	2U	3	0	0	0	0
62	2W	4	0	0	0	0
62	2X	5	0	0	0	0
62	2Z	2	0	0	0	0
62	2a	205	0	0	21	0
62	2c	1	0	0	0	0
62	2i	1	0	0	0	0
62	2j	3	0	0	0	0
62	2l	4	0	0	1	0
62	2r	1	0	0	0	0
62	2t	2	0	0	0	0
62	2v	2	0	0	0	0
62	2w	1	0	0	0	0
62	2x	7	0	0	0	0
All	All	300046	0	196682	4057	1

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

The worst 5 of 4057 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	1.25	1.32
1:1A:1054:A:N6	1:1A:1105:U:H3	1.39	1.19
54:1w:50:A:N6	54:1w:64:U:H3	1.43	1.16
54:2w:8:4SU:HN3	54:2w:14:A:H62	1.08	1.02
1:1A:1082:U:O4	1:1A:1086:A:N1	1.95	0.98

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:368:U:O4	8:2I:82:ARG:NE[2_655]	2.18	0.02

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	1D	273/276 (99%)	256 (94%)	16 (6%)	1 (0%)	30 39
3	2D	273/276 (99%)	256 (94%)	16 (6%)	1 (0%)	30 39
4	1E	202/206 (98%)	192 (95%)	9 (4%)	1 (0%)	24 34
4	2E	202/206 (98%)	193 (96%)	8 (4%)	1 (0%)	24 34
5	1F	200/210 (95%)	193 (96%)	6 (3%)	1 (0%)	24 34
5	2F	200/210 (95%)	187 (94%)	12 (6%)	1 (0%)	24 34
6	1G	179/182 (98%)	166 (93%)	11 (6%)	2 (1%)	11 15
6	2G	179/182 (98%)	150 (84%)	25 (14%)	4 (2%)	5 5
7	1H	172/180 (96%)	162 (94%)	9 (5%)	1 (1%)	21 29
7	2H	172/180 (96%)	155 (90%)	17 (10%)	0	100 100
8	1I	144/148 (97%)	128 (89%)	15 (10%)	1 (1%)	18 25
8	2I	144/148 (97%)	120 (83%)	22 (15%)	2 (1%)	9 11
9	1N	138/140 (99%)	130 (94%)	8 (6%)	0	100 100
9	2N	138/140 (99%)	132 (96%)	6 (4%)	0	100 100
10	1O	120/122 (98%)	114 (95%)	6 (5%)	0	100 100
10	2O	120/122 (98%)	110 (92%)	9 (8%)	1 (1%)	16 22
11	1P	147/150 (98%)	133 (90%)	12 (8%)	2 (1%)	9 11
11	2P	147/150 (98%)	131 (89%)	12 (8%)	4 (3%)	4 3
12	1Q	139/141 (99%)	133 (96%)	6 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
12	2Q	139/141 (99%)	127 (91%)	12 (9%)	0	100 100
13	1R	116/118 (98%)	110 (95%)	6 (5%)	0	100 100
13	2R	116/118 (98%)	112 (97%)	4 (3%)	0	100 100
14	1S	108/112 (96%)	104 (96%)	4 (4%)	0	100 100
14	2S	108/112 (96%)	100 (93%)	4 (4%)	4 (4%)	2 1
15	1T	129/146 (88%)	123 (95%)	4 (3%)	2 (2%)	7 9
15	2T	129/146 (88%)	122 (95%)	7 (5%)	0	100 100
16	1U	114/118 (97%)	114 (100%)	0	0	100 100
16	2U	114/118 (97%)	113 (99%)	1 (1%)	0	100 100
17	1V	99/101 (98%)	95 (96%)	2 (2%)	2 (2%)	6 6
17	2V	99/101 (98%)	93 (94%)	5 (5%)	1 (1%)	12 17
18	1W	110/113 (97%)	109 (99%)	1 (1%)	0	100 100
18	2W	110/113 (97%)	108 (98%)	2 (2%)	0	100 100
19	1X	93/96 (97%)	89 (96%)	3 (3%)	1 (1%)	11 15
19	2X	93/96 (97%)	89 (96%)	4 (4%)	0	100 100
20	1Y	105/110 (96%)	99 (94%)	5 (5%)	1 (1%)	12 17
20	2Y	105/110 (96%)	97 (92%)	8 (8%)	0	100 100
21	1Z	148/206 (72%)	133 (90%)	13 (9%)	2 (1%)	9 11
21	2Z	156/206 (76%)	119 (76%)	34 (22%)	3 (2%)	6 7
22	10	81/85 (95%)	78 (96%)	3 (4%)	0	100 100
22	20	81/85 (95%)	78 (96%)	3 (4%)	0	100 100
23	11	95/98 (97%)	92 (97%)	2 (2%)	1 (1%)	11 15
23	21	95/98 (97%)	90 (95%)	4 (4%)	1 (1%)	11 15
24	12	68/72 (94%)	67 (98%)	1 (2%)	0	100 100
24	22	68/72 (94%)	68 (100%)	0	0	100 100
25	13	57/60 (95%)	55 (96%)	2 (4%)	0	100 100
25	23	57/60 (95%)	54 (95%)	2 (4%)	1 (2%)	6 7
26	14	67/71 (94%)	52 (78%)	9 (13%)	6 (9%)	0 0
26	24	67/71 (94%)	50 (75%)	15 (22%)	2 (3%)	3 2
27	15	57/60 (95%)	56 (98%)	1 (2%)	0	100 100
27	25	57/60 (95%)	55 (96%)	2 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
28	16	51/54 (94%)	50 (98%)	1 (2%)	0	100 100
28	26	51/54 (94%)	46 (90%)	5 (10%)	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%)	60 (97%)	2 (3%)	0	100 100
31	19	35/37 (95%)	35 (100%)	0	0	100 100
31	29	35/37 (95%)	34 (97%)	1 (3%)	0	100 100
33	1b	229/256 (90%)	188 (82%)	32 (14%)	9 (4%)	2 1
33	2b	229/256 (90%)	184 (80%)	37 (16%)	8 (4%)	3 1
34	1c	204/239 (85%)	193 (95%)	11 (5%)	0	100 100
34	2c	204/239 (85%)	176 (86%)	26 (13%)	2 (1%)	12 17
35	1d	206/209 (99%)	189 (92%)	16 (8%)	1 (0%)	24 34
35	2d	206/209 (99%)	190 (92%)	15 (7%)	1 (0%)	24 34
36	1e	146/162 (90%)	131 (90%)	14 (10%)	1 (1%)	18 25
36	2e	146/162 (90%)	127 (87%)	15 (10%)	4 (3%)	4 3
37	1f	98/101 (97%)	91 (93%)	7 (7%)	0	100 100
37	2f	98/101 (97%)	98 (100%)	0	0	100 100
38	1g	153/156 (98%)	140 (92%)	12 (8%)	1 (1%)	18 25
38	2g	153/156 (98%)	139 (91%)	10 (6%)	4 (3%)	4 3
39	1h	135/138 (98%)	126 (93%)	8 (6%)	1 (1%)	18 25
39	2h	135/138 (98%)	124 (92%)	10 (7%)	1 (1%)	18 25
40	1i	125/128 (98%)	111 (89%)	12 (10%)	2 (2%)	7 9
40	2i	125/128 (98%)	108 (86%)	16 (13%)	1 (1%)	16 22
41	1j	95/105 (90%)	76 (80%)	16 (17%)	3 (3%)	3 2
41	2j	94/105 (90%)	79 (84%)	12 (13%)	3 (3%)	3 2
42	1k	112/129 (87%)	106 (95%)	3 (3%)	3 (3%)	4 3
42	2k	112/129 (87%)	101 (90%)	9 (8%)	2 (2%)	6 7
43	1l	119/132 (90%)	113 (95%)	5 (4%)	1 (1%)	16 22
43	2l	119/132 (90%)	109 (92%)	8 (7%)	2 (2%)	7 8
44	1m	121/126 (96%)	105 (87%)	14 (12%)	2 (2%)	7 8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
44	2m	120/126 (95%)	107 (89%)	11 (9%)	2 (2%)	7 8
45	1n	58/61 (95%)	55 (95%)	3 (5%)	0	100 100
45	2n	58/61 (95%)	53 (91%)	3 (5%)	2 (3%)	3 1
46	1o	86/89 (97%)	82 (95%)	2 (2%)	2 (2%)	5 4
46	2o	86/89 (97%)	79 (92%)	6 (7%)	1 (1%)	10 13
47	1p	80/88 (91%)	70 (88%)	10 (12%)	0	100 100
47	2p	80/88 (91%)	73 (91%)	7 (9%)	0	100 100
48	1q	97/105 (92%)	90 (93%)	6 (6%)	1 (1%)	12 17
48	2q	97/105 (92%)	86 (89%)	9 (9%)	2 (2%)	5 5
49	1r	66/88 (75%)	61 (92%)	4 (6%)	1 (2%)	8 10
49	2r	66/88 (75%)	59 (89%)	6 (9%)	1 (2%)	8 10
50	1s	81/93 (87%)	74 (91%)	7 (9%)	0	100 100
50	2s	81/93 (87%)	65 (80%)	14 (17%)	2 (2%)	4 4
51	1t	94/106 (89%)	84 (89%)	8 (8%)	2 (2%)	5 5
51	2t	94/106 (89%)	83 (88%)	10 (11%)	1 (1%)	11 15
52	1u	21/27 (78%)	19 (90%)	2 (10%)	0	100 100
52	2u	21/27 (78%)	18 (86%)	3 (14%)	0	100 100
All	All	11368/12128 (94%)	10432 (92%)	817 (7%)	119 (1%)	12 17

5 of 119 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	1F	130	ALA
6	1G	43	LEU
19	1X	93	GLU
21	1Z	52	SER
26	14	47	GLN

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	1D	215/218 (99%)	207 (96%)	8 (4%)	30 45
3	2D	215/218 (99%)	200 (93%)	15 (7%)	14 19
4	1E	164/166 (99%)	155 (94%)	9 (6%)	19 29
4	2E	164/166 (99%)	155 (94%)	9 (6%)	19 29
5	1F	160/166 (96%)	142 (89%)	18 (11%)	5 6
5	2F	159/166 (96%)	144 (91%)	15 (9%)	8 10
6	1G	143/156 (92%)	128 (90%)	15 (10%)	6 8
6	2G	143/156 (92%)	127 (89%)	16 (11%)	6 6
7	1H	144/148 (97%)	132 (92%)	12 (8%)	10 14
7	2H	144/148 (97%)	128 (89%)	16 (11%)	6 6
8	1I	113/124 (91%)	94 (83%)	19 (17%)	2 2
8	2I	105/124 (85%)	91 (87%)	14 (13%)	4 4
9	1N	118/119 (99%)	108 (92%)	10 (8%)	10 13
9	2N	118/119 (99%)	106 (90%)	12 (10%)	7 8
10	1O	100/100 (100%)	95 (95%)	5 (5%)	22 33
10	2O	100/100 (100%)	97 (97%)	3 (3%)	36 53
11	1P	115/116 (99%)	105 (91%)	10 (9%)	9 13
11	2P	115/116 (99%)	106 (92%)	9 (8%)	11 16
12	1Q	111/111 (100%)	108 (97%)	3 (3%)	39 58
12	2Q	111/111 (100%)	105 (95%)	6 (5%)	20 30
13	1R	101/101 (100%)	93 (92%)	8 (8%)	11 16
13	2R	101/101 (100%)	94 (93%)	7 (7%)	14 20
14	1S	86/88 (98%)	79 (92%)	7 (8%)	11 15
14	2S	85/88 (97%)	74 (87%)	11 (13%)	4 4
15	1T	115/127 (91%)	108 (94%)	7 (6%)	17 25
15	2T	113/127 (89%)	107 (95%)	6 (5%)	20 31
16	1U	93/94 (99%)	88 (95%)	5 (5%)	20 30
16	2U	93/94 (99%)	87 (94%)	6 (6%)	15 22
17	1V	80/82 (98%)	77 (96%)	3 (4%)	29 44
17	2V	80/82 (98%)	74 (92%)	6 (8%)	12 17
18	1W	90/92 (98%)	84 (93%)	6 (7%)	15 21
18	2W	90/92 (98%)	86 (96%)	4 (4%)	25 38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
19	1X	77/78 (99%)	75 (97%)	2 (3%)	40 59
19	2X	77/78 (99%)	74 (96%)	3 (4%)	28 43
20	1Y	85/91 (93%)	80 (94%)	5 (6%)	18 27
20	2Y	85/91 (93%)	76 (89%)	9 (11%)	6 7
21	1Z	135/179 (75%)	126 (93%)	9 (7%)	15 21
21	2Z	137/179 (76%)	120 (88%)	17 (12%)	4 4
22	10	65/67 (97%)	65 (100%)	0	100 100
22	20	65/67 (97%)	63 (97%)	2 (3%)	35 53
23	11	80/83 (96%)	79 (99%)	1 (1%)	61 76
23	21	80/83 (96%)	77 (96%)	3 (4%)	29 44
24	12	65/67 (97%)	61 (94%)	4 (6%)	16 24
24	22	65/67 (97%)	59 (91%)	6 (9%)	8 10
25	13	51/52 (98%)	43 (84%)	8 (16%)	2 2
25	23	50/52 (96%)	48 (96%)	2 (4%)	28 42
26	14	59/63 (94%)	48 (81%)	11 (19%)	1 1
26	24	53/63 (84%)	47 (89%)	6 (11%)	5 6
27	15	50/52 (96%)	46 (92%)	4 (8%)	11 15
27	25	50/52 (96%)	48 (96%)	2 (4%)	28 42
28	16	51/52 (98%)	49 (96%)	2 (4%)	28 43
28	26	50/52 (96%)	46 (92%)	4 (8%)	11 15
29	17	41/42 (98%)	37 (90%)	4 (10%)	7 9
29	27	41/42 (98%)	35 (85%)	6 (15%)	3 2
30	18	54/55 (98%)	53 (98%)	1 (2%)	50 69
30	28	54/55 (98%)	53 (98%)	1 (2%)	50 69
31	19	34/34 (100%)	33 (97%)	1 (3%)	37 55
31	29	34/34 (100%)	31 (91%)	3 (9%)	9 12
33	1b	192/220 (87%)	168 (88%)	24 (12%)	4 4
33	2b	187/220 (85%)	162 (87%)	25 (13%)	4 3
34	1c	142/188 (76%)	131 (92%)	11 (8%)	12 17
34	2c	140/188 (74%)	130 (93%)	10 (7%)	13 19
35	1d	169/181 (93%)	152 (90%)	17 (10%)	7 8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
35	2d	173/181 (96%)	149 (86%)	24 (14%)	3 3
36	1e	113/123 (92%)	104 (92%)	9 (8%)	11 15
36	2e	114/123 (93%)	103 (90%)	11 (10%)	8 9
37	1f	84/90 (93%)	78 (93%)	6 (7%)	13 19
37	2f	85/90 (94%)	81 (95%)	4 (5%)	23 36
38	1g	119/127 (94%)	103 (87%)	16 (13%)	4 3
38	2g	120/127 (94%)	109 (91%)	11 (9%)	8 10
39	1h	114/119 (96%)	108 (95%)	6 (5%)	20 31
39	2h	114/119 (96%)	104 (91%)	10 (9%)	9 12
40	1i	90/99 (91%)	76 (84%)	14 (16%)	2 2
40	2i	89/99 (90%)	76 (85%)	13 (15%)	3 2
41	1j	66/92 (72%)	55 (83%)	11 (17%)	2 2
41	2j	69/92 (75%)	54 (78%)	15 (22%)	1 1
42	1k	82/99 (83%)	73 (89%)	9 (11%)	6 6
42	2k	83/99 (84%)	76 (92%)	7 (8%)	10 14
43	1l	96/108 (89%)	94 (98%)	2 (2%)	47 66
43	2l	96/108 (89%)	88 (92%)	8 (8%)	10 14
44	1m	93/101 (92%)	81 (87%)	12 (13%)	4 4
44	2m	92/101 (91%)	83 (90%)	9 (10%)	7 9
45	1n	49/50 (98%)	46 (94%)	3 (6%)	17 25
45	2n	49/50 (98%)	44 (90%)	5 (10%)	7 8
46	1o	78/80 (98%)	72 (92%)	6 (8%)	12 17
46	2o	78/80 (98%)	72 (92%)	6 (8%)	12 17
47	1p	69/74 (93%)	62 (90%)	7 (10%)	7 8
47	2p	68/74 (92%)	61 (90%)	7 (10%)	7 8
48	1q	94/97 (97%)	85 (90%)	9 (10%)	8 9
48	2q	94/97 (97%)	87 (93%)	7 (7%)	13 17
49	1r	59/77 (77%)	57 (97%)	2 (3%)	32 48
49	2r	59/77 (77%)	54 (92%)	5 (8%)	10 13
50	1s	69/80 (86%)	63 (91%)	6 (9%)	9 13
50	2s	67/80 (84%)	59 (88%)	8 (12%)	5 5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
51	1t	70/82 (85%)	65 (93%)	5 (7%)	13 19
51	2t	70/82 (85%)	65 (93%)	5 (7%)	13 19
52	1u	18/22 (82%)	18 (100%)	0	100 100
52	2u	18/22 (82%)	18 (100%)	0	100 100
All	All	9303/10064 (92%)	8522 (92%)	781 (8%)	10 14

5 of 781 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	2N	43	THR
26	24	59	PHE
11	2P	95	VAL
9	2N	38	HIS
17	2V	61	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 133 such sidechains are listed below:

Mol	Chain	Res	Type
41	2j	13	HIS
42	2k	26	ASN
50	2s	69	HIS
40	1i	124	GLN
40	1i	87	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2864/2915 (98%)	421 (14%)	26 (0%)
1	2A	2791/2915 (95%)	461 (16%)	24 (0%)
2	1B	119/121 (98%)	6 (5%)	0
2	2B	118/121 (97%)	28 (23%)	0
32	1a	1497/1521 (98%)	240 (16%)	0
32	2a	1501/1521 (98%)	277 (18%)	0
53	1v	12/24 (50%)	3 (25%)	0
53	2v	12/24 (50%)	3 (25%)	0
54	1w	70/74 (94%)	24 (34%)	0
54	2w	68/74 (91%)	29 (42%)	0
55	1x	75/77 (97%)	7 (9%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
55	2x	75/77 (97%)	9 (12%)	0
56	1y	71/74 (95%)	27 (38%)	0
56	2y	71/74 (95%)	32 (45%)	0
All	All	9344/9612 (97%)	1567 (16%)	50 (0%)

5 of 1567 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	12	U
1	1A	34	C
1	1A	45	C
1	1A	63	U
1	1A	71	A

5 of 50 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2A	266	G
1	2A	856	C
1	2A	2689	U
1	2A	271(K)	U
1	2A	528	A

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

72 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	PSU	1A	2605	57,1	18,21,22	1.41	3 (16%)	21,30,33	1.95	5 (23%)
32	PSU	1a	516	32	18,21,22	1.44	2 (11%)	21,30,33	2.03	3 (14%)
32	5MC	1a	1407	32	19,22,23	1.79	3 (15%)	26,32,35	1.18	4 (15%)
55	5MC	1x	32	55	19,22,23	1.48	3 (15%)	26,32,35	1.24	2 (7%)
32	5MC	1a	1400	32	19,22,23	1.70	3 (15%)	26,32,35	1.17	4 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
55	PSU	2x	55	55	18,21,22	1.38	2 (11%)	21,30,33	2.08	4 (19%)
43	0TD	2l	92	43	8,9,10	4.63	2 (25%)	6,11,13	4.99	2 (33%)
32	5MC	1a	967	32	19,22,23	1.54	3 (15%)	26,32,35	1.07	2 (7%)
1	5MC	2A	1962	57,1	19,22,23	1.65	3 (15%)	26,32,35	1.14	3 (11%)
32	5MC	1a	1404	32	19,22,23	1.65	3 (15%)	26,32,35	1.10	2 (7%)
1	5MC	2A	1942	1	19,22,23	1.64	2 (10%)	26,32,35	1.16	3 (11%)
1	PSU	2A	1911	1	18,21,22	1.36	2 (11%)	21,30,33	1.93	3 (14%)
32	PSU	2a	516	32	18,21,22	1.36	2 (11%)	21,30,33	1.95	3 (14%)
32	G7M	2a	527	32,57	23,26,27	1.49	3 (13%)	34,39,42	1.67	5 (14%)
55	5MU	1x	54	55	19,22,23	1.45	5 (26%)	27,32,35	1.99	5 (18%)
56	5MU	1y	54	56	19,22,23	1.42	5 (26%)	27,32,35	1.96	7 (25%)
56	PSU	2y	55	56	18,21,22	1.42	2 (11%)	21,30,33	1.98	3 (14%)
1	2MA	2A	2503	57,1	22,25,26	1.47	4 (18%)	32,37,40	2.30	8 (25%)
56	4SU	1y	8	56	18,21,22	1.88	6 (33%)	25,30,33	1.69	5 (20%)
32	G7M	1a	527	32,57	23,26,27	1.47	4 (17%)	34,39,42	1.68	5 (14%)
1	OMU	2A	2552	57,1	19,22,23	1.26	2 (10%)	25,31,34	1.76	6 (24%)
32	UR3	1a	1498	32	19,22,23	1.02	1 (5%)	26,32,35	1.83	4 (15%)
54	4SU	1w	8	54	18,21,22	1.90	5 (27%)	25,30,33	1.95	5 (20%)
54	L3X	1w	76	54,1	24,28,29	1.42	3 (12%)	27,40,43	2.10	9 (33%)
1	PSU	1A	1917	1	18,21,22	1.34	2 (11%)	21,30,33	2.01	4 (19%)
54	5MU	2w	54	54	19,22,23	1.38	4 (21%)	27,32,35	1.73	6 (22%)
55	4SU	1x	8	55	18,21,22	2.14	6 (33%)	25,30,33	1.65	7 (28%)
1	5MC	1A	1942	1	19,22,23	1.68	3 (15%)	26,32,35	1.15	2 (7%)
1	OMC	2A	1920	1	19,22,23	0.78	0	25,31,34	0.96	1 (4%)
1	OMG	1A	2251	57,55,1	23,26,27	1.31	3 (13%)	32,38,41	1.97	6 (18%)
32	UR3	2a	1498	32	19,22,23	1.01	1 (5%)	26,32,35	1.76	3 (11%)
55	PSU	1x	55	55	18,21,22	1.37	2 (11%)	21,30,33	2.03	3 (14%)
56	4SU	2y	8	56	18,21,22	1.79	5 (27%)	25,30,33	1.93	5 (20%)
43	0TD	1l	92	43	8,9,10	4.56	1 (12%)	6,11,13	2.89	2 (33%)
1	5MU	2A	1915	1	19,22,23	1.41	5 (26%)	27,32,35	2.15	6 (22%)
56	PSU	1y	55	56	18,21,22	1.40	2 (11%)	21,30,33	2.12	4 (19%)
1	2MA	1A	2503	57,1	22,25,26	1.42	5 (22%)	32,37,40	2.30	10 (31%)
54	5MU	1w	54	54	19,22,23	1.38	4 (21%)	27,32,35	1.90	6 (22%)
32	M2G	1a	966	32	24,27,28	1.30	4 (16%)	33,40,43	1.87	6 (18%)
32	MA6	1a	1518	32	23,26,27	0.42	0	33,38,41	2.00	9 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
32	M2G	2a	966	32	24,27,28	1.31	4 (16%)	33,40,43	1.90	6 (18%)
1	5MC	1A	1962	57,1	19,22,23	1.74	3 (15%)	26,32,35	1.17	3 (11%)
32	4OC	2a	1402	32,57	20,23,24	0.75	0	25,32,35	1.09	2 (8%)
32	2MG	1a	1207	32	23,26,27	1.24	3 (13%)	33,38,41	2.25	10 (30%)
32	5MC	2a	1407	32	19,22,23	1.67	3 (15%)	26,32,35	1.24	3 (11%)
54	PSU	2w	55	54,57	18,21,22	1.36	2 (11%)	21,30,33	2.03	4 (19%)
55	31H	2x	76	57,55	31,34,35	1.20	3 (9%)	35,47,50	2.11	13 (37%)
32	MA6	2a	1519	32	23,26,27	0.44	0	33,38,41	2.09	10 (30%)
54	PSU	1w	55	54,57	18,21,22	1.40	2 (11%)	21,30,33	2.04	3 (14%)
1	PSU	2A	1917	1	18,21,22	1.39	2 (11%)	21,30,33	2.01	4 (19%)
1	PSU	1A	1911	1	18,21,22	1.38	2 (11%)	21,30,33	2.12	4 (19%)
32	5MC	2a	1400	32	19,22,23	1.67	3 (15%)	26,32,35	1.18	3 (11%)
1	5MU	2A	1939	1	19,22,23	1.34	5 (26%)	27,32,35	2.37	6 (22%)
32	MA6	2a	1518	32	23,26,27	0.42	0	33,38,41	2.04	9 (27%)
32	5MC	2a	967	32	19,22,23	1.64	2 (10%)	26,32,35	1.07	2 (7%)
55	5MC	2x	32	55	19,22,23	1.74	3 (15%)	26,32,35	1.28	3 (11%)
32	5MC	2a	1404	32	19,22,23	1.62	3 (15%)	26,32,35	1.23	3 (11%)
55	31H	1x	76	57,55	31,34,35	1.18	3 (9%)	35,47,50	2.09	11 (31%)
1	OMU	1A	2552	57,1	19,22,23	1.21	2 (10%)	25,31,34	1.93	5 (20%)
54	L3X	2w	76	54,1	24,28,29	1.40	3 (12%)	27,40,43	2.14	9 (33%)
56	5MU	2y	54	56	19,22,23	1.48	4 (21%)	27,32,35	1.91	8 (29%)
1	OMG	2A	2251	55,1	23,26,27	1.23	3 (13%)	32,38,41	1.97	7 (21%)
1	PSU	2A	2605	1	18,21,22	1.29	2 (11%)	21,30,33	2.06	4 (19%)
32	4OC	1a	1402	32	20,23,24	0.76	0	25,32,35	0.96	1 (4%)
1	OMC	1A	1920	1	19,22,23	0.77	0	25,31,34	0.93	1 (4%)
32	MA6	1a	1519	32	23,26,27	0.46	0	33,38,41	2.09	9 (27%)
32	2MG	2a	1207	32	23,26,27	1.27	3 (13%)	33,38,41	2.11	6 (18%)
54	4SU	2w	8	54	18,21,22	1.77	4 (22%)	25,30,33	3.15	6 (24%)
55	4SU	2x	8	55	18,21,22	2.00	7 (38%)	25,30,33	1.32	3 (12%)
55	5MU	2x	54	55	19,22,23	1.38	4 (21%)	27,32,35	2.07	6 (22%)
1	5MU	1A	1915	1	19,22,23	1.38	5 (26%)	27,32,35	2.09	5 (18%)
1	5MU	1A	1939	57,1	19,22,23	1.41	5 (26%)	27,32,35	2.30	6 (22%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	1A	2605	57,1	-	0/7/25/26	0/2/2/2
32	PSU	1a	516	32	-	0/7/25/26	0/2/2/2
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
55	5MC	1x	32	55	-	0/7/25/26	0/2/2/2
32	5MC	1a	1400	32	-	2/7/25/26	0/2/2/2
55	PSU	2x	55	55	-	0/7/25/26	0/2/2/2
43	0TD	2l	92	43	-	2/7/12/14	-
32	5MC	1a	967	32	-	1/7/25/26	0/2/2/2
1	5MC	2A	1962	57,1	-	2/7/25/26	0/2/2/2
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
32	PSU	2a	516	32	-	0/7/25/26	0/2/2/2
32	G7M	2a	527	32,57	-	2/7/25/26	0/3/3/3
55	5MU	1x	54	55	-	0/7/25/26	0/2/2/2
56	5MU	1y	54	56	-	0/7/25/26	0/2/2/2
56	PSU	2y	55	56	-	2/7/25/26	0/2/2/2
1	2MA	2A	2503	57,1	-	1/7/25/26	0/3/3/3
56	4SU	1y	8	56	-	1/7/25/26	0/2/2/2
32	G7M	1a	527	32,57	-	3/7/25/26	0/3/3/3
1	OMU	2A	2552	57,1	-	0/9/27/28	0/2/2/2
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
54	4SU	1w	8	54	-	0/7/25/26	0/2/2/2
54	L3X	1w	76	54,1	-	1/13/31/32	0/3/3/3
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
54	5MU	2w	54	54	-	0/7/25/26	0/2/2/2
55	4SU	1x	8	55	-	0/7/25/26	0/2/2/2
1	5MC	1A	1942	1	-	0/7/25/26	0/2/2/2
1	OMC	2A	1920	1	-	0/9/27/28	0/2/2/2
1	OMG	1A	2251	57,55,1	-	0/9/27/28	0/3/3/3
32	UR3	2a	1498	32	-	0/7/25/26	0/2/2/2
55	PSU	1x	55	55	-	2/7/25/26	0/2/2/2
56	4SU	2y	8	56	-	3/7/25/26	0/2/2/2
43	0TD	1l	92	43	-	1/7/12/14	-
1	5MU	2A	1915	1	-	0/7/25/26	0/2/2/2
56	PSU	1y	55	56	-	1/7/25/26	0/2/2/2
1	2MA	1A	2503	57,1	-	1/7/25/26	0/3/3/3
54	5MU	1w	54	54	-	0/7/25/26	0/2/2/2
32	M2G	1a	966	32	-	0/11/29/30	0/3/3/3

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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	M2G	2a	966	32	-	0/11/29/30	0/3/3/3
1	5MC	1A	1962	57,1	-	0/7/25/26	0/2/2/2
32	4OC	2a	1402	32,57	-	3/9/29/30	0/2/2/2
32	2MG	1a	1207	32	-	2/9/27/28	0/3/3/3
32	5MC	2a	1407	32	-	0/7/25/26	0/2/2/2
54	PSU	2w	55	54,57	-	0/7/25/26	0/2/2/2
55	31H	2x	76	57,55	-	4/22/40/41	0/3/3/3
32	MA6	2a	1519	32	-	3/11/29/30	0/3/3/3
54	PSU	1w	55	54,57	-	0/7/25/26	0/2/2/2
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
32	5MC	2a	1400	32	-	0/7/25/26	0/2/2/2
1	5MU	2A	1939	1	-	0/7/25/26	0/2/2/2
32	MA6	2a	1518	32	-	0/11/29/30	0/3/3/3
32	5MC	2a	967	32	-	0/7/25/26	0/2/2/2
55	5MC	2x	32	55	-	0/7/25/26	0/2/2/2
32	5MC	2a	1404	32	-	0/7/25/26	0/2/2/2
55	31H	1x	76	57,55	-	5/22/40/41	0/3/3/3
1	OMU	1A	2552	57,1	-	0/9/27/28	0/2/2/2
54	L3X	2w	76	54,1	-	2/13/31/32	0/3/3/3
56	5MU	2y	54	56	-	3/7/25/26	0/2/2/2
1	OMG	2A	2251	55,1	-	0/9/27/28	0/3/3/3
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
32	4OC	1a	1402	32	-	2/9/29/30	0/2/2/2
1	OMC	1A	1920	1	-	0/9/27/28	0/2/2/2
32	MA6	1a	1519	32	-	3/11/29/30	0/3/3/3
32	2MG	2a	1207	32	-	1/9/27/28	0/3/3/3
54	4SU	2w	8	54	-	0/7/25/26	0/2/2/2
55	4SU	2x	8	55	-	0/7/25/26	0/2/2/2
55	5MU	2x	54	55	-	0/7/25/26	0/2/2/2
1	5MU	1A	1915	1	-	0/7/25/26	0/2/2/2
1	5MU	1A	1939	57,1	-	0/7/25/26	0/2/2/2

The worst 5 of 205 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	2l	92	0TD	CB-SB	-12.51	1.69	1.82
43	1l	92	0TD	CB-SB	-12.39	1.69	1.82
32	1a	1407	5MC	C5-C4	6.88	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	1962	5MC	C5-C4	6.37	1.48	1.44
55	2x	32	5MC	C5-C4	6.34	1.48	1.44

The worst 5 of 357 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	2l	92	0TD	CSB-SB-CB	-11.56	81.58	102.36
54	2w	8	4SU	C4-N3-C2	-9.28	118.42	127.31
1	2A	2503	2MA	C5-C4-N3	-8.13	118.62	127.18
54	2w	8	4SU	C5-C4-S4	-7.47	115.78	124.31
1	1A	2503	2MA	C5-C4-N3	-7.38	119.40	127.18

There are no chirality outliers.

5 of 53 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	1a	1207	2MG	N1-C2-N2-CM2
32	1a	1207	2MG	N3-C2-N2-CM2
32	1a	1519	MA6	O4'-C4'-C5'-O5'
32	2a	1207	2MG	N3-C2-N2-CM2
32	2a	1402	4OC	O4'-C4'-C5'-O5'

There are no ring outliers.

29 monomers are involved in 47 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
43	2l	92	0TD	1	0
1	2A	2503	2MA	1	0
56	1y	8	4SU	2	0
1	2A	2552	OMU	1	0
54	1w	8	4SU	1	0
54	1w	76	L3X	1	0
54	2w	54	5MU	2	0
55	1x	8	4SU	2	0
56	2y	8	4SU	2	0
1	2A	1915	5MU	1	0
54	1w	54	5MU	1	0
32	1a	966	M2G	1	0
32	1a	1518	MA6	2	0
32	2a	1402	4OC	2	0
55	2x	76	31H	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	2a	1519	MA6	3	0
54	1w	55	PSU	3	0
32	2a	1518	MA6	3	0
32	2a	1404	5MC	2	0
55	1x	76	31H	2	0
1	1A	2552	OMU	2	0
54	2w	76	L3X	2	0
56	2y	54	5MU	1	0
1	2A	2251	OMG	1	0
32	1a	1402	4OC	2	0
32	1a	1519	MA6	1	0
54	2w	8	4SU	7	0
1	1A	1915	5MU	2	0
1	1A	1939	5MU	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2761 ligands modelled in this entry, 2757 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
59	CLM	2A	3863	-	20,20,20	1.01	1 (5%)	23,27,27	1.02	2 (8%)
61	SF4	1d	501	35	0,12,12	-	-	-		
59	CLM	1A	4097	-	20,20,20	0.97	2 (10%)	23,27,27	1.22	2 (8%)
61	SF4	2d	303	35	0,12,12	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	CLM	2A	3863	-	-	0/20/22/22	0/1/1/1
61	SF4	1d	501	35	-	-	0/6/5/5
59	CLM	1A	4097	-	-	2/20/22/22	0/1/1/1
61	SF4	2d	303	35	-	-	0/6/5/5

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	1A	4097	CLM	C6-C5	-2.43	1.48	1.51
59	2A	3863	CLM	C6-C5	-2.37	1.48	1.51
59	1A	4097	CLM	C9-N9	-2.34	1.39	1.45

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
59	1A	4097	CLM	O5-C5-C6	-3.43	103.76	111.20
59	2A	3863	CLM	C6-C5-C3	2.65	116.48	111.72
59	1A	4097	CLM	C6-C5-C3	2.54	116.27	111.72
59	2A	3863	CLM	O5-C5-C6	-2.02	106.82	111.20

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
59	1A	4097	CLM	N2-C3-C4-O4
59	1A	4097	CLM	C5-C3-C4-O4

There are no ring outliers.

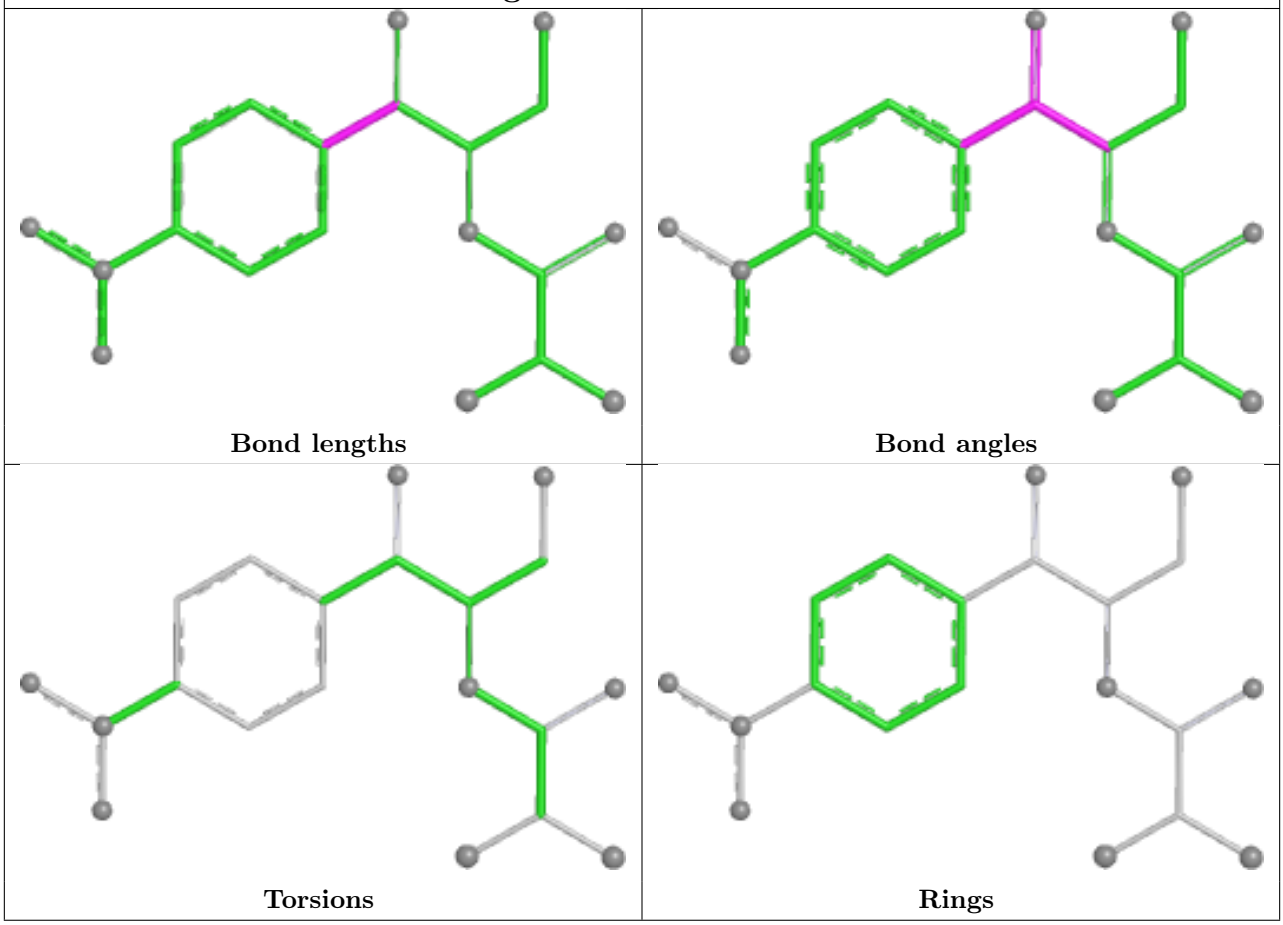
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
59	1A	4097	CLM	1	0
61	2d	303	SF4	1	0

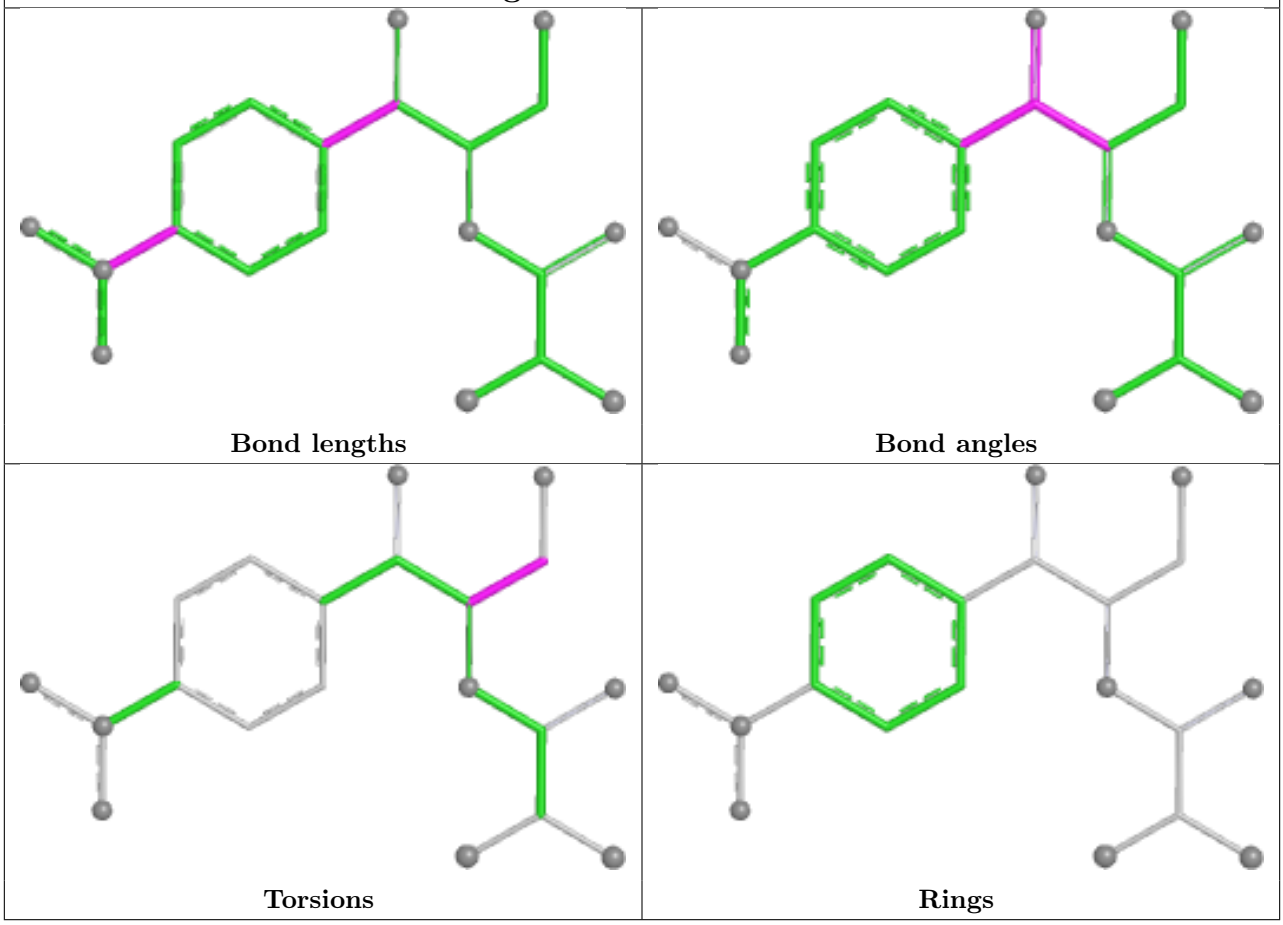
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand CLM 2A 3863



Ligand CLM 1A 4097



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	2860/2915 (98%)	-0.45	125 (4%) 39 39	23, 38, 94, 106	0
1	2A	2789/2915 (95%)	0.08	116 (4%) 40 41	34, 60, 92, 105	0
2	1B	120/121 (99%)	-0.33	0 100 100	31, 52, 67, 87	0
2	2B	120/121 (99%)	0.81	0 100 100	65, 79, 87, 91	0
3	1D	275/276 (99%)	0.05	4 (1%) 72 73	24, 40, 54, 72	0
3	2D	275/276 (99%)	0.48	8 (2%) 53 55	33, 53, 66, 81	0
4	1E	204/206 (99%)	-0.05	1 (0%) 87 89	20, 42, 61, 73	0
4	2E	204/206 (99%)	0.53	4 (1%) 65 65	36, 60, 71, 83	0
5	1F	202/210 (96%)	0.10	1 (0%) 87 89	21, 45, 68, 80	0
5	2F	202/210 (96%)	0.61	3 (1%) 72 73	39, 70, 80, 86	0
6	1G	181/182 (99%)	0.75	13 (7%) 21 20	43, 61, 75, 86	0
6	2G	181/182 (99%)	1.39	33 (18%) 3 3	70, 79, 85, 91	0
7	1H	174/180 (96%)	0.38	3 (1%) 69 69	40, 54, 66, 72	0
7	2H	174/180 (96%)	1.44	39 (22%) 2 2	70, 81, 88, 95	0
8	1I	146/148 (98%)	0.85	6 (4%) 41 42	43, 73, 81, 84	0
8	2I	146/148 (98%)	1.37	28 (19%) 3 2	59, 74, 81, 84	0
9	1N	140/140 (100%)	0.06	2 (1%) 73 74	27, 40, 60, 72	0
9	2N	140/140 (100%)	0.95	10 (7%) 22 21	47, 66, 77, 84	0
10	1O	122/122 (100%)	0.16	1 (0%) 82 84	32, 42, 60, 66	0
10	2O	122/122 (100%)	0.53	0 100 100	45, 59, 71, 75	0
11	1P	149/150 (99%)	0.20	2 (1%) 75 75	23, 48, 67, 74	0
11	2P	149/150 (99%)	0.80	7 (4%) 36 36	41, 69, 82, 87	0
12	1Q	141/141 (100%)	0.03	1 (0%) 84 86	26, 43, 58, 72	0
12	2Q	141/141 (100%)	1.02	11 (7%) 19 18	48, 67, 76, 83	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	1R	118/118 (100%)	-0.04	0 100 100	27, 37, 50, 60	0
13	2R	118/118 (100%)	0.57	2 (1%) 69 69	42, 55, 64, 71	0
14	1S	110/112 (98%)	0.29	1 (0%) 81 83	41, 52, 63, 67	0
14	2S	110/112 (98%)	1.54	31 (28%) 1 1	64, 74, 80, 83	0
15	1T	131/146 (89%)	0.26	4 (3%) 51 52	32, 47, 68, 79	0
15	2T	131/146 (89%)	0.70	4 (3%) 51 52	51, 61, 76, 80	0
16	1U	116/118 (98%)	-0.23	1 (0%) 81 83	23, 33, 49, 61	0
16	2U	116/118 (98%)	0.80	2 (1%) 69 69	48, 62, 75, 79	0
17	1V	101/101 (100%)	0.03	2 (1%) 65 65	26, 42, 58, 70	0
17	2V	101/101 (100%)	1.04	8 (7%) 18 18	47, 70, 76, 87	0
18	1W	112/113 (99%)	-0.10	2 (1%) 67 68	27, 35, 53, 75	0
18	2W	112/113 (99%)	0.48	3 (2%) 56 57	41, 51, 69, 90	0
19	1X	95/96 (98%)	0.14	3 (3%) 50 51	29, 40, 64, 81	0
19	2X	95/96 (98%)	0.90	7 (7%) 20 19	48, 62, 77, 86	0
20	1Y	107/110 (97%)	0.33	1 (0%) 81 83	38, 51, 68, 79	0
20	2Y	107/110 (97%)	1.15	16 (14%) 5 5	63, 71, 80, 86	0
21	1Z	154/206 (74%)	0.84	14 (9%) 15 14	42, 64, 85, 88	0
21	2Z	160/206 (77%)	1.51	43 (26%) 1 1	64, 80, 89, 93	0
22	10	83/85 (97%)	0.17	3 (3%) 46 47	29, 40, 57, 64	0
22	20	83/85 (97%)	1.29	12 (14%) 6 5	46, 65, 74, 80	0
23	11	97/98 (98%)	0.33	1 (1%) 79 80	28, 47, 71, 74	0
23	21	97/98 (98%)	0.96	6 (6%) 26 26	40, 59, 74, 78	0
24	12	70/72 (97%)	0.37	1 (1%) 73 74	38, 50, 62, 73	0
24	22	70/72 (97%)	0.91	3 (4%) 40 40	61, 71, 77, 79	0
25	13	59/60 (98%)	-0.01	0 100 100	28, 39, 58, 70	0
25	23	59/60 (98%)	0.93	4 (6%) 23 22	58, 67, 75, 79	0
26	14	69/71 (97%)	1.28	14 (20%) 3 2	53, 76, 86, 88	0
26	24	69/71 (97%)	1.76	24 (34%) 1 0	78, 85, 90, 94	0
27	15	59/60 (98%)	-0.15	0 100 100	21, 35, 51, 59	0
27	25	59/60 (98%)	0.56	0 100 100	39, 53, 68, 75	0
28	16	53/54 (98%)	-0.04	0 100 100	33, 45, 59, 63	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
28	26	53/54 (98%)	0.78	5 (9%) 14 13	55, 64, 70, 71	0
29	17	48/49 (97%)	-0.10	4 (8%) 17 17	24, 31, 53, 64	0
29	27	48/49 (97%)	0.36	3 (6%) 26 25	34, 44, 64, 76	0
30	18	64/65 (98%)	-0.11	0 100 100	27, 37, 45, 57	0
30	28	64/65 (98%)	0.75	1 (1%) 70 71	45, 58, 64, 68	0
31	19	37/37 (100%)	-0.13	0 100 100	33, 42, 56, 63	0
31	29	37/37 (100%)	1.08	4 (10%) 11 10	61, 68, 74, 80	0
32	1a	1488/1521 (97%)	0.26	27 (1%) 67 68	38, 69, 92, 102	0
32	2a	1491/1521 (98%)	0.69	89 (5%) 27 27	52, 79, 94, 104	0
33	1b	231/256 (90%)	1.36	49 (21%) 2 2	66, 78, 85, 90	0
33	2b	231/256 (90%)	1.66	73 (31%) 1 0	73, 84, 89, 94	0
34	1c	206/239 (86%)	1.06	22 (10%) 11 10	59, 73, 82, 88	0
34	2c	206/239 (86%)	1.93	88 (42%) 0 0	76, 84, 88, 92	0
35	1d	208/209 (99%)	1.31	39 (18%) 3 2	59, 70, 78, 81	0
35	2d	208/209 (99%)	1.21	29 (13%) 6 5	63, 74, 81, 85	0
36	1e	148/162 (91%)	0.80	5 (3%) 48 49	49, 66, 74, 77	0
36	2e	148/162 (91%)	1.35	25 (16%) 4 3	67, 77, 83, 86	0
37	1f	100/101 (99%)	0.86	2 (2%) 65 65	60, 70, 77, 80	0
37	2f	100/101 (99%)	1.02	6 (6%) 27 27	62, 73, 79, 80	0
38	1g	155/156 (99%)	0.98	16 (10%) 12 11	63, 73, 83, 89	0
38	2g	155/156 (99%)	1.63	44 (28%) 1 1	73, 80, 86, 91	0
39	1h	137/138 (99%)	0.87	5 (3%) 46 47	59, 67, 74, 77	0
39	2h	137/138 (99%)	1.30	19 (13%) 6 5	69, 77, 82, 86	0
40	1i	127/128 (99%)	1.32	20 (15%) 5 4	56, 77, 83, 85	0
40	2i	127/128 (99%)	2.40	77 (60%) 0 0	73, 84, 89, 92	0
41	1j	97/105 (92%)	1.68	33 (34%) 1 0	62, 78, 84, 86	0
41	2j	96/105 (91%)	2.26	53 (55%) 0 0	72, 84, 89, 93	0
42	1k	114/129 (88%)	0.86	7 (6%) 27 26	45, 68, 77, 86	0
42	2k	114/129 (88%)	1.27	15 (13%) 7 6	57, 74, 82, 84	0
43	1l	121/132 (91%)	0.86	6 (4%) 34 33	50, 60, 69, 81	0
43	2l	121/132 (91%)	1.41	28 (23%) 2 1	61, 72, 78, 81	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
44	1m	123/126 (97%)	1.23	12 (9%) 13 12	60, 72, 80, 91	0
44	2m	122/126 (96%)	1.77	33 (27%) 1 1	73, 82, 88, 93	0
45	1n	60/61 (98%)	1.19	7 (11%) 9 8	60, 70, 76, 78	0
45	2n	60/61 (98%)	2.59	37 (61%) 0 0	77, 84, 89, 90	0
46	1o	88/89 (98%)	0.94	6 (6%) 23 22	51, 66, 76, 78	0
46	2o	88/89 (98%)	0.93	8 (9%) 15 14	64, 74, 81, 84	0
47	1p	82/88 (93%)	1.46	16 (19%) 3 2	56, 72, 78, 81	0
47	2p	82/88 (93%)	1.09	7 (8%) 16 16	62, 71, 78, 83	0
48	1q	99/105 (94%)	1.29	16 (16%) 4 3	54, 69, 77, 80	0
48	2q	99/105 (94%)	1.05	7 (7%) 22 21	64, 74, 80, 87	0
49	1r	68/88 (77%)	0.69	1 (1%) 72 73	57, 68, 75, 78	0
49	2r	68/88 (77%)	1.14	6 (8%) 15 15	68, 75, 80, 82	0
50	1s	83/93 (89%)	1.34	11 (13%) 7 6	67, 75, 82, 84	0
50	2s	83/93 (89%)	2.36	54 (65%) 0 0	78, 86, 91, 94	0
51	1t	96/106 (90%)	1.32	17 (17%) 4 3	64, 72, 79, 82	0
51	2t	96/106 (90%)	0.94	6 (6%) 26 25	60, 72, 82, 84	0
52	1u	23/27 (85%)	1.27	4 (17%) 4 3	65, 71, 76, 79	0
52	2u	23/27 (85%)	2.08	11 (47%) 0 0	76, 81, 85, 86	0
53	1v	13/24 (54%)	1.15	5 (38%) 1 0	50, 71, 91, 94	0
53	2v	13/24 (54%)	2.06	5 (38%) 1 0	72, 85, 99, 101	0
54	1w	69/74 (93%)	1.25	12 (17%) 4 3	49, 93, 100, 101	0
54	2w	68/74 (91%)	1.56	10 (14%) 6 5	66, 96, 100, 101	0
55	1x	72/77 (93%)	0.42	1 (1%) 73 74	30, 68, 84, 88	0
55	2x	72/77 (93%)	0.86	3 (4%) 40 41	50, 82, 91, 97	0
56	1y	70/74 (94%)	2.19	41 (58%) 0 0	60, 98, 103, 105	0
56	2y	70/74 (94%)	2.15	42 (60%) 0 0	70, 99, 104, 104	0
All	All	20885/21740 (96%)	0.54	1802 (8%) 16 15	20, 66, 89, 106	0

The worst 5 of 1802 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
44	2m	124	PRO	10.4
44	1m	124	PRO	9.7

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Mol	Chain	Res	Type	RSRZ
44	1m	123	ALA	8.4
1	2A	2111	C	7.2
44	2m	123	ALA	6.7

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
56	4SU	2y	8	20/21	0.44	0.18	93,99,108,115	0
56	4SU	1y	8	20/21	0.51	0.17	92,98,101,118	0
56	5MU	2y	54	21/22	0.52	0.17	96,99,105,120	0
56	PSU	2y	55	20/21	0.56	0.17	96,103,107,108	0
56	PSU	1y	55	20/21	0.62	0.15	94,98,104,112	0
54	4SU	2w	8	20/21	0.62	0.15	90,97,110,116	0
56	5MU	1y	54	21/22	0.63	0.13	90,94,100,113	0
54	5MU	2w	54	21/22	0.69	0.14	83,91,95,98	0
54	PSU	2w	55	20/21	0.70	0.13	88,94,103,103	0
54	4SU	1w	8	20/21	0.71	0.13	94,96,106,110	0
54	PSU	1w	55	20/21	0.78	0.13	81,90,98,98	0
32	2MG	2a	1207	24/25	0.78	0.16	82,88,96,101	0
54	5MU	1w	54	21/22	0.83	0.12	72,83,88,93	0
1	5MU	2A	1915	21/22	0.85	0.14	75,77,81,91	0
55	5MU	2x	54	21/22	0.86	0.14	79,86,90,97	0
32	PSU	2a	516	20/21	0.87	0.13	76,83,88,91	0
55	PSU	2x	55	20/21	0.87	0.12	77,82,88,96	0
32	M2G	2a	966	25/26	0.88	0.16	60,70,81,88	0
55	PSU	1x	55	20/21	0.88	0.12	60,65,77,78	0
55	4SU	2x	8	20/21	0.88	0.12	77,81,87,88	0
32	5MC	2a	967	21/22	0.89	0.13	68,74,80,83	0
43	0TD	1l	92	10/11	0.89	0.14	54,56,61,70	0
55	5MU	1x	54	21/22	0.90	0.12	65,74,76,83	0
1	PSU	2A	1917	20/21	0.90	0.12	67,75,84,85	0
55	5MC	2x	32	21/22	0.91	0.15	66,78,80,80	0
32	5MC	2a	1404	21/22	0.92	0.13	54,61,67,72	0
55	4SU	1x	8	20/21	0.92	0.11	58,64,79,80	0
32	G7M	2a	527	24/25	0.92	0.12	65,72,80,82	0
32	2MG	1a	1207	24/25	0.92	0.10	68,73,79,87	0
32	PSU	1a	516	20/21	0.92	0.10	62,66,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	PSU	2A	1911	20/21	0.92	0.11	64,69,77,81	0
32	5MC	2a	1400	21/22	0.92	0.15	68,76,80,86	0
32	4OC	2a	1402	22/23	0.93	0.12	56,64,68,72	0
54	L3X	2w	76	26/27	0.93	0.12	52,59,63,64	0
1	5MU	1A	1915	21/22	0.93	0.10	51,60,65,69	0
32	5MC	2a	1407	21/22	0.93	0.12	54,60,67,75	0
1	OMC	2A	1920	21/22	0.93	0.13	58,67,71,79	0
55	5MC	1x	32	21/22	0.94	0.12	51,57,64,66	0
43	0TD	2l	92	10/11	0.94	0.12	67,72,77,86	0
32	MA6	2a	1518	24/25	0.94	0.12	56,69,73,76	0
32	UR3	2a	1498	21/22	0.95	0.11	59,63,69,71	0
55	31H	2x	76	32/33	0.95	0.12	42,54,62,74	0
32	M2G	1a	966	25/26	0.95	0.12	55,60,70,72	0
32	MA6	2a	1519	24/25	0.95	0.13	56,65,71,72	0
32	5MC	1a	967	21/22	0.96	0.09	55,61,68,71	0
1	5MC	1A	1942	21/22	0.96	0.09	36,42,49,61	0
1	5MU	2A	1939	21/22	0.96	0.08	34,38,45,47	0
1	5MC	2A	1942	21/22	0.96	0.09	54,59,65,73	0
55	31H	1x	76	32/33	0.96	0.10	24,38,45,54	10
1	5MC	2A	1962	21/22	0.96	0.09	47,51,61,72	0
54	L3X	1w	76	26/27	0.96	0.08	37,42,48,51	0
1	2MA	2A	2503	23/24	0.96	0.10	34,42,44,45	0
32	5MC	1a	1404	21/22	0.96	0.09	39,44,47,47	0
1	PSU	1A	1911	20/21	0.96	0.09	44,49,58,58	0
32	G7M	1a	527	24/25	0.96	0.09	49,54,59,63	0
1	PSU	1A	1917	20/21	0.96	0.08	48,56,61,64	0
32	5MC	1a	1407	21/22	0.97	0.08	34,43,45,46	0
32	MA6	1a	1519	24/25	0.97	0.09	40,45,50,55	0
1	OMC	1A	1920	21/22	0.97	0.08	37,46,49,52	0
32	5MC	1a	1400	21/22	0.97	0.08	41,50,53,55	0
1	OMG	2A	2251	24/25	0.97	0.08	38,44,50,55	0
32	4OC	1a	1402	22/23	0.97	0.07	36,46,53,58	0
1	OMU	2A	2552	21/22	0.97	0.08	37,42,48,51	0
1	PSU	2A	2605	20/21	0.97	0.07	39,45,51,52	0
1	PSU	1A	2605	20/21	0.97	0.07	24,30,35,38	0
1	5MC	1A	1962	21/22	0.98	0.06	27,38,41,46	0
1	OMG	1A	2251	24/25	0.98	0.06	23,28,33,34	0
1	2MA	1A	2503	23/24	0.98	0.06	19,24,28,31	0
1	OMU	1A	2552	21/22	0.98	0.07	26,30,33,37	0
32	UR3	1a	1498	21/22	0.98	0.07	35,44,47,50	0
32	MA6	1a	1518	24/25	0.98	0.09	40,46,49,51	0
1	5MU	1A	1939	21/22	0.98	0.06	24,28,33,34	0

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
57	MG	2j	201	1/1	0.47	0.21	88,88,88,88	0
57	MG	2A	3669	1/1	0.49	0.27	83,83,83,83	0
57	MG	2A	3573	1/1	0.51	0.26	86,86,86,86	0
57	MG	2A	3752	1/1	0.54	0.17	80,80,80,80	0
57	MG	1A	3880	1/1	0.55	0.35	80,80,80,80	0
57	MG	1w	105	1/1	0.56	0.22	88,88,88,88	0
57	MG	1A	3798	1/1	0.58	0.16	61,61,61,61	0
57	MG	2w	101	1/1	0.60	0.21	83,83,83,83	0
57	MG	1B	229	1/1	0.61	0.29	86,86,86,86	0
57	MG	2A	3513	1/1	0.64	0.37	85,85,85,85	0
57	MG	2A	3681	1/1	0.65	0.19	70,70,70,70	0
57	MG	2B	201	1/1	0.66	0.26	82,82,82,82	0
57	MG	2A	3858	1/1	0.67	0.25	75,75,75,75	0
57	MG	2A	3424	1/1	0.68	0.48	88,88,88,88	0
57	MG	2A	3710	1/1	0.68	0.18	71,71,71,71	0
57	MG	2A	3278	1/1	0.68	0.15	75,75,75,75	0
57	MG	2A	3801	1/1	0.68	0.18	71,71,71,71	0
57	MG	2A	3325	1/1	0.68	0.41	79,79,79,79	0
57	MG	2A	3660	1/1	0.68	0.18	78,78,78,78	0
57	MG	2A	3364	1/1	0.68	0.23	77,77,77,77	0
57	MG	2A	3672	1/1	0.68	0.12	76,76,76,76	0
57	MG	2A	3691	1/1	0.69	0.26	74,74,74,74	0
57	MG	2A	3706	1/1	0.69	0.22	76,76,76,76	0
57	MG	1A	3997	1/1	0.69	0.15	64,64,64,64	0
57	MG	2a	1805	1/1	0.69	0.24	71,71,71,71	0
57	MG	2A	3106	1/1	0.69	0.25	71,71,71,71	0
57	MG	2A	3757	1/1	0.69	0.21	66,66,66,66	0
57	MG	2A	3662	1/1	0.70	0.27	70,70,70,70	0
57	MG	1A	3640	1/1	0.70	0.19	80,80,80,80	0
57	MG	2a	1747	1/1	0.70	0.33	77,77,77,77	0
57	MG	2A	3299	1/1	0.71	0.29	84,84,84,84	0
57	MG	1B	231	1/1	0.71	0.14	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3539	1/1	0.71	0.19	62,62,62,62	0
57	MG	2A	3817	1/1	0.71	0.18	60,60,60,60	0
57	MG	1A	3360	1/1	0.71	0.24	77,77,77,77	0
57	MG	1A	4064	1/1	0.72	0.15	69,69,69,69	0
57	MG	1x	103	1/1	0.72	0.24	70,70,70,70	0
57	MG	2A	3099	1/1	0.72	0.16	76,76,76,76	0
57	MG	1A	3684	1/1	0.72	0.21	81,81,81,81	0
57	MG	1A	3999	1/1	0.72	0.15	63,63,63,63	0
57	MG	2a	1636	1/1	0.72	0.29	75,75,75,75	0
57	MG	2a	1739	1/1	0.72	0.32	72,72,72,72	0
57	MG	1a	1679	1/1	0.72	0.24	82,82,82,82	0
57	MG	2A	3657	1/1	0.72	0.12	85,85,85,85	0
57	MG	2A	3730	1/1	0.72	0.14	73,73,73,73	0
57	MG	2A	3312	1/1	0.72	0.29	76,76,76,76	0
57	MG	2A	3606	1/1	0.73	0.26	68,68,68,68	0
57	MG	1w	101	1/1	0.73	0.16	81,81,81,81	0
57	MG	2A	3777	1/1	0.73	0.21	75,75,75,75	0
57	MG	1A	3877	1/1	0.73	0.23	72,72,72,72	0
57	MG	1R	207	1/1	0.73	0.20	45,45,45,45	0
57	MG	2A	3336	1/1	0.73	0.11	75,75,75,75	0
57	MG	10	108	1/1	0.73	0.27	74,74,74,74	0
57	MG	1A	3210	1/1	0.73	0.11	79,79,79,79	0
57	MG	2a	1642	1/1	0.73	0.32	83,83,83,83	0
57	MG	2A	3112	1/1	0.73	0.31	83,83,83,83	0
57	MG	2A	3200	1/1	0.73	0.22	74,74,74,74	0
57	MG	1a	1682	1/1	0.73	0.24	80,80,80,80	0
57	MG	2A	3585	1/1	0.73	0.28	75,75,75,75	0
57	MG	2A	3751	1/1	0.73	0.21	50,50,50,50	0
57	MG	2A	3349	1/1	0.74	0.20	59,59,59,59	0
57	MG	2A	3735	1/1	0.74	0.28	72,72,72,72	0
57	MG	2G	201	1/1	0.74	0.34	81,81,81,81	0
57	MG	2A	3255	1/1	0.74	0.20	74,74,74,74	0
57	MG	2a	1638	1/1	0.74	0.36	84,84,84,84	0
57	MG	2A	3371	1/1	0.74	0.29	74,74,74,74	0
57	MG	2a	1709	1/1	0.74	0.27	76,76,76,76	0
57	MG	2A	3686	1/1	0.74	0.14	67,67,67,67	0
57	MG	1A	3707	1/1	0.74	0.20	54,54,54,54	0
57	MG	2a	1787	1/1	0.74	0.26	76,76,76,76	0
57	MG	2A	3332	1/1	0.74	0.27	81,81,81,81	0
57	MG	1A	3520	1/1	0.74	0.28	75,75,75,75	0
57	MG	2A	3845	1/1	0.74	0.32	76,76,76,76	0
57	MG	2A	3294	1/1	0.75	0.17	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	16	102	1/1	0.75	0.30	64,64,64,64	0
57	MG	2A	3069	1/1	0.75	0.23	70,70,70,70	0
57	MG	1A	3712	1/1	0.75	0.23	68,68,68,68	0
57	MG	2A	3644	1/1	0.75	0.18	47,47,47,47	0
57	MG	1B	210	1/1	0.75	0.21	71,71,71,71	0
57	MG	2a	1707	1/1	0.75	0.28	81,81,81,81	0
57	MG	1a	1703	1/1	0.75	0.26	73,73,73,73	0
57	MG	2A	3197	1/1	0.75	0.33	86,86,86,86	0
57	MG	1a	1722	1/1	0.75	0.45	75,75,75,75	0
57	MG	2A	3215	1/1	0.75	0.23	67,67,67,67	0
57	MG	2A	3810	1/1	0.75	0.16	59,59,59,59	0
57	MG	1U	210	1/1	0.75	0.43	66,66,66,66	0
57	MG	1A	3938	1/1	0.75	0.17	69,69,69,69	0
57	MG	1E	310	1/1	0.76	0.23	80,80,80,80	0
57	MG	2B	214	1/1	0.76	0.17	79,79,79,79	0
57	MG	1w	103	1/1	0.76	0.17	78,78,78,78	0
57	MG	2a	1608	1/1	0.76	0.26	75,75,75,75	0
57	MG	2A	3372	1/1	0.76	0.18	70,70,70,70	0
57	MG	2A	3195	1/1	0.76	0.19	69,69,69,69	0
57	MG	2A	3496	1/1	0.76	0.18	77,77,77,77	0
57	MG	2A	3258	1/1	0.76	0.18	74,74,74,74	0
57	MG	2A	3676	1/1	0.76	0.22	65,65,65,65	0
57	MG	2a	1712	1/1	0.76	0.31	78,78,78,78	0
57	MG	1a	1793	1/1	0.76	0.27	78,78,78,78	0
57	MG	2A	3199	1/1	0.76	0.35	70,70,70,70	0
57	MG	2A	3352	1/1	0.76	0.28	77,77,77,77	0
57	MG	2A	3705	1/1	0.76	0.20	79,79,79,79	0
57	MG	2a	1821	1/1	0.76	0.23	75,75,75,75	0
57	MG	2A	3850	1/1	0.76	0.21	65,65,65,65	0
57	MG	2v	103	1/1	0.76	0.43	79,79,79,79	0
57	MG	2A	3357	1/1	0.76	0.32	63,63,63,63	0
57	MG	2a	1622	1/1	0.77	0.26	81,81,81,81	0
57	MG	2A	3218	1/1	0.77	0.40	73,73,73,73	0
57	MG	2A	3485	1/1	0.77	0.24	69,69,69,69	0
57	MG	1A	3851	1/1	0.77	0.16	83,83,83,83	0
57	MG	2a	1699	1/1	0.77	0.15	71,71,71,71	0
57	MG	1A	3806	1/1	0.77	0.20	70,70,70,70	0
57	MG	1A	4010	1/1	0.77	0.11	77,77,77,77	0
57	MG	2A	3683	1/1	0.77	0.20	79,79,79,79	0
57	MG	2a	1714	1/1	0.77	0.38	71,71,71,71	0
57	MG	2A	3279	1/1	0.77	0.19	68,68,68,68	0
57	MG	2A	3062	1/1	0.77	0.13	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3214	1/1	0.77	0.23	62,62,62,62	0
57	MG	2a	1804	1/1	0.77	0.22	76,76,76,76	0
57	MG	2A	3609	1/1	0.77	0.23	65,65,65,65	0
57	MG	2A	3166	1/1	0.77	0.12	74,74,74,74	0
57	MG	2i	201	1/1	0.77	0.11	77,77,77,77	0
57	MG	2A	3321	1/1	0.77	0.25	69,69,69,69	0
57	MG	2A	3388	1/1	0.77	0.22	71,71,71,71	0
57	MG	2A	3741	1/1	0.77	0.20	67,67,67,67	0
57	MG	2A	3770	1/1	0.78	0.18	50,50,50,50	0
57	MG	2A	3704	1/1	0.78	0.18	74,74,74,74	0
57	MG	1a	1720	1/1	0.78	0.31	71,71,71,71	0
57	MG	1A	3858	1/1	0.78	0.21	62,62,62,62	0
57	MG	2A	3277	1/1	0.78	0.39	73,73,73,73	0
57	MG	2A	3711	1/1	0.78	0.21	73,73,73,73	0
57	MG	2A	3719	1/1	0.78	0.20	70,70,70,70	0
57	MG	2A	3857	1/1	0.78	0.17	66,66,66,66	0
57	MG	2A	3720	1/1	0.78	0.19	60,60,60,60	0
57	MG	1a	1784	1/1	0.78	0.13	81,81,81,81	0
57	MG	2A	3333	1/1	0.78	0.38	76,76,76,76	0
57	MG	2B	216	1/1	0.78	0.15	64,64,64,64	0
57	MG	2a	1817	1/1	0.78	0.21	74,74,74,74	0
57	MG	2a	1820	1/1	0.78	0.25	69,69,69,69	0
57	MG	2F	307	1/1	0.78	0.15	72,72,72,72	0
57	MG	1A	3678	1/1	0.78	0.14	63,63,63,63	0
57	MG	2A	3630	1/1	0.78	0.24	64,64,64,64	0
57	MG	2t	201	1/1	0.78	0.19	66,66,66,66	0
57	MG	2A	3175	1/1	0.78	0.19	58,58,58,58	0
57	MG	1a	1636	1/1	0.78	0.42	89,89,89,89	0
57	MG	2y	101	1/1	0.78	0.18	78,78,78,78	0
57	MG	2A	3687	1/1	0.79	0.33	78,78,78,78	0
57	MG	2A	3274	1/1	0.79	0.11	77,77,77,77	0
57	MG	2a	1808	1/1	0.79	0.20	77,77,77,77	0
57	MG	2a	1812	1/1	0.79	0.15	79,79,79,79	0
57	MG	2a	1671	1/1	0.79	0.16	71,71,71,71	0
57	MG	2A	3378	1/1	0.79	0.14	69,69,69,69	0
57	MG	2A	3675	1/1	0.79	0.19	64,64,64,64	0
57	MG	2A	3115	1/1	0.79	0.23	77,77,77,77	0
57	MG	20	101	1/1	0.79	0.27	74,74,74,74	0
57	MG	2q	202	1/1	0.79	0.12	81,81,81,81	0
57	MG	2A	3324	1/1	0.79	0.20	66,66,66,66	0
57	MG	2A	3481	1/1	0.79	0.31	76,76,76,76	0
57	MG	2a	1626	1/1	0.79	0.25	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1a	1799	1/1	0.79	0.12	72,72,72,72	0
57	MG	1A	3809	1/1	0.80	0.12	49,49,49,49	0
57	MG	2A	3209	1/1	0.80	0.17	72,72,72,72	0
57	MG	2A	3627	1/1	0.80	0.18	84,84,84,84	0
57	MG	2A	3342	1/1	0.80	0.31	81,81,81,81	0
57	MG	2a	1645	1/1	0.80	0.14	64,64,64,64	0
57	MG	2a	1656	1/1	0.80	0.34	76,76,76,76	0
57	MG	1A	4001	1/1	0.80	0.12	46,46,46,46	0
57	MG	1A	3831	1/1	0.80	0.21	73,73,73,73	0
57	MG	1x	101	1/1	0.80	0.31	71,71,71,71	0
57	MG	2A	3363	1/1	0.80	0.28	64,64,64,64	0
57	MG	2A	3664	1/1	0.80	0.13	67,67,67,67	0
57	MG	1A	4026	1/1	0.80	0.12	71,71,71,71	0
57	MG	2a	1730	1/1	0.80	0.21	83,83,83,83	0
57	MG	1a	1677	1/1	0.80	0.28	78,78,78,78	0
57	MG	1A	3347	1/1	0.80	0.25	65,65,65,65	0
57	MG	2a	1769	1/1	0.80	0.19	83,83,83,83	0
57	MG	2A	3837	1/1	0.80	0.14	71,71,71,71	0
57	MG	2a	1789	1/1	0.80	0.24	86,86,86,86	0
57	MG	1A	3545	1/1	0.80	0.23	60,60,60,60	0
57	MG	1A	3607	1/1	0.80	0.16	38,38,38,38	0
57	MG	2A	3392	1/1	0.80	0.17	75,75,75,75	0
57	MG	1a	1707	1/1	0.80	0.18	80,80,80,80	0
57	MG	2a	1815	1/1	0.80	0.19	77,77,77,77	0
57	MG	2A	3436	1/1	0.80	0.28	64,64,64,64	0
57	MG	2B	211	1/1	0.80	0.31	83,83,83,83	0
57	MG	1B	230	1/1	0.80	0.20	73,73,73,73	0
57	MG	1A	3219	1/1	0.80	0.19	65,65,65,65	0
57	MG	2A	3167	1/1	0.80	0.22	78,78,78,78	0
57	MG	1a	1759	1/1	0.80	0.16	68,68,68,68	0
57	MG	2T	3502	1/1	0.80	0.22	76,76,76,76	0
57	MG	1A	3514	1/1	0.80	0.22	68,68,68,68	0
57	MG	1O	205	1/1	0.80	0.13	76,76,76,76	0
57	MG	1A	3807	1/1	0.80	0.22	51,51,51,51	0
57	MG	1A	4022	1/1	0.81	0.15	84,84,84,84	0
57	MG	2A	3446	1/1	0.81	0.28	75,75,75,75	0
57	MG	1A	3305	1/1	0.81	0.27	52,52,52,52	0
57	MG	2A	3168	1/1	0.81	0.19	76,76,76,76	0
57	MG	1A	4048	1/1	0.81	0.16	58,58,58,58	0
57	MG	2A	3190	1/1	0.81	0.36	77,77,77,77	0
57	MG	2a	1746	1/1	0.81	0.28	75,75,75,75	0
57	MG	1A	3314	1/1	0.81	0.16	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	1t	201	1/1	0.81	0.26	69,69,69,69	0
57	MG	1a	1676	1/1	0.81	0.20	70,70,70,70	0
57	MG	2E	307	1/1	0.81	0.16	60,60,60,60	0
57	MG	2a	1795	1/1	0.81	0.16	64,64,64,64	0
57	MG	2A	3597	1/1	0.81	0.15	71,71,71,71	0
57	MG	1A	3532	1/1	0.81	0.24	79,79,79,79	0
57	MG	1A	3040	1/1	0.81	0.26	61,61,61,61	0
57	MG	1A	3976	1/1	0.81	0.20	69,69,69,69	0
57	MG	1a	1685	1/1	0.81	0.24	73,73,73,73	0
57	MG	2a	1610	1/1	0.81	0.26	69,69,69,69	0
57	MG	2A	3051	1/1	0.81	0.18	75,75,75,75	0
57	MG	1A	3169	1/1	0.81	0.23	66,66,66,66	0
57	MG	1A	3382	1/1	0.81	0.18	57,57,57,57	0
57	MG	2A	3088	1/1	0.81	0.12	65,65,65,65	0
57	MG	1A	3425	1/1	0.81	0.19	73,73,73,73	0
57	MG	1A	3479	1/1	0.81	0.26	75,75,75,75	0
57	MG	1a	1728	1/1	0.81	0.26	59,59,59,59	0
57	MG	2A	3422	1/1	0.81	0.29	66,66,66,66	0
57	MG	2w	104	1/1	0.81	0.19	82,82,82,82	0
57	MG	1a	1734	1/1	0.81	0.22	80,80,80,80	0
57	MG	1A	3583	1/1	0.82	0.19	67,67,67,67	0
57	MG	1s	101	1/1	0.82	0.17	78,78,78,78	0
57	MG	2T	3503	1/1	0.82	0.19	52,52,52,52	0
57	MG	2W	201	1/1	0.82	0.14	72,72,72,72	0
57	MG	1A	3079	1/1	0.82	0.19	64,64,64,64	0
57	MG	1a	1631	1/1	0.82	0.43	75,75,75,75	0
57	MG	2A	3208	1/1	0.82	0.11	68,68,68,68	0
57	MG	1A	3502	1/1	0.82	0.20	66,66,66,66	0
57	MG	1A	3646	1/1	0.82	0.12	64,64,64,64	0
57	MG	2A	3384	1/1	0.82	0.32	65,65,65,65	0
57	MG	2A	3386	1/1	0.82	0.18	69,69,69,69	0
57	MG	1A	3510	1/1	0.82	0.16	65,65,65,65	0
57	MG	1A	3399	1/1	0.82	0.11	55,55,55,55	0
57	MG	2A	3231	1/1	0.82	0.43	56,56,56,56	0
57	MG	2a	1669	1/1	0.82	0.31	70,70,70,70	0
57	MG	2A	3709	1/1	0.82	0.13	43,43,43,43	0
57	MG	2A	3244	1/1	0.82	0.15	63,63,63,63	0
57	MG	2A	3426	1/1	0.82	0.26	62,62,62,62	0
57	MG	2A	3427	1/1	0.82	0.27	57,57,57,57	0
57	MG	1x	111	1/1	0.82	0.15	65,65,65,65	0
57	MG	1B	213	1/1	0.82	0.20	75,75,75,75	0
57	MG	2a	1721	1/1	0.82	0.27	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3472	1/1	0.82	0.15	64,64,64,64	0
57	MG	2a	1738	1/1	0.82	0.32	65,65,65,65	0
57	MG	1B	225	1/1	0.82	0.13	62,62,62,62	0
57	MG	2A	3748	1/1	0.82	0.21	66,66,66,66	0
57	MG	1A	3933	1/1	0.82	0.13	58,58,58,58	0
57	MG	2a	1760	1/1	0.82	0.21	85,85,85,85	0
57	MG	1A	3405	1/1	0.82	0.15	74,74,74,74	0
57	MG	2A	3510	1/1	0.82	0.15	56,56,56,56	0
57	MG	1A	3246	1/1	0.82	0.36	73,73,73,73	0
57	MG	2a	1793	1/1	0.82	0.14	67,67,67,67	0
57	MG	2A	3289	1/1	0.82	0.29	68,68,68,68	0
57	MG	2A	3559	1/1	0.82	0.20	48,48,48,48	0
57	MG	1A	3985	1/1	0.82	0.12	69,69,69,69	0
57	MG	1A	3430	1/1	0.82	0.18	65,65,65,65	0
57	MG	1A	3549	1/1	0.82	0.29	60,60,60,60	0
57	MG	2A	3152	1/1	0.82	0.27	73,73,73,73	0
57	MG	1a	1737	1/1	0.82	0.35	83,83,83,83	0
57	MG	2A	3617	1/1	0.82	0.25	77,77,77,77	0
57	MG	1A	3554	1/1	0.82	0.13	54,54,54,54	0
57	MG	2A	3861	1/1	0.82	0.23	76,76,76,76	0
57	MG	1V	207	1/1	0.82	0.20	63,63,63,63	0
57	MG	2B	206	1/1	0.82	0.21	83,83,83,83	0
57	MG	2A	3170	1/1	0.82	0.19	84,84,84,84	0
57	MG	1a	1792	1/1	0.82	0.18	70,70,70,70	0
57	MG	2A	3338	1/1	0.82	0.20	60,60,60,60	0
57	MG	2A	3187	1/1	0.82	0.19	72,72,72,72	0
57	MG	1Y	202	1/1	0.82	0.10	64,64,64,64	0
57	MG	1O	204	1/1	0.83	0.14	66,66,66,66	0
57	MG	2a	1612	1/1	0.83	0.27	72,72,72,72	0
57	MG	2A	3101	1/1	0.83	0.20	74,74,74,74	0
57	MG	2A	3102	1/1	0.83	0.18	80,80,80,80	0
57	MG	2a	1631	1/1	0.83	0.23	63,63,63,63	0
57	MG	1A	3835	1/1	0.83	0.13	71,71,71,71	0
57	MG	1A	3331	1/1	0.83	0.18	59,59,59,59	0
57	MG	1S	201	1/1	0.83	0.22	43,43,43,43	0
57	MG	2A	3453	1/1	0.83	0.32	79,79,79,79	0
57	MG	2A	3120	1/1	0.83	0.25	79,79,79,79	0
57	MG	2A	3290	1/1	0.83	0.18	73,73,73,73	0
57	MG	2A	3484	1/1	0.83	0.18	62,62,62,62	0
57	MG	2a	1680	1/1	0.83	0.23	77,77,77,77	0
57	MG	2a	1682	1/1	0.83	0.15	65,65,65,65	0
57	MG	2a	1688	1/1	0.83	0.32	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2a	1689	1/1	0.83	0.20	73,73,73,73	0
57	MG	2A	3123	1/1	0.83	0.16	81,81,81,81	0
57	MG	2A	3744	1/1	0.83	0.16	76,76,76,76	0
57	MG	2A	3297	1/1	0.83	0.22	74,74,74,74	0
57	MG	2A	3148	1/1	0.83	0.29	71,71,71,71	0
57	MG	1A	3381	1/1	0.83	0.19	60,60,60,60	0
57	MG	2a	1720	1/1	0.83	0.28	72,72,72,72	0
57	MG	1A	3874	1/1	0.83	0.24	52,52,52,52	0
57	MG	2A	3761	1/1	0.83	0.14	72,72,72,72	0
57	MG	2a	1736	1/1	0.83	0.23	75,75,75,75	0
57	MG	1a	1788	1/1	0.83	0.16	83,83,83,83	0
57	MG	1A	3481	1/1	0.83	0.12	62,62,62,62	0
57	MG	2A	3790	1/1	0.83	0.16	74,74,74,74	0
57	MG	1A	3636	1/1	0.83	0.18	61,61,61,61	0
57	MG	2a	1750	1/1	0.83	0.20	87,87,87,87	0
57	MG	1A	3639	1/1	0.83	0.20	62,62,62,62	0
57	MG	2a	1761	1/1	0.83	0.14	70,70,70,70	0
57	MG	1a	1800	1/1	0.83	0.15	51,51,51,51	0
57	MG	2a	1786	1/1	0.83	0.11	85,85,85,85	0
57	MG	2A	3337	1/1	0.83	0.13	72,72,72,72	0
57	MG	1A	4070	1/1	0.83	0.11	70,70,70,70	0
57	MG	1B	202	1/1	0.83	0.18	59,59,59,59	0
57	MG	2A	3344	1/1	0.83	0.13	61,61,61,61	0
57	MG	1a	1659	1/1	0.83	0.27	78,78,78,78	0
57	MG	1B	207	1/1	0.83	0.14	75,75,75,75	0
57	MG	2A	3354	1/1	0.83	0.17	79,79,79,79	0
57	MG	1A	3489	1/1	0.83	0.14	71,71,71,71	0
57	MG	1A	3944	1/1	0.83	0.11	30,30,30,30	0
57	MG	1A	3950	1/1	0.83	0.18	83,83,83,83	0
57	MG	1A	3026	1/1	0.83	0.18	73,73,73,73	0
57	MG	1a	1692	1/1	0.83	0.17	86,86,86,86	0
57	MG	1A	3978	1/1	0.83	0.14	70,70,70,70	0
57	MG	2A	3221	1/1	0.83	0.21	63,63,63,63	0
57	MG	1A	3814	1/1	0.83	0.18	65,65,65,65	0
57	MG	1A	3508	1/1	0.83	0.21	71,71,71,71	0
57	MG	2A	3389	1/1	0.83	0.15	69,69,69,69	0
57	MG	2A	3253	1/1	0.83	0.12	78,78,78,78	0
57	MG	2w	102	1/1	0.83	0.21	71,71,71,71	0
57	MG	2a	1603	1/1	0.83	0.14	83,83,83,83	0
57	MG	2A	3693	1/1	0.83	0.19	58,58,58,58	0
57	MG	1A	3945	1/1	0.84	0.13	66,66,66,66	0
57	MG	2A	3796	1/1	0.84	0.20	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3470	1/1	0.84	0.18	67,67,67,67	0
57	MG	1D	311	1/1	0.84	0.29	78,78,78,78	0
57	MG	2a	1700	1/1	0.84	0.39	80,80,80,80	0
57	MG	2a	1701	1/1	0.84	0.24	69,69,69,69	0
57	MG	1A	3255	1/1	0.84	0.28	57,57,57,57	0
57	MG	2a	1708	1/1	0.84	0.22	70,70,70,70	0
57	MG	2A	3405	1/1	0.84	0.27	60,60,60,60	0
57	MG	1w	107	1/1	0.84	0.09	69,69,69,69	0
57	MG	1A	3811	1/1	0.84	0.15	65,65,65,65	0
57	MG	2a	1719	1/1	0.84	0.21	74,74,74,74	0
57	MG	2A	3316	1/1	0.84	0.18	51,51,51,51	0
57	MG	1A	4067	1/1	0.84	0.16	66,66,66,66	0
57	MG	1A	4069	1/1	0.84	0.10	50,50,50,50	0
57	MG	1A	3982	1/1	0.84	0.11	74,74,74,74	0
57	MG	2A	3204	1/1	0.84	0.16	64,64,64,64	0
57	MG	2A	3454	1/1	0.84	0.29	63,63,63,63	0
57	MG	1T	201	1/1	0.84	0.28	69,69,69,69	0
57	MG	2A	3334	1/1	0.84	0.22	73,73,73,73	0
57	MG	2B	219	1/1	0.84	0.25	78,78,78,78	0
57	MG	2A	3700	1/1	0.84	0.14	59,59,59,59	0
57	MG	2A	3702	1/1	0.84	0.10	65,65,65,65	0
57	MG	2a	1768	1/1	0.84	0.09	87,87,87,87	0
57	MG	1U	203	1/1	0.84	0.13	60,60,60,60	0
57	MG	1A	4075	1/1	0.84	0.22	58,58,58,58	0
57	MG	1A	3426	1/1	0.84	0.11	56,56,56,56	0
57	MG	2A	3498	1/1	0.84	0.28	77,77,77,77	0
57	MG	1A	3993	1/1	0.84	0.14	40,40,40,40	0
57	MG	1A	3930	1/1	0.84	0.12	47,47,47,47	0
57	MG	2a	1801	1/1	0.84	0.15	75,75,75,75	0
57	MG	2A	3535	1/1	0.84	0.16	74,74,74,74	0
57	MG	1a	1780	1/1	0.84	0.18	80,80,80,80	0
57	MG	2A	3724	1/1	0.84	0.15	68,68,68,68	0
57	MG	1A	3728	1/1	0.84	0.14	58,58,58,58	0
57	MG	1a	1624	1/1	0.84	0.14	59,59,59,59	0
57	MG	2a	1630	1/1	0.84	0.25	78,78,78,78	0
57	MG	1A	3423	1/1	0.84	0.18	67,67,67,67	0
57	MG	1B	228	1/1	0.84	0.13	74,74,74,74	0
57	MG	2a	1825	1/1	0.84	0.26	72,72,72,72	0
57	MG	2A	3273	1/1	0.84	0.25	75,75,75,75	0
57	MG	2A	3607	1/1	0.84	0.16	66,66,66,66	0
57	MG	1a	1647	1/1	0.84	0.14	62,62,62,62	0
57	MG	2a	1648	1/1	0.84	0.25	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3464	1/1	0.84	0.14	63,63,63,63	0
57	MG	1a	1825	1/1	0.84	0.25	69,69,69,69	0
57	MG	1a	1662	1/1	0.84	0.12	74,74,74,74	0
57	MG	2a	1679	1/1	0.84	0.15	75,75,75,75	0
57	MG	2x	102	1/1	0.84	0.31	75,75,75,75	0
57	MG	2A	3637	1/1	0.84	0.18	47,47,47,47	0
57	MG	2A	3701	1/1	0.85	0.16	62,62,62,62	0
57	MG	1A	3359	1/1	0.85	0.13	62,62,62,62	0
57	MG	2A	3703	1/1	0.85	0.16	68,68,68,68	0
57	MG	2a	1644	1/1	0.85	0.14	77,77,77,77	0
57	MG	2A	3070	1/1	0.85	0.10	47,47,47,47	0
57	MG	1A	3182	1/1	0.85	0.33	58,58,58,58	0
57	MG	2a	1650	1/1	0.85	0.19	80,80,80,80	0
57	MG	2A	3266	1/1	0.85	0.23	78,78,78,78	0
57	MG	2A	3094	1/1	0.85	0.10	74,74,74,74	0
57	MG	1A	3812	1/1	0.85	0.24	72,72,72,72	0
57	MG	1A	3695	1/1	0.85	0.10	31,31,31,31	0
57	MG	1a	1752	1/1	0.85	0.18	62,62,62,62	0
57	MG	1A	4077	1/1	0.85	0.12	60,60,60,60	0
57	MG	1a	1765	1/1	0.85	0.28	68,68,68,68	0
57	MG	1A	3962	1/1	0.85	0.09	24,24,24,24	0
57	MG	2a	1694	1/1	0.85	0.18	77,77,77,77	0
57	MG	1a	1783	1/1	0.85	0.11	75,75,75,75	0
57	MG	15	106	1/1	0.85	0.15	72,72,72,72	0
57	MG	1a	1787	1/1	0.85	0.19	77,77,77,77	0
57	MG	2a	1706	1/1	0.85	0.20	76,76,76,76	0
57	MG	1A	3972	1/1	0.85	0.19	64,64,64,64	0
57	MG	1a	1790	1/1	0.85	0.13	61,61,61,61	0
57	MG	2A	3318	1/1	0.85	0.26	72,72,72,72	0
57	MG	1A	3621	1/1	0.85	0.18	50,50,50,50	0
57	MG	1a	1629	1/1	0.85	0.33	77,77,77,77	0
57	MG	1A	3539	1/1	0.85	0.17	63,63,63,63	0
57	MG	2A	3775	1/1	0.85	0.18	69,69,69,69	0
57	MG	1B	221	1/1	0.85	0.21	64,64,64,64	0
57	MG	2A	3183	1/1	0.85	0.14	55,55,55,55	0
57	MG	1a	1823	1/1	0.85	0.17	63,63,63,63	0
57	MG	2A	3592	1/1	0.85	0.20	75,75,75,75	0
57	MG	1B	222	1/1	0.85	0.17	59,59,59,59	0
57	MG	1A	3716	1/1	0.85	0.15	62,62,62,62	0
57	MG	1A	3638	1/1	0.85	0.09	18,18,18,18	0
57	MG	1v	101	1/1	0.85	0.18	75,75,75,75	0
57	MG	1A	3862	1/1	0.85	0.15	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3347	1/1	0.85	0.10	68,68,68,68	0
57	MG	2a	1767	1/1	0.85	0.11	75,75,75,75	0
57	MG	1A	3732	1/1	0.85	0.20	64,64,64,64	0
57	MG	2A	3634	1/1	0.85	0.12	62,62,62,62	0
57	MG	2a	1781	1/1	0.85	0.23	88,88,88,88	0
57	MG	1A	3788	1/1	0.85	0.15	89,89,89,89	0
57	MG	2A	3353	1/1	0.85	0.18	73,73,73,73	0
57	MG	2A	3652	1/1	0.85	0.11	49,49,49,49	0
57	MG	2a	1791	1/1	0.85	0.14	67,67,67,67	0
57	MG	2A	3654	1/1	0.85	0.31	74,74,74,74	0
57	MG	1A	3297	1/1	0.85	0.20	70,70,70,70	0
57	MG	2A	3355	1/1	0.85	0.10	61,61,61,61	0
57	MG	2E	301	1/1	0.85	0.20	61,61,61,61	0
57	MG	2E	303	1/1	0.85	0.18	74,74,74,74	0
57	MG	2A	3213	1/1	0.85	0.26	54,54,54,54	0
57	MG	1A	3881	1/1	0.85	0.13	29,29,29,29	0
57	MG	1A	3893	1/1	0.85	0.22	79,79,79,79	0
57	MG	2Q	202	1/1	0.85	0.25	67,67,67,67	0
57	MG	2A	3366	1/1	0.85	0.30	77,77,77,77	0
57	MG	2A	3370	1/1	0.85	0.34	70,70,70,70	0
57	MG	1x	107	1/1	0.85	0.10	68,68,68,68	0
57	MG	1A	3899	1/1	0.85	0.21	73,73,73,73	0
57	MG	21	101	1/1	0.85	0.40	59,59,59,59	0
57	MG	2A	3682	1/1	0.85	0.17	78,78,78,78	0
57	MG	2A	3373	1/1	0.85	0.12	66,66,66,66	0
57	MG	2A	3685	1/1	0.85	0.12	64,64,64,64	0
57	MG	1A	3357	1/1	0.85	0.16	66,66,66,66	0
57	MG	2A	3240	1/1	0.85	0.33	65,65,65,65	0
57	MG	2A	3241	1/1	0.85	0.31	54,54,54,54	0
57	MG	1A	3397	1/1	0.85	0.24	32,32,32,32	0
57	MG	2A	3249	1/1	0.85	0.39	79,79,79,79	0
57	MG	23	101	1/1	0.86	0.30	78,78,78,78	0
57	MG	1a	1794	1/1	0.86	0.10	73,73,73,73	0
57	MG	1A	4089	1/1	0.86	0.18	42,42,42,42	0
57	MG	1A	3006	1/1	0.86	0.26	70,70,70,70	0
57	MG	1a	1804	1/1	0.86	0.12	51,51,51,51	0
57	MG	2a	1614	1/1	0.86	0.17	65,65,65,65	0
57	MG	1A	3376	1/1	0.86	0.17	54,54,54,54	0
57	MG	2A	3665	1/1	0.86	0.14	73,73,73,73	0
57	MG	1A	3350	1/1	0.86	0.18	59,59,59,59	0
57	MG	1l	201	1/1	0.86	0.28	73,73,73,73	0
57	MG	1B	211	1/1	0.86	0.13	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3979	1/1	0.86	0.14	70,70,70,70	0
57	MG	2a	1641	1/1	0.86	0.17	80,80,80,80	0
57	MG	2A	3207	1/1	0.86	0.15	67,67,67,67	0
57	MG	1A	3499	1/1	0.86	0.28	58,58,58,58	0
57	MG	1a	1665	1/1	0.86	0.12	61,61,61,61	0
57	MG	2a	1647	1/1	0.86	0.14	73,73,73,73	0
57	MG	1w	102	1/1	0.86	0.21	74,74,74,74	0
57	MG	1A	3558	1/1	0.86	0.12	61,61,61,61	0
57	MG	2a	1651	1/1	0.86	0.15	62,62,62,62	0
57	MG	1w	104	1/1	0.86	0.13	74,74,74,74	0
57	MG	2a	1660	1/1	0.86	0.13	67,67,67,67	0
57	MG	2a	1667	1/1	0.86	0.12	67,67,67,67	0
57	MG	1A	3329	1/1	0.86	0.20	56,56,56,56	0
57	MG	1A	3995	1/1	0.86	0.11	56,56,56,56	0
57	MG	2a	1672	1/1	0.86	0.22	65,65,65,65	0
57	MG	1A	3593	1/1	0.86	0.35	71,71,71,71	0
57	MG	2A	3379	1/1	0.86	0.15	67,67,67,67	0
57	MG	2A	3382	1/1	0.86	0.13	76,76,76,76	0
57	MG	1A	3358	1/1	0.86	0.07	43,43,43,43	0
57	MG	1A	3745	1/1	0.86	0.11	55,55,55,55	0
57	MG	2A	3242	1/1	0.86	0.14	67,67,67,67	0
57	MG	1a	1695	1/1	0.86	0.26	63,63,63,63	0
57	MG	2A	3020	1/1	0.86	0.16	68,68,68,68	0
57	MG	2A	3040	1/1	0.86	0.21	65,65,65,65	0
57	MG	2A	3411	1/1	0.86	0.12	56,56,56,56	0
57	MG	1a	1697	1/1	0.86	0.11	63,63,63,63	0
57	MG	1A	4004	1/1	0.86	0.11	33,33,33,33	0
57	MG	2A	3261	1/1	0.86	0.12	53,53,53,53	0
57	MG	1A	4009	1/1	0.86	0.14	66,66,66,66	0
57	MG	2A	3435	1/1	0.86	0.34	65,65,65,65	0
57	MG	1A	3197	1/1	0.86	0.29	58,58,58,58	0
57	MG	1A	3623	1/1	0.86	0.20	64,64,64,64	0
57	MG	1A	3469	1/1	0.86	0.10	64,64,64,64	0
57	MG	2a	1722	1/1	0.86	0.25	70,70,70,70	0
57	MG	2a	1727	1/1	0.86	0.29	74,74,74,74	0
57	MG	2a	1728	1/1	0.86	0.11	63,63,63,63	0
57	MG	2A	3098	1/1	0.86	0.27	77,77,77,77	0
57	MG	2A	3465	1/1	0.86	0.23	60,60,60,60	0
57	MG	2A	3467	1/1	0.86	0.20	57,57,57,57	0
57	MG	1A	3404	1/1	0.86	0.28	69,69,69,69	0
57	MG	2A	3475	1/1	0.86	0.30	68,68,68,68	0
57	MG	2A	3281	1/1	0.86	0.15	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3283	1/1	0.86	0.16	61,61,61,61	0
57	MG	1A	3529	1/1	0.86	0.15	62,62,62,62	0
57	MG	2A	3486	1/1	0.86	0.25	52,52,52,52	0
57	MG	2A	3798	1/1	0.86	0.10	80,80,80,80	0
57	MG	2A	3489	1/1	0.86	0.33	64,64,64,64	0
57	MG	1A	4066	1/1	0.86	0.07	19,19,19,19	0
57	MG	2A	3105	1/1	0.86	0.17	62,62,62,62	0
57	MG	1a	1753	1/1	0.86	0.13	60,60,60,60	0
57	MG	1A	3531	1/1	0.86	0.24	75,75,75,75	0
57	MG	2A	3534	1/1	0.86	0.20	60,60,60,60	0
57	MG	2A	3301	1/1	0.86	0.26	81,81,81,81	0
57	MG	2A	3305	1/1	0.86	0.15	60,60,60,60	0
57	MG	2A	3549	1/1	0.86	0.15	53,53,53,53	0
57	MG	2A	3307	1/1	0.86	0.15	63,63,63,63	0
57	MG	2B	203	1/1	0.86	0.26	79,79,79,79	0
57	MG	2A	3569	1/1	0.86	0.11	38,38,38,38	0
57	MG	1A	3476	1/1	0.86	0.21	59,59,59,59	0
57	MG	2A	3315	1/1	0.86	0.15	62,62,62,62	0
57	MG	1A	3664	1/1	0.86	0.10	33,33,33,33	0
57	MG	1A	3957	1/1	0.86	0.10	56,56,56,56	0
57	MG	2a	1818	1/1	0.86	0.13	87,87,87,87	0
57	MG	2A	3604	1/1	0.86	0.15	74,74,74,74	0
57	MG	2A	3319	1/1	0.86	0.12	57,57,57,57	0
57	MG	1A	3825	1/1	0.86	0.14	55,55,55,55	0
57	MG	2A	3323	1/1	0.86	0.20	64,64,64,64	0
57	MG	1A	4088	1/1	0.86	0.15	44,44,44,44	0
57	MG	2A	3159	1/1	0.86	0.19	64,64,64,64	0
57	MG	2R	202	1/1	0.86	0.16	64,64,64,64	0
57	MG	2T	3501	1/1	0.86	0.20	71,71,71,71	0
57	MG	1a	1601	1/1	0.86	0.27	72,72,72,72	0
57	MG	1a	1613	1/1	0.86	0.28	68,68,68,68	0
57	MG	1a	1614	1/1	0.86	0.10	63,63,63,63	0
57	MG	1a	1619	1/1	0.86	0.13	46,46,46,46	0
57	MG	2A	3171	1/1	0.86	0.18	61,61,61,61	0
57	MG	2a	1606	1/1	0.87	0.35	79,79,79,79	0
57	MG	2A	3653	1/1	0.87	0.22	70,70,70,70	0
57	MG	1A	3581	1/1	0.87	0.17	50,50,50,50	0
57	MG	2a	1611	1/1	0.87	0.18	66,66,66,66	0
57	MG	1A	3800	1/1	0.87	0.12	56,56,56,56	0
57	MG	1a	1669	1/1	0.87	0.10	54,54,54,54	0
57	MG	1a	1673	1/1	0.87	0.24	68,68,68,68	0
57	MG	1A	3472	1/1	0.87	0.11	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	1627	1/1	0.87	0.32	71,71,71,71	0
57	MG	1A	3344	1/1	0.87	0.19	63,63,63,63	0
57	MG	2A	3668	1/1	0.87	0.14	50,50,50,50	0
57	MG	1A	3082	1/1	0.87	0.20	44,44,44,44	0
57	MG	2A	3232	1/1	0.87	0.22	46,46,46,46	0
57	MG	2A	3236	1/1	0.87	0.20	68,68,68,68	0
57	MG	1a	1680	1/1	0.87	0.25	74,74,74,74	0
57	MG	1A	3290	1/1	0.87	0.28	48,48,48,48	0
57	MG	1A	3102	1/1	0.87	0.18	60,60,60,60	0
57	MG	2A	3008	1/1	0.87	0.14	57,57,57,57	0
57	MG	2A	3247	1/1	0.87	0.19	61,61,61,61	0
57	MG	2a	1649	1/1	0.87	0.18	73,73,73,73	0
57	MG	1A	3148	1/1	0.87	0.33	42,42,42,42	0
57	MG	2A	3391	1/1	0.87	0.15	78,78,78,78	0
57	MG	2A	3252	1/1	0.87	0.24	71,71,71,71	0
57	MG	2a	1657	1/1	0.87	0.18	86,86,86,86	0
57	MG	2A	3395	1/1	0.87	0.14	71,71,71,71	0
57	MG	2A	3404	1/1	0.87	0.23	48,48,48,48	0
57	MG	1A	3312	1/1	0.87	0.21	56,56,56,56	0
57	MG	1A	3830	1/1	0.87	0.15	61,61,61,61	0
57	MG	2A	3414	1/1	0.87	0.26	68,68,68,68	0
57	MG	2A	3419	1/1	0.87	0.21	65,65,65,65	0
57	MG	1A	3157	1/1	0.87	0.16	33,33,33,33	0
57	MG	1F	310	1/1	0.87	0.13	55,55,55,55	0
57	MG	1a	1710	1/1	0.87	0.17	69,69,69,69	0
57	MG	2A	3086	1/1	0.87	0.28	73,73,73,73	0
57	MG	2A	3433	1/1	0.87	0.13	69,69,69,69	0
57	MG	2A	3087	1/1	0.87	0.19	59,59,59,59	0
57	MG	2A	3275	1/1	0.87	0.28	77,77,77,77	0
57	MG	1A	3361	1/1	0.87	0.12	74,74,74,74	0
57	MG	1A	3845	1/1	0.87	0.09	62,62,62,62	0
57	MG	1a	1725	1/1	0.87	0.10	58,58,58,58	0
57	MG	1R	205	1/1	0.87	0.21	54,54,54,54	0
57	MG	1A	3364	1/1	0.87	0.16	58,58,58,58	0
57	MG	2A	3285	1/1	0.87	0.15	62,62,62,62	0
57	MG	1A	3657	1/1	0.87	0.08	32,32,32,32	0
57	MG	2a	1715	1/1	0.87	0.28	77,77,77,77	0
57	MG	2A	3480	1/1	0.87	0.27	68,68,68,68	0
57	MG	1a	1746	1/1	0.87	0.13	73,73,73,73	0
57	MG	1A	3433	1/1	0.87	0.13	58,58,58,58	0
57	MG	2A	3766	1/1	0.87	0.20	77,77,77,77	0
57	MG	1A	3866	1/1	0.87	0.18	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	4032	1/1	0.87	0.12	61,61,61,61	0
57	MG	2A	3117	1/1	0.87	0.16	52,52,52,52	0
57	MG	2a	1733	1/1	0.87	0.12	64,64,64,64	0
57	MG	2A	3778	1/1	0.87	0.23	79,79,79,79	0
57	MG	1A	3441	1/1	0.87	0.14	56,56,56,56	0
57	MG	1A	4049	1/1	0.87	0.14	52,52,52,52	0
57	MG	2A	3506	1/1	0.87	0.16	74,74,74,74	0
57	MG	1A	3445	1/1	0.87	0.11	53,53,53,53	0
57	MG	2A	3511	1/1	0.87	0.15	42,42,42,42	0
57	MG	2A	3149	1/1	0.87	0.23	68,68,68,68	0
57	MG	1A	3446	1/1	0.87	0.20	60,60,60,60	0
57	MG	1A	3698	1/1	0.87	0.14	64,64,64,64	0
57	MG	2A	3536	1/1	0.87	0.23	63,63,63,63	0
57	MG	1A	3459	1/1	0.87	0.10	58,58,58,58	0
57	MG	2A	3543	1/1	0.87	0.14	71,71,71,71	0
57	MG	1a	1605	1/1	0.87	0.09	71,71,71,71	0
57	MG	2A	3556	1/1	0.87	0.10	69,69,69,69	0
57	MG	1a	1611	1/1	0.87	0.13	70,70,70,70	0
57	MG	2B	205	1/1	0.87	0.12	68,68,68,68	0
57	MG	1A	3541	1/1	0.87	0.17	47,47,47,47	0
57	MG	1A	3462	1/1	0.87	0.29	69,69,69,69	0
57	MG	2A	3582	1/1	0.87	0.23	69,69,69,69	0
57	MG	2A	3584	1/1	0.87	0.12	67,67,67,67	0
57	MG	1A	3225	1/1	0.87	0.17	51,51,51,51	0
57	MG	1A	3380	1/1	0.87	0.33	69,69,69,69	0
57	MG	1a	1628	1/1	0.87	0.11	58,58,58,58	0
57	MG	2A	3189	1/1	0.87	0.14	62,62,62,62	0
57	MG	1a	1815	1/1	0.87	0.15	74,74,74,74	0
57	MG	1A	3734	1/1	0.87	0.12	65,65,65,65	0
57	MG	1a	1824	1/1	0.87	0.21	68,68,68,68	0
57	MG	2A	3198	1/1	0.87	0.13	60,60,60,60	0
57	MG	1A	4093	1/1	0.87	0.17	52,52,52,52	0
57	MG	1a	1635	1/1	0.87	0.26	79,79,79,79	0
57	MG	2A	3632	1/1	0.87	0.18	65,65,65,65	0
57	MG	1A	3557	1/1	0.87	0.12	66,66,66,66	0
57	MG	2A	3205	1/1	0.87	0.14	63,63,63,63	0
57	MG	1A	3052	1/1	0.87	0.10	50,50,50,50	0
57	MG	2A	3650	1/1	0.87	0.18	81,81,81,81	0
57	MG	25	105	1/1	0.87	0.15	63,63,63,63	0
57	MG	2w	103	1/1	0.87	0.19	75,75,75,75	0
57	MG	26	101	1/1	0.87	0.27	78,78,78,78	0
57	MG	27	102	1/1	0.87	0.14	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3795	1/1	0.87	0.11	28,28,28,28	0
57	MG	1A	3440	1/1	0.88	0.20	65,65,65,65	0
57	MG	1h	201	1/1	0.88	0.10	66,66,66,66	0
57	MG	1A	3546	1/1	0.88	0.22	61,61,61,61	0
57	MG	1n	102	1/1	0.88	0.21	62,62,62,62	0
57	MG	1a	1643	1/1	0.88	0.11	73,73,73,73	0
57	MG	2A	3645	1/1	0.88	0.14	52,52,52,52	0
57	MG	1A	3296	1/1	0.88	0.15	51,51,51,51	0
57	MG	2A	3210	1/1	0.88	0.22	74,74,74,74	0
57	MG	2A	3212	1/1	0.88	0.28	73,73,73,73	0
57	MG	1a	1655	1/1	0.88	0.24	72,72,72,72	0
57	MG	2A	3656	1/1	0.88	0.14	64,64,64,64	0
57	MG	2a	1618	1/1	0.88	0.11	64,64,64,64	0
57	MG	1B	220	1/1	0.88	0.21	72,72,72,72	0
57	MG	1A	3823	1/1	0.88	0.08	38,38,38,38	0
57	MG	2A	3661	1/1	0.88	0.19	72,72,72,72	0
57	MG	2a	1628	1/1	0.88	0.20	68,68,68,68	0
57	MG	1A	3682	1/1	0.88	0.10	44,44,44,44	0
57	MG	2A	3381	1/1	0.88	0.20	64,64,64,64	0
57	MG	1a	1666	1/1	0.88	0.19	71,71,71,71	0
57	MG	1A	3984	1/1	0.88	0.12	66,66,66,66	0
57	MG	2A	3385	1/1	0.88	0.23	74,74,74,74	0
57	MG	1A	3551	1/1	0.88	0.21	66,66,66,66	0
57	MG	1A	3493	1/1	0.88	0.20	47,47,47,47	0
57	MG	1A	3089	1/1	0.88	0.10	37,37,37,37	0
57	MG	1x	105	1/1	0.88	0.20	71,71,71,71	0
57	MG	1A	3837	1/1	0.88	0.12	52,52,52,52	0
57	MG	1A	3998	1/1	0.88	0.11	64,64,64,64	0
57	MG	2A	3403	1/1	0.88	0.28	55,55,55,55	0
57	MG	1E	307	1/1	0.88	0.14	59,59,59,59	0
57	MG	1A	3095	1/1	0.88	0.14	61,61,61,61	0
57	MG	2A	3027	1/1	0.88	0.14	63,63,63,63	0
57	MG	1F	303	1/1	0.88	0.11	59,59,59,59	0
57	MG	2A	3694	1/1	0.88	0.14	59,59,59,59	0
57	MG	2A	3416	1/1	0.88	0.18	60,60,60,60	0
57	MG	1A	3709	1/1	0.88	0.10	58,58,58,58	0
57	MG	2A	3256	1/1	0.88	0.24	57,57,57,57	0
57	MG	2A	3056	1/1	0.88	0.32	74,74,74,74	0
57	MG	1O	202	1/1	0.88	0.17	66,66,66,66	0
57	MG	2A	3263	1/1	0.88	0.17	65,65,65,65	0
57	MG	2A	3264	1/1	0.88	0.27	65,65,65,65	0
57	MG	2A	3708	1/1	0.88	0.15	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	2a	1693	1/1	0.88	0.19	67,67,67,67	0
57	MG	2A	3265	1/1	0.88	0.18	65,65,65,65	0
57	MG	2a	1697	1/1	0.88	0.22	68,68,68,68	0
57	MG	1A	3226	1/1	0.88	0.16	46,46,46,46	0
57	MG	2A	3443	1/1	0.88	0.17	50,50,50,50	0
57	MG	1A	3065	1/1	0.88	0.11	56,56,56,56	0
57	MG	2A	3083	1/1	0.88	0.13	62,62,62,62	0
57	MG	1A	3721	1/1	0.88	0.20	73,73,73,73	0
57	MG	2A	3457	1/1	0.88	0.12	72,72,72,72	0
57	MG	2A	3733	1/1	0.88	0.16	72,72,72,72	0
57	MG	1a	1711	1/1	0.88	0.27	62,62,62,62	0
57	MG	1R	206	1/1	0.88	0.11	32,32,32,32	0
57	MG	1A	3418	1/1	0.88	0.35	69,69,69,69	0
57	MG	1A	4023	1/1	0.88	0.12	53,53,53,53	0
57	MG	2A	3476	1/1	0.88	0.27	68,68,68,68	0
57	MG	1A	3466	1/1	0.88	0.19	58,58,58,58	0
57	MG	2A	3754	1/1	0.88	0.08	44,44,44,44	0
57	MG	2a	1723	1/1	0.88	0.30	66,66,66,66	0
57	MG	2a	1725	1/1	0.88	0.45	75,75,75,75	0
57	MG	1a	1733	1/1	0.88	0.40	79,79,79,79	0
57	MG	1T	203	1/1	0.88	0.18	54,54,54,54	0
57	MG	1a	1735	1/1	0.88	0.30	53,53,53,53	0
57	MG	1A	3614	1/1	0.88	0.09	15,15,15,15	0
57	MG	1A	4036	1/1	0.88	0.09	52,52,52,52	0
57	MG	1A	3737	1/1	0.88	0.09	65,65,65,65	0
57	MG	2A	3497	1/1	0.88	0.25	49,49,49,49	0
57	MG	1A	3739	1/1	0.88	0.11	22,22,22,22	0
57	MG	2A	3302	1/1	0.88	0.33	64,64,64,64	0
57	MG	1a	1757	1/1	0.88	0.20	50,50,50,50	0
57	MG	2A	3121	1/1	0.88	0.14	60,60,60,60	0
57	MG	1A	3129	1/1	0.88	0.18	53,53,53,53	0
57	MG	2A	3523	1/1	0.88	0.14	63,63,63,63	0
57	MG	2A	3527	1/1	0.88	0.13	70,70,70,70	0
57	MG	2A	3842	1/1	0.88	0.13	76,76,76,76	0
57	MG	2a	1775	1/1	0.88	0.14	67,67,67,67	0
57	MG	2a	1777	1/1	0.88	0.13	75,75,75,75	0
57	MG	2A	3530	1/1	0.88	0.08	43,43,43,43	0
57	MG	2a	1785	1/1	0.88	0.15	80,80,80,80	0
57	MG	2A	3136	1/1	0.88	0.13	68,68,68,68	0
57	MG	1A	3915	1/1	0.88	0.15	38,38,38,38	0
57	MG	2a	1788	1/1	0.88	0.27	77,77,77,77	0
57	MG	1a	1776	1/1	0.88	0.21	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3926	1/1	0.88	0.11	32,32,32,32	0
57	MG	18	105	1/1	0.88	0.14	52,52,52,52	0
57	MG	1A	3768	1/1	0.88	0.09	23,23,23,23	0
57	MG	1a	1603	1/1	0.88	0.11	67,67,67,67	0
57	MG	1a	1604	1/1	0.88	0.11	59,59,59,59	0
57	MG	2A	3566	1/1	0.88	0.16	64,64,64,64	0
57	MG	2A	3328	1/1	0.88	0.20	68,68,68,68	0
57	MG	2B	215	1/1	0.88	0.16	73,73,73,73	0
57	MG	1A	3530	1/1	0.88	0.16	45,45,45,45	0
57	MG	1A	3258	1/1	0.88	0.11	79,79,79,79	0
57	MG	1A	3334	1/1	0.88	0.14	49,49,49,49	0
57	MG	2A	3178	1/1	0.88	0.14	60,60,60,60	0
57	MG	2A	3586	1/1	0.88	0.14	69,69,69,69	0
57	MG	1A	3272	1/1	0.88	0.16	52,52,52,52	0
57	MG	2e	201	1/1	0.88	0.12	72,72,72,72	0
57	MG	2A	3594	1/1	0.88	0.24	69,69,69,69	0
57	MG	2O	201	1/1	0.88	0.20	57,57,57,57	0
57	MG	2l	201	1/1	0.88	0.16	64,64,64,64	0
57	MG	1A	3946	1/1	0.88	0.13	72,72,72,72	0
57	MG	1A	3087	1/1	0.88	0.19	34,34,34,34	0
57	MG	1a	1627	1/1	0.88	0.28	59,59,59,59	0
57	MG	1a	1805	1/1	0.88	0.08	58,58,58,58	0
57	MG	1A	4094	1/1	0.88	0.11	52,52,52,52	0
57	MG	2A	3616	1/1	0.88	0.10	36,36,36,36	0
57	MG	2Z	301	1/1	0.88	0.10	82,82,82,82	0
57	MG	1A	3542	1/1	0.88	0.23	59,59,59,59	0
57	MG	2x	103	1/1	0.88	0.15	81,81,81,81	0
57	MG	1A	3654	1/1	0.88	0.16	52,52,52,52	0
57	MG	1A	3383	1/1	0.89	0.20	44,44,44,44	0
57	MG	1A	4082	1/1	0.89	0.11	23,23,23,23	0
57	MG	1a	1779	1/1	0.89	0.17	65,65,65,65	0
57	MG	1A	3535	1/1	0.89	0.27	58,58,58,58	0
57	MG	25	103	1/1	0.89	0.24	61,61,61,61	0
57	MG	1A	3661	1/1	0.89	0.10	57,57,57,57	0
57	MG	2A	3621	1/1	0.89	0.15	53,53,53,53	0
57	MG	2A	3623	1/1	0.89	0.10	60,60,60,60	0
57	MG	2a	1602	1/1	0.89	0.10	70,70,70,70	0
57	MG	1A	3299	1/1	0.89	0.16	56,56,56,56	0
57	MG	2a	1605	1/1	0.89	0.34	77,77,77,77	0
57	MG	1A	3960	1/1	0.89	0.09	38,38,38,38	0
57	MG	2a	1607	1/1	0.89	0.12	58,58,58,58	0
57	MG	1a	1615	1/1	0.89	0.19	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1a	1789	1/1	0.89	0.11	71,71,71,71	0
57	MG	1A	3467	1/1	0.89	0.17	34,34,34,34	0
57	MG	1A	3968	1/1	0.89	0.12	57,57,57,57	0
57	MG	1a	1625	1/1	0.89	0.21	62,62,62,62	0
57	MG	2a	1616	1/1	0.89	0.16	72,72,72,72	0
57	MG	2a	1617	1/1	0.89	0.31	73,73,73,73	0
57	MG	1A	3680	1/1	0.89	0.12	63,63,63,63	0
57	MG	1A	3260	1/1	0.89	0.06	30,30,30,30	0
57	MG	2A	3194	1/1	0.89	0.19	58,58,58,58	0
57	MG	1A	3269	1/1	0.89	0.20	63,63,63,63	0
57	MG	2A	3367	1/1	0.89	0.11	60,60,60,60	0
57	MG	2A	3196	1/1	0.89	0.32	58,58,58,58	0
57	MG	1A	3248	1/1	0.89	0.22	68,68,68,68	0
57	MG	1A	3834	1/1	0.89	0.09	55,55,55,55	0
57	MG	1A	3319	1/1	0.89	0.17	53,53,53,53	0
57	MG	1a	1637	1/1	0.89	0.12	52,52,52,52	0
57	MG	2A	3203	1/1	0.89	0.08	66,66,66,66	0
57	MG	2a	1643	1/1	0.89	0.12	60,60,60,60	0
57	MG	1a	1639	1/1	0.89	0.30	65,65,65,65	0
57	MG	1A	3320	1/1	0.89	0.08	46,46,46,46	0
57	MG	1a	1646	1/1	0.89	0.10	66,66,66,66	0
57	MG	1A	3252	1/1	0.89	0.12	76,76,76,76	0
57	MG	1l	202	1/1	0.89	0.16	68,68,68,68	0
57	MG	1A	3994	1/1	0.89	0.17	65,65,65,65	0
57	MG	1A	3484	1/1	0.89	0.12	46,46,46,46	0
57	MG	2a	1652	1/1	0.89	0.13	64,64,64,64	0
57	MG	2a	1653	1/1	0.89	0.26	65,65,65,65	0
57	MG	2a	1655	1/1	0.89	0.12	81,81,81,81	0
57	MG	1A	3857	1/1	0.89	0.32	42,42,42,42	0
57	MG	1a	1663	1/1	0.89	0.14	64,64,64,64	0
57	MG	2a	1658	1/1	0.89	0.16	68,68,68,68	0
57	MG	1A	3121	1/1	0.89	0.10	46,46,46,46	0
57	MG	2a	1662	1/1	0.89	0.12	76,76,76,76	0
57	MG	2a	1664	1/1	0.89	0.24	69,69,69,69	0
57	MG	2A	3399	1/1	0.89	0.25	59,59,59,59	0
57	MG	2A	3216	1/1	0.89	0.20	64,64,64,64	0
57	MG	1A	3428	1/1	0.89	0.25	53,53,53,53	0
57	MG	1E	308	1/1	0.89	0.11	30,30,30,30	0
57	MG	2A	3695	1/1	0.89	0.14	52,52,52,52	0
57	MG	2A	3406	1/1	0.89	0.19	45,45,45,45	0
57	MG	1a	1670	1/1	0.89	0.25	72,72,72,72	0
57	MG	2a	1683	1/1	0.89	0.15	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	0.89	0.09	34,34,34,34	0
57	MG	2A	3235	1/1	0.89	0.13	62,62,62,62	0
57	MG	1A	3723	1/1	0.89	0.15	60,60,60,60	0
57	MG	2A	3421	1/1	0.89	0.49	70,70,70,70	0
57	MG	2a	1695	1/1	0.89	0.23	80,80,80,80	0
57	MG	1A	3870	1/1	0.89	0.17	40,40,40,40	0
57	MG	1A	3496	1/1	0.89	0.14	50,50,50,50	0
57	MG	1x	104	1/1	0.89	0.17	69,69,69,69	0
57	MG	1A	3024	1/1	0.89	0.30	64,64,64,64	0
57	MG	2a	1703	1/1	0.89	0.16	75,75,75,75	0
57	MG	2A	3432	1/1	0.89	0.22	50,50,50,50	0
57	MG	1A	3365	1/1	0.89	0.17	66,66,66,66	0
57	MG	1x	109	1/1	0.89	0.17	74,74,74,74	0
57	MG	1x	110	1/1	0.89	0.25	63,63,63,63	0
57	MG	2a	1711	1/1	0.89	0.13	68,68,68,68	0
57	MG	2A	3729	1/1	0.89	0.16	66,66,66,66	0
57	MG	2a	1713	1/1	0.89	0.25	80,80,80,80	0
57	MG	2A	3439	1/1	0.89	0.15	72,72,72,72	0
57	MG	1a	1683	1/1	0.89	0.12	57,57,57,57	0
57	MG	2a	1718	1/1	0.89	0.22	72,72,72,72	0
57	MG	2A	3001	1/1	0.89	0.35	62,62,62,62	0
57	MG	1A	4025	1/1	0.89	0.13	57,57,57,57	0
57	MG	1a	1691	1/1	0.89	0.22	78,78,78,78	0
57	MG	1A	3366	1/1	0.89	0.12	48,48,48,48	0
57	MG	1a	1693	1/1	0.89	0.14	68,68,68,68	0
57	MG	2A	3041	1/1	0.89	0.18	68,68,68,68	0
57	MG	2A	3468	1/1	0.89	0.15	62,62,62,62	0
57	MG	2A	3045	1/1	0.89	0.22	74,74,74,74	0
57	MG	2A	3048	1/1	0.89	0.23	67,67,67,67	0
57	MG	2A	3763	1/1	0.89	0.09	65,65,65,65	0
57	MG	2A	3267	1/1	0.89	0.12	59,59,59,59	0
57	MG	1A	3338	1/1	0.89	0.14	50,50,50,50	0
57	MG	1A	4033	1/1	0.89	0.09	61,61,61,61	0
57	MG	2a	1741	1/1	0.89	0.26	62,62,62,62	0
57	MG	2A	3060	1/1	0.89	0.13	65,65,65,65	0
57	MG	2A	3061	1/1	0.89	0.10	76,76,76,76	0
57	MG	1a	1699	1/1	0.89	0.18	53,53,53,53	0
57	MG	2A	3064	1/1	0.89	0.27	59,59,59,59	0
57	MG	1a	1700	1/1	0.89	0.31	59,59,59,59	0
57	MG	2a	1764	1/1	0.89	0.09	89,89,89,89	0
57	MG	2A	3282	1/1	0.89	0.14	64,64,64,64	0
57	MG	2A	3807	1/1	0.89	0.10	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1S	203	1/1	0.89	0.13	68,68,68,68	0
57	MG	2A	3816	1/1	0.89	0.08	54,54,54,54	0
57	MG	2A	3505	1/1	0.89	0.20	63,63,63,63	0
57	MG	2A	3818	1/1	0.89	0.11	43,43,43,43	0
57	MG	2A	3823	1/1	0.89	0.14	70,70,70,70	0
57	MG	2A	3829	1/1	0.89	0.14	45,45,45,45	0
57	MG	2A	3077	1/1	0.89	0.10	53,53,53,53	0
57	MG	2A	3287	1/1	0.89	0.12	65,65,65,65	0
57	MG	1A	3895	1/1	0.89	0.23	39,39,39,39	0
57	MG	2a	1790	1/1	0.89	0.20	67,67,67,67	0
57	MG	1T	202	1/1	0.89	0.26	68,68,68,68	0
57	MG	2a	1792	1/1	0.89	0.25	66,66,66,66	0
57	MG	1A	3896	1/1	0.89	0.13	64,64,64,64	0
57	MG	1a	1712	1/1	0.89	0.10	85,85,85,85	0
57	MG	2a	1800	1/1	0.89	0.12	83,83,83,83	0
57	MG	1A	3512	1/1	0.89	0.17	58,58,58,58	0
57	MG	2a	1802	1/1	0.89	0.16	76,76,76,76	0
57	MG	2A	3097	1/1	0.89	0.20	63,63,63,63	0
57	MG	1A	4053	1/1	0.89	0.08	59,59,59,59	0
57	MG	1A	3633	1/1	0.89	0.08	21,21,21,21	0
57	MG	1A	3378	1/1	0.89	0.23	50,50,50,50	0
57	MG	2B	208	1/1	0.89	0.21	65,65,65,65	0
57	MG	2A	3310	1/1	0.89	0.12	61,61,61,61	0
57	MG	2A	3548	1/1	0.89	0.10	54,54,54,54	0
57	MG	2a	1819	1/1	0.89	0.25	74,74,74,74	0
57	MG	1Z	301	1/1	0.89	0.16	77,77,77,77	0
57	MG	10	105	1/1	0.89	0.28	65,65,65,65	0
57	MG	2a	1822	1/1	0.89	0.26	67,67,67,67	0
57	MG	1A	3339	1/1	0.89	0.09	36,36,36,36	0
57	MG	13	101	1/1	0.89	0.08	49,49,49,49	0
57	MG	2A	3114	1/1	0.89	0.18	63,63,63,63	0
57	MG	1a	1742	1/1	0.89	0.17	61,61,61,61	0
57	MG	2F	302	1/1	0.89	0.18	72,72,72,72	0
57	MG	2A	3575	1/1	0.89	0.11	43,43,43,43	0
57	MG	1A	3340	1/1	0.89	0.27	63,63,63,63	0
57	MG	1A	3460	1/1	0.89	0.11	57,57,57,57	0
57	MG	1A	4071	1/1	0.89	0.12	47,47,47,47	0
57	MG	2R	201	1/1	0.89	0.23	66,66,66,66	0
57	MG	2A	3327	1/1	0.89	0.12	71,71,71,71	0
57	MG	1a	1755	1/1	0.89	0.15	82,82,82,82	0
57	MG	2A	3331	1/1	0.89	0.13	60,60,60,60	0
57	MG	18	106	1/1	0.89	0.13	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3342	1/1	0.89	0.12	71,71,71,71	0
57	MG	1A	3533	1/1	0.90	0.16	54,54,54,54	0
57	MG	1a	1701	1/1	0.90	0.29	68,68,68,68	0
57	MG	2A	3223	1/1	0.90	0.10	79,79,79,79	0
57	MG	2A	3227	1/1	0.90	0.13	50,50,50,50	0
57	MG	2A	3229	1/1	0.90	0.10	53,53,53,53	0
57	MG	1A	3477	1/1	0.90	0.08	66,66,66,66	0
57	MG	1Z	302	1/1	0.90	0.09	65,65,65,65	0
57	MG	2A	3037	1/1	0.90	0.27	71,71,71,71	0
57	MG	1a	1708	1/1	0.90	0.17	68,68,68,68	0
57	MG	2A	3390	1/1	0.90	0.09	68,68,68,68	0
57	MG	2a	1620	1/1	0.90	0.11	73,73,73,73	0
57	MG	1A	3343	1/1	0.90	0.12	58,58,58,58	0
57	MG	2a	1623	1/1	0.90	0.32	73,73,73,73	0
57	MG	1A	3480	1/1	0.90	0.18	58,58,58,58	0
57	MG	2A	3393	1/1	0.90	0.25	67,67,67,67	0
57	MG	2A	3671	1/1	0.90	0.15	56,56,56,56	0
57	MG	11	103	1/1	0.90	0.09	67,67,67,67	0
57	MG	2A	3049	1/1	0.90	0.07	52,52,52,52	0
57	MG	2a	1633	1/1	0.90	0.24	62,62,62,62	0
57	MG	2a	1635	1/1	0.90	0.15	69,69,69,69	0
57	MG	1a	1714	1/1	0.90	0.16	64,64,64,64	0
57	MG	1A	3439	1/1	0.90	0.30	73,73,73,73	0
57	MG	2a	1640	1/1	0.90	0.18	72,72,72,72	0
57	MG	2A	3057	1/1	0.90	0.24	58,58,58,58	0
57	MG	1A	3313	1/1	0.90	0.26	54,54,54,54	0
57	MG	2A	3410	1/1	0.90	0.11	48,48,48,48	0
57	MG	1A	3285	1/1	0.90	0.10	42,42,42,42	0
57	MG	17	105	1/1	0.90	0.14	49,49,49,49	0
57	MG	2a	1646	1/1	0.90	0.11	63,63,63,63	0
57	MG	2A	3690	1/1	0.90	0.23	65,65,65,65	0
57	MG	1A	3158	1/1	0.90	0.10	56,56,56,56	0
57	MG	1A	4086	1/1	0.90	0.11	50,50,50,50	0
57	MG	1A	3817	1/1	0.90	0.13	49,49,49,49	0
57	MG	2A	3071	1/1	0.90	0.10	62,62,62,62	0
57	MG	2A	3696	1/1	0.90	0.07	70,70,70,70	0
57	MG	1A	3821	1/1	0.90	0.16	38,38,38,38	0
57	MG	2A	3425	1/1	0.90	0.14	55,55,55,55	0
57	MG	1A	4090	1/1	0.90	0.27	48,48,48,48	0
57	MG	1A	3356	1/1	0.90	0.21	43,43,43,43	0
57	MG	2A	3429	1/1	0.90	0.19	59,59,59,59	0
57	MG	2A	3268	1/1	0.90	0.22	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	3447	1/1	0.90	0.18	47,47,47,47	0
57	MG	1A	3964	1/1	0.90	0.11	53,53,53,53	0
57	MG	1B	206	1/1	0.90	0.21	49,49,49,49	0
57	MG	1A	3295	1/1	0.90	0.11	42,42,42,42	0
57	MG	1A	3689	1/1	0.90	0.09	26,26,26,26	0
57	MG	1A	3832	1/1	0.90	0.10	31,31,31,31	0
57	MG	2a	1677	1/1	0.90	0.14	67,67,67,67	0
57	MG	1a	1771	1/1	0.90	0.18	78,78,78,78	0
57	MG	1A	3506	1/1	0.90	0.11	58,58,58,58	0
57	MG	2a	1681	1/1	0.90	0.16	70,70,70,70	0
57	MG	1A	3567	1/1	0.90	0.06	54,54,54,54	0
57	MG	2A	3462	1/1	0.90	0.08	61,61,61,61	0
57	MG	2a	1686	1/1	0.90	0.19	81,81,81,81	0
57	MG	1A	3981	1/1	0.90	0.09	75,75,75,75	0
57	MG	2A	3286	1/1	0.90	0.30	60,60,60,60	0
57	MG	2a	1690	1/1	0.90	0.14	70,70,70,70	0
57	MG	2A	3740	1/1	0.90	0.08	52,52,52,52	0
57	MG	2A	3107	1/1	0.90	0.29	73,73,73,73	0
57	MG	2A	3111	1/1	0.90	0.28	69,69,69,69	0
57	MG	2A	3473	1/1	0.90	0.18	71,71,71,71	0
57	MG	1a	1782	1/1	0.90	0.10	91,91,91,91	0
57	MG	2A	3292	1/1	0.90	0.10	59,59,59,59	0
57	MG	1A	3836	1/1	0.90	0.14	57,57,57,57	0
57	MG	2A	3296	1/1	0.90	0.30	64,64,64,64	0
57	MG	2a	1704	1/1	0.90	0.15	72,72,72,72	0
57	MG	2A	3759	1/1	0.90	0.11	67,67,67,67	0
57	MG	2A	3483	1/1	0.90	0.09	59,59,59,59	0
57	MG	1B	223	1/1	0.90	0.16	63,63,63,63	0
57	MG	1a	1632	1/1	0.90	0.19	61,61,61,61	0
57	MG	2a	1710	1/1	0.90	0.14	72,72,72,72	0
57	MG	1A	3702	1/1	0.90	0.13	47,47,47,47	0
57	MG	2A	3772	1/1	0.90	0.20	68,68,68,68	0
57	MG	2A	3774	1/1	0.90	0.14	76,76,76,76	0
57	MG	1A	3839	1/1	0.90	0.27	67,67,67,67	0
57	MG	2A	3490	1/1	0.90	0.23	63,63,63,63	0
57	MG	2A	3491	1/1	0.90	0.33	70,70,70,70	0
57	MG	2A	3492	1/1	0.90	0.17	62,62,62,62	0
57	MG	2A	3495	1/1	0.90	0.39	72,72,72,72	0
57	MG	2A	3797	1/1	0.90	0.19	65,65,65,65	0
57	MG	1A	3575	1/1	0.90	0.17	44,44,44,44	0
57	MG	1A	3204	1/1	0.90	0.09	48,48,48,48	0
57	MG	2A	3802	1/1	0.90	0.12	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2a	1726	1/1	0.90	0.39	76,76,76,76	0
57	MG	1a	1640	1/1	0.90	0.29	71,71,71,71	0
57	MG	2A	3311	1/1	0.90	0.19	78,78,78,78	0
57	MG	1A	3209	1/1	0.90	0.10	46,46,46,46	0
57	MG	2a	1731	1/1	0.90	0.26	63,63,63,63	0
57	MG	1a	1795	1/1	0.90	0.18	65,65,65,65	0
57	MG	2a	1734	1/1	0.90	0.31	67,67,67,67	0
57	MG	1B	233	1/1	0.90	0.10	57,57,57,57	0
57	MG	1B	234	1/1	0.90	0.13	72,72,72,72	0
57	MG	1a	1649	1/1	0.90	0.16	62,62,62,62	0
57	MG	2a	1740	1/1	0.90	0.28	70,70,70,70	0
57	MG	1a	1650	1/1	0.90	0.24	77,77,77,77	0
57	MG	2A	3840	1/1	0.90	0.11	71,71,71,71	0
57	MG	1A	3588	1/1	0.90	0.11	53,53,53,53	0
57	MG	1A	3124	1/1	0.90	0.18	55,55,55,55	0
57	MG	1a	1660	1/1	0.90	0.19	66,66,66,66	0
57	MG	2A	3326	1/1	0.90	0.11	48,48,48,48	0
57	MG	2A	3537	1/1	0.90	0.17	54,54,54,54	0
57	MG	1A	3596	1/1	0.90	0.23	56,56,56,56	0
57	MG	2A	3862	1/1	0.90	0.25	65,65,65,65	0
57	MG	2A	3540	1/1	0.90	0.11	78,78,78,78	0
57	MG	2B	202	1/1	0.90	0.10	64,64,64,64	0
57	MG	1b	302	1/1	0.90	0.17	84,84,84,84	0
57	MG	1A	3336	1/1	0.90	0.09	49,49,49,49	0
57	MG	1A	3519	1/1	0.90	0.12	58,58,58,58	0
57	MG	2B	207	1/1	0.90	0.18	70,70,70,70	0
57	MG	1A	4005	1/1	0.90	0.11	23,23,23,23	0
57	MG	2A	3192	1/1	0.90	0.22	63,63,63,63	0
57	MG	1G	204	1/1	0.90	0.15	55,55,55,55	0
57	MG	1A	3617	1/1	0.90	0.12	70,70,70,70	0
57	MG	1a	1671	1/1	0.90	0.26	62,62,62,62	0
57	MG	2A	3339	1/1	0.90	0.11	61,61,61,61	0
57	MG	2B	220	1/1	0.90	0.30	73,73,73,73	0
57	MG	2A	3579	1/1	0.90	0.17	57,57,57,57	0
57	MG	1A	3876	1/1	0.90	0.14	37,37,37,37	0
57	MG	1A	3301	1/1	0.90	0.23	61,61,61,61	0
57	MG	1A	3303	1/1	0.90	0.25	36,36,36,36	0
57	MG	2a	1803	1/1	0.90	0.26	74,74,74,74	0
57	MG	1A	3626	1/1	0.90	0.07	32,32,32,32	0
57	MG	1A	3889	1/1	0.90	0.09	35,35,35,35	0
57	MG	2a	1807	1/1	0.90	0.29	67,67,67,67	0
57	MG	1A	3271	1/1	0.90	0.13	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2a	1810	1/1	0.90	0.14	63,63,63,63	0
57	MG	1A	3777	1/1	0.90	0.12	40,40,40,40	0
57	MG	2a	1814	1/1	0.90	0.16	70,70,70,70	0
57	MG	1A	3369	1/1	0.90	0.14	57,57,57,57	0
57	MG	2a	1816	1/1	0.90	0.12	74,74,74,74	0
57	MG	1a	1687	1/1	0.90	0.12	77,77,77,77	0
57	MG	2A	3358	1/1	0.90	0.10	62,62,62,62	0
57	MG	2A	3359	1/1	0.90	0.08	78,78,78,78	0
57	MG	2A	3610	1/1	0.90	0.16	72,72,72,72	0
57	MG	2U	202	1/1	0.90	0.19	51,51,51,51	0
57	MG	2V	201	1/1	0.90	0.10	75,75,75,75	0
57	MG	2A	3360	1/1	0.90	0.15	47,47,47,47	0
57	MG	2X	101	1/1	0.90	0.14	73,73,73,73	0
57	MG	2A	3361	1/1	0.90	0.12	75,75,75,75	0
57	MG	1A	3898	1/1	0.90	0.09	45,45,45,45	0
57	MG	1A	3094	1/1	0.90	0.13	49,49,49,49	0
57	MG	1A	3900	1/1	0.90	0.11	49,49,49,49	0
57	MG	23	102	1/1	0.90	0.21	70,70,70,70	0
57	MG	2v	101	1/1	0.90	0.25	72,72,72,72	0
57	MG	1A	4055	1/1	0.90	0.10	31,31,31,31	0
57	MG	2v	104	1/1	0.90	0.15	70,70,70,70	0
57	MG	2A	3368	1/1	0.90	0.12	60,60,60,60	0
57	MG	1A	3902	1/1	0.90	0.24	40,40,40,40	0
57	MG	1X	106	1/1	0.90	0.12	83,83,83,83	0
57	MG	27	103	1/1	0.90	0.12	58,58,58,58	0
57	MG	2A	3641	1/1	0.90	0.10	44,44,44,44	0
57	MG	1x	112	1/1	0.90	0.17	66,66,66,66	0
57	MG	2A	3217	1/1	0.90	0.14	58,58,58,58	0
58	K	2A	3451	1/1	0.90	0.12	71,71,71,71	0
57	MG	1A	3386	1/1	0.91	0.09	52,52,52,52	0
57	MG	2a	1619	1/1	0.91	0.13	74,74,74,74	0
57	MG	2A	3380	1/1	0.91	0.26	58,58,58,58	0
57	MG	1a	1686	1/1	0.91	0.22	58,58,58,58	0
57	MG	1V	206	1/1	0.91	0.23	60,60,60,60	0
57	MG	1A	3020	1/1	0.91	0.11	44,44,44,44	0
57	MG	1W	202	1/1	0.91	0.17	50,50,50,50	0
57	MG	1x	106	1/1	0.91	0.19	60,60,60,60	0
57	MG	1A	3045	1/1	0.91	0.07	36,36,36,36	0
57	MG	1x	108	1/1	0.91	0.12	33,33,33,33	0
57	MG	1A	3916	1/1	0.91	0.19	37,37,37,37	0
57	MG	1A	3919	1/1	0.91	0.12	71,71,71,71	0
57	MG	1A	3401	1/1	0.91	0.16	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3208	1/1	0.91	0.11	35,35,35,35	0
57	MG	1A	3140	1/1	0.91	0.18	47,47,47,47	0
57	MG	2A	3398	1/1	0.91	0.15	65,65,65,65	0
57	MG	2A	3230	1/1	0.91	0.10	50,50,50,50	0
57	MG	1A	4072	1/1	0.91	0.14	47,47,47,47	0
57	MG	2A	3016	1/1	0.91	0.11	70,70,70,70	0
57	MG	2A	3234	1/1	0.91	0.13	65,65,65,65	0
57	MG	1A	3414	1/1	0.91	0.16	62,62,62,62	0
57	MG	2A	3023	1/1	0.91	0.31	71,71,71,71	0
57	MG	13	104	1/1	0.91	0.15	52,52,52,52	0
57	MG	2A	3028	1/1	0.91	0.11	48,48,48,48	0
57	MG	2A	3029	1/1	0.91	0.19	62,62,62,62	0
57	MG	2A	3243	1/1	0.91	0.12	62,62,62,62	0
57	MG	2A	3420	1/1	0.91	0.25	66,66,66,66	0
57	MG	13	105	1/1	0.91	0.14	62,62,62,62	0
57	MG	2A	3039	1/1	0.91	0.31	70,70,70,70	0
57	MG	1A	3943	1/1	0.91	0.10	28,28,28,28	0
57	MG	2A	3250	1/1	0.91	0.40	68,68,68,68	0
57	MG	1A	3068	1/1	0.91	0.26	48,48,48,48	0
57	MG	2a	1659	1/1	0.91	0.07	80,80,80,80	0
57	MG	2A	3042	1/1	0.91	0.17	56,56,56,56	0
57	MG	1a	1713	1/1	0.91	0.17	73,73,73,73	0
57	MG	1A	3420	1/1	0.91	0.27	67,67,67,67	0
57	MG	1A	3422	1/1	0.91	0.18	38,38,38,38	0
57	MG	1a	1721	1/1	0.91	0.18	68,68,68,68	0
57	MG	2A	3052	1/1	0.91	0.21	70,70,70,70	0
57	MG	2A	3054	1/1	0.91	0.18	68,68,68,68	0
57	MG	2a	1674	1/1	0.91	0.20	64,64,64,64	0
57	MG	1A	3151	1/1	0.91	0.17	43,43,43,43	0
57	MG	1a	1723	1/1	0.91	0.17	55,55,55,55	0
57	MG	2A	3450	1/1	0.91	0.15	67,67,67,67	0
57	MG	19	101	1/1	0.91	0.21	54,54,54,54	0
57	MG	1A	3955	1/1	0.91	0.18	56,56,56,56	0
57	MG	1A	4092	1/1	0.91	0.13	69,69,69,69	0
57	MG	2A	3063	1/1	0.91	0.22	68,68,68,68	0
57	MG	1A	3153	1/1	0.91	0.11	37,37,37,37	0
57	MG	2A	3276	1/1	0.91	0.10	61,61,61,61	0
57	MG	1A	3550	1/1	0.91	0.20	53,53,53,53	0
57	MG	2a	1692	1/1	0.91	0.36	67,67,67,67	0
57	MG	1A	3482	1/1	0.91	0.11	42,42,42,42	0
57	MG	1a	1612	1/1	0.91	0.14	77,77,77,77	0
57	MG	1A	3688	1/1	0.91	0.14	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	3764	1/1	0.91	0.14	64,64,64,64	0
57	MG	2A	3080	1/1	0.91	0.14	61,61,61,61	0
57	MG	2A	3767	1/1	0.91	0.14	61,61,61,61	0
57	MG	1A	3552	1/1	0.91	0.16	55,55,55,55	0
57	MG	1A	3362	1/1	0.91	0.08	54,54,54,54	0
57	MG	2A	3482	1/1	0.91	0.21	56,56,56,56	0
57	MG	1A	3291	1/1	0.91	0.16	54,54,54,54	0
57	MG	1A	3491	1/1	0.91	0.08	45,45,45,45	0
57	MG	2A	3288	1/1	0.91	0.11	66,66,66,66	0
57	MG	1A	3566	1/1	0.91	0.17	36,36,36,36	0
57	MG	1a	1763	1/1	0.91	0.09	66,66,66,66	0
57	MG	2A	3291	1/1	0.91	0.36	75,75,75,75	0
57	MG	1A	3335	1/1	0.91	0.12	63,63,63,63	0
57	MG	1a	1769	1/1	0.91	0.08	55,55,55,55	0
57	MG	2A	3295	1/1	0.91	0.12	57,57,57,57	0
57	MG	1A	3847	1/1	0.91	0.14	62,62,62,62	0
57	MG	1a	1775	1/1	0.91	0.25	70,70,70,70	0
57	MG	1A	3983	1/1	0.91	0.10	51,51,51,51	0
57	MG	2A	3500	1/1	0.91	0.33	69,69,69,69	0
57	MG	1a	1630	1/1	0.91	0.23	70,70,70,70	0
57	MG	2A	3820	1/1	0.91	0.09	47,47,47,47	0
57	MG	1A	3568	1/1	0.91	0.18	61,61,61,61	0
57	MG	2a	1724	1/1	0.91	0.24	72,72,72,72	0
57	MG	2A	3828	1/1	0.91	0.10	66,66,66,66	0
57	MG	2A	3304	1/1	0.91	0.15	66,66,66,66	0
57	MG	2A	3109	1/1	0.91	0.11	60,60,60,60	0
57	MG	2A	3512	1/1	0.91	0.19	63,63,63,63	0
57	MG	1A	3292	1/1	0.91	0.13	59,59,59,59	0
57	MG	2A	3518	1/1	0.91	0.15	44,44,44,44	0
57	MG	2A	3308	1/1	0.91	0.15	68,68,68,68	0
57	MG	2A	3526	1/1	0.91	0.11	52,52,52,52	0
57	MG	2A	3309	1/1	0.91	0.11	63,63,63,63	0
57	MG	2a	1737	1/1	0.91	0.31	63,63,63,63	0
57	MG	1A	3986	1/1	0.91	0.11	76,76,76,76	0
57	MG	2A	3531	1/1	0.91	0.09	53,53,53,53	0
57	MG	1A	3717	1/1	0.91	0.29	60,60,60,60	0
57	MG	1A	3576	1/1	0.91	0.13	47,47,47,47	0
57	MG	2a	1745	1/1	0.91	0.18	70,70,70,70	0
57	MG	1A	3073	1/1	0.91	0.35	68,68,68,68	0
57	MG	2A	3119	1/1	0.91	0.20	61,61,61,61	0
57	MG	2a	1749	1/1	0.91	0.09	62,62,62,62	0
57	MG	1A	3864	1/1	0.91	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	1a	1641	1/1	0.91	0.20	73,73,73,73	0
57	MG	1A	3865	1/1	0.91	0.10	45,45,45,45	0
57	MG	2A	3129	1/1	0.91	0.14	78,78,78,78	0
57	MG	2B	213	1/1	0.91	0.21	62,62,62,62	0
57	MG	2A	3133	1/1	0.91	0.21	57,57,57,57	0
57	MG	1D	313	1/1	0.91	0.10	36,36,36,36	0
57	MG	2A	3138	1/1	0.91	0.29	61,61,61,61	0
57	MG	2B	217	1/1	0.91	0.17	71,71,71,71	0
57	MG	2A	3562	1/1	0.91	0.13	45,45,45,45	0
57	MG	2a	1784	1/1	0.91	0.16	68,68,68,68	0
57	MG	2A	3142	1/1	0.91	0.15	70,70,70,70	0
57	MG	2A	3144	1/1	0.91	0.18	45,45,45,45	0
57	MG	1A	3374	1/1	0.91	0.19	48,48,48,48	0
57	MG	2E	304	1/1	0.91	0.12	65,65,65,65	0
57	MG	1a	1648	1/1	0.91	0.21	63,63,63,63	0
57	MG	1A	3244	1/1	0.91	0.27	39,39,39,39	0
57	MG	2F	306	1/1	0.91	0.22	50,50,50,50	0
57	MG	2A	3157	1/1	0.91	0.17	64,64,64,64	0
57	MG	2A	3335	1/1	0.91	0.15	78,78,78,78	0
57	MG	1A	3100	1/1	0.91	0.20	72,72,72,72	0
57	MG	2a	1798	1/1	0.91	0.14	81,81,81,81	0
57	MG	1E	311	1/1	0.91	0.21	41,41,41,41	0
57	MG	2A	3590	1/1	0.91	0.14	67,67,67,67	0
57	MG	1a	1656	1/1	0.91	0.11	50,50,50,50	0
57	MG	1A	3509	1/1	0.91	0.09	50,50,50,50	0
57	MG	1A	4006	1/1	0.91	0.16	32,32,32,32	0
57	MG	2A	3603	1/1	0.91	0.10	46,46,46,46	0
57	MG	1A	3047	1/1	0.91	0.15	33,33,33,33	0
57	MG	2A	3345	1/1	0.91	0.09	67,67,67,67	0
57	MG	2a	1809	1/1	0.91	0.20	74,74,74,74	0
57	MG	2V	202	1/1	0.91	0.34	54,54,54,54	0
57	MG	2A	3346	1/1	0.91	0.08	65,65,65,65	0
57	MG	1A	3251	1/1	0.91	0.15	45,45,45,45	0
57	MG	2A	3176	1/1	0.91	0.20	69,69,69,69	0
57	MG	2A	3612	1/1	0.91	0.14	61,61,61,61	0
57	MG	1a	1826	1/1	0.91	0.14	62,62,62,62	0
57	MG	1b	301	1/1	0.91	0.09	82,82,82,82	0
57	MG	2A	3184	1/1	0.91	0.20	62,62,62,62	0
57	MG	23	103	1/1	0.91	0.11	56,56,56,56	0
57	MG	1a	1664	1/1	0.91	0.26	73,73,73,73	0
57	MG	1e	202	1/1	0.91	0.17	53,53,53,53	0
57	MG	1f	202	1/1	0.91	0.14	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	4020	1/1	0.91	0.07	44,44,44,44	0
57	MG	1A	3759	1/1	0.91	0.11	26,26,26,26	0
57	MG	2a	1601	1/1	0.91	0.16	75,75,75,75	0
57	MG	1A	3764	1/1	0.91	0.13	33,33,33,33	0
57	MG	1n	101	1/1	0.91	0.29	64,64,64,64	0
57	MG	2A	3642	1/1	0.91	0.14	57,57,57,57	0
57	MG	1A	3891	1/1	0.91	0.07	34,34,34,34	0
57	MG	1A	3892	1/1	0.91	0.13	24,24,24,24	0
57	MG	1A	3451	1/1	0.91	0.25	43,43,43,43	0
57	MG	2a	1609	1/1	0.91	0.09	78,78,78,78	0
57	MG	1A	3515	1/1	0.91	0.10	61,61,61,61	0
57	MG	1A	3781	1/1	0.91	0.07	63,63,63,63	0
57	MG	1A	4038	1/1	0.91	0.12	55,55,55,55	0
57	MG	1A	3050	1/1	0.91	0.10	27,27,27,27	0
57	MG	2a	1615	1/1	0.91	0.18	64,64,64,64	0
57	MG	1A	3195	1/1	0.91	0.12	30,30,30,30	0
57	MG	1U	205	1/1	0.91	0.15	38,38,38,38	0
57	MG	1A	3501	1/1	0.92	0.16	61,61,61,61	0
57	MG	1A	3924	1/1	0.92	0.11	51,51,51,51	0
57	MG	1B	203	1/1	0.92	0.06	37,37,37,37	0
57	MG	2A	3180	1/1	0.92	0.14	54,54,54,54	0
57	MG	1A	3747	1/1	0.92	0.10	45,45,45,45	0
57	MG	28	102	1/1	0.92	0.16	54,54,54,54	0
57	MG	1A	3928	1/1	0.92	0.08	46,46,46,46	0
57	MG	2A	3356	1/1	0.92	0.24	56,56,56,56	0
57	MG	1B	208	1/1	0.92	0.20	62,62,62,62	0
57	MG	1A	3233	1/1	0.92	0.08	56,56,56,56	0
57	MG	1f	201	1/1	0.92	0.18	50,50,50,50	0
57	MG	1A	3004	1/1	0.92	0.08	28,28,28,28	0
57	MG	1A	3595	1/1	0.92	0.13	37,37,37,37	0
57	MG	1B	218	1/1	0.92	0.16	49,49,49,49	0
57	MG	1A	3245	1/1	0.92	0.11	51,51,51,51	0
57	MG	1A	3601	1/1	0.92	0.09	35,35,35,35	0
57	MG	1A	3207	1/1	0.92	0.10	51,51,51,51	0
57	MG	2A	3646	1/1	0.92	0.12	58,58,58,58	0
57	MG	1a	1651	1/1	0.92	0.13	71,71,71,71	0
57	MG	1A	3789	1/1	0.92	0.14	54,54,54,54	0
57	MG	2A	3201	1/1	0.92	0.13	69,69,69,69	0
57	MG	1A	3794	1/1	0.92	0.08	30,30,30,30	0
57	MG	2A	3655	1/1	0.92	0.19	63,63,63,63	0
57	MG	1a	1657	1/1	0.92	0.21	55,55,55,55	0
57	MG	2a	1621	1/1	0.92	0.19	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3376	1/1	0.92	0.14	53,53,53,53	0
57	MG	2A	3377	1/1	0.92	0.15	67,67,67,67	0
57	MG	1A	3609	1/1	0.92	0.09	43,43,43,43	0
57	MG	1A	3610	1/1	0.92	0.09	43,43,43,43	0
57	MG	1A	3387	1/1	0.92	0.10	51,51,51,51	0
57	MG	2a	1629	1/1	0.92	0.07	81,81,81,81	0
57	MG	1A	3961	1/1	0.92	0.08	52,52,52,52	0
57	MG	1A	3616	1/1	0.92	0.08	35,35,35,35	0
57	MG	1A	3449	1/1	0.92	0.11	67,67,67,67	0
57	MG	2a	1634	1/1	0.92	0.26	70,70,70,70	0
57	MG	1D	305	1/1	0.92	0.16	48,48,48,48	0
57	MG	1A	3967	1/1	0.92	0.12	42,42,42,42	0
57	MG	2A	3387	1/1	0.92	0.09	58,58,58,58	0
57	MG	2a	1639	1/1	0.92	0.14	67,67,67,67	0
57	MG	1A	3618	1/1	0.92	0.12	28,28,28,28	0
57	MG	1A	3970	1/1	0.92	0.11	54,54,54,54	0
57	MG	1A	3388	1/1	0.92	0.11	47,47,47,47	0
57	MG	1a	1675	1/1	0.92	0.20	71,71,71,71	0
57	MG	2A	3684	1/1	0.92	0.10	43,43,43,43	0
57	MG	1A	3973	1/1	0.92	0.09	64,64,64,64	0
57	MG	2A	3222	1/1	0.92	0.14	65,65,65,65	0
57	MG	1A	3452	1/1	0.92	0.25	55,55,55,55	0
57	MG	2A	3688	1/1	0.92	0.10	59,59,59,59	0
57	MG	2A	3689	1/1	0.92	0.16	61,61,61,61	0
57	MG	1A	3813	1/1	0.92	0.08	32,32,32,32	0
57	MG	1A	3392	1/1	0.92	0.10	46,46,46,46	0
57	MG	2A	3692	1/1	0.92	0.12	59,59,59,59	0
57	MG	2A	3401	1/1	0.92	0.21	53,53,53,53	0
57	MG	1F	314	1/1	0.92	0.11	55,55,55,55	0
57	MG	2A	3007	1/1	0.92	0.15	61,61,61,61	0
57	MG	1G	203	1/1	0.92	0.08	59,59,59,59	0
57	MG	2A	3014	1/1	0.92	0.11	46,46,46,46	0
57	MG	2A	3407	1/1	0.92	0.46	65,65,65,65	0
57	MG	2A	3409	1/1	0.92	0.16	43,43,43,43	0
57	MG	1A	3394	1/1	0.92	0.23	61,61,61,61	0
57	MG	1I	201	1/1	0.92	0.08	66,66,66,66	0
57	MG	2a	1666	1/1	0.92	0.14	59,59,59,59	0
57	MG	2A	3413	1/1	0.92	0.27	70,70,70,70	0
57	MG	2A	3238	1/1	0.92	0.11	61,61,61,61	0
57	MG	2A	3415	1/1	0.92	0.20	70,70,70,70	0
57	MG	1A	3525	1/1	0.92	0.15	58,58,58,58	0
57	MG	2A	3417	1/1	0.92	0.26	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3418	1/1	0.92	0.30	60,60,60,60	0
57	MG	2A	3713	1/1	0.92	0.11	57,57,57,57	0
57	MG	2A	3718	1/1	0.92	0.20	66,66,66,66	0
57	MG	1A	3527	1/1	0.92	0.12	50,50,50,50	0
57	MG	1A	3171	1/1	0.92	0.26	43,43,43,43	0
57	MG	2A	3721	1/1	0.92	0.13	62,62,62,62	0
57	MG	1P	205	1/1	0.92	0.20	55,55,55,55	0
57	MG	2A	3725	1/1	0.92	0.10	58,58,58,58	0
57	MG	2A	3727	1/1	0.92	0.15	69,69,69,69	0
57	MG	1Q	205	1/1	0.92	0.09	55,55,55,55	0
57	MG	2A	3246	1/1	0.92	0.10	54,54,54,54	0
57	MG	1A	3829	1/1	0.92	0.12	52,52,52,52	0
57	MG	1A	3463	1/1	0.92	0.10	53,53,53,53	0
57	MG	2A	3738	1/1	0.92	0.20	71,71,71,71	0
57	MG	1A	3321	1/1	0.92	0.14	61,61,61,61	0
57	MG	2A	3251	1/1	0.92	0.15	75,75,75,75	0
57	MG	2A	3742	1/1	0.92	0.21	65,65,65,65	0
57	MG	1A	3172	1/1	0.92	0.09	49,49,49,49	0
57	MG	2A	3043	1/1	0.92	0.21	70,70,70,70	0
57	MG	2A	3434	1/1	0.92	0.19	53,53,53,53	0
57	MG	2A	3254	1/1	0.92	0.08	81,81,81,81	0
57	MG	1A	3403	1/1	0.92	0.16	65,65,65,65	0
57	MG	2A	3756	1/1	0.92	0.23	51,51,51,51	0
57	MG	1a	1704	1/1	0.92	0.27	63,63,63,63	0
57	MG	2A	3758	1/1	0.92	0.12	57,57,57,57	0
57	MG	1A	3534	1/1	0.92	0.13	52,52,52,52	0
57	MG	2A	3260	1/1	0.92	0.15	63,63,63,63	0
57	MG	1A	3468	1/1	0.92	0.08	50,50,50,50	0
57	MG	1A	3672	1/1	0.92	0.05	23,23,23,23	0
57	MG	2A	3053	1/1	0.92	0.23	57,57,57,57	0
57	MG	2a	1717	1/1	0.92	0.17	63,63,63,63	0
57	MG	1A	3673	1/1	0.92	0.16	27,27,27,27	0
57	MG	1A	3841	1/1	0.92	0.09	71,71,71,71	0
57	MG	1A	3088	1/1	0.92	0.09	47,47,47,47	0
57	MG	1V	202	1/1	0.92	0.31	31,31,31,31	0
57	MG	2A	3270	1/1	0.92	0.13	73,73,73,73	0
57	MG	2A	3271	1/1	0.92	0.17	77,77,77,77	0
57	MG	1A	3332	1/1	0.92	0.18	51,51,51,51	0
57	MG	2A	3784	1/1	0.92	0.09	62,62,62,62	0
57	MG	2A	3787	1/1	0.92	0.09	51,51,51,51	0
57	MG	2A	3788	1/1	0.92	0.10	66,66,66,66	0
57	MG	1A	3406	1/1	0.92	0.33	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	3793	1/1	0.92	0.13	62,62,62,62	0
57	MG	1A	3852	1/1	0.92	0.13	76,76,76,76	0
57	MG	2a	1732	1/1	0.92	0.32	64,64,64,64	0
57	MG	2A	3477	1/1	0.92	0.25	68,68,68,68	0
57	MG	1A	4014	1/1	0.92	0.08	28,28,28,28	0
57	MG	2A	3065	1/1	0.92	0.36	75,75,75,75	0
57	MG	2A	3068	1/1	0.92	0.23	62,62,62,62	0
57	MG	1A	3475	1/1	0.92	0.09	56,56,56,56	0
57	MG	1a	1727	1/1	0.92	0.22	53,53,53,53	0
57	MG	2A	3813	1/1	0.92	0.10	61,61,61,61	0
57	MG	1Y	203	1/1	0.92	0.28	52,52,52,52	0
57	MG	1A	3333	1/1	0.92	0.14	50,50,50,50	0
57	MG	1A	3415	1/1	0.92	0.13	45,45,45,45	0
57	MG	1A	3478	1/1	0.92	0.10	65,65,65,65	0
57	MG	1a	1736	1/1	0.92	0.21	60,60,60,60	0
57	MG	1A	3183	1/1	0.92	0.11	46,46,46,46	0
57	MG	1a	1739	1/1	0.92	0.10	65,65,65,65	0
57	MG	2A	3836	1/1	0.92	0.09	64,64,64,64	0
57	MG	2a	1762	1/1	0.92	0.10	62,62,62,62	0
57	MG	1A	3257	1/1	0.92	0.07	57,57,57,57	0
57	MG	1A	3706	1/1	0.92	0.10	39,39,39,39	0
57	MG	1A	3869	1/1	0.92	0.06	39,39,39,39	0
57	MG	1A	3081	1/1	0.92	0.13	46,46,46,46	0
57	MG	1A	3708	1/1	0.92	0.17	55,55,55,55	0
57	MG	2a	1776	1/1	0.92	0.15	60,60,60,60	0
57	MG	1A	3051	1/1	0.92	0.11	42,42,42,42	0
57	MG	1A	4051	1/1	0.92	0.06	31,31,31,31	0
57	MG	2a	1782	1/1	0.92	0.14	59,59,59,59	0
57	MG	1a	1760	1/1	0.92	0.09	63,63,63,63	0
57	MG	1A	3711	1/1	0.92	0.07	67,67,67,67	0
57	MG	1A	3878	1/1	0.92	0.10	40,40,40,40	0
57	MG	2A	3303	1/1	0.92	0.16	52,52,52,52	0
57	MG	2A	3521	1/1	0.92	0.15	60,60,60,60	0
57	MG	1A	4057	1/1	0.92	0.14	31,31,31,31	0
57	MG	1A	3371	1/1	0.92	0.11	57,57,57,57	0
57	MG	2A	3306	1/1	0.92	0.15	69,69,69,69	0
57	MG	1A	3564	1/1	0.92	0.18	35,35,35,35	0
57	MG	2B	209	1/1	0.92	0.20	65,65,65,65	0
57	MG	1A	3373	1/1	0.92	0.21	45,45,45,45	0
57	MG	2B	212	1/1	0.92	0.20	62,62,62,62	0
57	MG	1A	3302	1/1	0.92	0.34	70,70,70,70	0
57	MG	1a	1606	1/1	0.92	0.26	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3722	1/1	0.92	0.10	40,40,40,40	0
57	MG	1A	3232	1/1	0.92	0.26	50,50,50,50	0
57	MG	1A	3724	1/1	0.92	0.19	76,76,76,76	0
57	MG	2B	218	1/1	0.92	0.24	81,81,81,81	0
57	MG	2A	3124	1/1	0.92	0.23	54,54,54,54	0
57	MG	2A	3317	1/1	0.92	0.11	51,51,51,51	0
57	MG	1a	1785	1/1	0.92	0.07	58,58,58,58	0
57	MG	2A	3130	1/1	0.92	0.10	47,47,47,47	0
57	MG	1A	3726	1/1	0.92	0.13	62,62,62,62	0
57	MG	2A	3134	1/1	0.92	0.23	53,53,53,53	0
57	MG	2E	308	1/1	0.92	0.15	39,39,39,39	0
57	MG	2F	301	1/1	0.92	0.16	49,49,49,49	0
57	MG	2A	3561	1/1	0.92	0.09	38,38,38,38	0
57	MG	2F	303	1/1	0.92	0.12	50,50,50,50	0
57	MG	1A	3569	1/1	0.92	0.25	58,58,58,58	0
57	MG	1a	1616	1/1	0.92	0.12	57,57,57,57	0
57	MG	1A	4081	1/1	0.92	0.19	54,54,54,54	0
57	MG	1a	1622	1/1	0.92	0.14	67,67,67,67	0
57	MG	2A	3146	1/1	0.92	0.12	57,57,57,57	0
57	MG	2Q	203	1/1	0.92	0.08	46,46,46,46	0
57	MG	2f	202	1/1	0.92	0.14	77,77,77,77	0
57	MG	1a	1623	1/1	0.92	0.15	64,64,64,64	0
57	MG	2A	3581	1/1	0.92	0.08	61,61,61,61	0
57	MG	1A	3571	1/1	0.92	0.13	41,41,41,41	0
57	MG	2l	202	1/1	0.92	0.10	77,77,77,77	0
57	MG	2l	203	1/1	0.92	0.07	72,72,72,72	0
57	MG	2A	3583	1/1	0.92	0.09	32,32,32,32	0
57	MG	1A	3733	1/1	0.92	0.12	48,48,48,48	0
57	MG	1a	1798	1/1	0.92	0.11	71,71,71,71	0
57	MG	2v	102	1/1	0.92	0.35	77,77,77,77	0
57	MG	1A	3494	1/1	0.92	0.17	56,56,56,56	0
57	MG	2A	3163	1/1	0.92	0.15	54,54,54,54	0
57	MG	2A	3164	1/1	0.92	0.11	46,46,46,46	0
57	MG	2A	3593	1/1	0.92	0.08	67,67,67,67	0
57	MG	1A	3907	1/1	0.92	0.09	41,41,41,41	0
57	MG	1A	3910	1/1	0.92	0.15	42,42,42,42	0
57	MG	1A	3270	1/1	0.92	0.24	53,53,53,53	0
57	MG	1a	1809	1/1	0.92	0.08	69,69,69,69	0
57	MG	1A	3307	1/1	0.92	0.06	30,30,30,30	0
58	K	1A	3570	1/1	0.92	0.12	58,58,58,58	0
57	MG	2A	3172	1/1	0.92	0.12	60,60,60,60	0
57	MG	1A	3247	1/1	0.93	0.13	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3369	1/1	0.93	0.20	51,51,51,51	0
57	MG	27	101	1/1	0.93	0.25	66,66,66,66	0
57	MG	1A	3495	1/1	0.93	0.21	63,63,63,63	0
57	MG	2A	3643	1/1	0.93	0.19	68,68,68,68	0
57	MG	1A	3700	1/1	0.93	0.06	26,26,26,26	0
57	MG	1a	1661	1/1	0.93	0.09	67,67,67,67	0
57	MG	1A	3099	1/1	0.93	0.10	51,51,51,51	0
57	MG	2A	3647	1/1	0.93	0.10	45,45,45,45	0
57	MG	2a	1604	1/1	0.93	0.26	65,65,65,65	0
57	MG	1A	3989	1/1	0.93	0.08	38,38,38,38	0
57	MG	2A	3651	1/1	0.93	0.12	46,46,46,46	0
57	MG	1E	312	1/1	0.93	0.14	58,58,58,58	0
57	MG	2A	3202	1/1	0.93	0.16	61,61,61,61	0
57	MG	1A	3703	1/1	0.93	0.08	31,31,31,31	0
57	MG	1F	308	1/1	0.93	0.13	36,36,36,36	0
57	MG	1A	3437	1/1	0.93	0.12	50,50,50,50	0
57	MG	1A	3144	1/1	0.93	0.09	49,49,49,49	0
57	MG	2A	3383	1/1	0.93	0.18	63,63,63,63	0
57	MG	1A	3996	1/1	0.93	0.10	48,48,48,48	0
57	MG	1a	1672	1/1	0.93	0.09	66,66,66,66	0
57	MG	1A	3049	1/1	0.93	0.08	41,41,41,41	0
57	MG	1a	1674	1/1	0.93	0.27	75,75,75,75	0
57	MG	1A	3215	1/1	0.93	0.14	53,53,53,53	0
57	MG	1N	201	1/1	0.93	0.16	44,44,44,44	0
57	MG	1A	3585	1/1	0.93	0.20	66,66,66,66	0
57	MG	1A	3586	1/1	0.93	0.10	50,50,50,50	0
57	MG	1A	3443	1/1	0.93	0.11	55,55,55,55	0
57	MG	2a	1625	1/1	0.93	0.14	70,70,70,70	0
57	MG	1A	3590	1/1	0.93	0.11	42,42,42,42	0
57	MG	2A	3220	1/1	0.93	0.35	73,73,73,73	0
57	MG	1A	3868	1/1	0.93	0.22	34,34,34,34	0
57	MG	1A	3719	1/1	0.93	0.13	45,45,45,45	0
57	MG	2A	3006	1/1	0.93	0.19	68,68,68,68	0
57	MG	2A	3225	1/1	0.93	0.16	61,61,61,61	0
57	MG	1A	3027	1/1	0.93	0.12	77,77,77,77	0
57	MG	1A	4013	1/1	0.93	0.06	29,29,29,29	0
57	MG	2A	3010	1/1	0.93	0.08	66,66,66,66	0
57	MG	1A	3189	1/1	0.93	0.20	43,43,43,43	0
57	MG	2a	1637	1/1	0.93	0.25	73,73,73,73	0
57	MG	1A	3341	1/1	0.93	0.12	51,51,51,51	0
57	MG	2A	3018	1/1	0.93	0.18	64,64,64,64	0
57	MG	1A	3598	1/1	0.93	0.12	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1a	1694	1/1	0.93	0.14	55,55,55,55	0
57	MG	1A	3190	1/1	0.93	0.13	43,43,43,43	0
57	MG	1A	4024	1/1	0.93	0.07	47,47,47,47	0
57	MG	1A	3606	1/1	0.93	0.08	51,51,51,51	0
57	MG	2A	3034	1/1	0.93	0.10	61,61,61,61	0
57	MG	1A	3731	1/1	0.93	0.10	79,79,79,79	0
57	MG	1A	3885	1/1	0.93	0.09	46,46,46,46	0
57	MG	2A	3245	1/1	0.93	0.11	71,71,71,71	0
57	MG	1A	3888	1/1	0.93	0.11	32,32,32,32	0
57	MG	1V	205	1/1	0.93	0.19	55,55,55,55	0
57	MG	1a	1706	1/1	0.93	0.31	65,65,65,65	0
57	MG	1A	4035	1/1	0.93	0.07	75,75,75,75	0
57	MG	1A	3265	1/1	0.93	0.09	65,65,65,65	0
57	MG	2a	1654	1/1	0.93	0.14	74,74,74,74	0
57	MG	1a	1709	1/1	0.93	0.44	77,77,77,77	0
57	MG	1A	3308	1/1	0.93	0.07	43,43,43,43	0
57	MG	1A	4045	1/1	0.93	0.12	64,64,64,64	0
57	MG	2A	3716	1/1	0.93	0.13	44,44,44,44	0
57	MG	1Y	201	1/1	0.93	0.16	50,50,50,50	0
57	MG	1A	3457	1/1	0.93	0.26	39,39,39,39	0
57	MG	1A	3458	1/1	0.93	0.20	39,39,39,39	0
57	MG	2A	3259	1/1	0.93	0.10	55,55,55,55	0
57	MG	2A	3722	1/1	0.93	0.11	70,70,70,70	0
57	MG	2A	3438	1/1	0.93	0.24	58,58,58,58	0
57	MG	2A	3055	1/1	0.93	0.21	66,66,66,66	0
57	MG	2A	3440	1/1	0.93	0.32	58,58,58,58	0
57	MG	2A	3441	1/1	0.93	0.26	64,64,64,64	0
57	MG	2a	1673	1/1	0.93	0.11	66,66,66,66	0
57	MG	2A	3442	1/1	0.93	0.10	57,57,57,57	0
57	MG	2a	1675	1/1	0.93	0.13	75,75,75,75	0
57	MG	2a	1676	1/1	0.93	0.11	74,74,74,74	0
57	MG	2A	3732	1/1	0.93	0.11	65,65,65,65	0
57	MG	1a	1715	1/1	0.93	0.08	51,51,51,51	0
57	MG	2A	3734	1/1	0.93	0.10	67,67,67,67	0
57	MG	1a	1717	1/1	0.93	0.30	71,71,71,71	0
57	MG	1a	1718	1/1	0.93	0.22	53,53,53,53	0
57	MG	1A	4050	1/1	0.93	0.13	38,38,38,38	0
57	MG	2a	1684	1/1	0.93	0.21	61,61,61,61	0
57	MG	1A	3894	1/1	0.93	0.07	39,39,39,39	0
57	MG	2A	3456	1/1	0.93	0.13	62,62,62,62	0
57	MG	1A	4052	1/1	0.93	0.12	50,50,50,50	0
57	MG	2A	3745	1/1	0.93	0.14	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	10	106	1/1	0.93	0.10	56,56,56,56	0
57	MG	2A	3749	1/1	0.93	0.10	63,63,63,63	0
57	MG	2A	3463	1/1	0.93	0.15	61,61,61,61	0
57	MG	1A	3309	1/1	0.93	0.32	63,63,63,63	0
57	MG	2A	3066	1/1	0.93	0.15	59,59,59,59	0
57	MG	1A	3349	1/1	0.93	0.08	59,59,59,59	0
57	MG	2A	3470	1/1	0.93	0.09	64,64,64,64	0
57	MG	2A	3471	1/1	0.93	0.26	64,64,64,64	0
57	MG	2a	1702	1/1	0.93	0.14	80,80,80,80	0
57	MG	12	3702	1/1	0.93	0.10	45,45,45,45	0
57	MG	2A	3760	1/1	0.93	0.20	62,62,62,62	0
57	MG	1A	3395	1/1	0.93	0.24	56,56,56,56	0
57	MG	1A	3266	1/1	0.93	0.26	68,68,68,68	0
57	MG	1A	3351	1/1	0.93	0.12	47,47,47,47	0
57	MG	15	105	1/1	0.93	0.21	46,46,46,46	0
57	MG	1A	3400	1/1	0.93	0.38	49,49,49,49	0
57	MG	2A	3769	1/1	0.93	0.11	43,43,43,43	0
57	MG	1A	3228	1/1	0.93	0.10	52,52,52,52	0
57	MG	2A	3771	1/1	0.93	0.12	67,67,67,67	0
57	MG	1a	1741	1/1	0.93	0.18	67,67,67,67	0
57	MG	1A	3113	1/1	0.93	0.17	31,31,31,31	0
57	MG	2a	1716	1/1	0.93	0.23	68,68,68,68	0
57	MG	2A	3089	1/1	0.93	0.10	47,47,47,47	0
57	MG	2A	3091	1/1	0.93	0.16	50,50,50,50	0
57	MG	1a	1744	1/1	0.93	0.15	56,56,56,56	0
57	MG	2A	3487	1/1	0.93	0.26	60,60,60,60	0
57	MG	18	101	1/1	0.93	0.27	60,60,60,60	0
57	MG	1a	1747	1/1	0.93	0.08	56,56,56,56	0
57	MG	1a	1751	1/1	0.93	0.07	57,57,57,57	0
57	MG	1A	3783	1/1	0.93	0.08	33,33,33,33	0
57	MG	2A	3794	1/1	0.93	0.11	68,68,68,68	0
57	MG	1A	3637	1/1	0.93	0.07	25,25,25,25	0
57	MG	1A	3918	1/1	0.93	0.08	34,34,34,34	0
57	MG	1A	3537	1/1	0.93	0.23	33,33,33,33	0
57	MG	1A	3791	1/1	0.93	0.10	51,51,51,51	0
57	MG	1A	3317	1/1	0.93	0.12	49,49,49,49	0
57	MG	2A	3298	1/1	0.93	0.08	63,63,63,63	0
57	MG	2A	3808	1/1	0.93	0.07	59,59,59,59	0
57	MG	2A	3809	1/1	0.93	0.17	64,64,64,64	0
57	MG	2a	1735	1/1	0.93	0.31	63,63,63,63	0
57	MG	1A	3927	1/1	0.93	0.08	42,42,42,42	0
57	MG	2A	3812	1/1	0.93	0.08	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	4087	1/1	0.93	0.08	51,51,51,51	0
57	MG	1a	1608	1/1	0.93	0.32	63,63,63,63	0
57	MG	1A	3061	1/1	0.93	0.12	45,45,45,45	0
57	MG	1A	3643	1/1	0.93	0.07	29,29,29,29	0
57	MG	2a	1744	1/1	0.93	0.20	69,69,69,69	0
57	MG	2A	3515	1/1	0.93	0.10	61,61,61,61	0
57	MG	2A	3118	1/1	0.93	0.21	76,76,76,76	0
57	MG	1A	3235	1/1	0.93	0.18	54,54,54,54	0
57	MG	1A	3649	1/1	0.93	0.08	43,43,43,43	0
57	MG	1A	3652	1/1	0.93	0.09	41,41,41,41	0
57	MG	2a	1754	1/1	0.93	0.10	85,85,85,85	0
57	MG	2a	1757	1/1	0.93	0.08	50,50,50,50	0
57	MG	2A	3122	1/1	0.93	0.07	54,54,54,54	0
57	MG	2A	3528	1/1	0.93	0.08	47,47,47,47	0
57	MG	2A	3529	1/1	0.93	0.10	52,52,52,52	0
57	MG	1A	3653	1/1	0.93	0.12	48,48,48,48	0
57	MG	2a	1766	1/1	0.93	0.12	73,73,73,73	0
57	MG	2A	3848	1/1	0.93	0.08	52,52,52,52	0
57	MG	1A	4096	1/1	0.93	0.11	59,59,59,59	0
57	MG	2A	3851	1/1	0.93	0.12	56,56,56,56	0
57	MG	2A	3852	1/1	0.93	0.14	51,51,51,51	0
57	MG	2A	3853	1/1	0.93	0.14	48,48,48,48	0
57	MG	2A	3533	1/1	0.93	0.14	69,69,69,69	0
57	MG	2a	1778	1/1	0.93	0.19	74,74,74,74	0
57	MG	1a	1621	1/1	0.93	0.32	77,77,77,77	0
57	MG	2A	3313	1/1	0.93	0.23	68,68,68,68	0
57	MG	1B	201	1/1	0.93	0.17	63,63,63,63	0
57	MG	1A	3409	1/1	0.93	0.20	43,43,43,43	0
57	MG	1A	3413	1/1	0.93	0.08	49,49,49,49	0
57	MG	1A	3659	1/1	0.93	0.08	26,26,26,26	0
57	MG	1a	1626	1/1	0.93	0.26	64,64,64,64	0
57	MG	2A	3544	1/1	0.93	0.10	47,47,47,47	0
57	MG	1A	3239	1/1	0.93	0.12	47,47,47,47	0
57	MG	1A	3956	1/1	0.93	0.07	45,45,45,45	0
57	MG	2A	3551	1/1	0.93	0.08	52,52,52,52	0
57	MG	2B	210	1/1	0.93	0.14	75,75,75,75	0
57	MG	1A	3322	1/1	0.93	0.21	55,55,55,55	0
57	MG	2a	1797	1/1	0.93	0.18	70,70,70,70	0
57	MG	2A	3558	1/1	0.93	0.09	45,45,45,45	0
57	MG	2a	1799	1/1	0.93	0.16	79,79,79,79	0
57	MG	1A	3958	1/1	0.93	0.09	57,57,57,57	0
57	MG	1a	1796	1/1	0.93	0.12	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3668	1/1	0.93	0.09	42,42,42,42	0
57	MG	2A	3153	1/1	0.93	0.16	43,43,43,43	0
57	MG	2A	3155	1/1	0.93	0.14	65,65,65,65	0
57	MG	2A	3570	1/1	0.93	0.13	53,53,53,53	0
57	MG	2a	1806	1/1	0.93	0.09	65,65,65,65	0
57	MG	1A	3670	1/1	0.93	0.06	22,22,22,22	0
57	MG	1A	3363	1/1	0.93	0.14	43,43,43,43	0
57	MG	2D	305	1/1	0.93	0.15	52,52,52,52	0
57	MG	2A	3576	1/1	0.93	0.11	50,50,50,50	0
57	MG	2a	1811	1/1	0.93	0.17	50,50,50,50	0
57	MG	2A	3161	1/1	0.93	0.12	43,43,43,43	0
57	MG	2A	3580	1/1	0.93	0.14	54,54,54,54	0
57	MG	2A	3162	1/1	0.93	0.33	60,60,60,60	0
57	MG	1a	1802	1/1	0.93	0.13	70,70,70,70	0
57	MG	1a	1803	1/1	0.93	0.11	67,67,67,67	0
57	MG	2A	3165	1/1	0.93	0.18	64,64,64,64	0
57	MG	1A	3827	1/1	0.93	0.17	50,50,50,50	0
57	MG	2F	305	1/1	0.93	0.21	50,50,50,50	0
57	MG	1A	3828	1/1	0.93	0.12	56,56,56,56	0
57	MG	1a	1806	1/1	0.93	0.09	81,81,81,81	0
57	MG	1a	1638	1/1	0.93	0.19	60,60,60,60	0
57	MG	2d	301	1/1	0.93	0.33	63,63,63,63	0
57	MG	2N	201	1/1	0.93	0.07	62,62,62,62	0
57	MG	1A	3326	1/1	0.93	0.09	35,35,35,35	0
57	MG	1B	224	1/1	0.93	0.09	57,57,57,57	0
57	MG	2A	3173	1/1	0.93	0.09	61,61,61,61	0
57	MG	2k	201	1/1	0.93	0.12	73,73,73,73	0
57	MG	2A	3350	1/1	0.93	0.12	65,65,65,65	0
57	MG	1A	3328	1/1	0.93	0.17	62,62,62,62	0
57	MG	1a	1642	1/1	0.93	0.19	70,70,70,70	0
57	MG	1A	3971	1/1	0.93	0.11	65,65,65,65	0
57	MG	2r	101	1/1	0.93	0.18	84,84,84,84	0
57	MG	1A	3679	1/1	0.93	0.07	30,30,30,30	0
57	MG	2U	201	1/1	0.93	0.14	63,63,63,63	0
57	MG	1A	3199	1/1	0.93	0.42	39,39,39,39	0
57	MG	1A	3833	1/1	0.93	0.08	38,38,38,38	0
57	MG	2A	3613	1/1	0.93	0.15	68,68,68,68	0
57	MG	1A	3368	1/1	0.93	0.08	48,48,48,48	0
57	MG	2A	3188	1/1	0.93	0.22	74,74,74,74	0
57	MG	1A	3085	1/1	0.93	0.23	34,34,34,34	0
57	MG	1A	3427	1/1	0.93	0.16	59,59,59,59	0
57	MG	2A	3624	1/1	0.93	0.15	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3191	1/1	0.93	0.09	68,68,68,68	0
57	MG	1D	310	1/1	0.93	0.17	28,28,28,28	0
57	MG	2A	3193	1/1	0.93	0.11	65,65,65,65	0
57	MG	1A	3086	1/1	0.93	0.21	30,30,30,30	0
57	MG	2A	3108	1/1	0.94	0.09	50,50,50,50	0
57	MG	2T	3504	1/1	0.94	0.16	59,59,59,59	0
57	MG	1A	3523	1/1	0.94	0.34	40,40,40,40	0
57	MG	1a	1730	1/1	0.94	0.20	54,54,54,54	0
57	MG	1A	3819	1/1	0.94	0.06	32,32,32,32	0
57	MG	1A	3083	1/1	0.94	0.25	46,46,46,46	0
57	MG	1U	208	1/1	0.94	0.19	36,36,36,36	0
57	MG	2W	202	1/1	0.94	0.09	43,43,43,43	0
57	MG	1A	3988	1/1	0.94	0.10	23,23,23,23	0
57	MG	1A	3318	1/1	0.94	0.12	53,53,53,53	0
57	MG	2A	3600	1/1	0.94	0.17	58,58,58,58	0
57	MG	20	102	1/1	0.94	0.13	68,68,68,68	0
57	MG	2A	3601	1/1	0.94	0.17	57,57,57,57	0
57	MG	1a	1738	1/1	0.94	0.29	62,62,62,62	0
57	MG	1A	3528	1/1	0.94	0.12	52,52,52,52	0
57	MG	1A	3250	1/1	0.94	0.16	69,69,69,69	0
57	MG	25	101	1/1	0.94	0.27	61,61,61,61	0
57	MG	1A	3647	1/1	0.94	0.09	53,53,53,53	0
57	MG	2A	3608	1/1	0.94	0.18	70,70,70,70	0
57	MG	1a	1743	1/1	0.94	0.14	65,65,65,65	0
57	MG	1A	3122	1/1	0.94	0.10	47,47,47,47	0
57	MG	2A	3127	1/1	0.94	0.14	53,53,53,53	0
57	MG	1X	105	1/1	0.94	0.07	51,51,51,51	0
57	MG	2A	3615	1/1	0.94	0.07	31,31,31,31	0
57	MG	1A	3377	1/1	0.94	0.22	40,40,40,40	0
57	MG	1A	3450	1/1	0.94	0.18	48,48,48,48	0
57	MG	2A	3618	1/1	0.94	0.11	54,54,54,54	0
57	MG	2A	3619	1/1	0.94	0.13	50,50,50,50	0
57	MG	1A	3018	1/1	0.94	0.11	33,33,33,33	0
57	MG	2A	3135	1/1	0.94	0.10	38,38,38,38	0
57	MG	1A	4000	1/1	0.94	0.11	46,46,46,46	0
57	MG	2A	3351	1/1	0.94	0.08	60,60,60,60	0
57	MG	1A	3655	1/1	0.94	0.14	59,59,59,59	0
57	MG	2A	3139	1/1	0.94	0.24	57,57,57,57	0
57	MG	2A	3141	1/1	0.94	0.14	59,59,59,59	0
57	MG	1A	4003	1/1	0.94	0.12	51,51,51,51	0
57	MG	1Z	303	1/1	0.94	0.18	57,57,57,57	0
57	MG	10	104	1/1	0.94	0.25	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	1761	1/1	0.94	0.13	68,68,68,68	0
57	MG	1A	3001	1/1	0.94	0.13	48,48,48,48	0
57	MG	2A	3150	1/1	0.94	0.10	54,54,54,54	0
57	MG	1A	3198	1/1	0.94	0.07	45,45,45,45	0
57	MG	2A	3362	1/1	0.94	0.17	70,70,70,70	0
57	MG	2A	3649	1/1	0.94	0.08	59,59,59,59	0
57	MG	1A	3130	1/1	0.94	0.12	38,38,38,38	0
57	MG	11	101	1/1	0.94	0.54	48,48,48,48	0
57	MG	2A	3156	1/1	0.94	0.09	74,74,74,74	0
57	MG	1A	3538	1/1	0.94	0.22	54,54,54,54	0
57	MG	12	3701	1/1	0.94	0.07	53,53,53,53	0
57	MG	1a	1777	1/1	0.94	0.10	55,55,55,55	0
57	MG	1a	1778	1/1	0.94	0.10	59,59,59,59	0
57	MG	1A	3200	1/1	0.94	0.10	49,49,49,49	0
57	MG	2A	3659	1/1	0.94	0.08	59,59,59,59	0
57	MG	1A	3540	1/1	0.94	0.25	46,46,46,46	0
57	MG	1A	3843	1/1	0.94	0.16	53,53,53,53	0
57	MG	1A	4016	1/1	0.94	0.08	30,30,30,30	0
57	MG	2A	3663	1/1	0.94	0.09	73,73,73,73	0
57	MG	1A	3844	1/1	0.94	0.09	52,52,52,52	0
57	MG	1A	3385	1/1	0.94	0.17	38,38,38,38	0
57	MG	2A	3666	1/1	0.94	0.12	69,69,69,69	0
57	MG	1a	1786	1/1	0.94	0.08	57,57,57,57	0
57	MG	1A	3330	1/1	0.94	0.12	48,48,48,48	0
57	MG	2A	3670	1/1	0.94	0.10	60,60,60,60	0
57	MG	1A	3850	1/1	0.94	0.15	42,42,42,42	0
57	MG	1A	3543	1/1	0.94	0.19	41,41,41,41	0
57	MG	1A	3261	1/1	0.94	0.06	33,33,33,33	0
57	MG	1A	4027	1/1	0.94	0.06	64,64,64,64	0
57	MG	2A	3679	1/1	0.94	0.11	57,57,57,57	0
57	MG	1A	4028	1/1	0.94	0.08	66,66,66,66	0
57	MG	2A	3179	1/1	0.94	0.20	59,59,59,59	0
57	MG	1A	4030	1/1	0.94	0.06	49,49,49,49	0
57	MG	2A	3182	1/1	0.94	0.23	66,66,66,66	0
57	MG	1a	1602	1/1	0.94	0.11	67,67,67,67	0
57	MG	1A	3264	1/1	0.94	0.23	67,67,67,67	0
57	MG	1A	3547	1/1	0.94	0.28	57,57,57,57	0
57	MG	1A	3859	1/1	0.94	0.14	52,52,52,52	0
57	MG	1A	3860	1/1	0.94	0.08	47,47,47,47	0
57	MG	1a	1801	1/1	0.94	0.10	63,63,63,63	0
57	MG	1A	4037	1/1	0.94	0.08	78,78,78,78	0
57	MG	1a	1609	1/1	0.94	0.10	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3400	1/1	0.94	0.19	47,47,47,47	0
57	MG	1A	3465	1/1	0.94	0.16	52,52,52,52	0
57	MG	2A	3402	1/1	0.94	0.25	55,55,55,55	0
57	MG	1A	4040	1/1	0.94	0.08	58,58,58,58	0
57	MG	2A	3699	1/1	0.94	0.08	65,65,65,65	0
57	MG	1A	3138	1/1	0.94	0.28	39,39,39,39	0
57	MG	1A	4047	1/1	0.94	0.08	42,42,42,42	0
57	MG	1a	1811	1/1	0.94	0.13	76,76,76,76	0
57	MG	1A	3139	1/1	0.94	0.12	42,42,42,42	0
57	MG	1a	1817	1/1	0.94	0.07	64,64,64,64	0
57	MG	1A	3691	1/1	0.94	0.13	73,73,73,73	0
57	MG	1A	3694	1/1	0.94	0.09	42,42,42,42	0
57	MG	1A	3059	1/1	0.94	0.13	54,54,54,54	0
57	MG	2a	1678	1/1	0.94	0.17	65,65,65,65	0
57	MG	1A	3041	1/1	0.94	0.07	32,32,32,32	0
57	MG	1A	3555	1/1	0.94	0.22	58,58,58,58	0
57	MG	1A	3872	1/1	0.94	0.14	31,31,31,31	0
57	MG	2A	3712	1/1	0.94	0.07	68,68,68,68	0
57	MG	1e	201	1/1	0.94	0.10	68,68,68,68	0
57	MG	1A	3022	1/1	0.94	0.06	46,46,46,46	0
57	MG	1A	3214	1/1	0.94	0.15	55,55,55,55	0
57	MG	2a	1687	1/1	0.94	0.15	68,68,68,68	0
57	MG	1A	3704	1/1	0.94	0.13	31,31,31,31	0
57	MG	1A	3275	1/1	0.94	0.12	46,46,46,46	0
57	MG	1A	3277	1/1	0.94	0.07	48,48,48,48	0
57	MG	2a	1691	1/1	0.94	0.12	44,44,44,44	0
57	MG	1A	3090	1/1	0.94	0.10	32,32,32,32	0
57	MG	1A	3882	1/1	0.94	0.08	32,32,32,32	0
57	MG	1A	3884	1/1	0.94	0.11	28,28,28,28	0
57	MG	1A	3289	1/1	0.94	0.26	47,47,47,47	0
57	MG	2A	3428	1/1	0.94	0.09	77,77,77,77	0
57	MG	1A	3886	1/1	0.94	0.10	52,52,52,52	0
57	MG	2A	3430	1/1	0.94	0.13	51,51,51,51	0
57	MG	1A	3710	1/1	0.94	0.12	59,59,59,59	0
57	MG	1A	3216	1/1	0.94	0.20	61,61,61,61	0
57	MG	1A	3046	1/1	0.94	0.05	40,40,40,40	0
57	MG	1A	3224	1/1	0.94	0.17	38,38,38,38	0
57	MG	2a	1705	1/1	0.94	0.09	74,74,74,74	0
57	MG	1A	3002	1/1	0.94	0.07	53,53,53,53	0
57	MG	2A	3226	1/1	0.94	0.12	56,56,56,56	0
57	MG	1A	3579	1/1	0.94	0.39	42,42,42,42	0
57	MG	1w	106	1/1	0.94	0.08	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3483	1/1	0.94	0.16	57,57,57,57	0
57	MG	1a	1645	1/1	0.94	0.10	60,60,60,60	0
57	MG	1A	3078	1/1	0.94	0.08	26,26,26,26	0
57	MG	2A	3444	1/1	0.94	0.07	62,62,62,62	0
57	MG	1A	3897	1/1	0.94	0.07	31,31,31,31	0
57	MG	2A	3447	1/1	0.94	0.14	58,58,58,58	0
57	MG	1A	3488	1/1	0.94	0.14	41,41,41,41	0
57	MG	1A	3416	1/1	0.94	0.11	44,44,44,44	0
57	MG	1A	3490	1/1	0.94	0.10	54,54,54,54	0
57	MG	1A	3417	1/1	0.94	0.15	41,41,41,41	0
57	MG	1A	3905	1/1	0.94	0.07	32,32,32,32	0
57	MG	2A	3458	1/1	0.94	0.10	62,62,62,62	0
57	MG	2A	3459	1/1	0.94	0.20	45,45,45,45	0
57	MG	1A	3591	1/1	0.94	0.10	39,39,39,39	0
57	MG	1A	3592	1/1	0.94	0.16	35,35,35,35	0
57	MG	1A	3492	1/1	0.94	0.09	39,39,39,39	0
57	MG	2A	3466	1/1	0.94	0.10	39,39,39,39	0
57	MG	1B	209	1/1	0.94	0.14	37,37,37,37	0
57	MG	2A	3003	1/1	0.94	0.23	48,48,48,48	0
57	MG	2a	1729	1/1	0.94	0.41	73,73,73,73	0
57	MG	2A	3005	1/1	0.94	0.21	67,67,67,67	0
57	MG	1A	3594	1/1	0.94	0.24	59,59,59,59	0
57	MG	1A	3917	1/1	0.94	0.21	54,54,54,54	0
57	MG	1A	3735	1/1	0.94	0.06	52,52,52,52	0
57	MG	1A	3164	1/1	0.94	0.16	58,58,58,58	0
57	MG	2A	3011	1/1	0.94	0.12	58,58,58,58	0
57	MG	2A	3785	1/1	0.94	0.08	43,43,43,43	0
57	MG	2A	3013	1/1	0.94	0.11	50,50,50,50	0
57	MG	1A	3298	1/1	0.94	0.14	54,54,54,54	0
57	MG	2A	3789	1/1	0.94	0.07	48,48,48,48	0
57	MG	1A	3925	1/1	0.94	0.09	58,58,58,58	0
57	MG	1A	3743	1/1	0.94	0.19	61,61,61,61	0
57	MG	1A	3597	1/1	0.94	0.09	34,34,34,34	0
57	MG	1A	3421	1/1	0.94	0.13	57,57,57,57	0
57	MG	2A	3025	1/1	0.94	0.09	47,47,47,47	0
57	MG	1A	3757	1/1	0.94	0.12	45,45,45,45	0
57	MG	1A	3599	1/1	0.94	0.12	43,43,43,43	0
57	MG	2A	3488	1/1	0.94	0.29	72,72,72,72	0
57	MG	2a	1751	1/1	0.94	0.09	83,83,83,83	0
57	MG	2A	3805	1/1	0.94	0.08	56,56,56,56	0
57	MG	2a	1755	1/1	0.94	0.12	70,70,70,70	0
57	MG	2a	1756	1/1	0.94	0.11	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3806	1/1	0.94	0.13	62,62,62,62	0
57	MG	1A	3761	1/1	0.94	0.06	29,29,29,29	0
57	MG	1A	3763	1/1	0.94	0.10	31,31,31,31	0
57	MG	1A	3167	1/1	0.94	0.10	39,39,39,39	0
57	MG	1A	3766	1/1	0.94	0.11	32,32,32,32	0
57	MG	1a	1678	1/1	0.94	0.29	65,65,65,65	0
57	MG	1A	3603	1/1	0.94	0.11	28,28,28,28	0
57	MG	2A	3272	1/1	0.94	0.08	72,72,72,72	0
57	MG	1B	235	1/1	0.94	0.08	48,48,48,48	0
57	MG	2a	1770	1/1	0.94	0.11	70,70,70,70	0
57	MG	2A	3499	1/1	0.94	0.37	67,67,67,67	0
57	MG	1a	1681	1/1	0.94	0.13	64,64,64,64	0
57	MG	2A	3502	1/1	0.94	0.08	69,69,69,69	0
57	MG	2A	3825	1/1	0.94	0.08	60,60,60,60	0
57	MG	2a	1779	1/1	0.94	0.22	67,67,67,67	0
57	MG	1A	3605	1/1	0.94	0.07	28,28,28,28	0
57	MG	1D	309	1/1	0.94	0.11	41,41,41,41	0
57	MG	2A	3833	1/1	0.94	0.11	45,45,45,45	0
57	MG	2A	3507	1/1	0.94	0.05	39,39,39,39	0
57	MG	1A	3952	1/1	0.94	0.09	49,49,49,49	0
57	MG	2A	3838	1/1	0.94	0.09	59,59,59,59	0
57	MG	1A	3953	1/1	0.94	0.07	63,63,63,63	0
57	MG	1A	3048	1/1	0.94	0.11	24,24,24,24	0
57	MG	1a	1688	1/1	0.94	0.11	63,63,63,63	0
57	MG	2A	3847	1/1	0.94	0.06	47,47,47,47	0
57	MG	1a	1690	1/1	0.94	0.16	61,61,61,61	0
57	MG	2A	3516	1/1	0.94	0.12	28,28,28,28	0
57	MG	1A	3500	1/1	0.94	0.07	47,47,47,47	0
57	MG	2a	1796	1/1	0.94	0.20	71,71,71,71	0
57	MG	1A	3785	1/1	0.94	0.08	49,49,49,49	0
57	MG	2A	3522	1/1	0.94	0.10	52,52,52,52	0
57	MG	2A	3856	1/1	0.94	0.15	67,67,67,67	0
57	MG	1A	3786	1/1	0.94	0.06	42,42,42,42	0
57	MG	2A	3525	1/1	0.94	0.14	58,58,58,58	0
57	MG	2A	3860	1/1	0.94	0.11	66,66,66,66	0
57	MG	2A	3058	1/1	0.94	0.17	55,55,55,55	0
57	MG	1A	3959	1/1	0.94	0.09	43,43,43,43	0
57	MG	1A	3025	1/1	0.94	0.08	38,38,38,38	0
57	MG	1A	3236	1/1	0.94	0.12	63,63,63,63	0
57	MG	1A	3790	1/1	0.94	0.08	48,48,48,48	0
57	MG	2B	204	1/1	0.94	0.13	76,76,76,76	0
57	MG	1A	3237	1/1	0.94	0.26	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3293	1/1	0.94	0.18	54,54,54,54	0
57	MG	1F	312	1/1	0.94	0.14	48,48,48,48	0
57	MG	1F	313	1/1	0.94	0.11	35,35,35,35	0
57	MG	1A	3965	1/1	0.94	0.06	45,45,45,45	0
57	MG	1A	3966	1/1	0.94	0.09	27,27,27,27	0
57	MG	1A	3111	1/1	0.94	0.09	46,46,46,46	0
57	MG	1A	3241	1/1	0.94	0.07	37,37,37,37	0
57	MG	2A	3541	1/1	0.94	0.14	51,51,51,51	0
57	MG	2A	3542	1/1	0.94	0.07	51,51,51,51	0
57	MG	1A	3969	1/1	0.94	0.23	52,52,52,52	0
57	MG	1A	3007	1/1	0.94	0.08	40,40,40,40	0
57	MG	2A	3546	1/1	0.94	0.12	48,48,48,48	0
57	MG	2a	1823	1/1	0.94	0.13	70,70,70,70	0
57	MG	2A	3547	1/1	0.94	0.10	58,58,58,58	0
57	MG	1A	3436	1/1	0.94	0.10	53,53,53,53	0
57	MG	2d	302	1/1	0.94	0.09	70,70,70,70	0
57	MG	2A	3085	1/1	0.94	0.28	67,67,67,67	0
57	MG	1A	3802	1/1	0.94	0.07	22,22,22,22	0
57	MG	2A	3555	1/1	0.94	0.15	59,59,59,59	0
57	MG	1A	3116	1/1	0.94	0.19	42,42,42,42	0
57	MG	2A	3557	1/1	0.94	0.14	47,47,47,47	0
57	MG	2E	306	1/1	0.94	0.09	34,34,34,34	0
57	MG	1Q	201	1/1	0.94	0.34	42,42,42,42	0
57	MG	1A	3975	1/1	0.94	0.07	60,60,60,60	0
57	MG	2q	201	1/1	0.94	0.12	77,77,77,77	0
57	MG	1a	1716	1/1	0.94	0.14	56,56,56,56	0
57	MG	1Q	207	1/1	0.94	0.08	35,35,35,35	0
57	MG	2A	3563	1/1	0.94	0.16	64,64,64,64	0
57	MG	2A	3564	1/1	0.94	0.08	52,52,52,52	0
57	MG	2A	3096	1/1	0.94	0.09	51,51,51,51	0
57	MG	1A	3186	1/1	0.94	0.06	39,39,39,39	0
57	MG	1a	1719	1/1	0.94	0.19	56,56,56,56	0
57	MG	2A	3314	1/1	0.94	0.29	65,65,65,65	0
57	MG	1A	3977	1/1	0.94	0.10	55,55,55,55	0
57	MG	2P	201	1/1	0.94	0.17	60,60,60,60	0
57	MG	1A	3628	1/1	0.94	0.06	21,21,21,21	0
57	MG	1A	3631	1/1	0.94	0.10	62,62,62,62	0
57	MG	2A	3103	1/1	0.94	0.10	59,59,59,59	0
57	MG	2x	104	1/1	0.94	0.11	69,69,69,69	0
57	MG	1A	3517	1/1	0.94	0.07	49,49,49,49	0
57	MG	1A	3187	1/1	0.94	0.08	50,50,50,50	0
57	MG	1A	3370	1/1	0.94	0.09	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	ZN	2n	501	1/1	0.94	0.07	106,106,106,106	0
57	MG	2A	3110	1/1	0.95	0.12	61,61,61,61	0
57	MG	2A	3602	1/1	0.95	0.13	51,51,51,51	0
57	MG	1A	3818	1/1	0.95	0.06	27,27,27,27	0
57	MG	2A	3340	1/1	0.95	0.11	61,61,61,61	0
57	MG	2A	3605	1/1	0.95	0.11	62,62,62,62	0
57	MG	2A	3341	1/1	0.95	0.18	64,64,64,64	0
57	MG	1U	202	1/1	0.95	0.25	42,42,42,42	0
57	MG	2Y	201	1/1	0.95	0.21	56,56,56,56	0
57	MG	2A	3343	1/1	0.95	0.18	64,64,64,64	0
57	MG	2A	3113	1/1	0.95	0.14	60,60,60,60	0
57	MG	1A	3019	1/1	0.95	0.14	50,50,50,50	0
57	MG	1A	3990	1/1	0.95	0.12	40,40,40,40	0
57	MG	1U	206	1/1	0.95	0.17	37,37,37,37	0
57	MG	2A	3614	1/1	0.95	0.09	60,60,60,60	0
57	MG	1A	3010	1/1	0.95	0.05	34,34,34,34	0
57	MG	1U	209	1/1	0.95	0.29	36,36,36,36	0
57	MG	1A	3348	1/1	0.95	0.21	49,49,49,49	0
57	MG	25	104	1/1	0.95	0.11	51,51,51,51	0
57	MG	1V	201	1/1	0.95	0.19	30,30,30,30	0
57	MG	1A	3642	1/1	0.95	0.08	31,31,31,31	0
57	MG	2A	3620	1/1	0.95	0.10	44,44,44,44	0
57	MG	1A	3522	1/1	0.95	0.18	35,35,35,35	0
57	MG	2A	3622	1/1	0.95	0.17	66,66,66,66	0
57	MG	28	101	1/1	0.95	0.14	61,61,61,61	0
57	MG	1a	1748	1/1	0.95	0.05	35,35,35,35	0
57	MG	1A	3644	1/1	0.95	0.07	32,32,32,32	0
57	MG	1A	3645	1/1	0.95	0.06	30,30,30,30	0
57	MG	2A	3629	1/1	0.95	0.06	38,38,38,38	0
57	MG	1A	3091	1/1	0.95	0.14	60,60,60,60	0
57	MG	2A	3131	1/1	0.95	0.12	49,49,49,49	0
57	MG	2A	3633	1/1	0.95	0.07	34,34,34,34	0
57	MG	2A	3132	1/1	0.95	0.06	49,49,49,49	0
57	MG	1a	1754	1/1	0.95	0.06	54,54,54,54	0
57	MG	1A	3274	1/1	0.95	0.20	36,36,36,36	0
57	MG	1A	3092	1/1	0.95	0.09	49,49,49,49	0
57	MG	1A	3431	1/1	0.95	0.08	44,44,44,44	0
57	MG	1A	3432	1/1	0.95	0.07	46,46,46,46	0
57	MG	2a	1613	1/1	0.95	0.10	73,73,73,73	0
57	MG	1A	3355	1/1	0.95	0.16	38,38,38,38	0
57	MG	1A	3435	1/1	0.95	0.10	35,35,35,35	0
57	MG	1a	1764	1/1	0.95	0.13	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3648	1/1	0.95	0.09	55,55,55,55	0
57	MG	2A	3143	1/1	0.95	0.17	53,53,53,53	0
57	MG	1A	4007	1/1	0.95	0.08	21,21,21,21	0
57	MG	1a	1768	1/1	0.95	0.10	66,66,66,66	0
57	MG	1A	3029	1/1	0.95	0.07	38,38,38,38	0
57	MG	2A	3375	1/1	0.95	0.13	56,56,56,56	0
57	MG	1a	1770	1/1	0.95	0.20	75,75,75,75	0
57	MG	2a	1624	1/1	0.95	0.08	65,65,65,65	0
57	MG	10	103	1/1	0.95	0.08	51,51,51,51	0
57	MG	2A	3151	1/1	0.95	0.07	55,55,55,55	0
57	MG	1A	3658	1/1	0.95	0.08	25,25,25,25	0
57	MG	1A	3150	1/1	0.95	0.23	42,42,42,42	0
57	MG	1A	3288	1/1	0.95	0.12	54,54,54,54	0
57	MG	10	107	1/1	0.95	0.16	61,61,61,61	0
57	MG	1A	3662	1/1	0.95	0.08	53,53,53,53	0
57	MG	10	109	1/1	0.95	0.08	46,46,46,46	0
57	MG	2A	3160	1/1	0.95	0.13	55,55,55,55	0
57	MG	1A	3217	1/1	0.95	0.12	34,34,34,34	0
57	MG	1A	3846	1/1	0.95	0.13	48,48,48,48	0
57	MG	1A	3536	1/1	0.95	0.10	38,38,38,38	0
57	MG	1A	3218	1/1	0.95	0.14	46,46,46,46	0
57	MG	1A	3074	1/1	0.95	0.09	27,27,27,27	0
57	MG	1A	3444	1/1	0.95	0.17	41,41,41,41	0
57	MG	1A	3853	1/1	0.95	0.06	26,26,26,26	0
57	MG	2A	3674	1/1	0.95	0.09	66,66,66,66	0
57	MG	1A	3220	1/1	0.95	0.20	47,47,47,47	0
57	MG	1A	3293	1/1	0.95	0.19	53,53,53,53	0
57	MG	2A	3677	1/1	0.95	0.10	65,65,65,65	0
57	MG	2A	3396	1/1	0.95	0.14	57,57,57,57	0
57	MG	2A	3397	1/1	0.95	0.13	44,44,44,44	0
57	MG	1A	3221	1/1	0.95	0.14	45,45,45,45	0
57	MG	17	104	1/1	0.95	0.15	58,58,58,58	0
57	MG	1A	3448	1/1	0.95	0.08	56,56,56,56	0
57	MG	1A	3861	1/1	0.95	0.07	47,47,47,47	0
57	MG	1A	3544	1/1	0.95	0.23	51,51,51,51	0
57	MG	1A	3222	1/1	0.95	0.06	38,38,38,38	0
57	MG	1A	3096	1/1	0.95	0.15	41,41,41,41	0
57	MG	1A	3367	1/1	0.95	0.25	64,64,64,64	0
57	MG	1A	3548	1/1	0.95	0.10	26,26,26,26	0
57	MG	1A	3867	1/1	0.95	0.09	42,42,42,42	0
57	MG	2A	3408	1/1	0.95	0.30	64,64,64,64	0
57	MG	1A	3075	1/1	0.95	0.06	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	3697	1/1	0.95	0.12	27,27,27,27	0
57	MG	1A	3456	1/1	0.95	0.21	39,39,39,39	0
57	MG	2A	3412	1/1	0.95	0.34	59,59,59,59	0
57	MG	2A	3698	1/1	0.95	0.08	64,64,64,64	0
57	MG	1A	3699	1/1	0.95	0.10	36,36,36,36	0
57	MG	1A	3873	1/1	0.95	0.28	42,42,42,42	0
57	MG	1a	1610	1/1	0.95	0.05	27,27,27,27	0
57	MG	1A	3076	1/1	0.95	0.27	50,50,50,50	0
57	MG	1A	4054	1/1	0.95	0.07	55,55,55,55	0
57	MG	1a	1818	1/1	0.95	0.06	52,52,52,52	0
57	MG	1a	1820	1/1	0.95	0.07	65,65,65,65	0
57	MG	1a	1822	1/1	0.95	0.21	63,63,63,63	0
57	MG	1A	3227	1/1	0.95	0.10	43,43,43,43	0
57	MG	1A	4056	1/1	0.95	0.14	39,39,39,39	0
57	MG	1A	3553	1/1	0.95	0.07	49,49,49,49	0
57	MG	1A	4062	1/1	0.95	0.07	53,53,53,53	0
57	MG	1a	1618	1/1	0.95	0.06	60,60,60,60	0
57	MG	1A	3163	1/1	0.95	0.21	52,52,52,52	0
57	MG	1A	3230	1/1	0.95	0.21	32,32,32,32	0
57	MG	2A	3717	1/1	0.95	0.12	47,47,47,47	0
57	MG	2a	1685	1/1	0.95	0.21	57,57,57,57	0
57	MG	1A	3556	1/1	0.95	0.07	55,55,55,55	0
57	MG	1A	3101	1/1	0.95	0.08	41,41,41,41	0
57	MG	1A	3035	1/1	0.95	0.09	47,47,47,47	0
57	MG	1A	3108	1/1	0.95	0.17	39,39,39,39	0
57	MG	1A	3011	1/1	0.95	0.16	44,44,44,44	0
57	MG	1A	4074	1/1	0.95	0.06	43,43,43,43	0
57	MG	1A	3379	1/1	0.95	0.12	55,55,55,55	0
57	MG	2A	3726	1/1	0.95	0.10	43,43,43,43	0
57	MG	1A	3715	1/1	0.95	0.06	35,35,35,35	0
57	MG	1A	3310	1/1	0.95	0.08	45,45,45,45	0
57	MG	1A	3017	1/1	0.95	0.09	52,52,52,52	0
57	MG	2a	1698	1/1	0.95	0.15	64,64,64,64	0
57	MG	1A	3173	1/1	0.95	0.12	41,41,41,41	0
57	MG	1A	3572	1/1	0.95	0.27	33,33,33,33	0
57	MG	1A	3175	1/1	0.95	0.24	33,33,33,33	0
57	MG	1A	3471	1/1	0.95	0.11	35,35,35,35	0
57	MG	2A	3445	1/1	0.95	0.11	42,42,42,42	0
57	MG	1A	3577	1/1	0.95	0.16	44,44,44,44	0
57	MG	1A	3578	1/1	0.95	0.10	39,39,39,39	0
57	MG	2A	3448	1/1	0.95	0.06	49,49,49,49	0
57	MG	2A	3743	1/1	0.95	0.08	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	3384	1/1	0.95	0.10	49,49,49,49	0
57	MG	1A	3474	1/1	0.95	0.09	40,40,40,40	0
57	MG	1A	3582	1/1	0.95	0.30	39,39,39,39	0
57	MG	1x	102	1/1	0.95	0.11	52,52,52,52	0
57	MG	2A	3228	1/1	0.95	0.19	46,46,46,46	0
57	MG	1A	3315	1/1	0.95	0.16	60,60,60,60	0
57	MG	1a	1644	1/1	0.95	0.10	67,67,67,67	0
57	MG	2A	3460	1/1	0.95	0.07	54,54,54,54	0
57	MG	2A	3461	1/1	0.95	0.07	70,70,70,70	0
57	MG	1A	3181	1/1	0.95	0.13	38,38,38,38	0
57	MG	1A	3042	1/1	0.95	0.14	35,35,35,35	0
57	MG	1A	3911	1/1	0.95	0.26	37,37,37,37	0
57	MG	1A	3914	1/1	0.95	0.06	25,25,25,25	0
57	MG	1A	3120	1/1	0.95	0.17	44,44,44,44	0
57	MG	1A	3589	1/1	0.95	0.22	42,42,42,42	0
57	MG	2A	3765	1/1	0.95	0.09	58,58,58,58	0
57	MG	1A	3740	1/1	0.95	0.06	27,27,27,27	0
57	MG	1A	3742	1/1	0.95	0.07	20,20,20,20	0
57	MG	1B	212	1/1	0.95	0.08	42,42,42,42	0
57	MG	2A	3002	1/1	0.95	0.22	52,52,52,52	0
57	MG	2A	3474	1/1	0.95	0.50	66,66,66,66	0
57	MG	1A	3390	1/1	0.95	0.09	45,45,45,45	0
57	MG	2A	3004	1/1	0.95	0.32	61,61,61,61	0
57	MG	1a	1658	1/1	0.95	0.13	60,60,60,60	0
57	MG	2A	3478	1/1	0.95	0.28	68,68,68,68	0
57	MG	2A	3479	1/1	0.95	0.14	52,52,52,52	0
57	MG	2A	3783	1/1	0.95	0.07	58,58,58,58	0
57	MG	1B	214	1/1	0.95	0.06	55,55,55,55	0
57	MG	1B	216	1/1	0.95	0.10	53,53,53,53	0
57	MG	2A	3786	1/1	0.95	0.10	64,64,64,64	0
57	MG	1B	217	1/1	0.95	0.09	45,45,45,45	0
57	MG	1A	3391	1/1	0.95	0.20	60,60,60,60	0
57	MG	1A	3746	1/1	0.95	0.11	42,42,42,42	0
57	MG	1A	3184	1/1	0.95	0.08	58,58,58,58	0
57	MG	2a	1743	1/1	0.95	0.16	68,68,68,68	0
57	MG	1A	3748	1/1	0.95	0.07	58,58,58,58	0
57	MG	1A	3754	1/1	0.95	0.11	52,52,52,52	0
57	MG	2A	3795	1/1	0.95	0.10	50,50,50,50	0
57	MG	1a	1667	1/1	0.95	0.15	58,58,58,58	0
57	MG	2a	1748	1/1	0.95	0.08	70,70,70,70	0
57	MG	2A	3257	1/1	0.95	0.10	67,67,67,67	0
57	MG	2A	3019	1/1	0.95	0.09	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	2A	3800	1/1	0.95	0.07	76,76,76,76	0
57	MG	1a	1668	1/1	0.95	0.07	70,70,70,70	0
57	MG	1A	3756	1/1	0.95	0.07	18,18,18,18	0
57	MG	2A	3803	1/1	0.95	0.06	72,72,72,72	0
57	MG	2A	3493	1/1	0.95	0.33	64,64,64,64	0
57	MG	1A	3054	1/1	0.95	0.07	43,43,43,43	0
57	MG	2A	3262	1/1	0.95	0.09	63,63,63,63	0
57	MG	1B	226	1/1	0.95	0.10	67,67,67,67	0
57	MG	1A	3043	1/1	0.95	0.27	38,38,38,38	0
57	MG	1A	3323	1/1	0.95	0.16	36,36,36,36	0
57	MG	2A	3030	1/1	0.95	0.08	45,45,45,45	0
57	MG	2A	3031	1/1	0.95	0.10	53,53,53,53	0
57	MG	2A	3032	1/1	0.95	0.07	50,50,50,50	0
57	MG	2A	3269	1/1	0.95	0.07	55,55,55,55	0
57	MG	2a	1772	1/1	0.95	0.18	65,65,65,65	0
57	MG	1A	3762	1/1	0.95	0.08	35,35,35,35	0
57	MG	2A	3508	1/1	0.95	0.10	76,76,76,76	0
57	MG	2A	3035	1/1	0.95	0.07	47,47,47,47	0
57	MG	1A	3485	1/1	0.95	0.13	42,42,42,42	0
57	MG	1B	232	1/1	0.95	0.08	60,60,60,60	0
57	MG	2a	1780	1/1	0.95	0.07	60,60,60,60	0
57	MG	1A	3060	1/1	0.95	0.07	38,38,38,38	0
57	MG	2A	3831	1/1	0.95	0.08	42,42,42,42	0
57	MG	2a	1783	1/1	0.95	0.16	57,57,57,57	0
57	MG	2A	3514	1/1	0.95	0.06	33,33,33,33	0
57	MG	1A	3947	1/1	0.95	0.06	55,55,55,55	0
57	MG	1A	3765	1/1	0.95	0.11	44,44,44,44	0
57	MG	1A	3327	1/1	0.95	0.07	44,44,44,44	0
57	MG	1D	308	1/1	0.95	0.12	52,52,52,52	0
57	MG	2A	3047	1/1	0.95	0.15	36,36,36,36	0
57	MG	1A	3125	1/1	0.95	0.18	38,38,38,38	0
57	MG	1A	3954	1/1	0.95	0.07	51,51,51,51	0
57	MG	1A	3769	1/1	0.95	0.06	65,65,65,65	0
57	MG	1A	3770	1/1	0.95	0.08	24,24,24,24	0
57	MG	1E	301	1/1	0.95	0.18	41,41,41,41	0
57	MG	1E	306	1/1	0.95	0.08	46,46,46,46	0
57	MG	1A	3775	1/1	0.95	0.05	29,29,29,29	0
57	MG	2A	3855	1/1	0.95	0.07	64,64,64,64	0
57	MG	1A	3402	1/1	0.95	0.09	71,71,71,71	0
57	MG	1A	3779	1/1	0.95	0.14	68,68,68,68	0
57	MG	1A	3192	1/1	0.95	0.17	38,38,38,38	0
57	MG	1A	3256	1/1	0.95	0.12	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	3193	1/1	0.95	0.07	42,42,42,42	0
57	MG	1F	307	1/1	0.95	0.07	46,46,46,46	0
57	MG	2A	3538	1/1	0.95	0.12	53,53,53,53	0
57	MG	1A	3963	1/1	0.95	0.05	46,46,46,46	0
57	MG	1A	3127	1/1	0.95	0.22	36,36,36,36	0
57	MG	1A	3608	1/1	0.95	0.10	43,43,43,43	0
57	MG	1A	3259	1/1	0.95	0.10	28,28,28,28	0
57	MG	2A	3067	1/1	0.95	0.13	43,43,43,43	0
57	MG	2A	3300	1/1	0.95	0.16	72,72,72,72	0
57	MG	1A	3412	1/1	0.95	0.09	45,45,45,45	0
57	MG	2a	1813	1/1	0.95	0.20	74,74,74,74	0
57	MG	1G	201	1/1	0.95	0.15	41,41,41,41	0
57	MG	1A	3611	1/1	0.95	0.11	60,60,60,60	0
57	MG	1A	3792	1/1	0.95	0.05	20,20,20,20	0
57	MG	2A	3072	1/1	0.95	0.18	67,67,67,67	0
57	MG	2A	3073	1/1	0.95	0.19	56,56,56,56	0
57	MG	2A	3074	1/1	0.95	0.12	47,47,47,47	0
57	MG	1A	3008	1/1	0.95	0.08	24,24,24,24	0
57	MG	1A	3063	1/1	0.95	0.21	50,50,50,50	0
57	MG	1N	202	1/1	0.95	0.09	45,45,45,45	0
57	MG	2A	3084	1/1	0.95	0.08	55,55,55,55	0
57	MG	1A	3796	1/1	0.95	0.06	43,43,43,43	0
57	MG	1A	3262	1/1	0.95	0.09	56,56,56,56	0
57	MG	2D	301	1/1	0.95	0.12	52,52,52,52	0
57	MG	2D	302	1/1	0.95	0.10	53,53,53,53	0
57	MG	1A	3263	1/1	0.95	0.15	55,55,55,55	0
57	MG	2A	3565	1/1	0.95	0.08	38,38,38,38	0
57	MG	2E	302	1/1	0.95	0.14	61,61,61,61	0
57	MG	1P	204	1/1	0.95	0.05	42,42,42,42	0
57	MG	1A	3507	1/1	0.95	0.14	40,40,40,40	0
57	MG	2A	3090	1/1	0.95	0.17	57,57,57,57	0
57	MG	2A	3572	1/1	0.95	0.17	56,56,56,56	0
57	MG	1A	3131	1/1	0.95	0.08	70,70,70,70	0
57	MG	2A	3092	1/1	0.95	0.06	40,40,40,40	0
57	MG	2A	3320	1/1	0.95	0.06	64,64,64,64	0
57	MG	2A	3093	1/1	0.95	0.13	69,69,69,69	0
57	MG	1Q	204	1/1	0.95	0.09	62,62,62,62	0
57	MG	1A	3132	1/1	0.95	0.08	43,43,43,43	0
57	MG	1A	3419	1/1	0.95	0.46	78,78,78,78	0
57	MG	1R	201	1/1	0.95	0.10	37,37,37,37	0
57	MG	1R	202	1/1	0.95	0.08	46,46,46,46	0
57	MG	1A	3810	1/1	0.95	0.07	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3511	1/1	0.95	0.07	60,60,60,60	0
57	MG	1A	3632	1/1	0.95	0.12	30,30,30,30	0
57	MG	2A	3591	1/1	0.95	0.16	65,65,65,65	0
57	MG	1A	3133	1/1	0.95	0.10	40,40,40,40	0
57	MG	1a	1729	1/1	0.95	0.24	61,61,61,61	0
57	MG	1A	3267	1/1	0.95	0.21	36,36,36,36	0
57	MG	1A	3136	1/1	0.95	0.08	49,49,49,49	0
57	MG	2A	3598	1/1	0.95	0.12	58,58,58,58	0
59	CLM	1A	4097	20/20	0.95	0.09	29,37,54,64	0
57	MG	1A	3987	1/1	0.95	0.08	52,52,52,52	0
57	MG	1A	3908	1/1	0.96	0.08	43,43,43,43	0
57	MG	1A	3909	1/1	0.96	0.06	55,55,55,55	0
57	MG	1A	3784	1/1	0.96	0.05	40,40,40,40	0
57	MG	1A	3016	1/1	0.96	0.18	54,54,54,54	0
57	MG	1W	203	1/1	0.96	0.17	50,50,50,50	0
57	MG	1a	1724	1/1	0.96	0.09	56,56,56,56	0
57	MG	1W	207	1/1	0.96	0.13	33,33,33,33	0
57	MG	1X	101	1/1	0.96	0.38	33,33,33,33	0
57	MG	2A	3464	1/1	0.96	0.14	71,71,71,71	0
57	MG	1X	103	1/1	0.96	0.09	46,46,46,46	0
57	MG	1A	3434	1/1	0.96	0.13	38,38,38,38	0
57	MG	1A	3177	1/1	0.96	0.05	32,32,32,32	0
57	MG	1A	4058	1/1	0.96	0.05	60,60,60,60	0
57	MG	2A	3469	1/1	0.96	0.07	37,37,37,37	0
57	MG	1A	4061	1/1	0.96	0.08	49,49,49,49	0
57	MG	1A	3660	1/1	0.96	0.06	23,23,23,23	0
57	MG	2A	3075	1/1	0.96	0.07	45,45,45,45	0
57	MG	1A	3064	1/1	0.96	0.12	34,34,34,34	0
57	MG	2A	3079	1/1	0.96	0.16	54,54,54,54	0
57	MG	2a	1632	1/1	0.96	0.27	54,54,54,54	0
57	MG	1A	4065	1/1	0.96	0.07	62,62,62,62	0
57	MG	2A	3081	1/1	0.96	0.10	48,48,48,48	0
57	MG	1A	3143	1/1	0.96	0.10	51,51,51,51	0
57	MG	10	101	1/1	0.96	0.16	43,43,43,43	0
57	MG	1A	3438	1/1	0.96	0.09	45,45,45,45	0
57	MG	2A	3280	1/1	0.96	0.08	62,62,62,62	0
57	MG	1A	4068	1/1	0.96	0.15	58,58,58,58	0
57	MG	1A	3920	1/1	0.96	0.07	64,64,64,64	0
57	MG	1A	3665	1/1	0.96	0.06	35,35,35,35	0
57	MG	1A	3573	1/1	0.96	0.05	27,27,27,27	0
57	MG	1A	3574	1/1	0.96	0.10	60,60,60,60	0
57	MG	1A	4073	1/1	0.96	0.06	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3797	1/1	0.96	0.05	45,45,45,45	0
57	MG	2A	3728	1/1	0.96	0.08	37,37,37,37	0
57	MG	1A	3498	1/1	0.96	0.14	47,47,47,47	0
57	MG	1A	4076	1/1	0.96	0.06	52,52,52,52	0
57	MG	1A	3337	1/1	0.96	0.07	47,47,47,47	0
57	MG	1A	3677	1/1	0.96	0.15	46,46,46,46	0
57	MG	1A	3936	1/1	0.96	0.06	40,40,40,40	0
57	MG	1A	3804	1/1	0.96	0.05	25,25,25,25	0
57	MG	2A	3736	1/1	0.96	0.12	65,65,65,65	0
57	MG	2A	3737	1/1	0.96	0.07	66,66,66,66	0
57	MG	15	101	1/1	0.96	0.24	35,35,35,35	0
57	MG	15	104	1/1	0.96	0.07	39,39,39,39	0
57	MG	1A	3805	1/1	0.96	0.27	32,32,32,32	0
57	MG	2A	3104	1/1	0.96	0.24	54,54,54,54	0
57	MG	1A	3294	1/1	0.96	0.17	35,35,35,35	0
57	MG	16	101	1/1	0.96	0.09	57,57,57,57	0
57	MG	2a	1661	1/1	0.96	0.10	67,67,67,67	0
57	MG	2A	3501	1/1	0.96	0.35	69,69,69,69	0
57	MG	2a	1663	1/1	0.96	0.10	65,65,65,65	0
57	MG	2A	3747	1/1	0.96	0.06	66,66,66,66	0
57	MG	1A	3254	1/1	0.96	0.11	59,59,59,59	0
57	MG	17	101	1/1	0.96	0.05	34,34,34,34	0
57	MG	17	103	1/1	0.96	0.14	37,37,37,37	0
57	MG	1A	3442	1/1	0.96	0.12	46,46,46,46	0
57	MG	2A	3753	1/1	0.96	0.13	61,61,61,61	0
57	MG	1A	3580	1/1	0.96	0.06	37,37,37,37	0
57	MG	2A	3755	1/1	0.96	0.06	54,54,54,54	0
57	MG	2A	3509	1/1	0.96	0.08	53,53,53,53	0
57	MG	1A	3503	1/1	0.96	0.18	52,52,52,52	0
57	MG	18	103	1/1	0.96	0.10	40,40,40,40	0
57	MG	18	104	1/1	0.96	0.12	47,47,47,47	0
57	MG	1A	3951	1/1	0.96	0.06	63,63,63,63	0
57	MG	1A	4095	1/1	0.96	0.05	44,44,44,44	0
57	MG	1A	3687	1/1	0.96	0.08	39,39,39,39	0
57	MG	1A	3505	1/1	0.96	0.17	31,31,31,31	0
57	MG	2A	3517	1/1	0.96	0.07	69,69,69,69	0
57	MG	1A	3032	1/1	0.96	0.19	25,25,25,25	0
57	MG	2A	3520	1/1	0.96	0.13	62,62,62,62	0
57	MG	2A	3768	1/1	0.96	0.06	43,43,43,43	0
57	MG	1A	3055	1/1	0.96	0.13	41,41,41,41	0
57	MG	1B	204	1/1	0.96	0.23	62,62,62,62	0
57	MG	1A	3693	1/1	0.96	0.11	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	3524	1/1	0.96	0.07	45,45,45,45	0
57	MG	2A	3773	1/1	0.96	0.07	65,65,65,65	0
57	MG	1A	3389	1/1	0.96	0.19	28,28,28,28	0
57	MG	2A	3125	1/1	0.96	0.19	71,71,71,71	0
57	MG	2A	3776	1/1	0.96	0.06	52,52,52,52	0
57	MG	2A	3126	1/1	0.96	0.06	49,49,49,49	0
57	MG	2a	1696	1/1	0.96	0.09	56,56,56,56	0
57	MG	1A	3149	1/1	0.96	0.19	31,31,31,31	0
57	MG	2A	3128	1/1	0.96	0.05	61,61,61,61	0
57	MG	2A	3322	1/1	0.96	0.12	57,57,57,57	0
57	MG	1A	3104	1/1	0.96	0.10	30,30,30,30	0
57	MG	1A	3126	1/1	0.96	0.20	38,38,38,38	0
57	MG	1A	3826	1/1	0.96	0.09	50,50,50,50	0
57	MG	1A	3345	1/1	0.96	0.07	66,66,66,66	0
57	MG	1A	3513	1/1	0.96	0.08	44,44,44,44	0
57	MG	1A	3346	1/1	0.96	0.15	36,36,36,36	0
57	MG	2A	3791	1/1	0.96	0.06	53,53,53,53	0
57	MG	1A	3152	1/1	0.96	0.16	44,44,44,44	0
57	MG	1A	3398	1/1	0.96	0.12	25,25,25,25	0
57	MG	1A	3518	1/1	0.96	0.17	49,49,49,49	0
57	MG	1A	3453	1/1	0.96	0.15	45,45,45,45	0
57	MG	2A	3140	1/1	0.96	0.13	41,41,41,41	0
57	MG	1a	1620	1/1	0.96	0.05	48,48,48,48	0
57	MG	2A	3799	1/1	0.96	0.07	79,79,79,79	0
57	MG	1A	3454	1/1	0.96	0.10	36,36,36,36	0
57	MG	1A	3455	1/1	0.96	0.12	46,46,46,46	0
57	MG	1A	3600	1/1	0.96	0.06	27,27,27,27	0
57	MG	1A	3106	1/1	0.96	0.08	38,38,38,38	0
57	MG	2A	3147	1/1	0.96	0.07	46,46,46,46	0
57	MG	2A	3550	1/1	0.96	0.06	56,56,56,56	0
57	MG	1A	3304	1/1	0.96	0.29	53,53,53,53	0
57	MG	1A	3128	1/1	0.96	0.24	40,40,40,40	0
57	MG	1A	3058	1/1	0.96	0.05	42,42,42,42	0
57	MG	1A	3109	1/1	0.96	0.16	38,38,38,38	0
57	MG	1A	3461	1/1	0.96	0.11	42,42,42,42	0
57	MG	1A	3034	1/1	0.96	0.20	34,34,34,34	0
57	MG	2A	3154	1/1	0.96	0.11	56,56,56,56	0
57	MG	1A	3165	1/1	0.96	0.06	33,33,33,33	0
57	MG	1A	3849	1/1	0.96	0.07	24,24,24,24	0
57	MG	1a	1634	1/1	0.96	0.10	63,63,63,63	0
57	MG	1A	3234	1/1	0.96	0.08	47,47,47,47	0
57	MG	1A	3612	1/1	0.96	0.05	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3567	1/1	0.96	0.07	38,38,38,38	0
57	MG	1D	301	1/1	0.96	0.18	37,37,37,37	0
57	MG	1D	302	1/1	0.96	0.19	37,37,37,37	0
57	MG	2A	3832	1/1	0.96	0.05	55,55,55,55	0
57	MG	2A	3571	1/1	0.96	0.07	45,45,45,45	0
57	MG	2A	3835	1/1	0.96	0.06	56,56,56,56	0
57	MG	1A	3725	1/1	0.96	0.05	53,53,53,53	0
57	MG	1A	3613	1/1	0.96	0.05	34,34,34,34	0
57	MG	1A	3854	1/1	0.96	0.10	22,22,22,22	0
57	MG	1A	3408	1/1	0.96	0.20	32,32,32,32	0
57	MG	2a	1742	1/1	0.96	0.27	65,65,65,65	0
57	MG	1A	3268	1/1	0.96	0.10	42,42,42,42	0
57	MG	1A	3411	1/1	0.96	0.10	37,37,37,37	0
57	MG	2A	3169	1/1	0.96	0.08	63,63,63,63	0
57	MG	1A	3991	1/1	0.96	0.07	26,26,26,26	0
57	MG	2A	3849	1/1	0.96	0.06	40,40,40,40	0
57	MG	2A	3365	1/1	0.96	0.07	47,47,47,47	0
57	MG	1E	304	1/1	0.96	0.09	33,33,33,33	0
57	MG	1A	3009	1/1	0.96	0.05	27,27,27,27	0
57	MG	1A	3203	1/1	0.96	0.15	35,35,35,35	0
57	MG	2a	1752	1/1	0.96	0.09	70,70,70,70	0
57	MG	2a	1753	1/1	0.96	0.09	68,68,68,68	0
57	MG	2A	3587	1/1	0.96	0.16	61,61,61,61	0
57	MG	1A	3622	1/1	0.96	0.11	60,60,60,60	0
57	MG	1E	309	1/1	0.96	0.10	33,33,33,33	0
57	MG	2A	3177	1/1	0.96	0.15	61,61,61,61	0
57	MG	2a	1758	1/1	0.96	0.15	61,61,61,61	0
57	MG	1A	3316	1/1	0.96	0.12	55,55,55,55	0
57	MG	1a	1652	1/1	0.96	0.08	54,54,54,54	0
57	MG	1A	3168	1/1	0.96	0.08	40,40,40,40	0
57	MG	2A	3181	1/1	0.96	0.08	46,46,46,46	0
57	MG	1A	3627	1/1	0.96	0.06	37,37,37,37	0
57	MG	1A	3741	1/1	0.96	0.07	37,37,37,37	0
57	MG	1F	305	1/1	0.96	0.19	33,33,33,33	0
57	MG	1F	306	1/1	0.96	0.07	36,36,36,36	0
57	MG	1A	3114	1/1	0.96	0.09	36,36,36,36	0
57	MG	1A	3629	1/1	0.96	0.06	32,32,32,32	0
57	MG	1A	4002	1/1	0.96	0.06	55,55,55,55	0
57	MG	1F	311	1/1	0.96	0.06	48,48,48,48	0
57	MG	1A	3744	1/1	0.96	0.07	56,56,56,56	0
57	MG	1A	3473	1/1	0.96	0.12	33,33,33,33	0
57	MG	1A	3871	1/1	0.96	0.21	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	1F	315	1/1	0.96	0.19	54,54,54,54	0
57	MG	1A	3273	1/1	0.96	0.19	41,41,41,41	0
57	MG	1G	202	1/1	0.96	0.16	58,58,58,58	0
57	MG	1A	3028	1/1	0.96	0.19	29,29,29,29	0
57	MG	1A	3634	1/1	0.96	0.07	41,41,41,41	0
57	MG	1A	3875	1/1	0.96	0.07	32,32,32,32	0
57	MG	2A	3394	1/1	0.96	0.11	61,61,61,61	0
57	MG	1A	4012	1/1	0.96	0.06	53,53,53,53	0
57	MG	1A	3753	1/1	0.96	0.15	59,59,59,59	0
57	MG	1N	204	1/1	0.96	0.21	51,51,51,51	0
57	MG	1N	205	1/1	0.96	0.14	38,38,38,38	0
57	MG	1O	201	1/1	0.96	0.15	53,53,53,53	0
57	MG	2A	3206	1/1	0.96	0.07	58,58,58,58	0
57	MG	1A	3243	1/1	0.96	0.13	26,26,26,26	0
57	MG	2a	1794	1/1	0.96	0.14	66,66,66,66	0
57	MG	1O	203	1/1	0.96	0.20	66,66,66,66	0
57	MG	1A	3755	1/1	0.96	0.11	44,44,44,44	0
57	MG	2A	3631	1/1	0.96	0.15	46,46,46,46	0
57	MG	1A	3276	1/1	0.96	0.12	39,39,39,39	0
57	MG	2A	3211	1/1	0.96	0.15	72,72,72,72	0
57	MG	1P	202	1/1	0.96	0.25	36,36,36,36	0
57	MG	2A	3635	1/1	0.96	0.14	56,56,56,56	0
57	MG	2A	3636	1/1	0.96	0.09	40,40,40,40	0
57	MG	1A	3137	1/1	0.96	0.13	28,28,28,28	0
57	MG	2A	3639	1/1	0.96	0.05	46,46,46,46	0
57	MG	2A	3640	1/1	0.96	0.13	41,41,41,41	0
57	MG	1A	3324	1/1	0.96	0.13	30,30,30,30	0
57	MG	1A	3280	1/1	0.96	0.17	37,37,37,37	0
57	MG	1Q	202	1/1	0.96	0.07	36,36,36,36	0
57	MG	1A	3641	1/1	0.96	0.10	25,25,25,25	0
57	MG	1a	1689	1/1	0.96	0.16	66,66,66,66	0
57	MG	2A	3219	1/1	0.96	0.30	63,63,63,63	0
57	MG	2A	3024	1/1	0.96	0.08	53,53,53,53	0
57	MG	1A	3372	1/1	0.96	0.08	43,43,43,43	0
57	MG	2A	3026	1/1	0.96	0.21	54,54,54,54	0
57	MG	1A	3281	1/1	0.96	0.27	42,42,42,42	0
57	MG	1A	3284	1/1	0.96	0.25	34,34,34,34	0
57	MG	1A	4029	1/1	0.96	0.06	69,69,69,69	0
57	MG	1R	204	1/1	0.96	0.36	35,35,35,35	0
57	MG	1A	3118	1/1	0.96	0.22	28,28,28,28	0
57	MG	1a	1696	1/1	0.96	0.23	69,69,69,69	0
57	MG	2V	203	1/1	0.96	0.18	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3423	1/1	0.96	0.19	58,58,58,58	0
57	MG	1A	4031	1/1	0.96	0.06	50,50,50,50	0
57	MG	2A	3658	1/1	0.96	0.15	44,44,44,44	0
57	MG	1a	1698	1/1	0.96	0.14	48,48,48,48	0
57	MG	1A	3767	1/1	0.96	0.06	30,30,30,30	0
57	MG	2A	3233	1/1	0.96	0.14	42,42,42,42	0
57	MG	2f	201	1/1	0.96	0.13	51,51,51,51	0
57	MG	2A	3038	1/1	0.96	0.14	61,61,61,61	0
57	MG	1A	3429	1/1	0.96	0.09	48,48,48,48	0
57	MG	1A	4034	1/1	0.96	0.08	45,45,45,45	0
57	MG	2A	3431	1/1	0.96	0.17	47,47,47,47	0
57	MG	1a	1702	1/1	0.96	0.32	62,62,62,62	0
57	MG	2A	3239	1/1	0.96	0.23	44,44,44,44	0
57	MG	1A	3486	1/1	0.96	0.09	43,43,43,43	0
57	MG	1A	3487	1/1	0.96	0.08	50,50,50,50	0
57	MG	2A	3044	1/1	0.96	0.08	62,62,62,62	0
57	MG	1A	3771	1/1	0.96	0.07	28,28,28,28	0
57	MG	1A	3773	1/1	0.96	0.07	68,68,68,68	0
57	MG	1A	3287	1/1	0.96	0.14	37,37,37,37	0
57	MG	1U	204	1/1	0.96	0.08	38,38,38,38	0
57	MG	2A	3050	1/1	0.96	0.09	61,61,61,61	0
57	MG	2A	3678	1/1	0.96	0.10	39,39,39,39	0
57	MG	1A	4041	1/1	0.96	0.08	59,59,59,59	0
57	MG	2A	3680	1/1	0.96	0.07	67,67,67,67	0
57	MG	1A	3776	1/1	0.96	0.05	26,26,26,26	0
57	MG	1U	207	1/1	0.96	0.26	37,37,37,37	0
57	MG	1A	3212	1/1	0.96	0.27	54,54,54,54	0
57	MG	1A	3559	1/1	0.96	0.17	30,30,30,30	0
57	MG	1A	3904	1/1	0.96	0.13	53,53,53,53	0
57	MG	2A	3449	1/1	0.96	0.22	48,48,48,48	0
57	MG	1A	3174	1/1	0.96	0.07	35,35,35,35	0
57	MG	1A	3656	1/1	0.96	0.09	37,37,37,37	0
57	MG	1V	203	1/1	0.96	0.12	37,37,37,37	0
59	CLM	2A	3863	20/20	0.96	0.09	42,47,57,60	0
60	ZN	14	501	1/1	0.96	0.10	106,106,106,106	0
60	ZN	24	501	1/1	0.96	0.11	117,117,117,117	0
57	MG	2A	3455	1/1	0.96	0.07	52,52,52,52	0
57	MG	2A	3859	1/1	0.97	0.10	53,53,53,53	0
57	MG	1A	3206	1/1	0.97	0.08	37,37,37,37	0
57	MG	2A	3248	1/1	0.97	0.08	71,71,71,71	0
57	MG	2A	3116	1/1	0.97	0.08	37,37,37,37	0
57	MG	1A	3718	1/1	0.97	0.08	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3147	1/1	0.97	0.07	42,42,42,42	0
57	MG	1A	3242	1/1	0.97	0.14	36,36,36,36	0
57	MG	1N	203	1/1	0.97	0.06	44,44,44,44	0
57	MG	1A	3424	1/1	0.97	0.13	40,40,40,40	0
57	MG	1A	3650	1/1	0.97	0.06	36,36,36,36	0
57	MG	1A	3974	1/1	0.97	0.04	51,51,51,51	0
57	MG	2A	3532	1/1	0.97	0.11	44,44,44,44	0
57	MG	1A	3651	1/1	0.97	0.06	64,64,64,64	0
57	MG	1A	3110	1/1	0.97	0.20	31,31,31,31	0
57	MG	1A	3062	1/1	0.97	0.28	61,61,61,61	0
57	MG	1A	3727	1/1	0.97	0.07	54,54,54,54	0
57	MG	1A	3112	1/1	0.97	0.09	34,34,34,34	0
57	MG	1P	203	1/1	0.97	0.18	29,29,29,29	0
57	MG	2A	3697	1/1	0.97	0.14	40,40,40,40	0
57	MG	1A	3980	1/1	0.97	0.07	51,51,51,51	0
57	MG	1a	1726	1/1	0.97	0.12	47,47,47,47	0
57	MG	1A	3808	1/1	0.97	0.05	35,35,35,35	0
57	MG	1A	3178	1/1	0.97	0.10	29,29,29,29	0
57	MG	1A	3352	1/1	0.97	0.24	39,39,39,39	0
57	MG	1Q	203	1/1	0.97	0.05	47,47,47,47	0
57	MG	2A	3545	1/1	0.97	0.06	58,58,58,58	0
57	MG	2D	304	1/1	0.97	0.37	42,42,42,42	0
57	MG	1A	4083	1/1	0.97	0.07	45,45,45,45	0
57	MG	1A	4085	1/1	0.97	0.07	48,48,48,48	0
57	MG	1A	3354	1/1	0.97	0.12	35,35,35,35	0
57	MG	1A	3890	1/1	0.97	0.06	22,22,22,22	0
57	MG	1A	3030	1/1	0.97	0.16	30,30,30,30	0
57	MG	2E	305	1/1	0.97	0.10	39,39,39,39	0
57	MG	1A	3602	1/1	0.97	0.07	54,54,54,54	0
57	MG	2A	3552	1/1	0.97	0.09	50,50,50,50	0
57	MG	2A	3553	1/1	0.97	0.07	35,35,35,35	0
57	MG	2A	3012	1/1	0.97	0.08	47,47,47,47	0
57	MG	1A	3736	1/1	0.97	0.06	44,44,44,44	0
57	MG	2A	3145	1/1	0.97	0.08	38,38,38,38	0
57	MG	2F	304	1/1	0.97	0.09	63,63,63,63	0
57	MG	1A	3815	1/1	0.97	0.28	33,33,33,33	0
57	MG	2A	3015	1/1	0.97	0.07	39,39,39,39	0
57	MG	1A	3816	1/1	0.97	0.06	37,37,37,37	0
57	MG	2A	3017	1/1	0.97	0.21	60,60,60,60	0
57	MG	1a	1633	1/1	0.97	0.06	31,31,31,31	0
57	MG	1A	3282	1/1	0.97	0.07	31,31,31,31	0
57	MG	1a	1745	1/1	0.97	0.09	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2P	202	1/1	0.97	0.10	66,66,66,66	0
57	MG	2Q	201	1/1	0.97	0.05	49,49,49,49	0
57	MG	1S	202	1/1	0.97	0.09	44,44,44,44	0
57	MG	1A	3992	1/1	0.97	0.06	32,32,32,32	0
57	MG	2A	3568	1/1	0.97	0.10	51,51,51,51	0
57	MG	1A	3604	1/1	0.97	0.07	42,42,42,42	0
57	MG	2A	3731	1/1	0.97	0.07	38,38,38,38	0
57	MG	1A	3393	1/1	0.97	0.08	55,55,55,55	0
57	MG	1A	3820	1/1	0.97	0.08	27,27,27,27	0
57	MG	1A	3056	1/1	0.97	0.20	46,46,46,46	0
57	MG	1A	3901	1/1	0.97	0.06	35,35,35,35	0
57	MG	2A	3574	1/1	0.97	0.06	47,47,47,47	0
57	MG	1A	3031	1/1	0.97	0.17	33,33,33,33	0
57	MG	1A	3666	1/1	0.97	0.06	24,24,24,24	0
57	MG	2A	3739	1/1	0.97	0.11	55,55,55,55	0
57	MG	2A	3577	1/1	0.97	0.07	37,37,37,37	0
57	MG	1A	3667	1/1	0.97	0.05	34,34,34,34	0
57	MG	1A	3286	1/1	0.97	0.17	46,46,46,46	0
57	MG	1A	3155	1/1	0.97	0.18	45,45,45,45	0
57	MG	2A	3036	1/1	0.97	0.08	31,31,31,31	0
57	MG	1A	3516	1/1	0.97	0.16	27,27,27,27	0
57	MG	2A	3746	1/1	0.97	0.14	39,39,39,39	0
57	MG	1A	3185	1/1	0.97	0.09	69,69,69,69	0
57	MG	1A	3752	1/1	0.97	0.05	38,38,38,38	0
57	MG	1a	1766	1/1	0.97	0.13	43,43,43,43	0
57	MG	2A	3437	1/1	0.97	0.24	60,60,60,60	0
57	MG	1A	3675	1/1	0.97	0.05	32,32,32,32	0
57	MG	1A	3561	1/1	0.97	0.09	51,51,51,51	0
57	MG	1A	3253	1/1	0.97	0.07	51,51,51,51	0
57	MG	1a	1653	1/1	0.97	0.10	49,49,49,49	0
57	MG	2a	1765	1/1	0.97	0.11	46,46,46,46	0
57	MG	1a	1654	1/1	0.97	0.07	56,56,56,56	0
57	MG	1A	3565	1/1	0.97	0.23	36,36,36,36	0
57	MG	1A	3067	1/1	0.97	0.05	31,31,31,31	0
57	MG	1A	3681	1/1	0.97	0.04	24,24,24,24	0
57	MG	1A	3838	1/1	0.97	0.04	39,39,39,39	0
57	MG	2a	1771	1/1	0.97	0.07	77,77,77,77	0
57	MG	1W	205	1/1	0.97	0.11	41,41,41,41	0
57	MG	1W	206	1/1	0.97	0.17	41,41,41,41	0
57	MG	1A	4015	1/1	0.97	0.05	33,33,33,33	0
57	MG	1A	3921	1/1	0.97	0.14	41,41,41,41	0
57	MG	2A	3452	1/1	0.97	0.10	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3185	1/1	0.97	0.05	56,56,56,56	0
57	MG	2A	3186	1/1	0.97	0.06	63,63,63,63	0
57	MG	1A	4019	1/1	0.97	0.04	36,36,36,36	0
57	MG	1X	104	1/1	0.97	0.10	32,32,32,32	0
57	MG	2A	3611	1/1	0.97	0.10	46,46,46,46	0
57	MG	1A	3922	1/1	0.97	0.06	30,30,30,30	0
57	MG	1A	4021	1/1	0.97	0.07	35,35,35,35	0
57	MG	2A	3059	1/1	0.97	0.06	43,43,43,43	0
57	MG	1A	3119	1/1	0.97	0.06	39,39,39,39	0
57	MG	1A	3840	1/1	0.97	0.04	39,39,39,39	0
57	MG	1a	1791	1/1	0.97	0.10	71,71,71,71	0
57	MG	1A	3521	1/1	0.97	0.15	35,35,35,35	0
57	MG	1A	3620	1/1	0.97	0.09	33,33,33,33	0
57	MG	1A	3188	1/1	0.97	0.09	44,44,44,44	0
57	MG	2A	3329	1/1	0.97	0.20	56,56,56,56	0
57	MG	2A	3330	1/1	0.97	0.09	58,58,58,58	0
57	MG	1A	3159	1/1	0.97	0.10	33,33,33,33	0
57	MG	1A	3524	1/1	0.97	0.21	33,33,33,33	0
57	MG	1A	3223	1/1	0.97	0.09	50,50,50,50	0
57	MG	1A	3937	1/1	0.97	0.04	30,30,30,30	0
57	MG	1A	3848	1/1	0.97	0.13	45,45,45,45	0
57	MG	1A	3940	1/1	0.97	0.04	46,46,46,46	0
57	MG	1A	3526	1/1	0.97	0.16	30,30,30,30	0
57	MG	1A	3103	1/1	0.97	0.08	37,37,37,37	0
57	MG	1A	3696	1/1	0.97	0.09	38,38,38,38	0
57	MG	1D	312	1/1	0.97	0.04	38,38,38,38	0
57	MG	2A	3076	1/1	0.97	0.06	26,26,26,26	0
57	MG	1A	3407	1/1	0.97	0.04	37,37,37,37	0
57	MG	2A	3638	1/1	0.97	0.14	46,46,46,46	0
57	MG	2A	3078	1/1	0.97	0.07	59,59,59,59	0
57	MG	1a	1807	1/1	0.97	0.05	64,64,64,64	0
57	MG	1A	3630	1/1	0.97	0.04	22,22,22,22	0
57	MG	2A	3804	1/1	0.97	0.12	48,48,48,48	0
57	MG	1a	1810	1/1	0.97	0.04	47,47,47,47	0
57	MG	1a	1684	1/1	0.97	0.18	55,55,55,55	0
57	MG	2A	3348	1/1	0.97	0.07	68,68,68,68	0
57	MG	1A	3036	1/1	0.97	0.06	39,39,39,39	0
57	MG	1a	1816	1/1	0.97	0.07	59,59,59,59	0
57	MG	1A	3855	1/1	0.97	0.08	32,32,32,32	0
57	MG	13	103	1/1	0.97	0.10	42,42,42,42	0
57	MG	1a	1819	1/1	0.97	0.05	59,59,59,59	0
57	MG	2A	3815	1/1	0.97	0.06	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	3856	1/1	0.97	0.06	52,52,52,52	0
57	MG	1A	4044	1/1	0.97	0.05	57,57,57,57	0
57	MG	1A	3053	1/1	0.97	0.07	53,53,53,53	0
57	MG	2a	1824	1/1	0.97	0.08	71,71,71,71	0
57	MG	2A	3819	1/1	0.97	0.06	58,58,58,58	0
57	MG	15	102	1/1	0.97	0.14	38,38,38,38	0
57	MG	2A	3224	1/1	0.97	0.17	42,42,42,42	0
57	MG	2A	3824	1/1	0.97	0.04	52,52,52,52	0
57	MG	15	103	1/1	0.97	0.21	26,26,26,26	0
57	MG	2A	3827	1/1	0.97	0.05	61,61,61,61	0
57	MG	1A	3166	1/1	0.97	0.17	38,38,38,38	0
57	MG	1A	3196	1/1	0.97	0.17	38,38,38,38	0
57	MG	2A	3830	1/1	0.97	0.06	47,47,47,47	0
57	MG	1A	3780	1/1	0.97	0.07	27,27,27,27	0
57	MG	1A	3635	1/1	0.97	0.07	32,32,32,32	0
57	MG	1A	3782	1/1	0.97	0.07	43,43,43,43	0
57	MG	2A	3503	1/1	0.97	0.10	57,57,57,57	0
57	MG	2A	3100	1/1	0.97	0.08	30,30,30,30	0
57	MG	1A	3107	1/1	0.97	0.06	30,30,30,30	0
57	MG	2a	1665	1/1	0.97	0.14	56,56,56,56	0
57	MG	1A	3084	1/1	0.97	0.20	30,30,30,30	0
57	MG	2A	3839	1/1	0.97	0.05	70,70,70,70	0
57	MG	1A	3023	1/1	0.97	0.07	16,16,16,16	0
57	MG	2a	1670	1/1	0.97	0.06	61,61,61,61	0
57	MG	1A	3584	1/1	0.97	0.13	40,40,40,40	0
57	MG	2A	3844	1/1	0.97	0.09	41,41,41,41	0
57	MG	2A	3667	1/1	0.97	0.06	33,33,33,33	0
57	MG	2A	3846	1/1	0.97	0.14	60,60,60,60	0
57	MG	2x	101	1/1	0.97	0.11	60,60,60,60	0
57	MG	1A	3170	1/1	0.97	0.05	28,28,28,28	0
57	MG	2A	3237	1/1	0.97	0.08	67,67,67,67	0
57	MG	1m	3001	1/1	0.97	0.09	67,67,67,67	0
57	MG	1A	3145	1/1	0.97	0.23	28,28,28,28	0
57	MG	1A	3146	1/1	0.97	0.06	31,31,31,31	0
57	MG	1a	1705	1/1	0.97	0.29	55,55,55,55	0
57	MG	1A	4059	1/1	0.97	0.06	43,43,43,43	0
57	MG	1A	4060	1/1	0.97	0.05	45,45,45,45	0
57	MG	1A	3205	1/1	0.97	0.12	19,19,19,19	0
60	ZN	2Y	202	1/1	0.97	0.06	89,89,89,89	0
57	MG	1A	3238	1/1	0.97	0.15	32,32,32,32	0
57	MG	1A	4063	1/1	0.97	0.06	29,29,29,29	0
57	MG	1A	3162	1/1	0.98	0.23	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3158	1/1	0.98	0.15	43,43,43,43	0
57	MG	1A	3013	1/1	0.98	0.09	28,28,28,28	0
57	MG	2D	303	1/1	0.98	0.04	30,30,30,30	0
57	MG	1A	3913	1/1	0.98	0.03	29,29,29,29	0
57	MG	1A	3690	1/1	0.98	0.04	26,26,26,26	0
57	MG	1a	1756	1/1	0.98	0.10	50,50,50,50	0
57	MG	1B	205	1/1	0.98	0.05	40,40,40,40	0
57	MG	1A	3141	1/1	0.98	0.04	29,29,29,29	0
57	MG	2A	3033	1/1	0.98	0.04	41,41,41,41	0
57	MG	1A	3692	1/1	0.98	0.07	27,27,27,27	0
57	MG	1A	3410	1/1	0.98	0.06	42,42,42,42	0
57	MG	2A	3578	1/1	0.98	0.07	45,45,45,45	0
57	MG	1A	3142	1/1	0.98	0.05	20,20,20,20	0
57	MG	1A	3191	1/1	0.98	0.17	32,32,32,32	0
57	MG	1A	3005	1/1	0.98	0.07	44,44,44,44	0
57	MG	1A	4011	1/1	0.98	0.04	71,71,71,71	0
57	MG	1A	3066	1/1	0.98	0.11	32,32,32,32	0
57	MG	1A	3497	1/1	0.98	0.11	45,45,45,45	0
57	MG	2A	3174	1/1	0.98	0.16	37,37,37,37	0
57	MG	1A	3923	1/1	0.98	0.05	63,63,63,63	0
57	MG	1A	3842	1/1	0.98	0.05	52,52,52,52	0
57	MG	2A	3588	1/1	0.98	0.08	58,58,58,58	0
57	MG	2A	3589	1/1	0.98	0.06	42,42,42,42	0
57	MG	1a	1772	1/1	0.98	0.05	60,60,60,60	0
57	MG	1a	1773	1/1	0.98	0.05	49,49,49,49	0
57	MG	2A	3046	1/1	0.98	0.12	50,50,50,50	0
57	MG	1a	1774	1/1	0.98	0.05	54,54,54,54	0
57	MG	1A	3194	1/1	0.98	0.11	33,33,33,33	0
57	MG	2A	3596	1/1	0.98	0.06	40,40,40,40	0
57	MG	1B	219	1/1	0.98	0.07	34,34,34,34	0
57	MG	1A	4017	1/1	0.98	0.06	28,28,28,28	0
57	MG	2A	3750	1/1	0.98	0.05	57,57,57,57	0
57	MG	2A	3599	1/1	0.98	0.11	54,54,54,54	0
57	MG	1A	3044	1/1	0.98	0.05	34,34,34,34	0
57	MG	1A	3375	1/1	0.98	0.19	41,41,41,41	0
57	MG	1A	3038	1/1	0.98	0.18	32,32,32,32	0
57	MG	1A	3929	1/1	0.98	0.04	41,41,41,41	0
57	MG	1W	201	1/1	0.98	0.05	45,45,45,45	0
57	MG	1A	3772	1/1	0.98	0.07	39,39,39,39	0
57	MG	1A	3932	1/1	0.98	0.03	19,19,19,19	0
57	MG	1W	204	1/1	0.98	0.23	40,40,40,40	0
57	MG	1A	3115	1/1	0.98	0.04	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	3774	1/1	0.98	0.05	47,47,47,47	0
57	MG	2A	3762	1/1	0.98	0.04	63,63,63,63	0
57	MG	1A	3072	1/1	0.98	0.03	12,12,12,12	0
57	MG	1A	3504	1/1	0.98	0.10	37,37,37,37	0
57	MG	1X	102	1/1	0.98	0.14	38,38,38,38	0
57	MG	1A	3117	1/1	0.98	0.10	41,41,41,41	0
57	MG	1A	3941	1/1	0.98	0.08	54,54,54,54	0
57	MG	1A	3942	1/1	0.98	0.04	43,43,43,43	0
57	MG	23	104	1/1	0.98	0.04	60,60,60,60	0
57	MG	1A	3778	1/1	0.98	0.06	50,50,50,50	0
57	MG	25	102	1/1	0.98	0.26	43,43,43,43	0
57	MG	1B	236	1/1	0.98	0.06	30,30,30,30	0
57	MG	1A	3300	1/1	0.98	0.07	34,34,34,34	0
57	MG	1A	3648	1/1	0.98	0.07	38,38,38,38	0
57	MG	1D	303	1/1	0.98	0.07	39,39,39,39	0
57	MG	1D	304	1/1	0.98	0.08	20,20,20,20	0
57	MG	1A	3231	1/1	0.98	0.17	32,32,32,32	0
57	MG	1D	306	1/1	0.98	0.21	31,31,31,31	0
57	MG	10	102	1/1	0.98	0.15	46,46,46,46	0
57	MG	2A	3625	1/1	0.98	0.11	43,43,43,43	0
57	MG	2A	3779	1/1	0.98	0.05	62,62,62,62	0
57	MG	2a	1763	1/1	0.98	0.04	74,74,74,74	0
57	MG	2A	3780	1/1	0.98	0.04	75,75,75,75	0
57	MG	1D	307	1/1	0.98	0.23	42,42,42,42	0
57	MG	2A	3628	1/1	0.98	0.06	50,50,50,50	0
57	MG	1A	3105	1/1	0.98	0.05	50,50,50,50	0
57	MG	1A	3949	1/1	0.98	0.05	57,57,57,57	0
57	MG	1a	1808	1/1	0.98	0.06	56,56,56,56	0
57	MG	1A	3713	1/1	0.98	0.03	15,15,15,15	0
57	MG	1A	3714	1/1	0.98	0.08	63,63,63,63	0
57	MG	2A	3082	1/1	0.98	0.07	49,49,49,49	0
57	MG	2a	1774	1/1	0.98	0.15	63,63,63,63	0
57	MG	1A	3201	1/1	0.98	0.17	26,26,26,26	0
57	MG	2A	3792	1/1	0.98	0.09	72,72,72,72	0
57	MG	1a	1812	1/1	0.98	0.03	47,47,47,47	0
57	MG	1A	3202	1/1	0.98	0.04	45,45,45,45	0
57	MG	1A	3787	1/1	0.98	0.08	24,24,24,24	0
57	MG	11	102	1/1	0.98	0.04	36,36,36,36	0
57	MG	1E	302	1/1	0.98	0.13	34,34,34,34	0
57	MG	1A	4046	1/1	0.98	0.04	52,52,52,52	0
57	MG	1E	305	1/1	0.98	0.13	36,36,36,36	0
57	MG	2A	3494	1/1	0.98	0.20	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	1821	1/1	0.98	0.05	60,60,60,60	0
57	MG	1A	3093	1/1	0.98	0.08	27,27,27,27	0
57	MG	13	102	1/1	0.98	0.03	30,30,30,30	0
57	MG	1A	3306	1/1	0.98	0.10	39,39,39,39	0
57	MG	2A	3095	1/1	0.98	0.14	48,48,48,48	0
57	MG	1A	3134	1/1	0.98	0.07	43,43,43,43	0
57	MG	1A	3720	1/1	0.98	0.08	27,27,27,27	0
57	MG	1A	3135	1/1	0.98	0.04	36,36,36,36	0
57	MG	1A	3793	1/1	0.98	0.05	20,20,20,20	0
57	MG	1A	3154	1/1	0.98	0.14	34,34,34,34	0
57	MG	1F	301	1/1	0.98	0.13	38,38,38,38	0
57	MG	1F	302	1/1	0.98	0.05	27,27,27,27	0
57	MG	2A	3814	1/1	0.98	0.11	51,51,51,51	0
57	MG	1A	3179	1/1	0.98	0.07	22,22,22,22	0
57	MG	1F	304	1/1	0.98	0.05	35,35,35,35	0
57	MG	1A	3560	1/1	0.98	0.08	26,26,26,26	0
57	MG	1A	3311	1/1	0.98	0.06	31,31,31,31	0
57	MG	2A	3374	1/1	0.98	0.09	67,67,67,67	0
57	MG	17	102	1/1	0.98	0.10	33,33,33,33	0
57	MG	2A	3821	1/1	0.98	0.04	40,40,40,40	0
57	MG	1A	3562	1/1	0.98	0.14	25,25,25,25	0
57	MG	1A	3563	1/1	0.98	0.28	34,34,34,34	0
57	MG	1A	3801	1/1	0.98	0.03	19,19,19,19	0
57	MG	1A	3663	1/1	0.98	0.09	38,38,38,38	0
57	MG	18	102	1/1	0.98	0.09	44,44,44,44	0
57	MG	1A	3803	1/1	0.98	0.05	47,47,47,47	0
57	MG	1A	3729	1/1	0.98	0.04	28,28,28,28	0
57	MG	1A	3879	1/1	0.98	0.05	43,43,43,43	0
57	MG	1A	3730	1/1	0.98	0.05	25,25,25,25	0
57	MG	1A	3240	1/1	0.98	0.12	29,29,29,29	0
57	MG	1A	3180	1/1	0.98	0.04	33,33,33,33	0
57	MG	1A	3039	1/1	0.98	0.21	37,37,37,37	0
57	MG	1A	3033	1/1	0.98	0.24	30,30,30,30	0
57	MG	1A	3211	1/1	0.98	0.06	38,38,38,38	0
57	MG	1A	3887	1/1	0.98	0.03	45,45,45,45	0
57	MG	1A	3278	1/1	0.98	0.16	40,40,40,40	0
57	MG	2A	3841	1/1	0.98	0.06	24,24,24,24	0
57	MG	1A	3671	1/1	0.98	0.07	30,30,30,30	0
57	MG	1A	3619	1/1	0.98	0.09	32,32,32,32	0
57	MG	1A	3279	1/1	0.98	0.12	29,29,29,29	0
57	MG	1A	3012	1/1	0.98	0.05	32,32,32,32	0
57	MG	1A	3676	1/1	0.98	0.05	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3213	1/1	0.98	0.19	34,34,34,34	0
57	MG	1A	4078	1/1	0.98	0.07	15,15,15,15	0
57	MG	1A	3123	1/1	0.98	0.14	34,34,34,34	0
57	MG	1P	201	1/1	0.98	0.15	31,31,31,31	0
57	MG	1a	1617	1/1	0.98	0.07	41,41,41,41	0
57	MG	2a	1668	1/1	0.98	0.17	55,55,55,55	0
57	MG	1a	1731	1/1	0.98	0.09	55,55,55,55	0
57	MG	2A	3854	1/1	0.98	0.04	61,61,61,61	0
57	MG	1a	1732	1/1	0.98	0.08	49,49,49,49	0
57	MG	1A	3624	1/1	0.98	0.08	25,25,25,25	0
57	MG	2A	3137	1/1	0.98	0.13	43,43,43,43	0
57	MG	1A	3625	1/1	0.98	0.06	54,54,54,54	0
57	MG	1A	4084	1/1	0.98	0.07	40,40,40,40	0
57	MG	1A	3160	1/1	0.98	0.09	30,30,30,30	0
57	MG	2A	3009	1/1	0.98	0.12	49,49,49,49	0
57	MG	1A	3822	1/1	0.98	0.04	29,29,29,29	0
57	MG	1A	3249	1/1	0.98	0.31	35,35,35,35	0
57	MG	1A	3824	1/1	0.98	0.14	40,40,40,40	0
57	MG	1A	3749	1/1	0.98	0.04	41,41,41,41	0
57	MG	1A	3903	1/1	0.98	0.21	22,22,22,22	0
57	MG	2A	3554	1/1	0.98	0.11	39,39,39,39	0
57	MG	1Q	206	1/1	0.98	0.20	40,40,40,40	0
57	MG	1A	3750	1/1	0.98	0.04	49,49,49,49	0
57	MG	1A	3751	1/1	0.98	0.06	23,23,23,23	0
57	MG	1A	3161	1/1	0.98	0.12	30,30,30,30	0
57	MG	2A	3707	1/1	0.98	0.06	64,64,64,64	0
57	MG	2A	3284	1/1	0.98	0.10	49,49,49,49	0
57	MG	2A	3560	1/1	0.98	0.08	44,44,44,44	0
57	MG	1R	203	1/1	0.98	0.28	38,38,38,38	0
57	MG	1A	3685	1/1	0.98	0.05	30,30,30,30	0
57	MG	2A	3021	1/1	0.98	0.06	29,29,29,29	0
57	MG	1a	1749	1/1	0.98	0.12	37,37,37,37	0
60	ZN	1n	103	1/1	0.98	0.04	71,71,71,71	0
57	MG	2A	3714	1/1	0.98	0.09	47,47,47,47	0
57	MG	1a	1750	1/1	0.98	0.07	43,43,43,43	0
60	ZN	26	102	1/1	0.98	0.04	60,60,60,60	0
57	MG	1A	3325	1/1	0.98	0.05	52,52,52,52	0
61	SF4	1d	501	8/8	0.98	0.05	62,70,75,80	0
61	SF4	2d	303	8/8	0.98	0.05	71,81,85,99	0
57	MG	1A	4008	1/1	0.99	0.03	32,32,32,32	0
57	MG	1A	4091	1/1	0.99	0.06	46,46,46,46	0
57	MG	1A	3705	1/1	0.99	0.04	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3939	1/1	0.99	0.06	37,37,37,37	0
57	MG	1A	3760	1/1	0.99	0.03	37,37,37,37	0
57	MG	1A	3906	1/1	0.99	0.07	38,38,38,38	0
57	MG	1A	3615	1/1	0.99	0.07	31,31,31,31	0
57	MG	1A	3080	1/1	0.99	0.12	44,44,44,44	0
57	MG	1A	3070	1/1	0.99	0.06	20,20,20,20	0
57	MG	1a	1813	1/1	0.99	0.03	61,61,61,61	0
57	MG	1a	1814	1/1	0.99	0.03	69,69,69,69	0
57	MG	1A	3683	1/1	0.99	0.02	30,30,30,30	0
57	MG	1A	3071	1/1	0.99	0.18	30,30,30,30	0
57	MG	2A	3673	1/1	0.99	0.03	41,41,41,41	0
57	MG	1A	4018	1/1	0.99	0.03	32,32,32,32	0
57	MG	1X	107	1/1	0.99	0.04	29,29,29,29	0
57	MG	1A	3912	1/1	0.99	0.05	28,28,28,28	0
57	MG	1a	1762	1/1	0.99	0.03	46,46,46,46	0
57	MG	1a	1607	1/1	0.99	0.06	51,51,51,51	0
57	MG	1E	303	1/1	0.99	0.18	31,31,31,31	0
57	MG	2A	3811	1/1	0.99	0.03	50,50,50,50	0
57	MG	1A	3948	1/1	0.99	0.03	40,40,40,40	0
57	MG	2A	3022	1/1	0.99	0.10	43,43,43,43	0
57	MG	1A	3283	1/1	0.99	0.15	31,31,31,31	0
57	MG	1a	1767	1/1	0.99	0.04	55,55,55,55	0
57	MG	1A	3686	1/1	0.99	0.07	26,26,26,26	0
57	MG	1A	3057	1/1	0.99	0.06	26,26,26,26	0
57	MG	1A	3353	1/1	0.99	0.09	36,36,36,36	0
57	MG	1A	3037	1/1	0.99	0.04	20,20,20,20	0
57	MG	1A	3799	1/1	0.99	0.03	46,46,46,46	0
57	MG	2A	3626	1/1	0.99	0.07	43,43,43,43	0
57	MG	1A	3176	1/1	0.99	0.10	31,31,31,31	0
57	MG	2A	3504	1/1	0.99	0.02	57,57,57,57	0
57	MG	1B	215	1/1	0.99	0.04	43,43,43,43	0
57	MG	2A	3826	1/1	0.99	0.07	46,46,46,46	0
57	MG	2a	1759	1/1	0.99	0.07	61,61,61,61	0
57	MG	1A	3021	1/1	0.99	0.12	27,27,27,27	0
57	MG	1A	3097	1/1	0.99	0.05	32,32,32,32	0
57	MG	1A	3098	1/1	0.99	0.12	20,20,20,20	0
57	MG	1A	3669	1/1	0.99	0.05	39,39,39,39	0
57	MG	1A	3015	1/1	0.99	0.05	36,36,36,36	0
57	MG	1A	3587	1/1	0.99	0.04	43,43,43,43	0
57	MG	1a	1781	1/1	0.99	0.05	46,46,46,46	0
57	MG	2A	3834	1/1	0.99	0.07	33,33,33,33	0
57	MG	1A	3396	1/1	0.99	0.29	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3003	1/1	0.99	0.03	29,29,29,29	0
57	MG	1U	201	1/1	0.99	0.13	31,31,31,31	0
57	MG	1F	309	1/1	0.99	0.16	30,30,30,30	0
57	MG	1A	3077	1/1	0.99	0.06	31,31,31,31	0
57	MG	2a	1773	1/1	0.99	0.06	63,63,63,63	0
57	MG	1A	3014	1/1	0.99	0.09	28,28,28,28	0
57	MG	2A	3519	1/1	0.99	0.06	49,49,49,49	0
57	MG	1A	3701	1/1	0.99	0.03	17,17,17,17	0
57	MG	2A	3843	1/1	0.99	0.03	58,58,58,58	0
57	MG	1B	227	1/1	0.99	0.04	39,39,39,39	0
57	MG	1A	4079	1/1	0.99	0.06	50,50,50,50	0
57	MG	1A	4080	1/1	0.99	0.08	31,31,31,31	0
57	MG	1A	4039	1/1	0.99	0.03	46,46,46,46	0
57	MG	1A	3931	1/1	0.99	0.02	45,45,45,45	0
57	MG	1A	3229	1/1	0.99	0.10	31,31,31,31	0
57	MG	1A	4042	1/1	0.99	0.05	43,43,43,43	0
57	MG	2A	3715	1/1	0.99	0.04	32,32,32,32	0
57	MG	2A	3782	1/1	0.99	0.04	55,55,55,55	0
60	ZN	1Y	204	1/1	0.99	0.02	60,60,60,60	0
57	MG	1a	1740	1/1	0.99	0.06	61,61,61,61	0
60	ZN	16	103	1/1	0.99	0.07	53,53,53,53	0
60	ZN	19	102	1/1	0.99	0.04	44,44,44,44	0
57	MG	1a	1797	1/1	0.99	0.06	54,54,54,54	0
57	MG	1A	4043	1/1	0.99	0.03	25,25,25,25	0
57	MG	1V	204	1/1	0.99	0.10	29,29,29,29	0
60	ZN	25	106	1/1	0.99	0.05	62,62,62,62	0
57	MG	1A	3069	1/1	0.99	0.11	25,25,25,25	0
60	ZN	29	501	1/1	0.99	0.04	68,68,68,68	0
57	MG	1A	3934	1/1	0.99	0.06	61,61,61,61	0
57	MG	1A	3156	1/1	0.99	0.13	26,26,26,26	0
57	MG	1A	3758	1/1	0.99	0.07	47,47,47,47	0
57	MG	1A	3883	1/1	1.00	0.06	33,33,33,33	0
57	MG	2A	3723	1/1	1.00	0.04	46,46,46,46	0
57	MG	1A	3935	1/1	1.00	0.05	28,28,28,28	0
57	MG	2A	3781	1/1	1.00	0.06	64,64,64,64	0
57	MG	2A	3822	1/1	1.00	0.06	41,41,41,41	0
57	MG	1A	3674	1/1	1.00	0.05	24,24,24,24	0
57	MG	1A	3738	1/1	1.00	0.05	49,49,49,49	0
57	MG	1a	1758	1/1	1.00	0.05	34,34,34,34	0
60	ZN	15	107	1/1	1.00	0.05	43,43,43,43	0
57	MG	2A	3595	1/1	1.00	0.04	37,37,37,37	0

6.5 Other polymers (i)

There are no such residues in this entry.