wwPDB X-ray Structure Validation Summary Report (i)

Aug 6, 2026 – 03:56 AM EDT

PDB ID	:	8VTU / pdb_00008vtu
Title	:	Crystal structure of the wild-type Thermus thermophilus 70S ribosome in complex with macrolone MCX-66, mRNA, aminoacylated A-site Phe-tRNAphe, aminoacylated P-site fMet-tRNAmet, and deacylated E-site tRNAphe at 2.40A resolution
Authors	:	Aleksandrova, E.V.; Ma, C.-X.; Klepacki, D.; Alizadeh, F.; Vazquez-Laslop, N.; Liang, J.-H.; Polikanov, Y.S.; Mankin, A.S.
Deposited on	:	2024-01-27
Resolution	:	2.40 Å(reported)

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

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

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

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

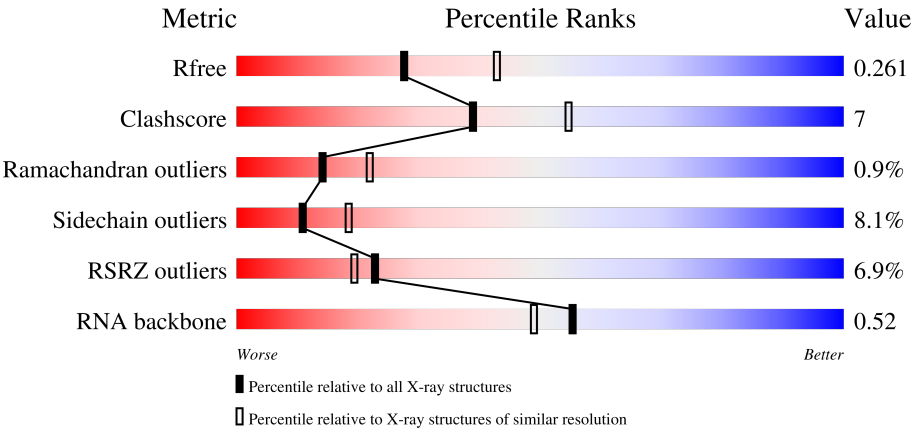
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.40 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	1A	2915	6% 70% 23% 5% •
1	2A	2915	5% 64% 26% 6% •

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Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

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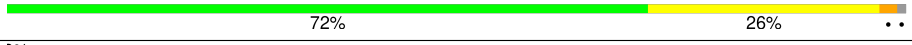
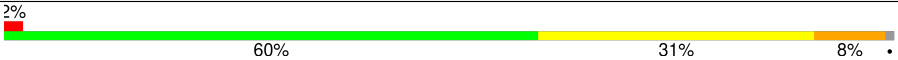
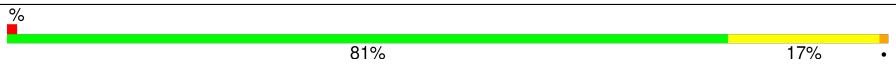
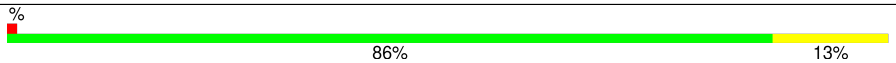
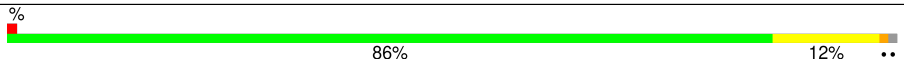
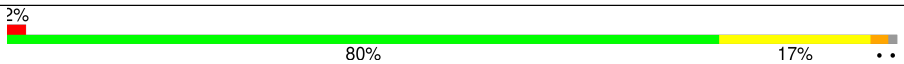
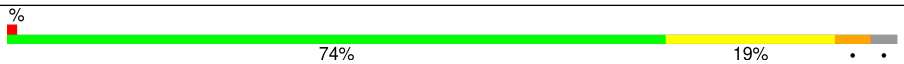
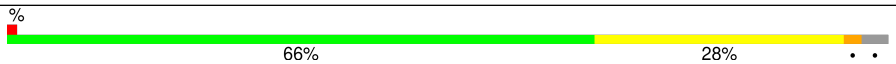
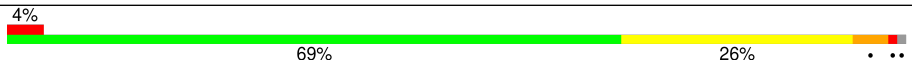
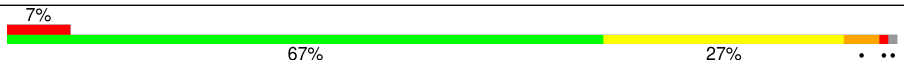
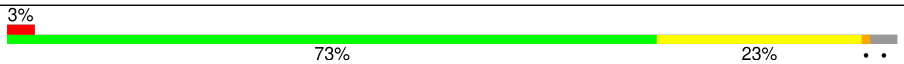
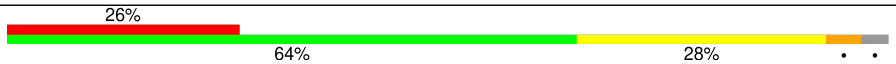
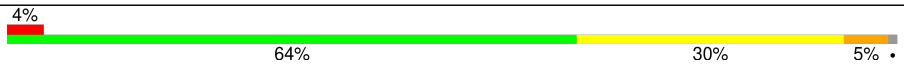
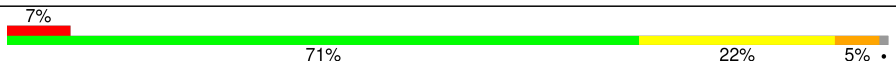
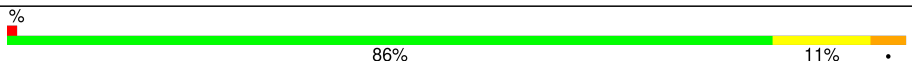
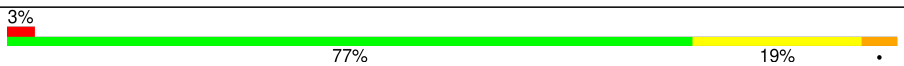
Mol	Chain	Length	Quality of chain
2	1B	121	
2	2B	121	
3	1D	276	
3	2D	276	
4	1E	206	
4	2E	206	
5	1F	210	
5	2F	210	
6	1G	182	
6	2G	182	
7	1H	180	
7	2H	180	
8	1I	148	
8	2I	148	
9	1N	140	
9	2N	140	
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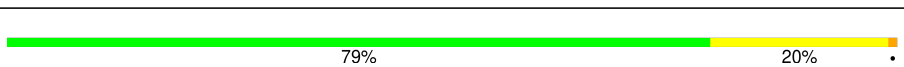
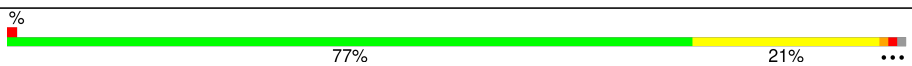
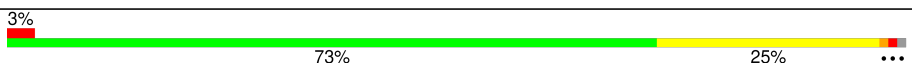
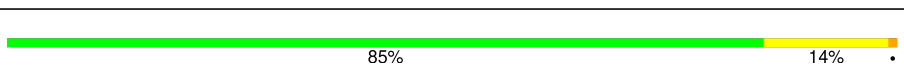
10	2O	122	
11	1P	150	
11	2P	150	
12	1Q	141	
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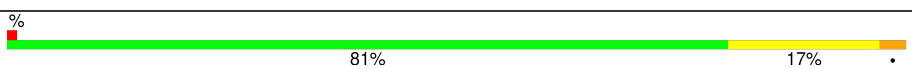
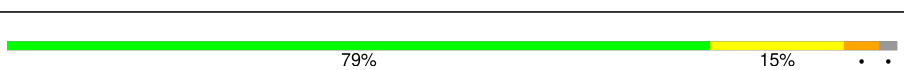
13	2R	118	
14	1S	112	

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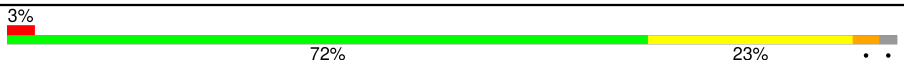
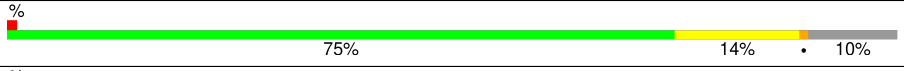
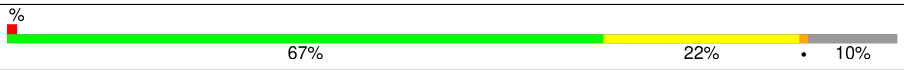
Mol	Chain	Length	Quality of chain
14	2S	112	
15	1T	146	
15	2T	146	
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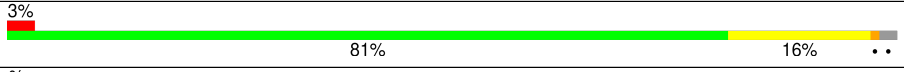
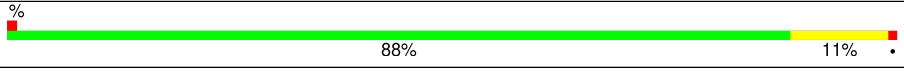
16	2U	118	
17	1V	101	
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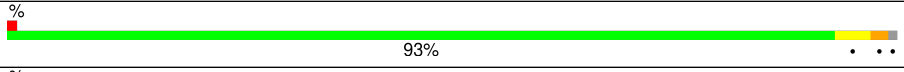
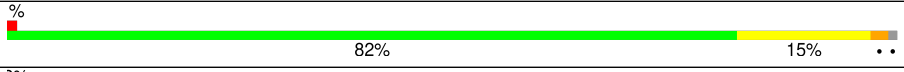
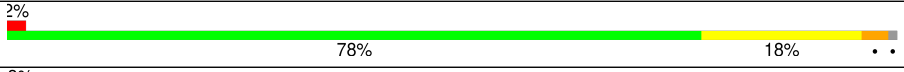
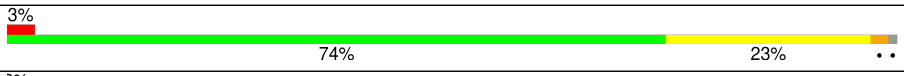
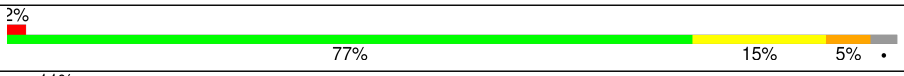
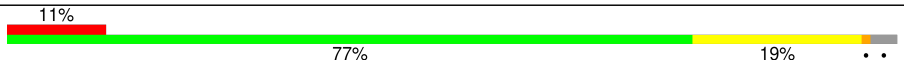
18	1W	113	
18	2W	113	
19	1X	96	
19	2X	96	
20	1Y	110	
20	2Y	110	
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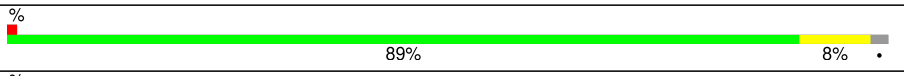
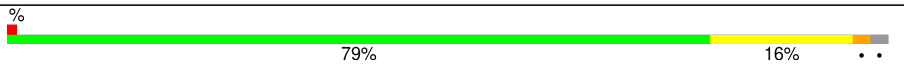
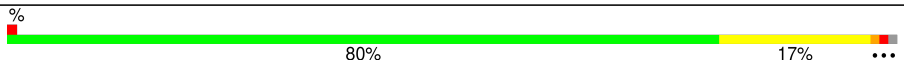
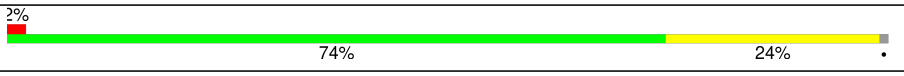
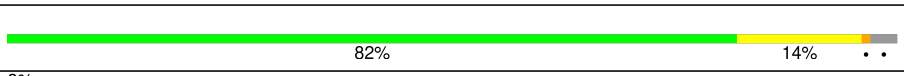
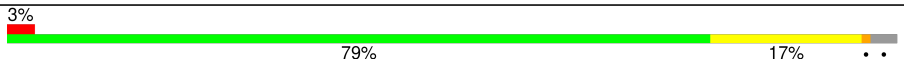
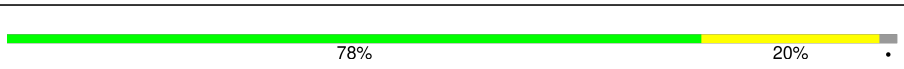
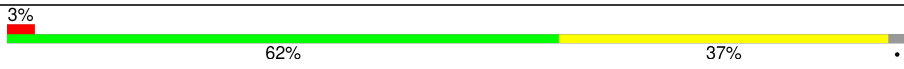
22	10	85	
22	20	85	
23	11	98	
23	21	98	
24	12	72	
24	22	72	
25	13	60	
25	23	60	
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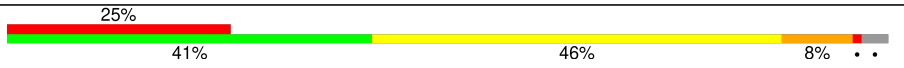
26	24	71	

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Mol	Chain	Length	Quality of chain
27	15	60	2% 87% 10%
27	25	60	3% 83% 13%
28	16	54	2% 78% 19%
28	26	54	69% 26%
29	17	49	6% 84% 12%
29	27	49	8% 78% 20%
30	18	65	74% 23%
30	28	65	69% 28%
31	19	37	78% 22%
31	29	37	5% 86% 14%
32	1a	1521	4% 64% 29% 6%
32	2a	1521	5% 59% 33% 6%
33	1b	256	20% 55% 29% 6% 10%
33	2b	256	22% 51% 33% 6% 10%
34	1c	239	6% 62% 23% 14%
34	2c	239	20% 56% 27% 14%
35	1d	209	12% 66% 28% 6%
35	2d	209	4% 73% 23%
36	1e	162	2% 57% 30% 9%
36	2e	162	4% 60% 28% 9%
37	1f	101	76% 21%
37	2f	101	2% 73% 22%
38	1g	156	8% 75% 21%
38	2g	156	13% 67% 26% 6%
39	1h	138	% 77% 20%

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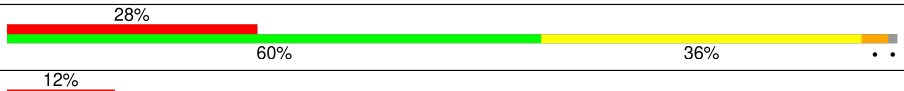
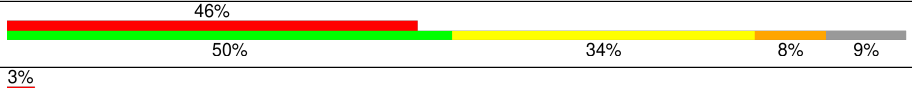
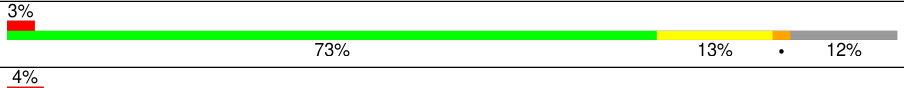
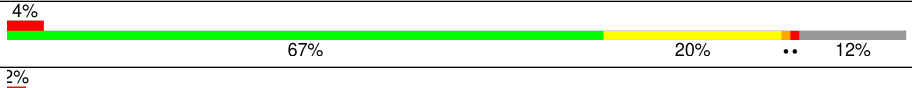
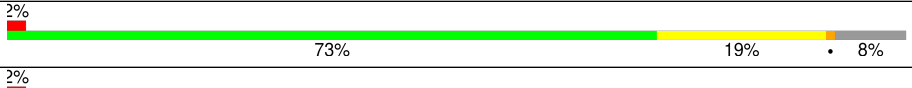
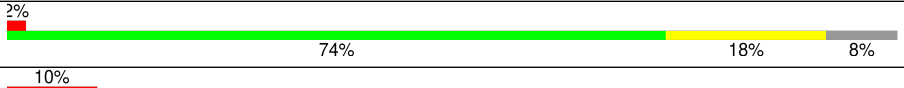
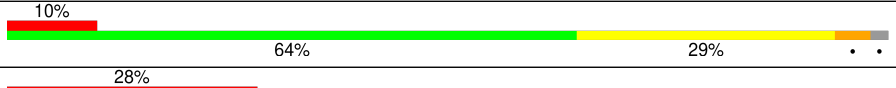
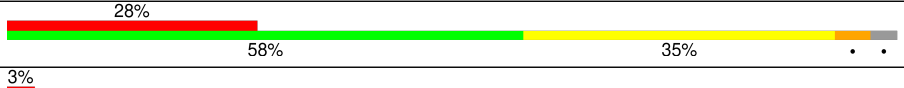
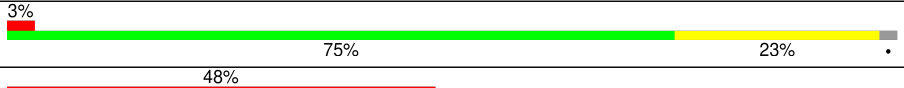
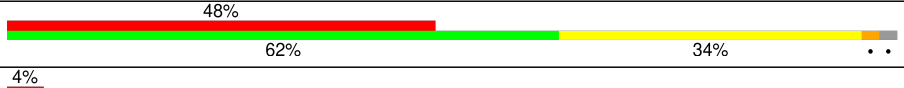
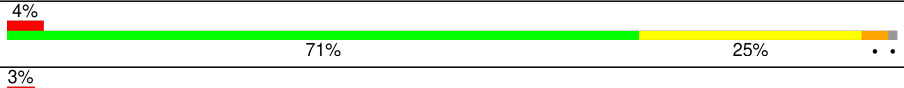
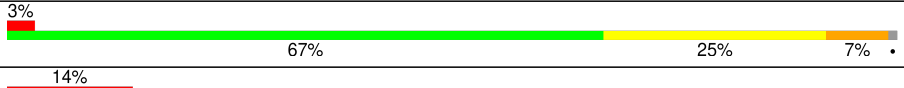
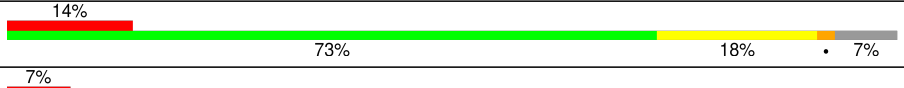
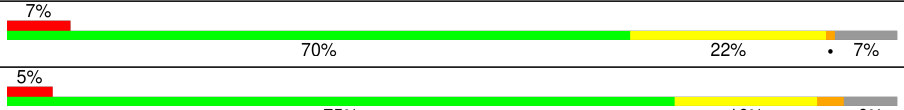
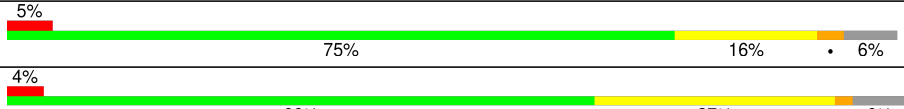
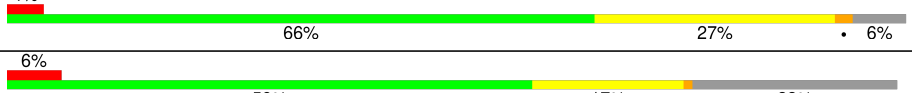
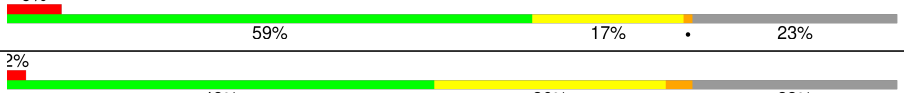
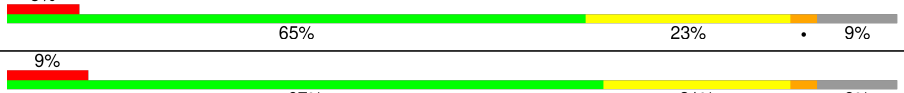
40	1i	128	
40	2i	128	
41	1j	105	
41	2j	105	
42	1k	129	
42	2k	129	
43	1l	132	
43	2l	132	
44	1m	126	
44	2m	126	
45	1n	61	
45	2n	61	
46	1o	89	
46	2o	89	
47	1p	88	
47	2p	88	
48	1q	105	
48	2q	105	
49	1r	88	
49	2r	88	
50	1s	93	
50	2s	93	
51	1t	106	
51	2t	106	

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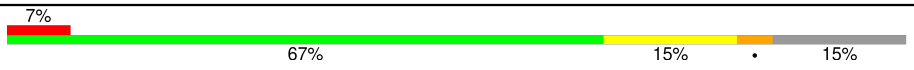
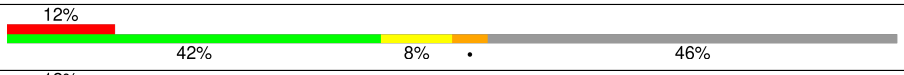
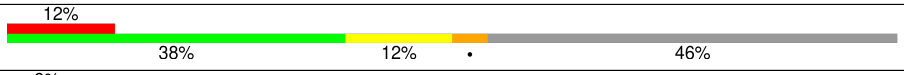
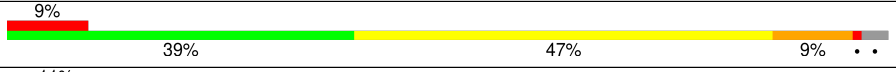
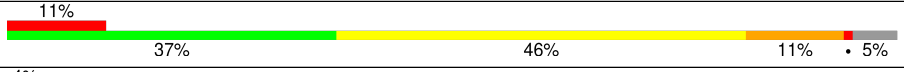
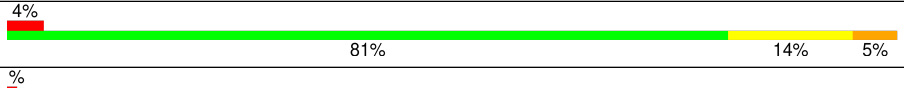
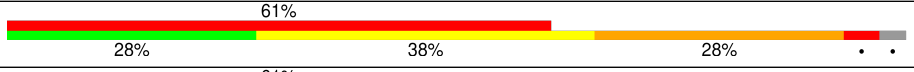
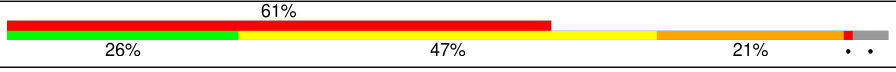
Mol	Chain	Length	Quality of chain
52	1u	27	
52	2u	27	
53	1v	24	
53	2v	24	
54	1w	76	
54	2w	76	
55	1x	77	
55	2x	77	
56	1y	76	
56	2y	76	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	10	107	-	-	-	X
57	MG	1U	211	-	-	-	X
57	MG	2A	3306	-	-	-	X
57	MG	2v	102	-	-	-	X

2 Entry composition (i)

There are 64 unique types of molecules in this entry. The entry contains 300455 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	203	Total	C	N	O	S	0	0	1
			1584	1009	298	275	2			
5	2F	203	Total	C	N	O	S	0	0	1
			1580	1007	297	274	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	1G	181	Total	C	N	O	S	0	0	0
			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 MF-mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	1v	13	Total	C	N	O	P	0	0	0
			277	125	51	88	13			
53	2v	13	Total	C	N	O	P	0	0	0
			277	125	51	88	13			

- Molecule 54 is a RNA chain called Aminoacylated Phe-tRNAphe.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
54	1w	74	Total	C	N	O	P	S	0	0	0
			1592	713	286	517	74	2			
54	2w	72	Total	C	N	O	P	S	0	0	0
			1544	690	279	501	72	2			

- Molecule 55 is a RNA chain called Aminoacylated fMet-tRNAmet.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
55	1x	77	Total	C	N	O	P	S	0	0	0
			1646	734	298	536	77	1			
55	2x	77	Total	C	N	O	P	S	0	0	0
			1646	734	298	536	77	1			

- Molecule 56 is a RNA chain called Deacylated tRNAphe.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
56	1y	74	Total	C	N	O	P	S	0	0	0
			1585	707	285	518	74	1			
56	2y	73	Total	C	N	O	P	S	0	0	0
			1565	698	283	510	73	1			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	1A	1117	Total	Mg	0	0
			1117	1117		
57	1B	37	Total	Mg	0	0
			37	37		
57	1D	15	Total	Mg	0	0
			15	15		
57	1E	15	Total	Mg	0	0
			15	15		
57	1F	12	Total	Mg	0	0
			12	12		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	1G	5	Total Mg 5 5	0	0
57	1I	1	Total Mg 1 1	0	0
57	1N	4	Total Mg 4 4	0	0
57	1O	6	Total Mg 6 6	0	0
57	1P	6	Total Mg 6 6	0	0
57	1Q	6	Total Mg 6 6	0	0
57	1R	6	Total Mg 6 6	0	0
57	1S	3	Total Mg 3 3	0	0
57	1T	2	Total Mg 2 2	0	0
57	1U	11	Total Mg 11 11	0	0
57	1V	7	Total Mg 7 7	0	0
57	1W	4	Total Mg 4 4	0	0
57	1X	6	Total Mg 6 6	0	0
57	1Y	2	Total Mg 2 2	0	0
57	1Z	4	Total Mg 4 4	0	0
57	10	9	Total Mg 9 9	0	0
57	11	5	Total Mg 5 5	0	0
57	12	2	Total Mg 2 2	0	0
57	13	4	Total Mg 4 4	0	0
57	14	1	Total Mg 1 1	0	0
57	15	7	Total Mg 7 7	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	16	1	Total Mg 1 1	0	0
57	17	5	Total Mg 5 5	0	0
57	18	5	Total Mg 5 5	0	0
57	19	1	Total Mg 1 1	0	0
57	1a	222	Total Mg 222 222	0	0
57	1b	1	Total Mg 1 1	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	1j	1	Total Mg 1 1	0	0
57	1k	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	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	9	Total Mg 9 9	0	0
57	1x	14	Total Mg 14 14	0	0
57	2A	842	Total Mg 842 842	0	0
57	2B	18	Total Mg 18 18	0	0
57	2D	9	Total Mg 9 9	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	2E	8	Total Mg 8 8	0	0
57	2F	8	Total Mg 8 8	0	0
57	2G	1	Total Mg 1 1	0	0
57	2N	1	Total Mg 1 1	0	0
57	2O	2	Total Mg 2 2	0	0
57	2P	1	Total Mg 1 1	0	0
57	2Q	3	Total Mg 3 3	0	0
57	2R	3	Total Mg 3 3	0	0
57	2T	4	Total Mg 4 4	0	0
57	2U	2	Total Mg 2 2	0	0
57	2V	2	Total Mg 2 2	0	0
57	2W	1	Total Mg 1 1	0	0
57	2X	2	Total Mg 2 2	0	0
57	2Y	1	Total Mg 1 1	0	0
57	2Z	1	Total Mg 1 1	0	0
57	20	1	Total Mg 1 1	0	0
57	21	3	Total Mg 3 3	0	0
57	23	2	Total Mg 2 2	0	0
57	25	4	Total Mg 4 4	0	0
57	27	2	Total Mg 2 2	0	0
57	28	2	Total Mg 2 2	0	0

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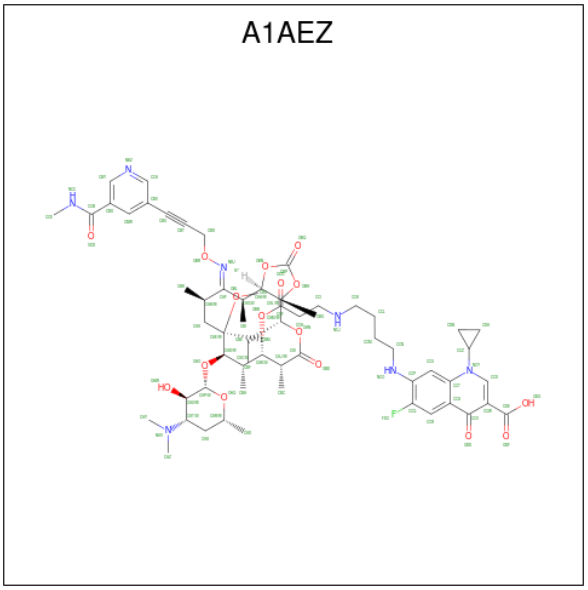
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	2a	231	Total Mg 231 231	0	0
57	2d	1	Total Mg 1 1	0	0
57	2e	1	Total Mg 1 1	0	0
57	2f	2	Total Mg 2 2	0	0
57	2g	1	Total Mg 1 1	0	0
57	2j	1	Total Mg 1 1	0	0
57	2l	4	Total Mg 4 4	0	0
57	2m	1	Total Mg 1 1	0	0
57	2q	2	Total Mg 2 2	0	0
57	2r	1	Total Mg 1 1	0	0
57	2t	1	Total Mg 1 1	0	0
57	2v	2	Total Mg 2 2	0	0
57	2w	7	Total Mg 7 7	0	0
57	2x	7	Total Mg 7 7	0	0
57	2y	2	Total Mg 2 2	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 1-cyclopropyl-7-[(4-{[3-({(3aR,4R,7R,8S,9S,10R,11R,13R,14E,15S,15aR)-10-{[(2S,3R,4S,6R)-4-(dimethylamino)-3-hydroxy-6-methyloxan-2-yl]oxy}-4-ethyl-11-methoxy-3a,7,9,11,13,15-hexamethyl-14-[({3-[5-(methylcarbamoyl)pyridin-3-yl]prop-2-yn-1-yl}oxy)imino]-2,6-dioxododecahydro-2H,4H-[1,3]dioxolo[4,5-c]oxacyclotetradecin-8-yl}ox

y)-3-oxopropyl]amino}butyl)amino]-6-fluoro-4-oxo-1,4-dihydroquinoline-3-carboxylic acid (non-preferred name) (CCD ID: A1AEZ) (formula: $C_{61}H_{84}FN_7O_{16}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
59	1A	1	Total	C	F	N	O	0	0
			85	61	1	7	16		
59	2A	1	Total	C	F	N	O	0	0
			85	61	1	7	16		

- 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		

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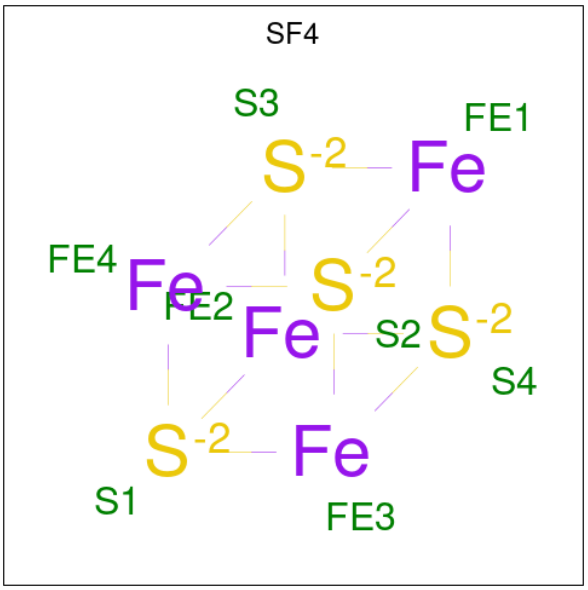
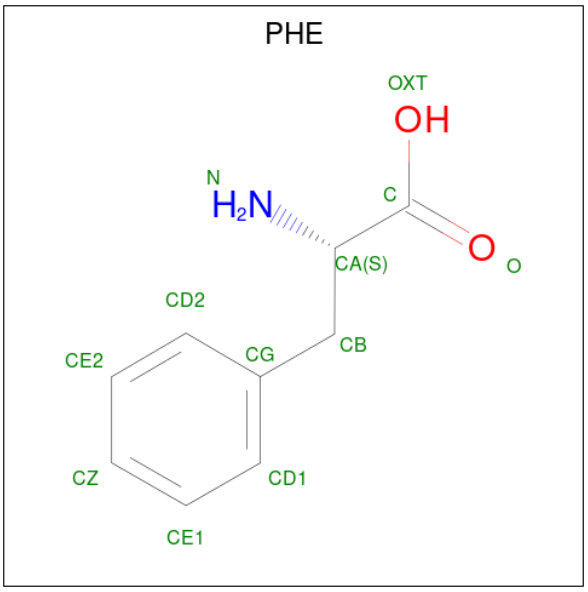
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	25	1	Total Zn 1 1	0	0
60	26	1	Total Zn 1 1	0	0
60	29	1	Total Zn 1 1	0	0
60	2n	1	Total Zn 1 1	0	0

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



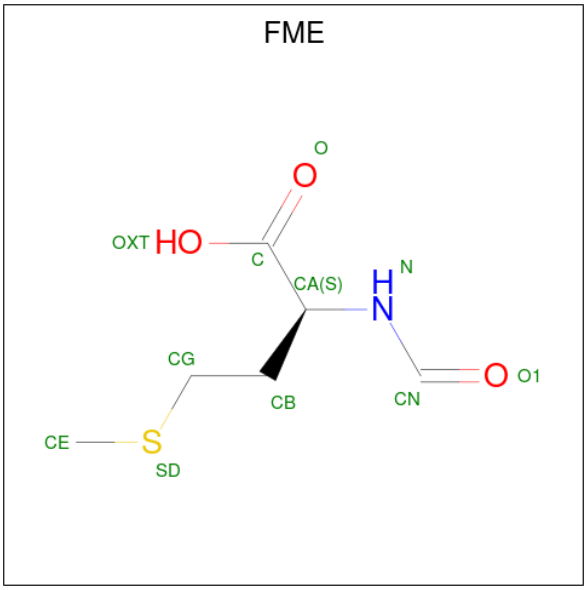
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1d	1	Total Fe S 8 4 4	0	0
61	2d	1	Total Fe S 8 4 4	0	0

- Molecule 62 is PHENYLALANINE (CCD ID: PHE) (formula: $C_9H_{11}NO_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
62	1w	1	Total C N O 11 9 1 1	0	0
62	2w	1	Total C N O 11 9 1 1	0	0

- Molecule 63 is N-FORMYLMETHIONINE (CCD ID: FME) (formula: $C_6H_{11}NO_3S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
63	1x	1	Total C N O S 10 6 1 2 1	0	0
63	2x	1	Total C N O S 10 6 1 2 1	0	0

- Molecule 64 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
64	1A	2052	Total O 2052 2052	0	0
64	1B	64	Total O 64 64	0	0
64	1D	31	Total O 31 31	0	0
64	1E	27	Total O 27 27	0	0
64	1F	19	Total O 19 19	0	0
64	1G	3	Total O 3 3	0	0
64	1H	2	Total O 2 2	0	0
64	1N	5	Total O 5 5	0	0
64	1O	6	Total O 6 6	0	0
64	1P	22	Total O 22 22	0	0
64	1Q	9	Total O 9 9	0	0
64	1R	9	Total O 9 9	0	0
64	1S	4	Total O 4 4	0	0
64	1T	8	Total O 8 8	0	0
64	1U	13	Total O 13 13	0	0
64	1V	8	Total O 8 8	0	0
64	1W	8	Total O 8 8	0	0
64	1X	4	Total O 4 4	0	0
64	1Y	2	Total O 2 2	0	0
64	1Z	1	Total O 1 1	0	0
64	10	12	Total O 12 12	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
64	11	9	Total O 9 9	0	0
64	12	3	Total O 3 3	0	0
64	13	4	Total O 4 4	0	0
64	14	1	Total O 1 1	0	0
64	15	6	Total O 6 6	0	0
64	16	2	Total O 2 2	0	0
64	17	9	Total O 9 9	0	0
64	18	10	Total O 10 10	0	0
64	1a	418	Total O 418 418	0	0
64	1b	1	Total O 1 1	0	0
64	1d	3	Total O 3 3	0	0
64	1e	1	Total O 1 1	0	0
64	1f	2	Total O 2 2	0	0
64	1g	1	Total O 1 1	0	0
64	1i	2	Total O 2 2	0	0
64	1j	2	Total O 2 2	0	0
64	1k	1	Total O 1 1	0	0
64	1l	5	Total O 5 5	0	0
64	1m	2	Total O 2 2	0	0
64	1p	1	Total O 1 1	0	0
64	1q	2	Total O 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
64	1r	1	Total O 1 1	0	0
64	1v	4	Total O 4 4	0	0
64	1w	15	Total O 15 15	0	0
64	1x	16	Total O 16 16	0	0
64	1y	1	Total O 1 1	0	0
64	2A	1183	Total O 1183 1183	0	0
64	2B	18	Total O 18 18	0	0
64	2D	22	Total O 22 22	0	0
64	2E	12	Total O 12 12	0	0
64	2F	12	Total O 12 12	0	0
64	2N	2	Total O 2 2	0	0
64	2O	2	Total O 2 2	0	0
64	2P	10	Total O 10 10	0	0
64	2Q	1	Total O 1 1	0	0
64	2R	4	Total O 4 4	0	0
64	2T	6	Total O 6 6	0	0
64	2U	2	Total O 2 2	0	0
64	2W	1	Total O 1 1	0	0
64	2X	2	Total O 2 2	0	0
64	2Y	2	Total O 2 2	0	0
64	20	2	Total O 2 2	0	0

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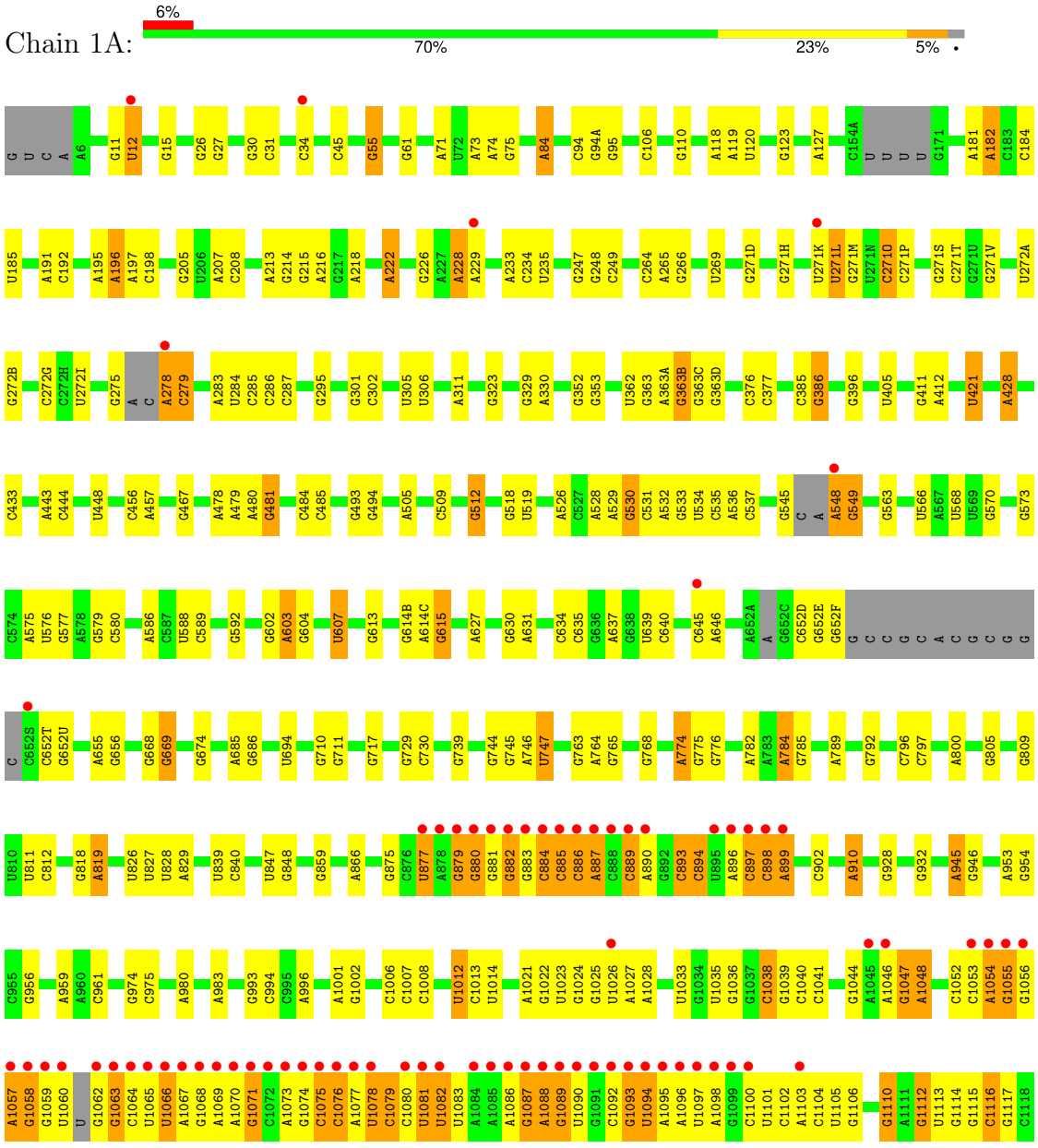
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
64	21	7	Total O 7 7	0	0
64	23	2	Total O 2 2	0	0
64	25	1	Total O 1 1	0	0
64	26	1	Total O 1 1	0	0
64	27	4	Total O 4 4	0	0
64	28	3	Total O 3 3	0	0
64	29	1	Total O 1 1	0	0
64	2a	265	Total O 265 265	0	0
64	2c	2	Total O 2 2	0	0
64	2d	3	Total O 3 3	0	0
64	2e	1	Total O 1 1	0	0
64	2g	1	Total O 1 1	0	0
64	2j	2	Total O 2 2	0	0
64	2l	6	Total O 6 6	0	0
64	2n	1	Total O 1 1	0	0
64	2p	1	Total O 1 1	0	0
64	2r	1	Total O 1 1	0	0
64	2t	5	Total O 5 5	0	0
64	2w	2	Total O 2 2	0	0
64	2x	7	Total O 7 7	0	0
64	2y	3	Total O 3 3	0	0

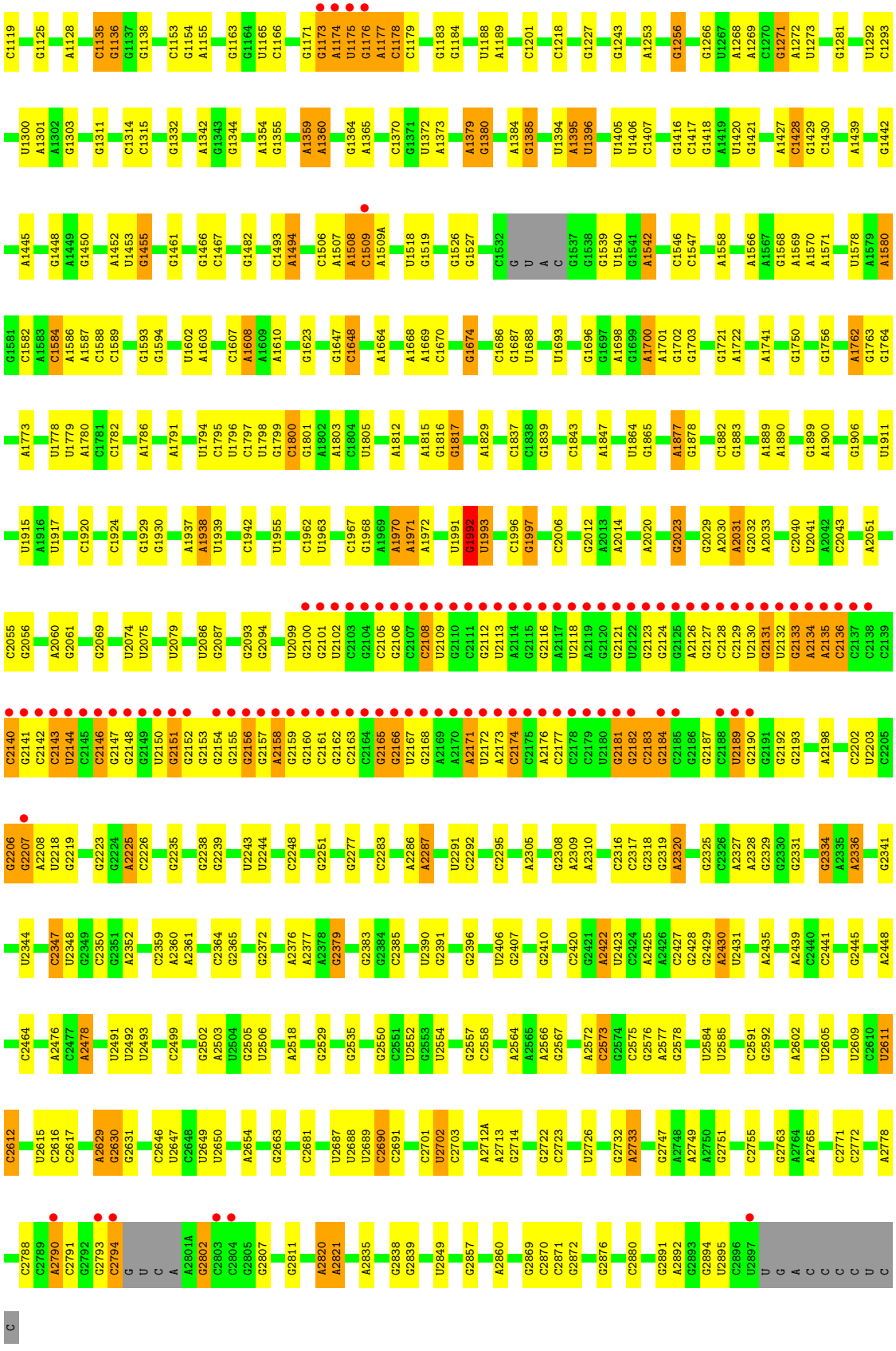
3 Residue-property plots (i)

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

- Molecule 1: 23S Ribosomal RNA

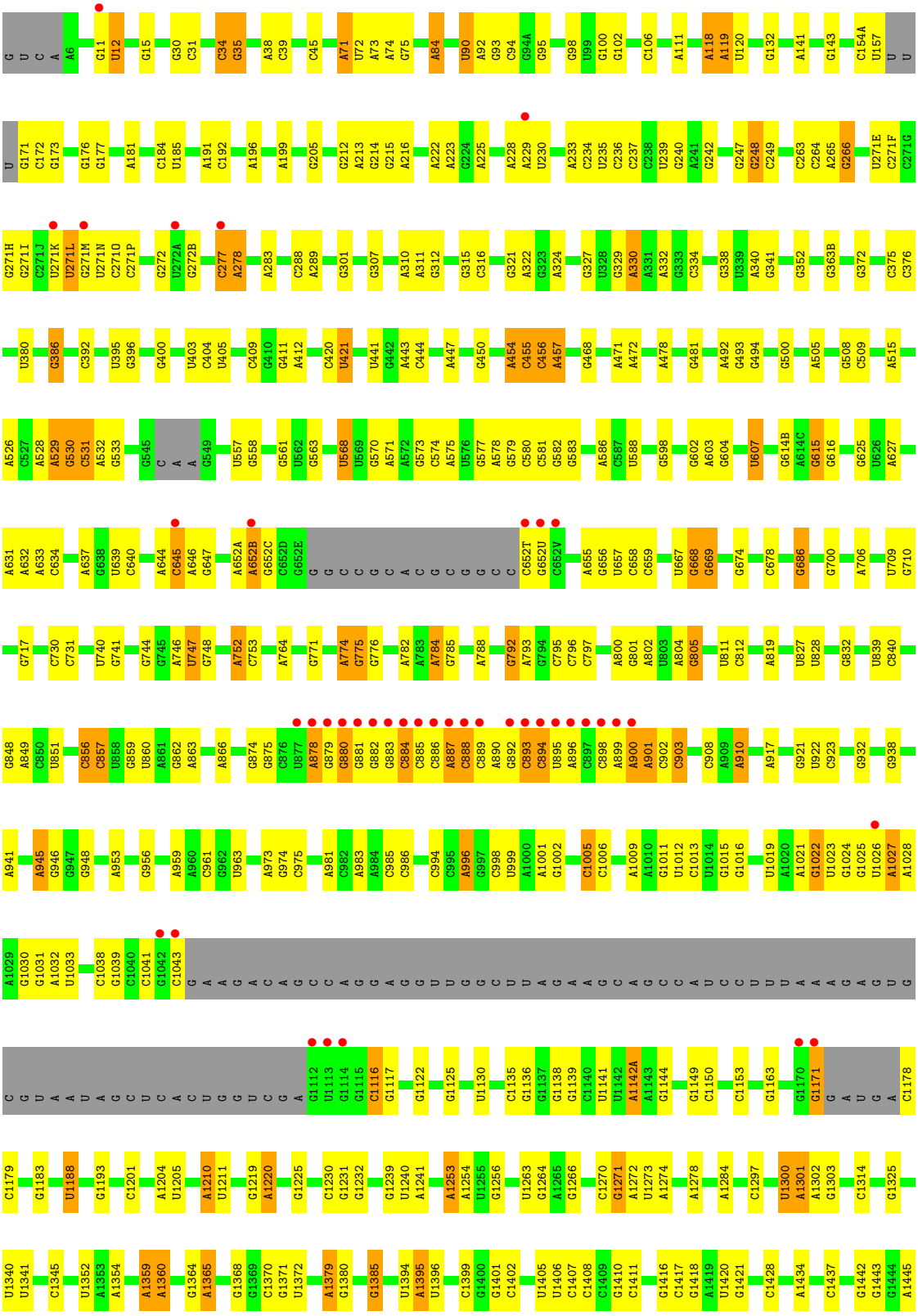
Chain 1A:

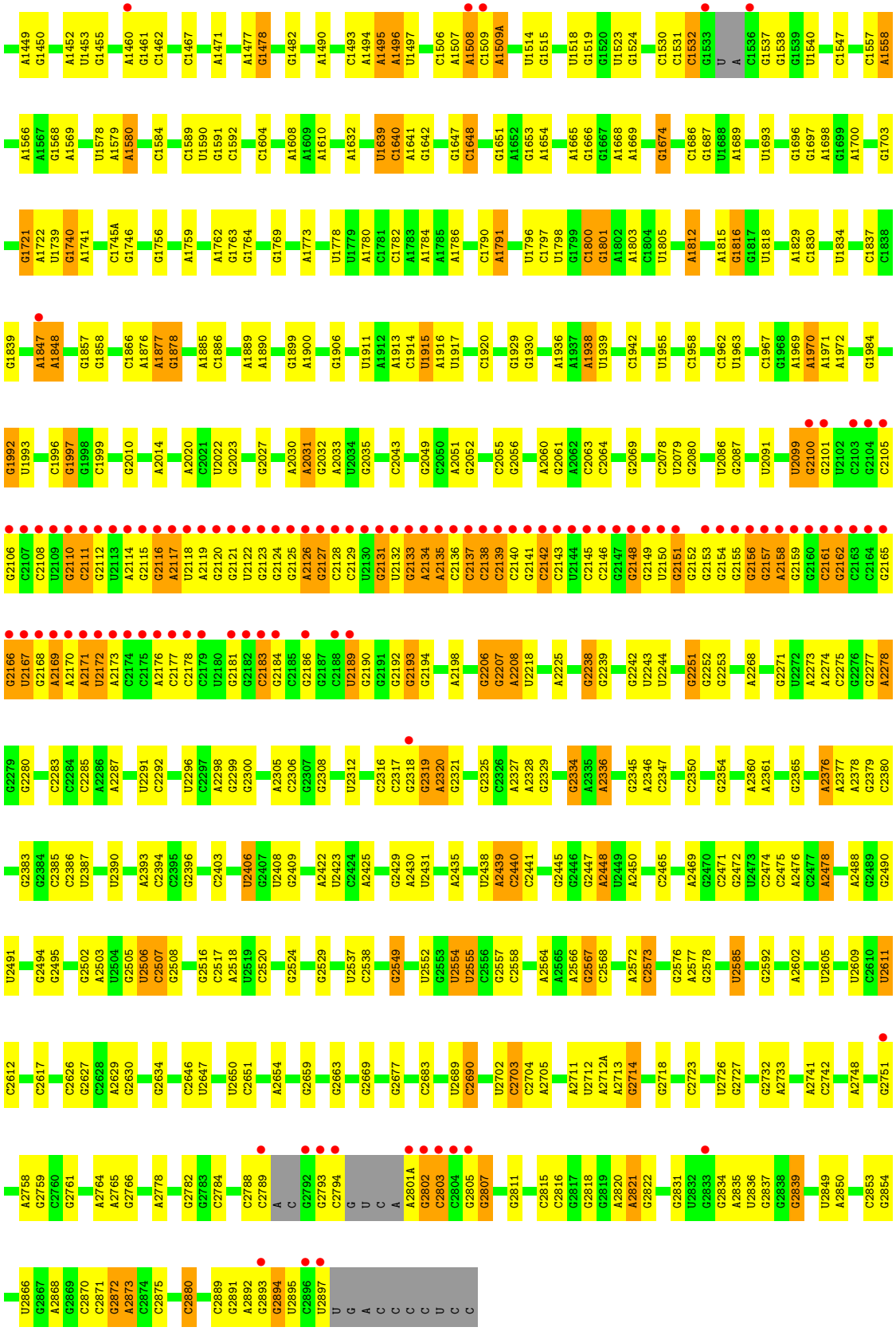




• Molecule 1: 23S Ribosomal RNA

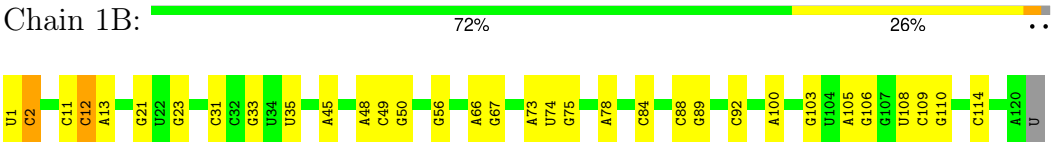
Chain 2A:





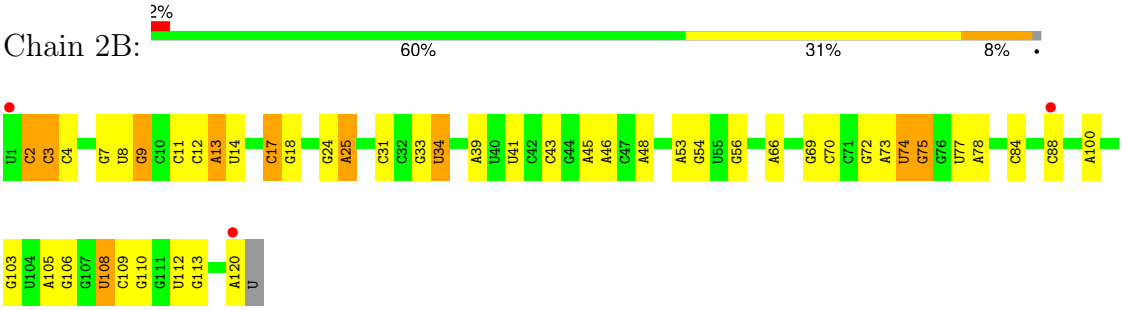
• Molecule 2: 5S Ribosomal RNA

Chain 1B:



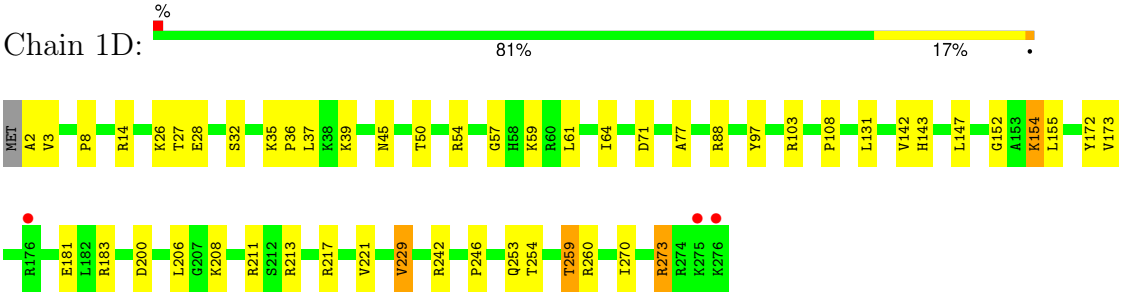
• Molecule 2: 5S Ribosomal RNA

Chain 2B:



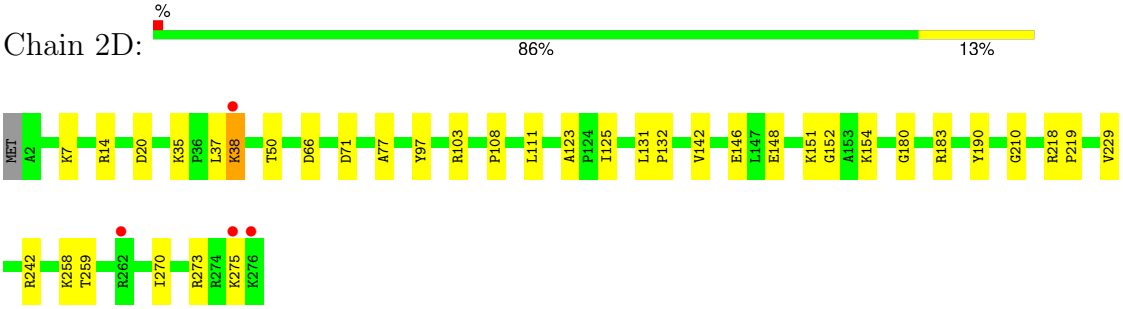
• Molecule 3: 50S ribosomal protein L2

Chain 1D:



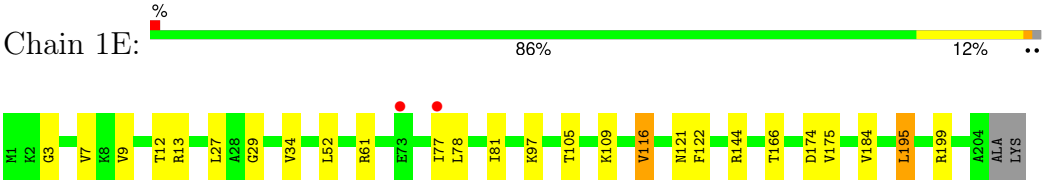
• Molecule 3: 50S ribosomal protein L2

Chain 2D:



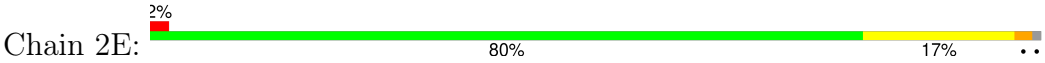
• Molecule 4: 50S ribosomal protein L3

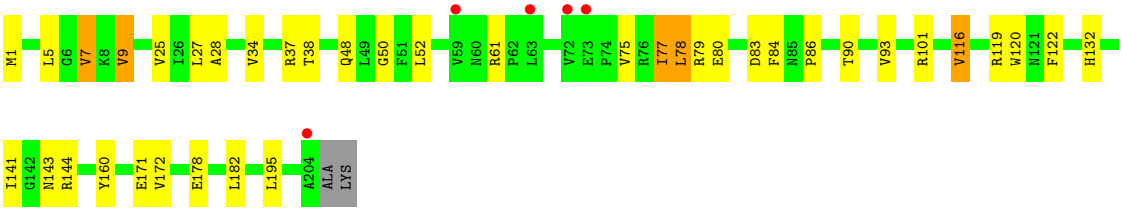
Chain 1E:



• Molecule 4: 50S ribosomal protein L3

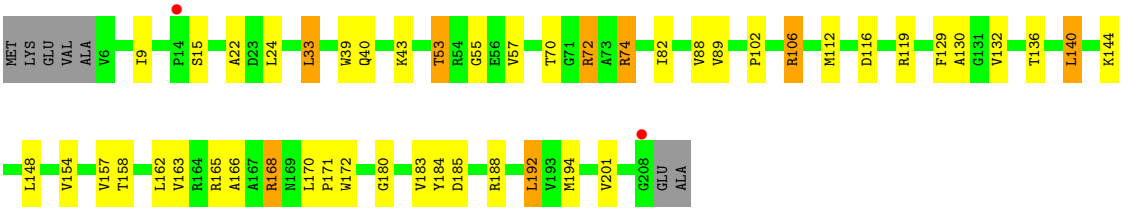
Chain 2E:





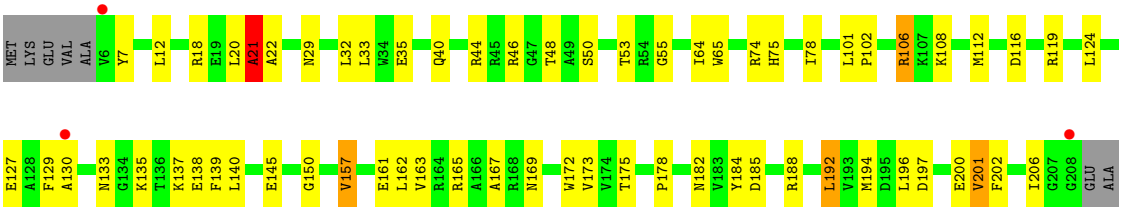
• Molecule 5: 50S ribosomal protein L4

Chain 1F:



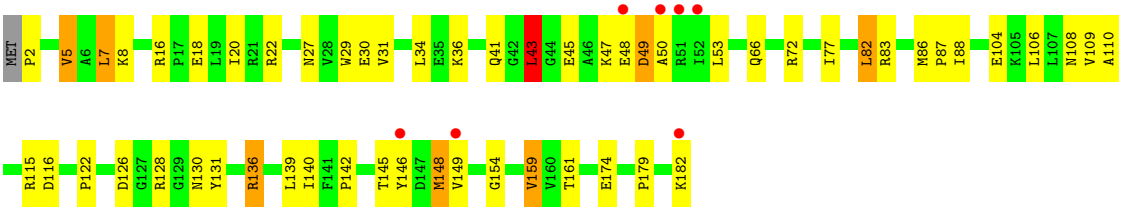
• Molecule 5: 50S ribosomal protein L4

Chain 2F:



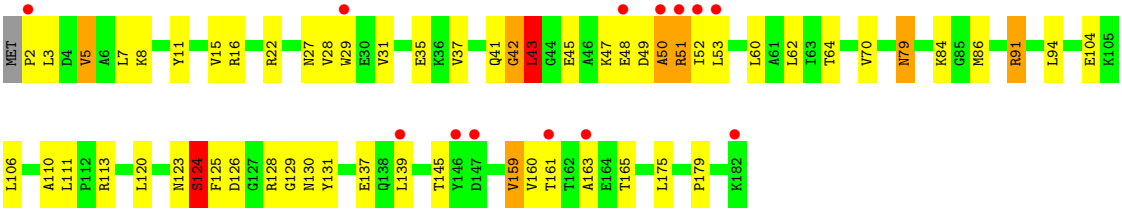
• Molecule 6: 50S ribosomal protein L5

Chain 1G:



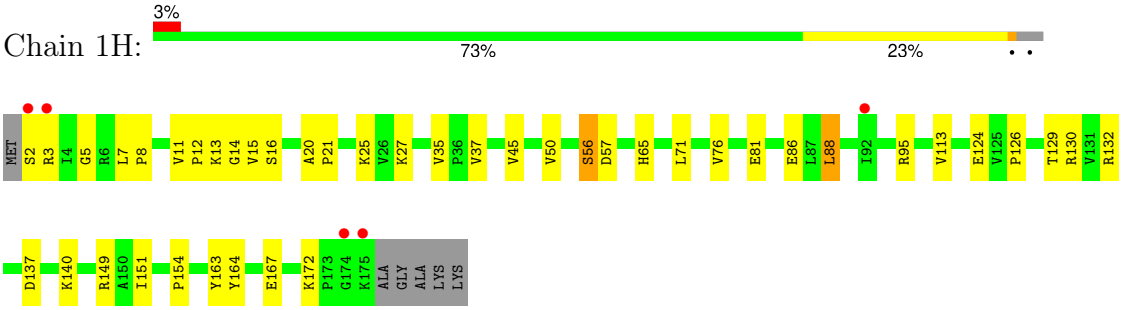
• Molecule 6: 50S ribosomal protein L5

Chain 2G:



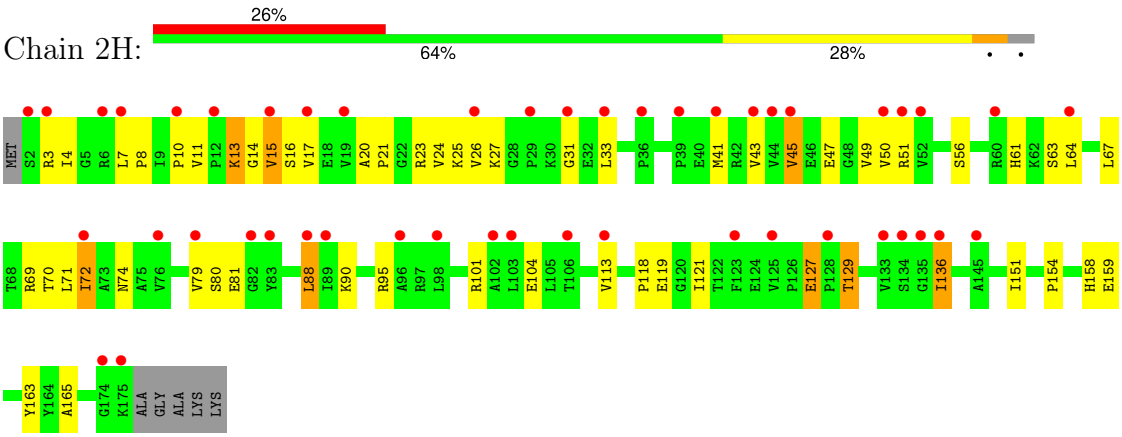
• Molecule 7: 50S ribosomal protein L6

Chain 1H:



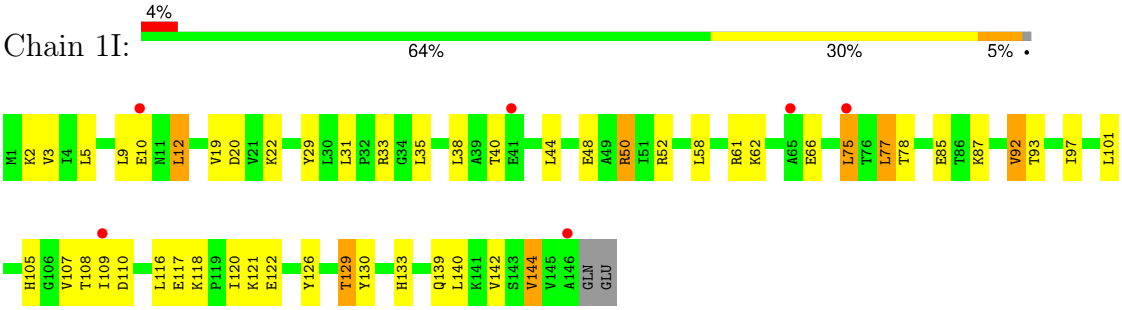
• Molecule 7: 50S ribosomal protein L6

Chain 2H:



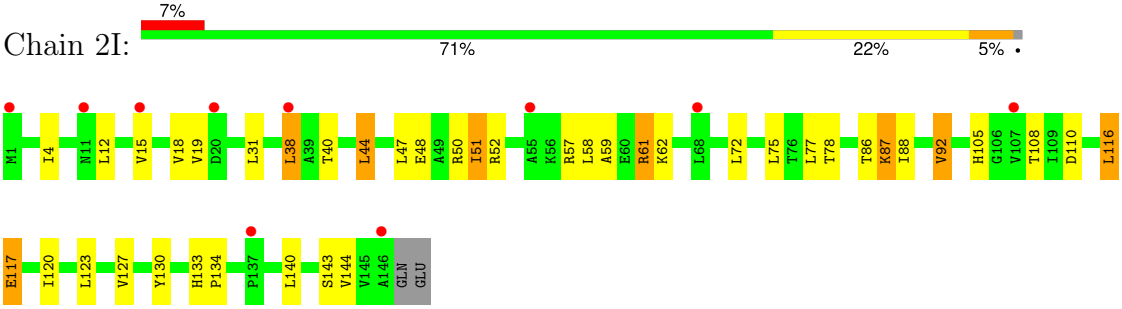
• Molecule 8: 50S ribosomal protein L9

Chain 1I:



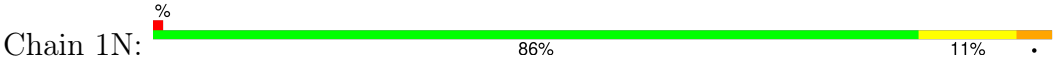
• Molecule 8: 50S ribosomal protein L9

Chain 2I:

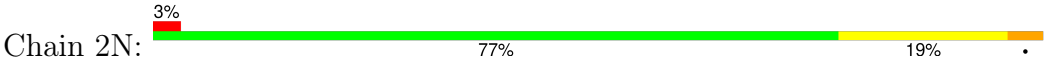


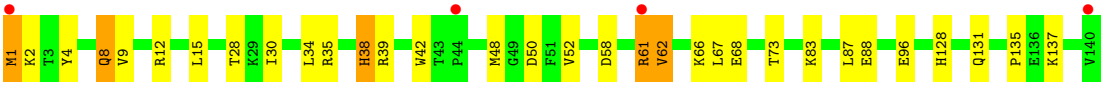
• Molecule 9: 50S ribosomal protein L13

Chain 1N:

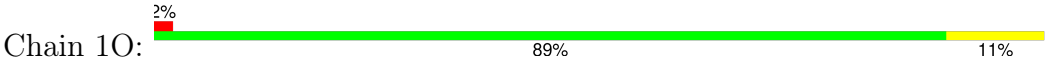


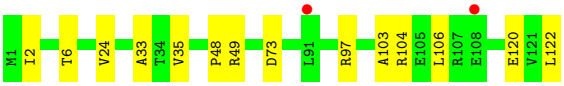
• Molecule 9: 50S ribosomal protein L13



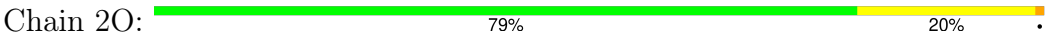


• Molecule 10: 50S ribosomal protein L14

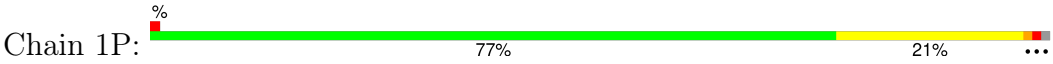


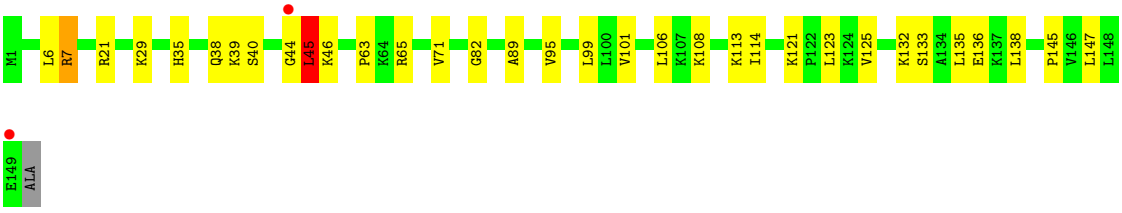


• Molecule 10: 50S ribosomal protein L14

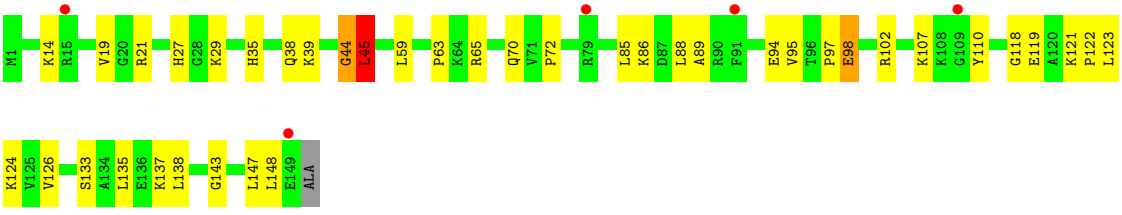


• Molecule 11: 50S ribosomal protein L15

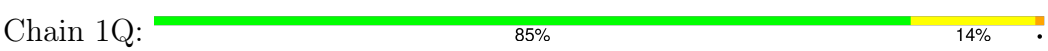


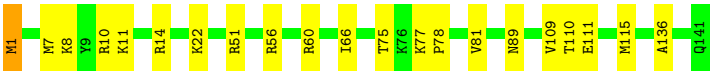


• Molecule 11: 50S ribosomal protein L15



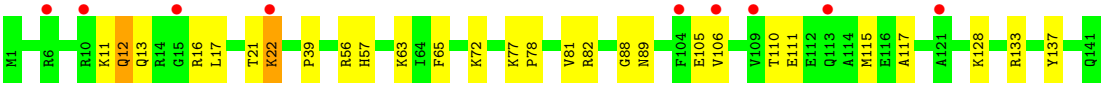
• Molecule 12: 50S ribosomal protein L16





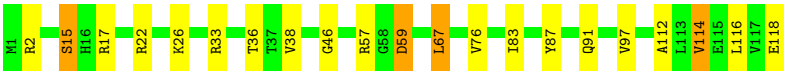
• Molecule 12: 50S ribosomal protein L16

Chain 2Q:



• Molecule 13: 50S ribosomal protein L17

Chain 1R:

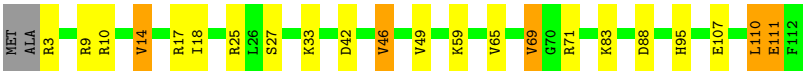


• Molecule 13: 50S ribosomal protein L17

Chain 2R:

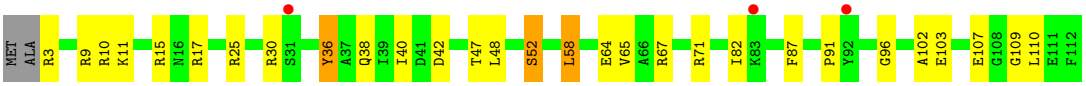
• Molecule 14: 50S ribosomal protein L18

Chain 1S:



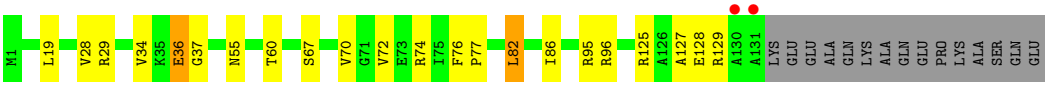
• Molecule 14: 50S ribosomal protein L18

Chain 2S:



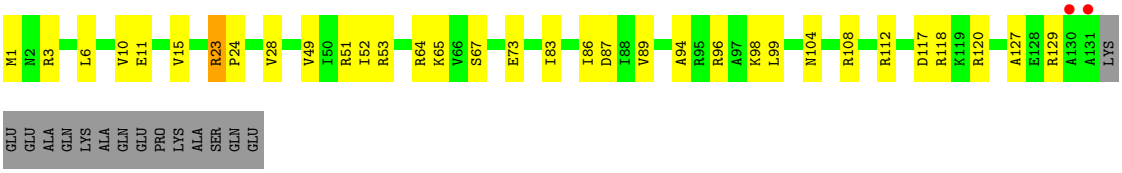
• Molecule 15: 50S ribosomal protein L19

Chain 1T:

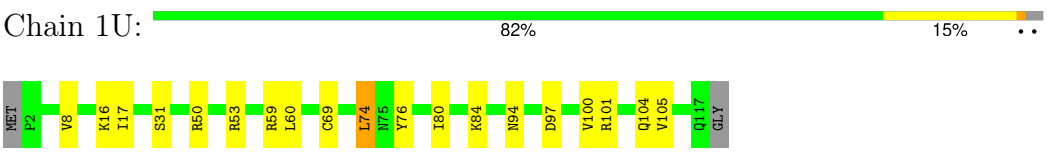


• Molecule 15: 50S ribosomal protein L19

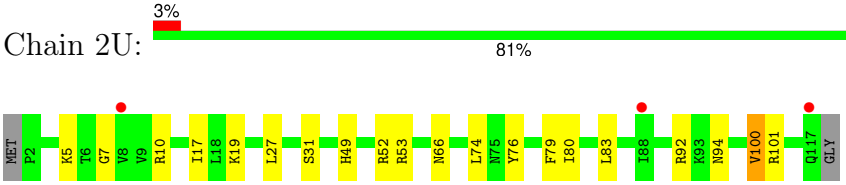
Chain 2T:



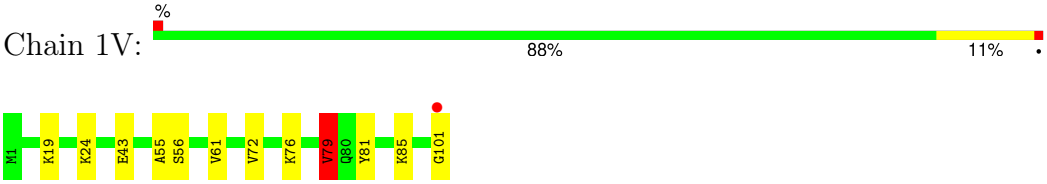
• Molecule 16: 50S ribosomal protein L20



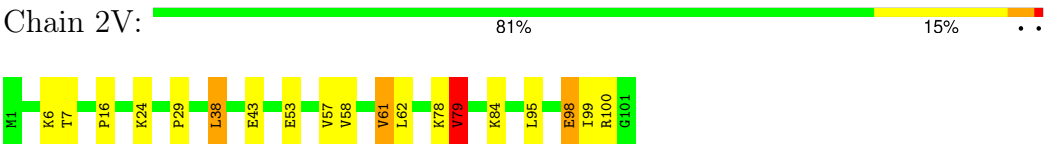
• Molecule 16: 50S ribosomal protein L20



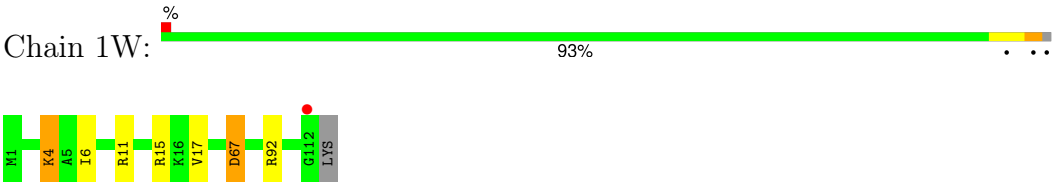
• Molecule 17: 50S ribosomal protein L21



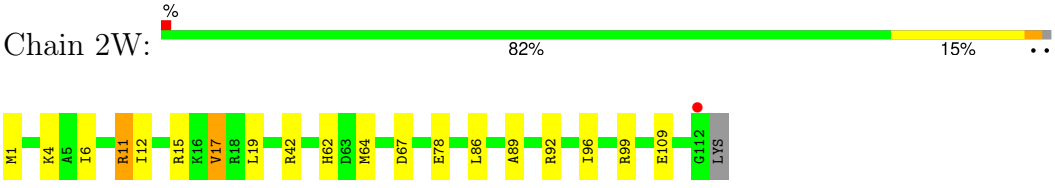
• Molecule 17: 50S ribosomal protein L21



• Molecule 18: 50S ribosomal protein L22

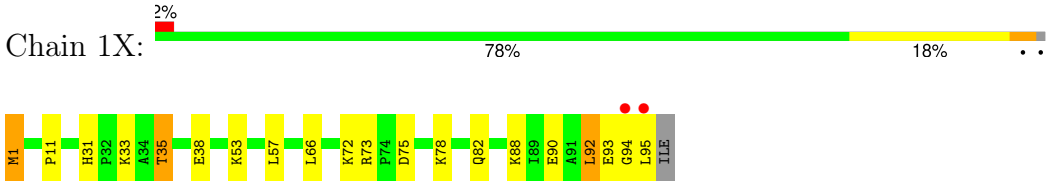


• Molecule 18: 50S ribosomal protein L22



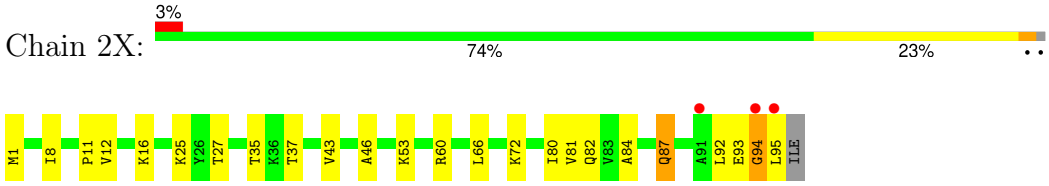
• Molecule 19: 50S ribosomal protein L23

Chain 1X:



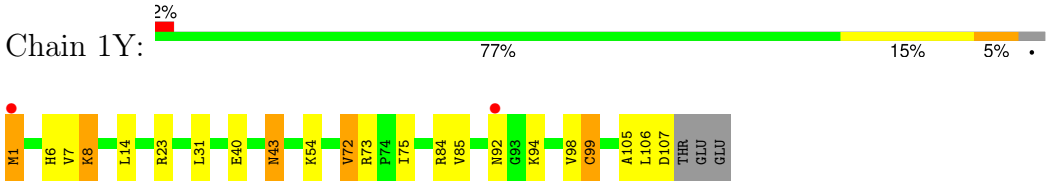
• Molecule 19: 50S ribosomal protein L23

Chain 2X:



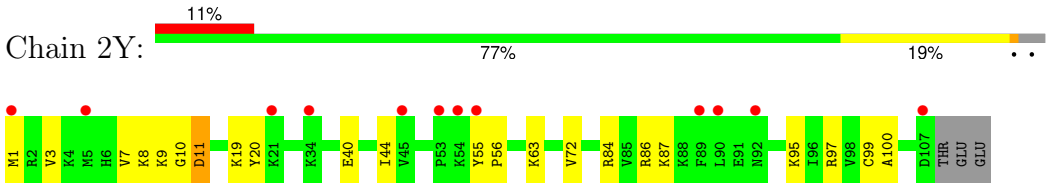
• Molecule 20: 50S ribosomal protein L24

Chain 1Y:



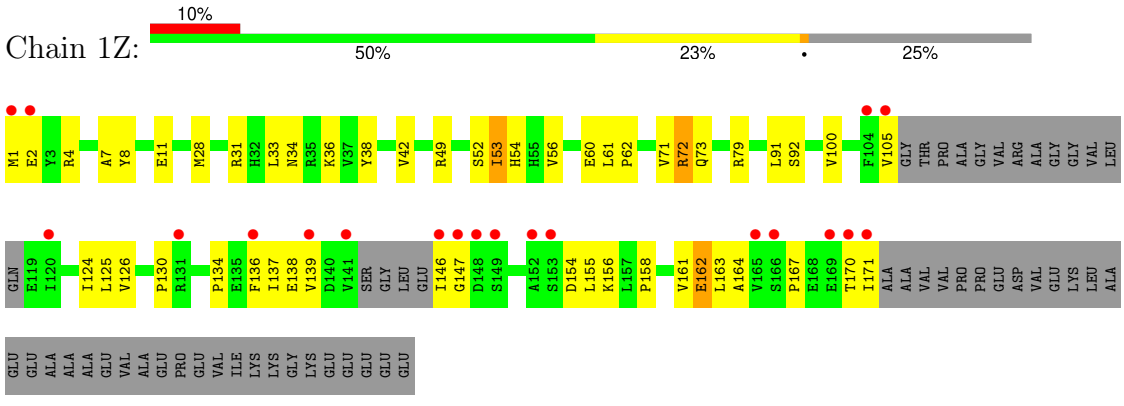
• Molecule 20: 50S ribosomal protein L24

Chain 2Y:



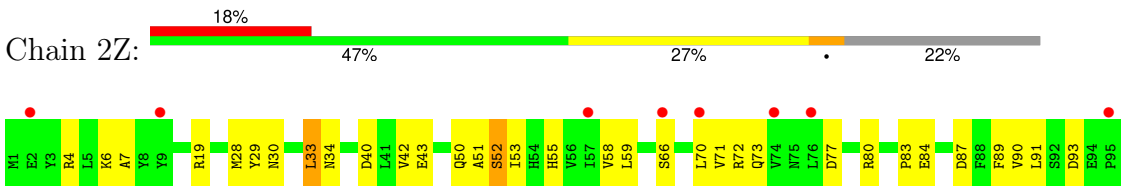
• Molecule 21: 50S ribosomal protein L25

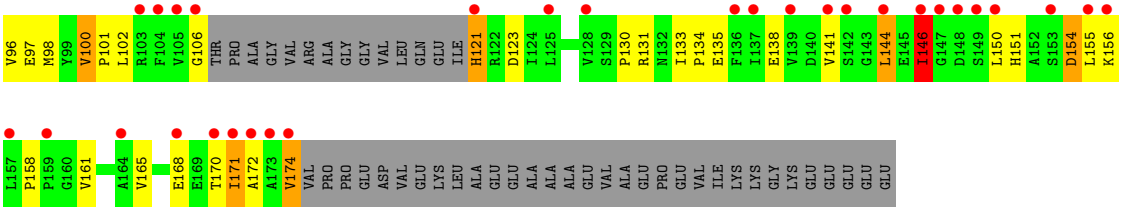
Chain 1Z:



• Molecule 21: 50S ribosomal protein L25

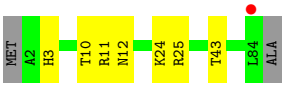
Chain 2Z:





• Molecule 22: 50S ribosomal protein L27

Chain 10:

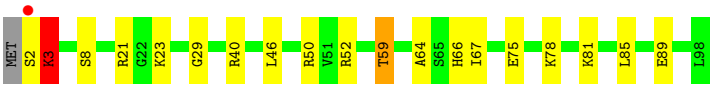


• Molecule 22: 50S ribosomal protein L27

Chain 20:

• Molecule 23: 50S ribosomal protein L28

Chain 11:

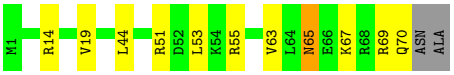


• Molecule 23: 50S ribosomal protein L28

Chain 21:

• Molecule 24: 50S ribosomal protein L29

Chain 12:

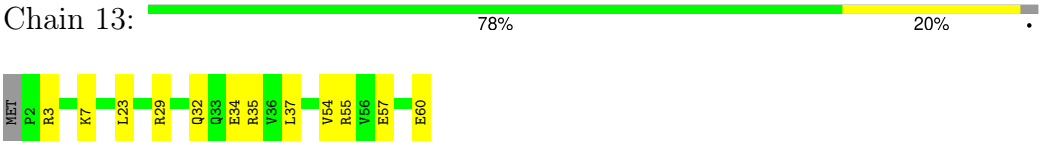


• Molecule 24: 50S ribosomal protein L29

Chain 22:

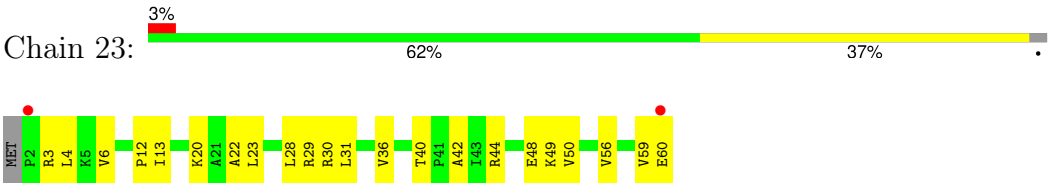
• Molecule 25: 50S ribosomal protein L30

Chain 13:



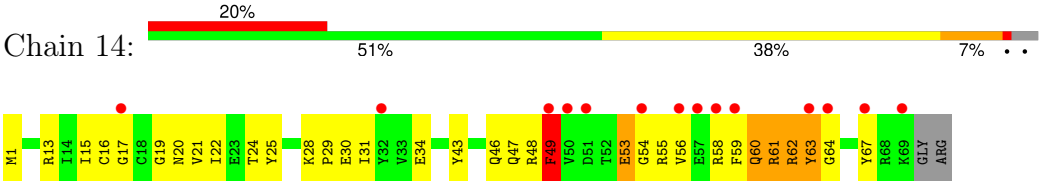
• Molecule 25: 50S ribosomal protein L30

Chain 23:



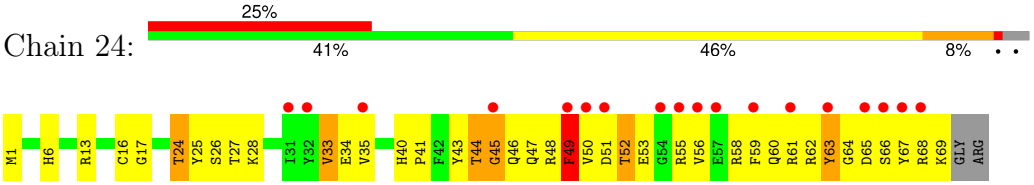
• Molecule 26: 50S ribosomal protein L31

Chain 14:



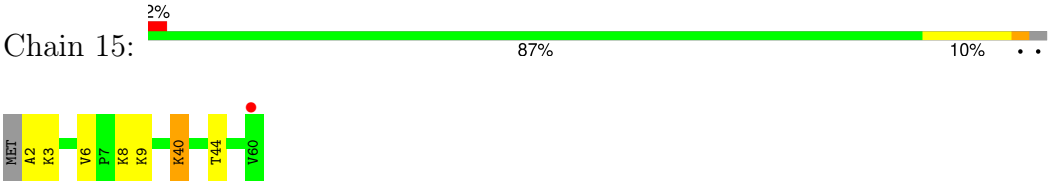
• Molecule 26: 50S ribosomal protein L31

Chain 24:



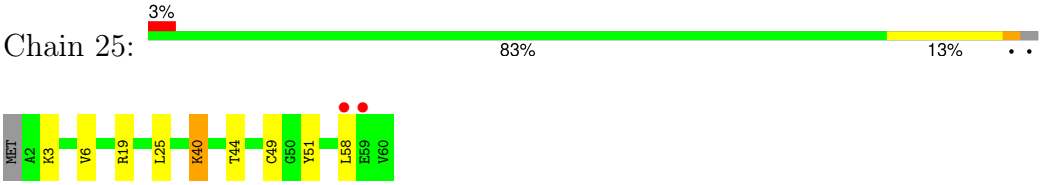
• Molecule 27: 50S ribosomal protein L32

Chain 15:



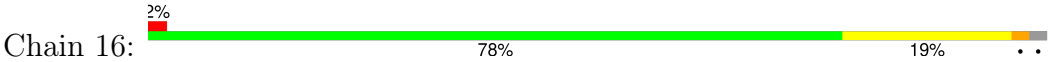
• Molecule 27: 50S ribosomal protein L32

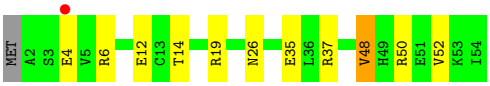
Chain 25:



• Molecule 28: 50S ribosomal protein L33

Chain 16:



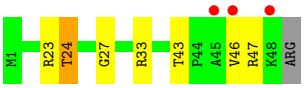


• Molecule 28: 50S ribosomal protein L33

Chain 26:

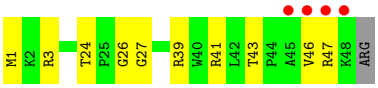
• Molecule 29: 50S ribosomal protein L34

Chain 17:



• Molecule 29: 50S ribosomal protein L34

Chain 27:

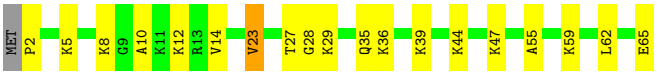


• Molecule 30: 50S ribosomal protein L35

Chain 18:

• Molecule 30: 50S ribosomal protein L35

Chain 28:

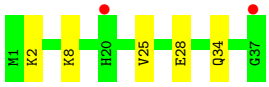


• Molecule 31: 50S ribosomal protein L36

Chain 19:

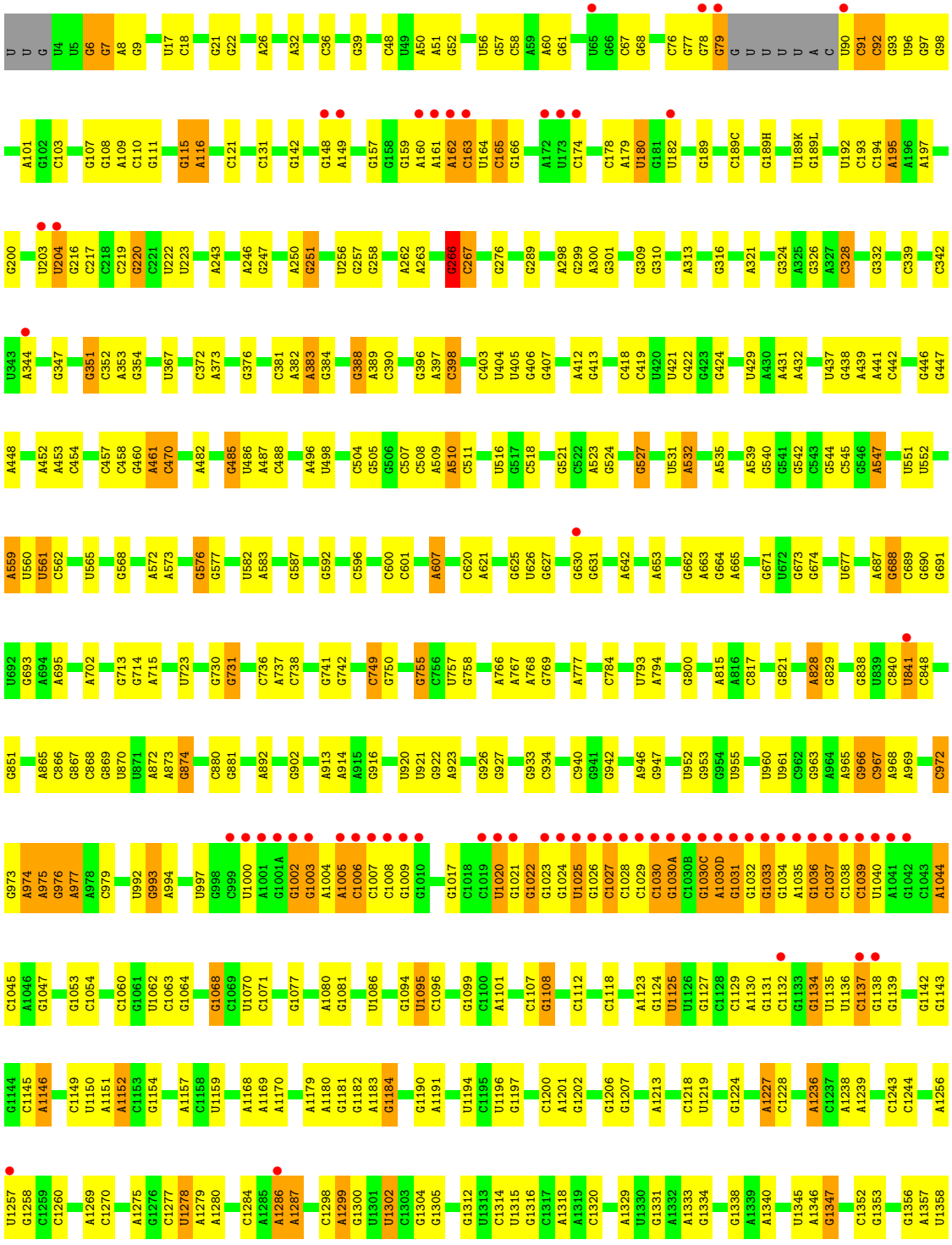
• Molecule 31: 50S ribosomal protein L36

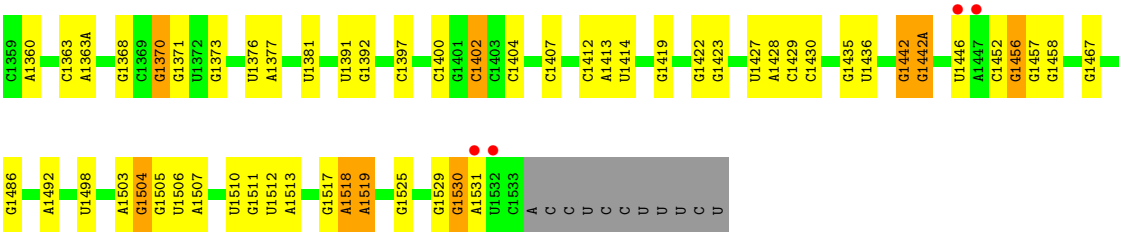
Chain 29:



• Molecule 32: 16S Ribosomal RNA

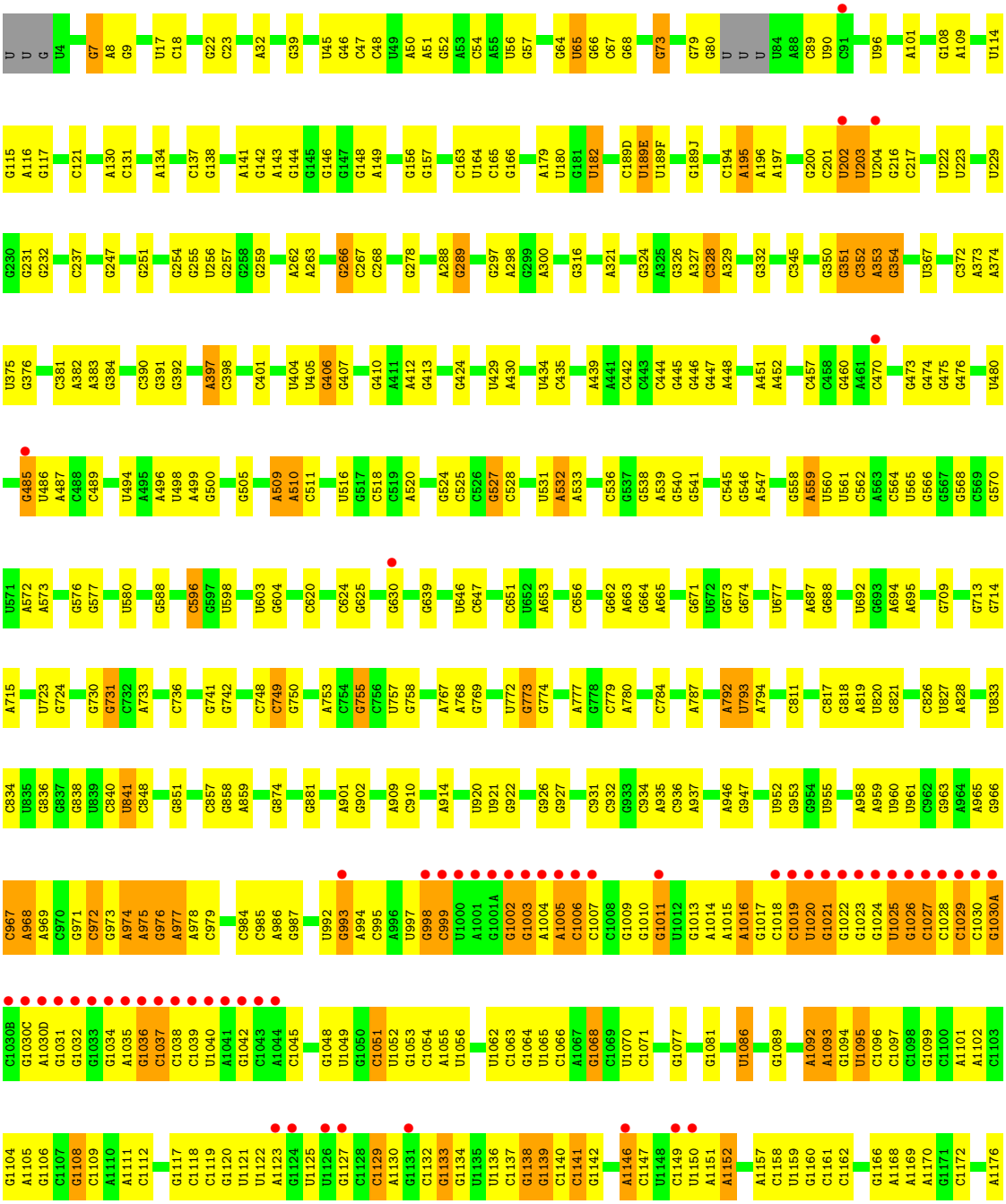
Chain 1a:

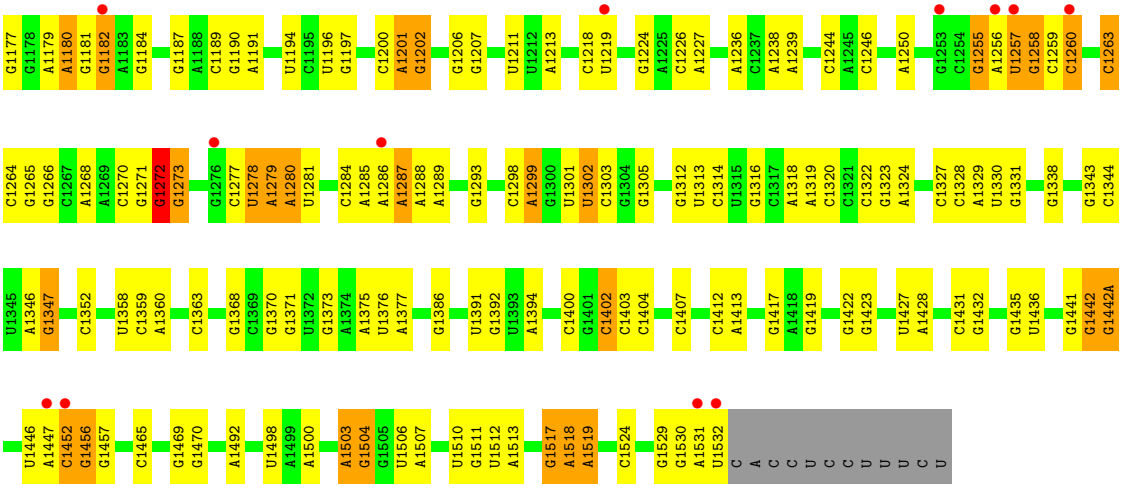




• Molecule 32: 16S Ribosomal RNA

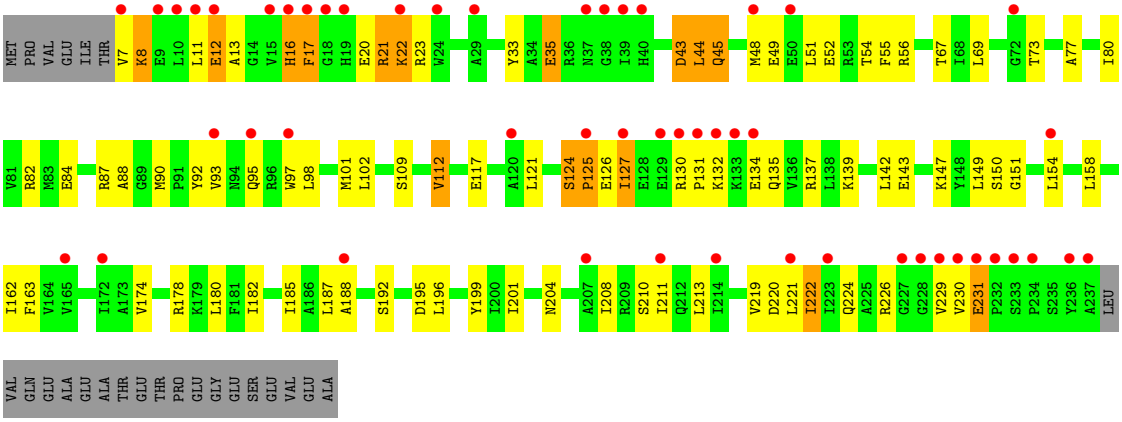
Chain 2a:





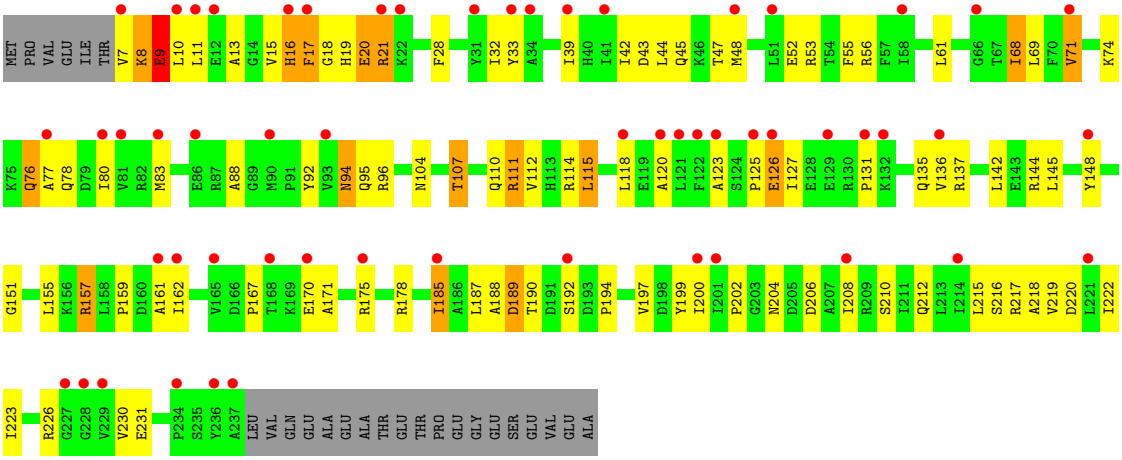
• Molecule 33: 30S ribosomal protein S2

Chain 1b:



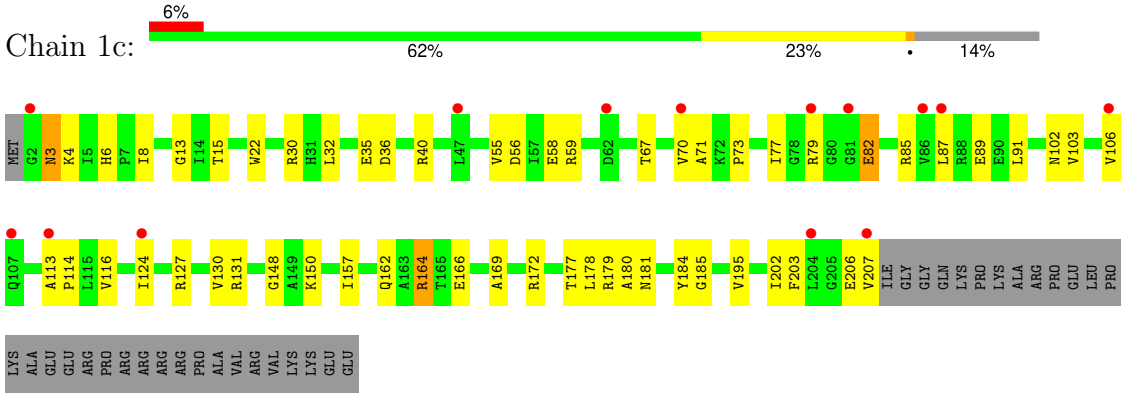
• Molecule 33: 30S ribosomal protein S2

Chain 2b:



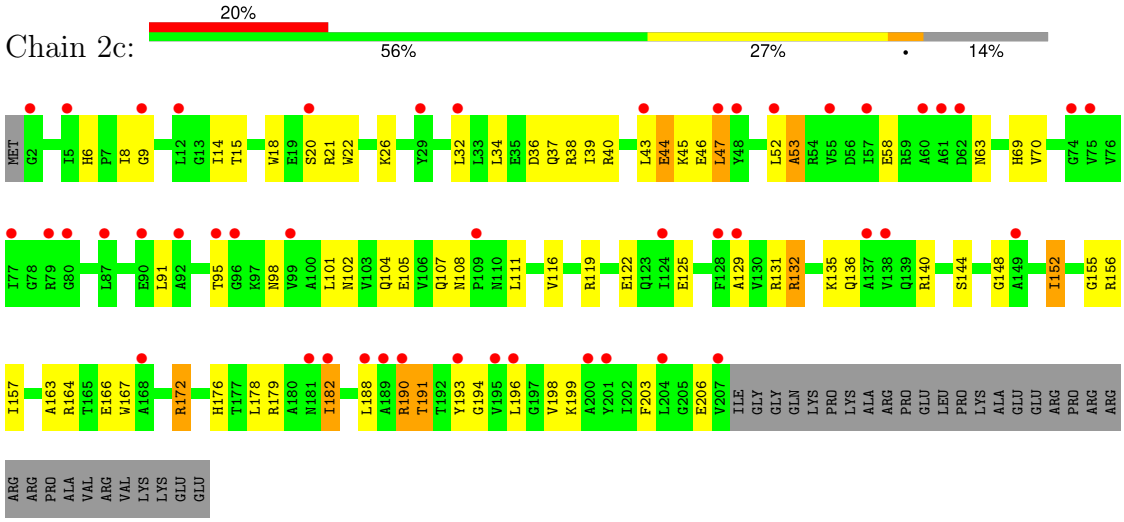
• Molecule 34: 30S ribosomal protein S3

Chain 1c:



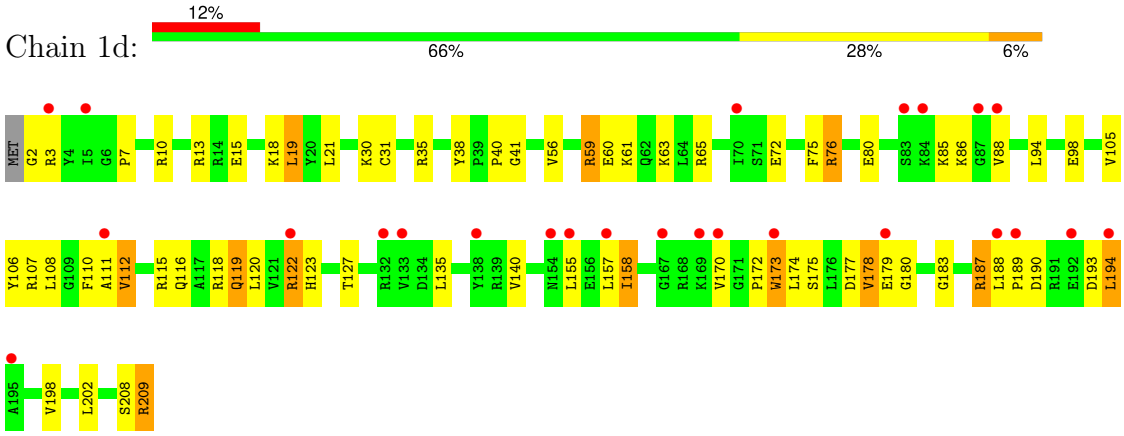
• Molecule 34: 30S ribosomal protein S3

Chain 2c:



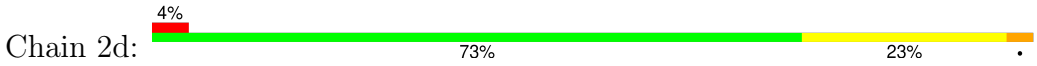
• Molecule 35: 30S ribosomal protein S4

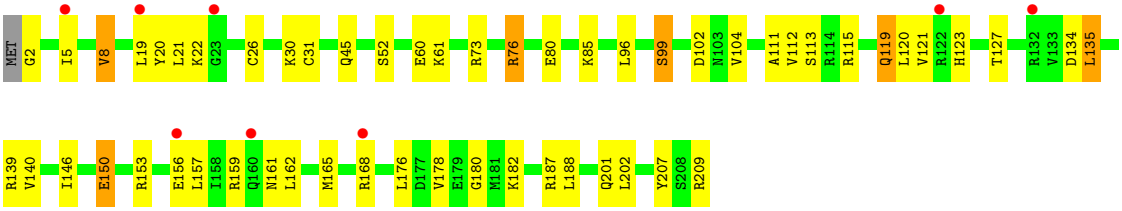
Chain 1d:



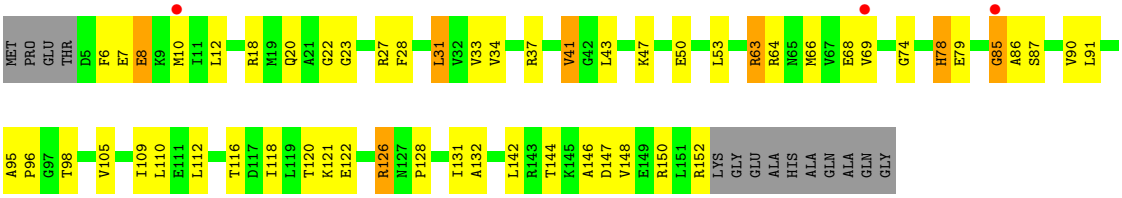
• Molecule 35: 30S ribosomal protein S4

Chain 2d:

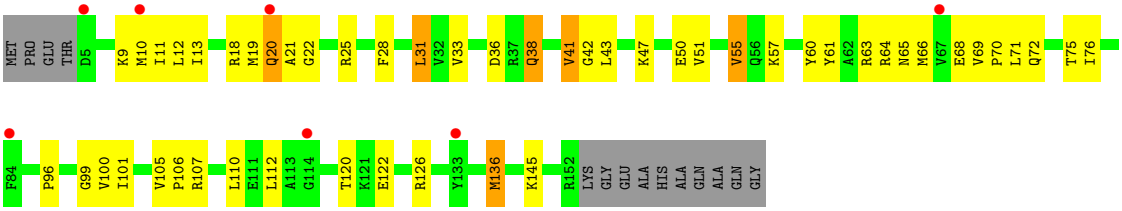




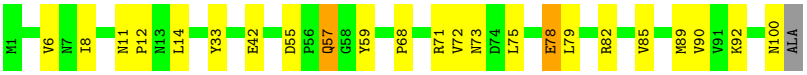
• Molecule 36: 30S ribosomal protein S5



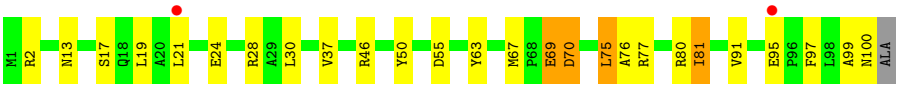
• Molecule 36: 30S ribosomal protein S5



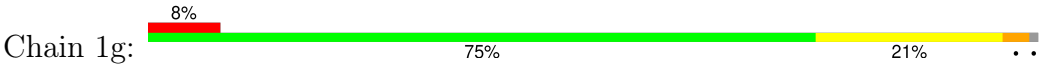
• Molecule 37: 30S ribosomal protein S6

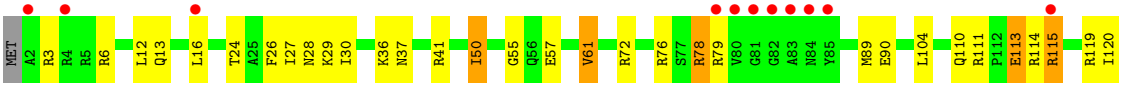


• Molecule 37: 30S ribosomal protein S6



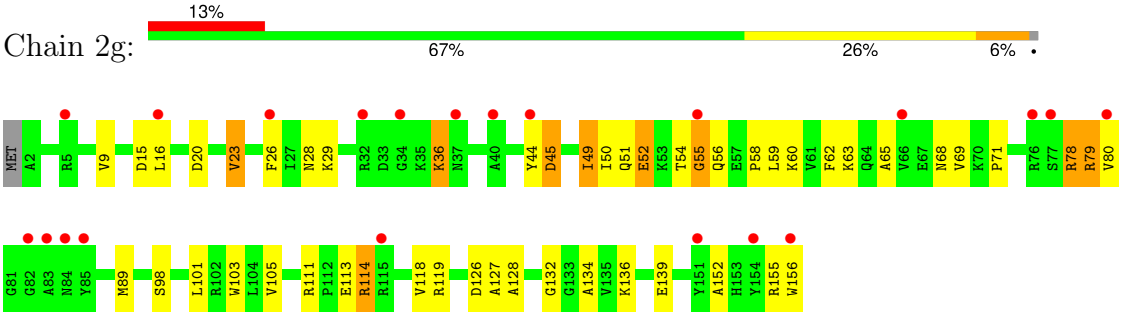
• Molecule 38: 30S ribosomal protein S7





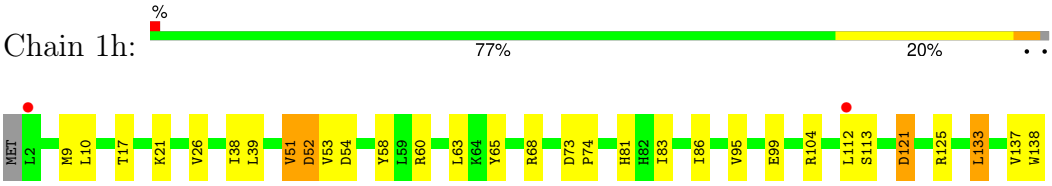
• Molecule 38: 30S ribosomal protein S7

Chain 2g:



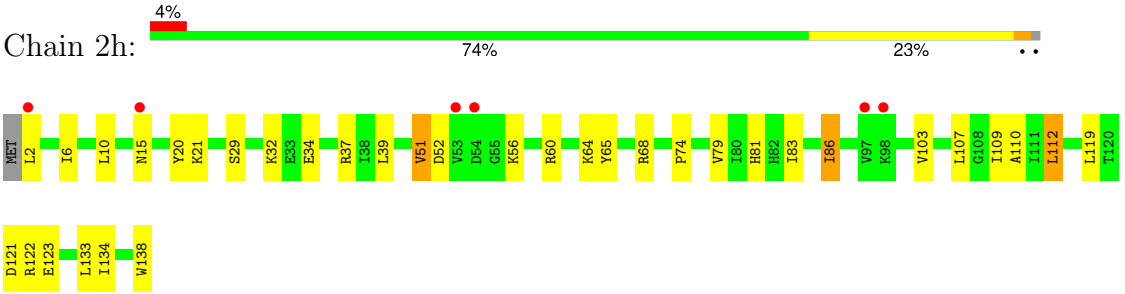
• Molecule 39: 30S ribosomal protein S8

Chain 1h:



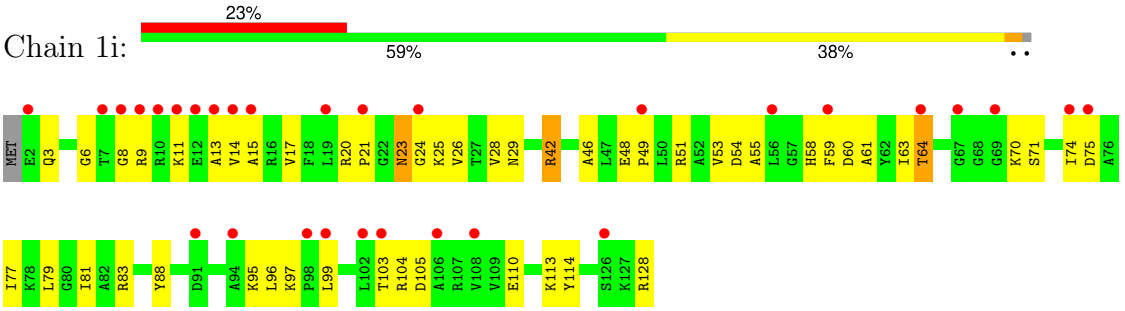
• Molecule 39: 30S ribosomal protein S8

Chain 2h:



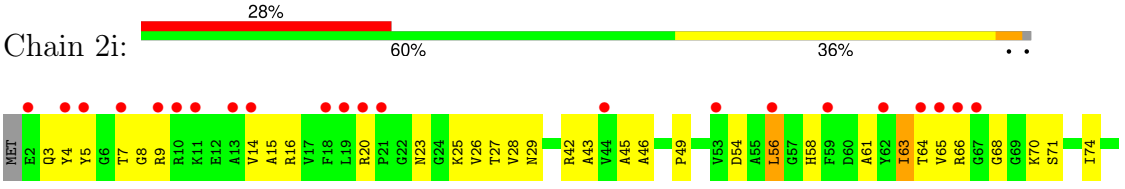
• Molecule 40: 30S ribosomal protein S9

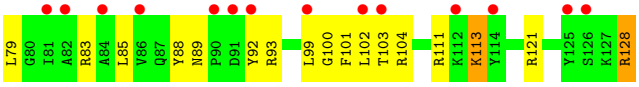
Chain 1i:



• Molecule 40: 30S ribosomal protein S9

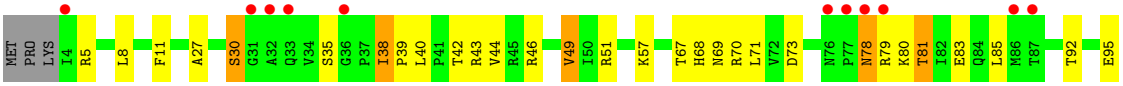
Chain 2i:

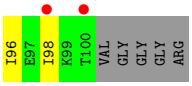




• Molecule 41: 30S ribosomal protein S10

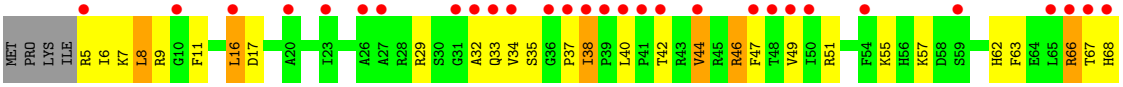
Chain 1j:

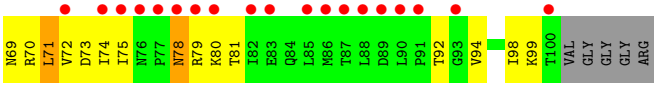




• Molecule 41: 30S ribosomal protein S10

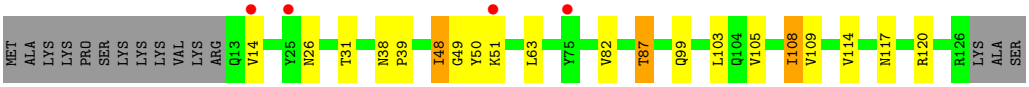
Chain 2j:





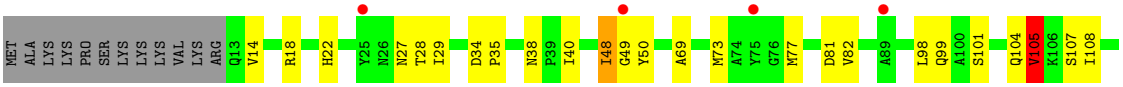
• Molecule 42: 30S ribosomal protein S11

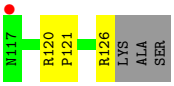
Chain 1k:



• Molecule 42: 30S ribosomal protein S11

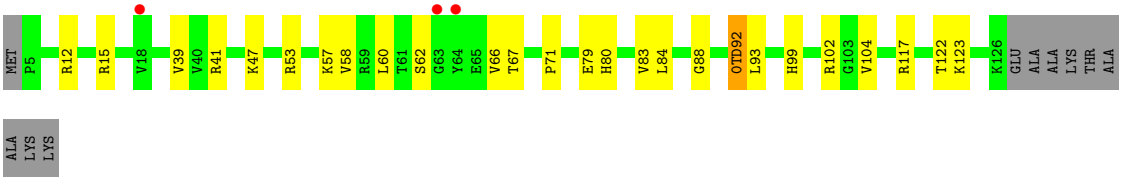
Chain 2k:





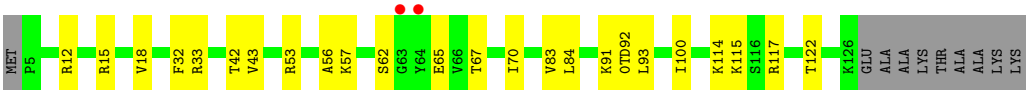
• Molecule 43: 30S ribosomal protein S12

Chain 1l:



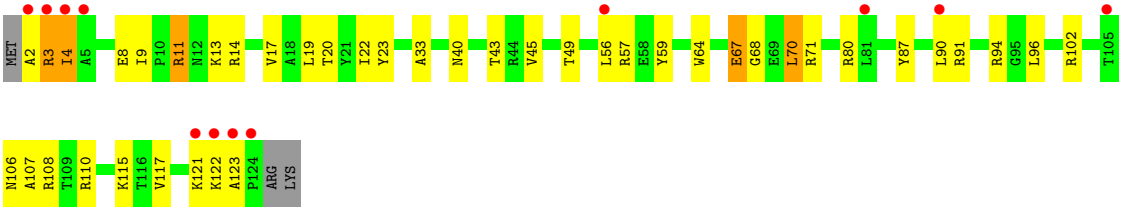
• Molecule 43: 30S ribosomal protein S12

Chain 2l:



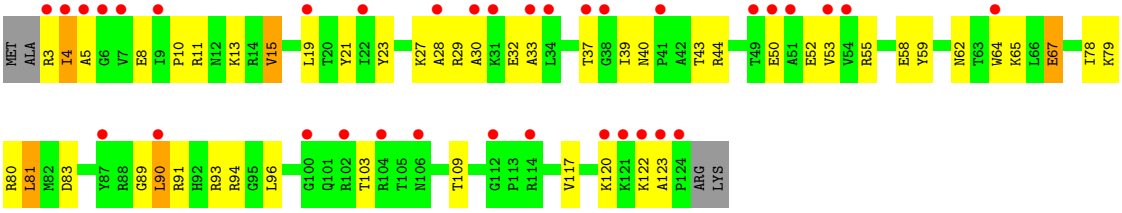
• Molecule 44: 30S ribosomal protein S13

Chain 1m:



• Molecule 44: 30S ribosomal protein S13

Chain 2m:

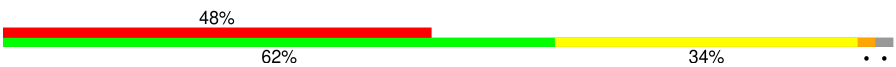


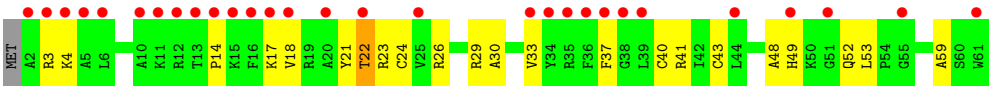
• Molecule 45: 30S ribosomal protein S14 type Z

Chain 1n:

• Molecule 45: 30S ribosomal protein S14 type Z

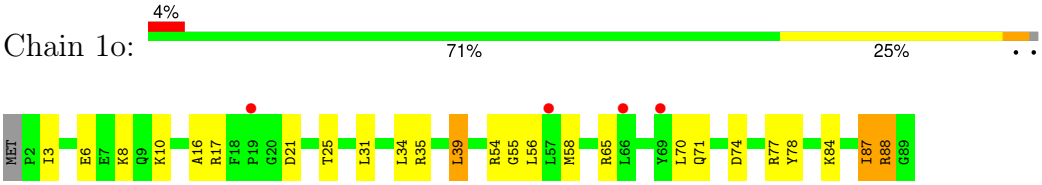
Chain 2n:





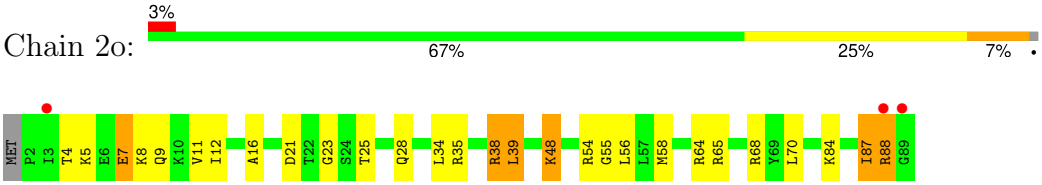
• Molecule 46: 30S ribosomal protein S15

Chain 1o:



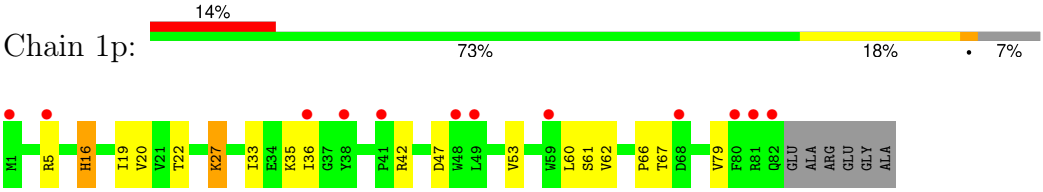
• Molecule 46: 30S ribosomal protein S15

Chain 2o:



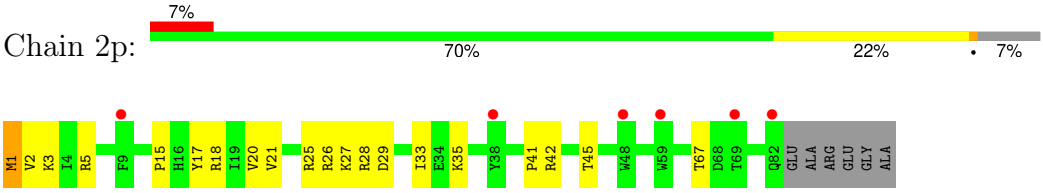
• Molecule 47: 30S ribosomal protein S16

Chain 1p:



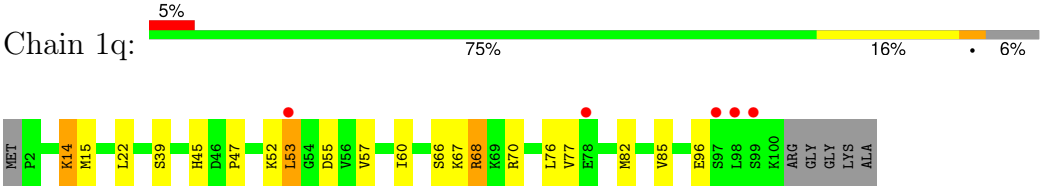
• Molecule 47: 30S ribosomal protein S16

Chain 2p:



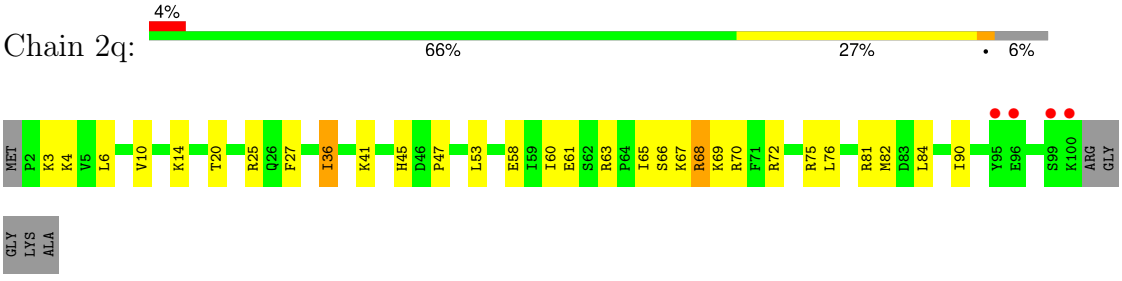
• Molecule 48: 30S ribosomal protein S17

Chain 1q:



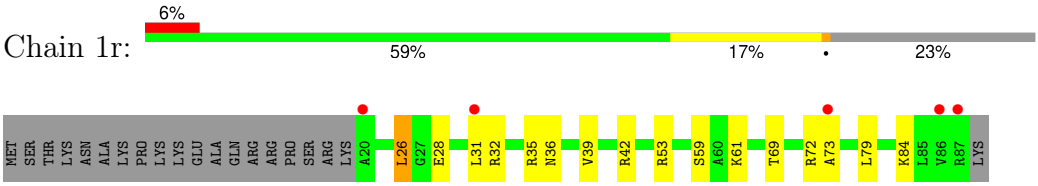
• Molecule 48: 30S ribosomal protein S17

Chain 2q:



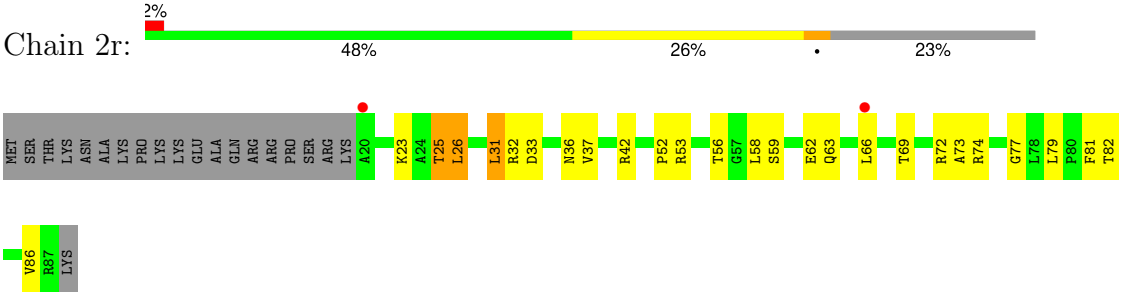
• Molecule 49: 30S ribosomal protein S18

Chain 1r:



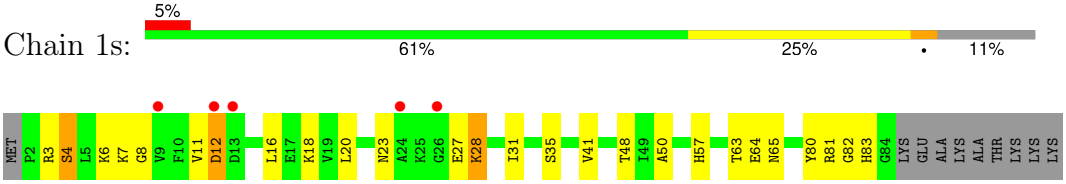
• Molecule 49: 30S ribosomal protein S18

Chain 2r:



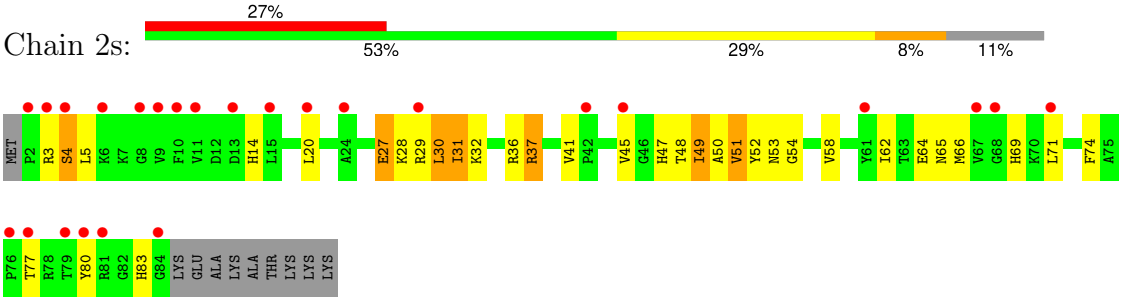
• Molecule 50: 30S ribosomal protein S19

Chain 1s:



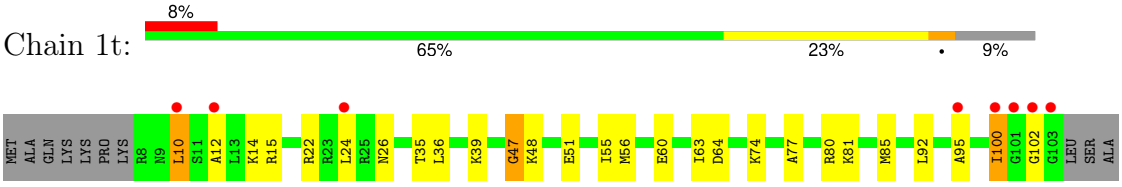
• Molecule 50: 30S ribosomal protein S19

Chain 2s:



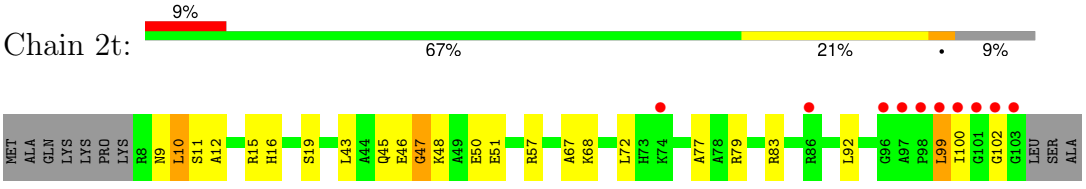
• Molecule 51: 30S ribosomal protein S20

Chain 1t:



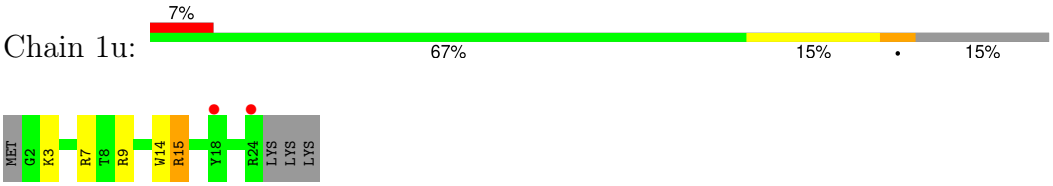
• Molecule 51: 30S ribosomal protein S20

Chain 2t:



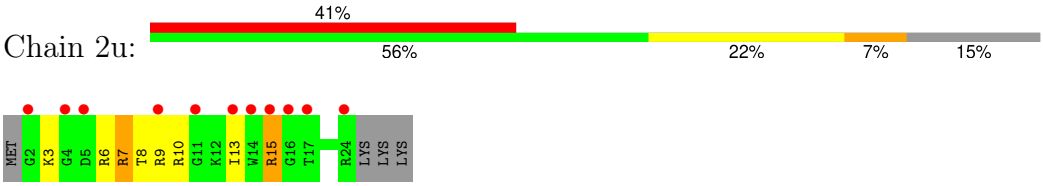
• Molecule 52: 30S ribosomal protein Thx

Chain 1u:



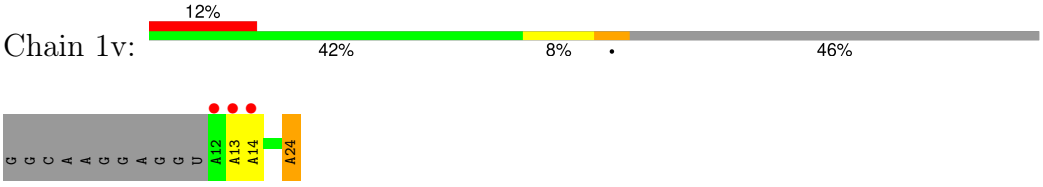
• Molecule 52: 30S ribosomal protein Thx

Chain 2u:



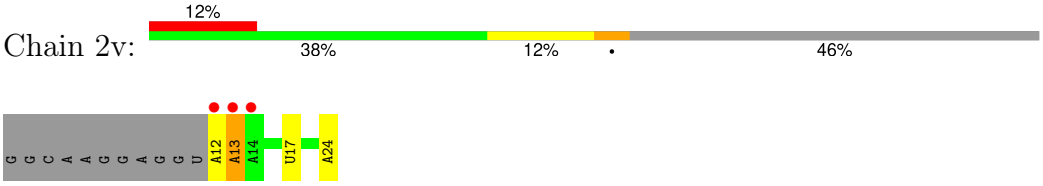
• Molecule 53: MF-mRNA

Chain 1v:



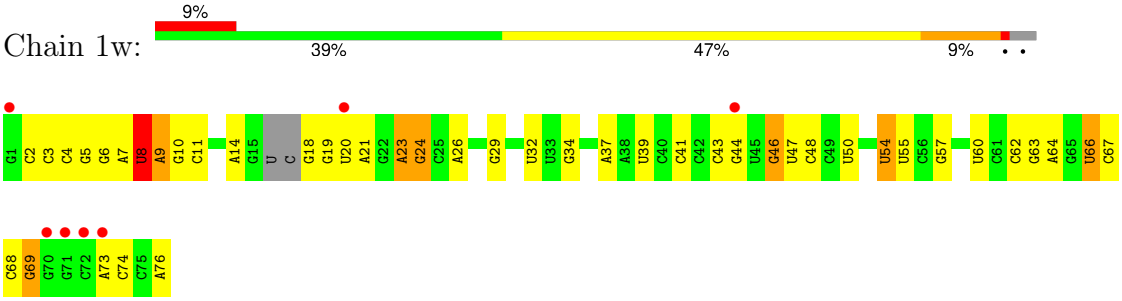
• Molecule 53: MF-mRNA

Chain 2v:



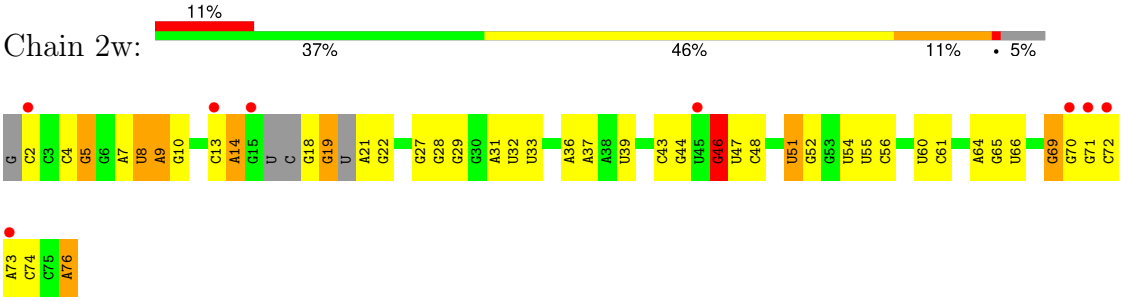
• Molecule 54: Aminoacylated Phe-tRNAphe

Chain 1w:



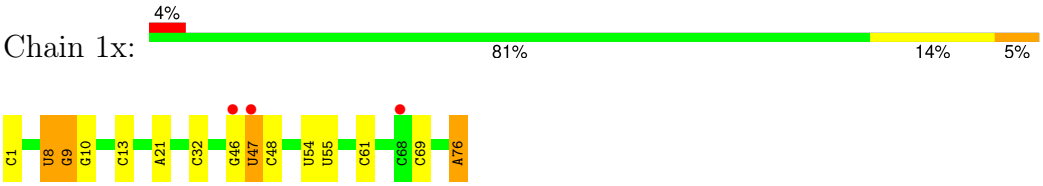
• Molecule 54: Aminoacylated Phe-tRNAphe

Chain 2w:



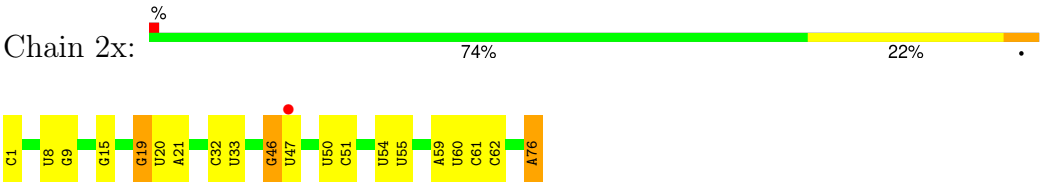
• Molecule 55: Aminoacylated fMet-tRNAmet

Chain 1x:



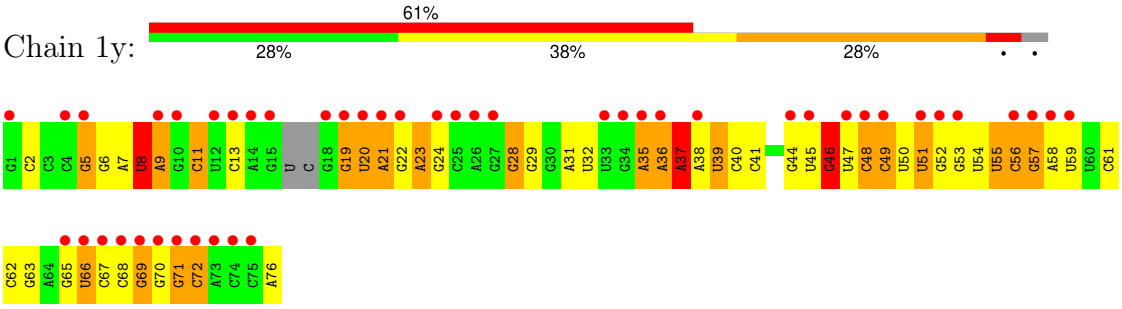
• Molecule 55: Aminoacylated fMet-tRNAmet

Chain 2x:



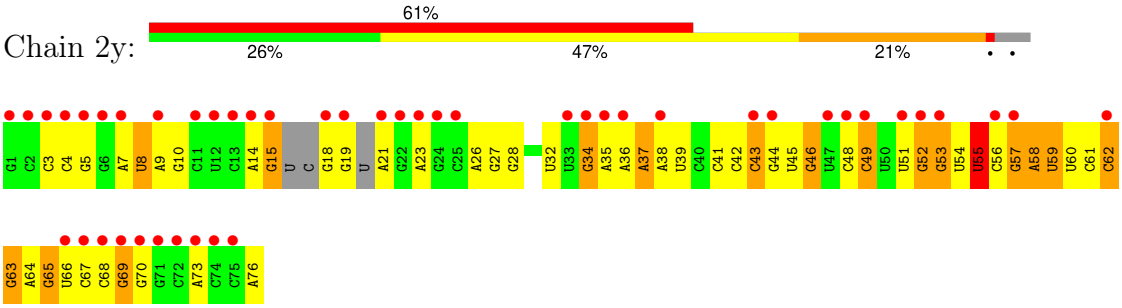
• Molecule 56: Deacylated tRNAphe

Chain 1y:



• Molecule 56: Deacylated tRNAphe

Chain 2y:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	209.98Å 450.78Å 623.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	107.27 – 2.40 107.27 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.9 (107.27-2.40) 98.8 (107.27-2.40)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.15 (at 2.40Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.221 , 0.260 0.223 , 0.261	Depositor DCC
R_{free} test set	112480 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å^2)	47.1	Xtriage
Anisotropy	0.130	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 45.6	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	0.93	EDS
Total number of atoms	300455	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.54% 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: 5MU, K, 5MC, 4OC, OMU, A1AEZ, 0TD, 2MA, 4SU, MG, FME, MA6, ZN, MIA, 2MG, OMG, UR3, M2G, 8AN, PSU, G7M, SF4, OMC

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	0/67295	0.40	1/105042 (0.0%)
2	1B	0.21	0/2882	0.39	0/4494
2	2B	0.19	0/2879	0.38	0/4487
3	1D	0.26	0/2186	0.51	0/2944
3	2D	0.23	0/2186	0.46	0/2944
4	1E	0.25	0/1592	0.49	0/2149
4	2E	0.20	0/1592	0.43	0/2149
5	1F	0.25	0/1619	0.51	0/2193
5	2F	0.19	0/1615	0.46	2/2188 (0.1%)
6	1G	0.22	0/1448	0.53	2/1957 (0.1%)
6	2G	0.19	0/1453	0.42	0/1963
7	1H	0.21	0/1356	0.40	0/1834
7	2H	0.20	0/1356	0.39	0/1834
8	1I	0.18	0/1112	0.41	0/1514
8	2I	0.18	0/1079	0.44	0/1475
9	1N	0.25	0/1144	0.46	0/1543
9	2N	0.18	0/1144	0.39	0/1543
10	1O	0.24	0/943	0.43	0/1269
10	2O	0.19	0/943	0.39	0/1269
11	1P	0.24	0/1152	0.55	0/1533
11	2P	0.21	0/1152	0.48	0/1533
12	1Q	0.26	0/1143	0.46	0/1527
12	2Q	0.19	0/1143	0.40	0/1527
13	1R	0.27	0/982	0.49	0/1312
13	2R	0.19	0/982	0.42	0/1312
14	1S	0.22	0/883	0.47	0/1176
14	2S	0.20	0/880	0.43	0/1172
15	1T	0.24	0/1105	0.47	0/1477
15	2T	0.20	0/1097	0.41	0/1468
16	1U	0.28	0/977	0.47	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
16	2U	0.19	0/977	0.40	0/1301
17	1V	0.25	0/782	0.49	0/1049
17	2V	0.19	0/782	0.42	0/1049
18	1W	0.26	0/897	0.45	0/1205
18	2W	0.21	0/897	0.40	0/1205
19	1X	0.27	0/764	0.55	0/1025
19	2X	0.21	0/764	0.49	2/1025 (0.2%)
20	1Y	0.22	0/819	0.50	0/1095
20	2Y	0.20	0/819	0.43	0/1095
21	1Z	0.24	0/1267	0.47	0/1717
21	2Z	0.21	0/1299	0.43	0/1763
22	10	0.25	0/662	0.50	0/881
22	20	0.20	0/662	0.45	0/881
23	11	0.23	0/762	0.41	0/1014
23	21	0.22	0/762	0.41	0/1014
24	12	0.24	0/590	0.44	0/781
24	22	0.19	0/590	0.39	0/781
25	13	0.26	0/474	0.47	0/635
25	23	0.18	0/469	0.41	0/630
26	14	0.26	0/565	0.60	1/761 (0.1%)
26	24	0.24	0/545	0.56	0/737
27	15	0.26	0/469	0.50	0/635
27	25	0.19	0/469	0.42	0/635
28	16	0.26	0/460	0.46	0/613
28	26	0.21	0/456	0.44	0/608
29	17	0.29	0/426	0.54	0/561
29	27	0.24	0/426	0.50	0/561
30	18	0.26	0/525	0.47	0/691
30	28	0.20	0/525	0.38	0/691
31	19	0.26	0/310	0.51	0/407
31	29	0.18	0/310	0.41	0/407
32	1a	0.20	0/35795	0.39	2/55864 (0.0%)
32	2a	0.19	0/35886	0.37	3/56005 (0.0%)
33	1b	0.20	0/1881	0.49	0/2542
33	2b	0.21	0/1860	0.48	0/2518
34	1c	0.20	0/1572	0.40	0/2126
34	2c	0.20	0/1566	0.41	0/2119
35	1d	0.19	0/1685	0.44	0/2262
35	2d	0.20	0/1704	0.42	0/2284
36	1e	0.21	0/1145	0.49	1/1543 (0.1%)
36	2e	0.20	0/1149	0.44	0/1548
37	1f	0.17	0/823	0.39	0/1115
37	2f	0.19	0/829	0.39	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
38	1g	0.19	0/1250	0.42	0/1679
38	2g	0.20	0/1254	0.44	0/1683
39	1h	0.19	0/1108	0.42	0/1494
39	2h	0.17	0/1108	0.41	0/1494
40	1i	0.20	0/1002	0.49	0/1346
40	2i	0.21	0/997	0.46	0/1343
41	1j	0.21	0/722	0.43	0/982
41	2j	0.21	0/727	0.48	0/988
42	1k	0.18	0/844	0.41	0/1145
42	2k	0.17	0/848	0.37	0/1149
43	1l	0.23	0/937	0.42	0/1260
43	2l	0.18	0/937	0.39	0/1260
44	1m	0.20	0/969	0.49	0/1302
44	2m	0.20	0/961	0.47	0/1291
45	1n	0.19	0/501	0.41	0/664
45	2n	0.20	0/501	0.42	0/664
46	1o	0.19	0/739	0.38	0/985
46	2o	0.18	0/739	0.37	0/985
47	1p	0.19	0/697	0.43	0/939
47	2p	0.18	0/693	0.45	0/935
48	1q	0.20	0/836	0.45	0/1117
48	2q	0.19	0/836	0.46	0/1117
49	1r	0.20	0/560	0.38	0/746
49	2r	0.18	0/560	0.40	0/746
50	1s	0.19	0/667	0.49	0/900
50	2s	0.27	0/661	0.57	2/893 (0.2%)
51	1t	0.19	0/730	0.45	0/965
51	2t	0.22	0/729	0.50	0/965
52	1u	0.18	0/203	0.43	0/266
52	2u	0.19	0/203	0.45	0/266
53	1v	0.22	0/310	0.33	0/480
53	2v	0.22	0/310	0.35	0/480
54	1w	0.28	1/1581 (0.1%)	0.43	0/2458
54	2w	0.29	2/1531 (0.1%)	0.39	0/2379
55	1x	0.27	0/1723	0.41	0/2684
55	2x	0.25	1/1723 (0.1%)	0.39	0/2684
56	1y	0.33	2/1606 (0.1%)	0.40	0/2497
56	2y	0.33	2/1583 (0.1%)	0.40	0/2459
All	All	0.23	8/316636 (0.0%)	0.43	18/474041 (0.0%)

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

sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
11	1P	0	1
11	2P	0	1
All	All	0	2

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	2y	46	G7M	O3'-P	5.73	1.61	1.56
56	2y	8	4SU	O3'-P	5.52	1.61	1.56
56	1y	46	G7M	O3'-P	5.49	1.61	1.56
54	2w	46	G7M	O3'-P	5.34	1.61	1.56
54	1w	46	G7M	O3'-P	5.25	1.61	1.56

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1A	1992	G	C2'-C3'-O3'	6.76	119.64	109.50
6	1G	49	ASP	CA-C-O	-6.59	111.09	120.51
1	2A	1992	G	C2'-C3'-O3'	6.39	119.08	109.50
26	14	60	GLN	N-CA-C	-6.07	106.23	113.21
32	2a	1272	G	N1-C2-N2	-5.89	98.52	116.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	1P	35	HIS	Peptide
11	2P	35	HIS	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1A	61852	0	31196	466	0
1	2A	60322	0	30428	523	0
2	1B	2577	0	1305	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	2B	2575	0	1303	31	0
3	1D	2136	0	2218	35	0
3	2D	2136	0	2218	29	0
4	1E	1559	0	1618	14	0
4	2E	1559	0	1618	26	0
5	1F	1584	0	1625	29	0
5	2F	1580	0	1619	43	0
6	1G	1423	0	1436	33	0
6	2G	1428	0	1438	36	0
7	1H	1330	0	1407	22	0
7	2H	1330	0	1407	28	0
8	1I	1097	0	1140	30	0
8	2I	1064	0	1082	25	0
9	1N	1117	0	1184	11	0
9	2N	1117	0	1184	20	0
10	1O	933	0	996	11	0
10	2O	933	0	996	15	0
11	1P	1135	0	1212	22	0
11	2P	1135	0	1212	23	0
12	1Q	1122	0	1179	12	0
12	2Q	1122	0	1179	18	0
13	1R	968	0	1033	13	0
13	2R	968	0	1033	15	0
14	1S	873	0	927	19	0
14	2S	870	0	923	24	0
15	1T	1091	0	1151	13	0
15	2T	1083	0	1136	20	0
16	1U	959	0	1019	11	0
16	2U	959	0	1019	13	0
17	1V	771	0	830	7	0
17	2V	771	0	829	11	0
18	1W	886	0	940	3	0
18	2W	886	0	940	11	0
19	1X	750	0	814	12	0
19	2X	750	0	814	17	0
20	1Y	806	0	881	12	0
20	2Y	806	0	881	11	0
21	1Z	1240	0	1240	31	0
21	2Z	1271	0	1273	47	0
22	10	653	0	674	9	0
22	20	653	0	674	12	0
23	11	755	0	826	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	21	755	0	826	18	0
24	12	588	0	643	5	0
24	22	588	0	643	6	0
25	13	469	0	518	8	0
25	23	464	0	514	12	0
26	14	552	0	533	30	0
26	24	532	0	503	28	0
27	15	455	0	465	5	0
27	25	455	0	465	5	0
28	16	453	0	473	6	0
28	26	449	0	469	8	0
29	17	418	0	467	4	0
29	27	418	0	467	7	0
30	18	517	0	582	12	0
30	28	517	0	582	14	0
31	19	307	0	335	5	0
31	29	307	0	335	3	0
32	1a	32246	0	16295	312	0
32	2a	32327	0	16338	368	0
33	1b	1846	0	1867	55	0
33	2b	1825	0	1828	69	0
34	1c	1548	0	1535	34	0
34	2c	1542	0	1517	53	0
35	1d	1655	0	1672	52	0
35	2d	1674	0	1714	34	0
36	1e	1129	0	1185	31	0
36	2e	1133	0	1191	32	0
37	1f	810	0	804	11	0
37	2f	816	0	808	19	0
38	1g	1231	0	1238	23	0
38	2g	1235	0	1249	31	0
39	1h	1088	0	1126	17	0
39	2h	1088	0	1126	20	0
40	1i	983	0	986	29	0
40	2i	978	0	966	34	0
41	1j	709	0	650	23	0
41	2j	714	0	672	33	0
42	1k	829	0	825	11	0
42	2k	833	0	836	15	0
43	1l	932	0	981	14	0
43	2l	932	0	981	11	0
44	1m	958	0	1002	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	2m	950	0	988	31	0
45	1n	492	0	529	10	0
45	2n	492	0	529	20	0
46	1o	728	0	760	14	0
46	2o	728	0	760	19	0
47	1p	681	0	697	9	0
47	2p	677	0	686	15	0
48	1q	823	0	891	11	0
48	2q	823	0	891	17	0
49	1r	555	0	618	7	0
49	2r	555	0	618	21	0
50	1s	652	0	662	17	0
50	2s	646	0	644	29	0
51	1t	728	0	798	19	0
51	2t	727	0	796	19	0
52	1u	199	0	208	4	0
52	2u	199	0	208	6	0
53	1v	277	0	140	1	0
53	2v	277	0	140	2	0
54	1w	1592	0	817	19	0
54	2w	1544	0	786	18	0
55	1x	1646	0	838	9	0
55	2x	1646	0	838	11	0
56	1y	1585	0	803	32	0
56	2y	1565	0	794	40	0
57	10	9	0	0	0	0
57	11	5	0	0	0	0
57	12	2	0	0	0	0
57	13	4	0	0	0	0
57	14	1	0	0	0	0
57	15	7	0	0	0	0
57	16	1	0	0	0	0
57	17	5	0	0	0	0
57	18	5	0	0	0	0
57	19	1	0	0	0	0
57	1A	1117	0	0	0	0
57	1B	37	0	0	0	0
57	1D	15	0	0	0	0
57	1E	15	0	0	0	0
57	1F	12	0	0	0	0
57	1G	5	0	0	0	0
57	1I	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	1N	4	0	0	0	0
57	1O	6	0	0	0	0
57	1P	6	0	0	0	0
57	1Q	6	0	0	0	0
57	1R	6	0	0	0	0
57	1S	3	0	0	0	0
57	1T	2	0	0	0	0
57	1U	11	0	0	0	0
57	1V	7	0	0	0	0
57	1W	4	0	0	0	0
57	1X	6	0	0	0	0
57	1Y	2	0	0	0	0
57	1Z	4	0	0	0	0
57	1a	222	0	0	0	0
57	1b	1	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	1j	1	0	0	0	0
57	1k	1	0	0	0	0
57	1l	2	0	0	0	0
57	1m	1	0	0	0	0
57	1n	1	0	0	0	0
57	1t	1	0	0	0	0
57	1v	1	0	0	0	0
57	1w	9	0	0	0	0
57	1x	14	0	0	0	0
57	20	1	0	0	0	0
57	21	3	0	0	0	0
57	23	2	0	0	0	0
57	25	4	0	0	0	0
57	27	2	0	0	0	0
57	28	2	0	0	0	0
57	2A	842	0	0	0	0
57	2B	18	0	0	0	0
57	2D	9	0	0	0	0
57	2E	8	0	0	0	0
57	2F	8	0	0	0	0
57	2G	1	0	0	0	0
57	2N	1	0	0	0	0
57	2O	2	0	0	0	0
57	2P	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	2Q	3	0	0	0	0
57	2R	3	0	0	0	0
57	2T	4	0	0	0	0
57	2U	2	0	0	0	0
57	2V	2	0	0	0	0
57	2W	1	0	0	0	0
57	2X	2	0	0	0	0
57	2Y	1	0	0	0	0
57	2Z	1	0	0	0	0
57	2a	231	0	0	0	0
57	2d	1	0	0	0	0
57	2e	1	0	0	0	0
57	2f	2	0	0	0	0
57	2g	1	0	0	0	0
57	2j	1	0	0	0	0
57	2l	4	0	0	0	0
57	2m	1	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	2	0	0	0	0
57	2w	7	0	0	0	0
57	2x	7	0	0	0	0
57	2y	2	0	0	0	0
58	1A	1	0	0	0	0
58	2A	1	0	0	0	0
59	1A	85	0	0	2	0
59	2A	85	0	0	1	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	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
62	1w	11	0	8	0	0
62	2w	11	0	8	1	0
63	1x	10	0	10	0	0
63	2x	10	0	10	0	0
64	10	12	0	0	2	0
64	11	9	0	0	0	0
64	12	3	0	0	0	0
64	13	4	0	0	0	0
64	14	1	0	0	0	0
64	15	6	0	0	0	0
64	16	2	0	0	0	0
64	17	9	0	0	1	0
64	18	10	0	0	1	0
64	1A	2052	0	0	67	0
64	1B	64	0	0	2	0
64	1D	31	0	0	0	0
64	1E	27	0	0	2	0
64	1F	19	0	0	1	0
64	1G	3	0	0	1	0
64	1H	2	0	0	0	0
64	1N	5	0	0	0	0
64	1O	6	0	0	0	0
64	1P	22	0	0	0	0
64	1Q	9	0	0	0	0
64	1R	9	0	0	1	0
64	1S	4	0	0	1	0
64	1T	8	0	0	0	0
64	1U	13	0	0	0	0
64	1V	8	0	0	0	0
64	1W	8	0	0	0	0
64	1X	4	0	0	0	0
64	1Y	2	0	0	0	0
64	1Z	1	0	0	0	0
64	1a	418	0	0	25	0
64	1b	1	0	0	0	0
64	1d	3	0	0	0	0
64	1e	1	0	0	0	0
64	1f	2	0	0	0	0
64	1g	1	0	0	0	0
64	1i	2	0	0	0	0
64	1j	2	0	0	0	0
64	1k	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
64	1l	5	0	0	0	0
64	1m	2	0	0	0	0
64	1p	1	0	0	0	0
64	1q	2	0	0	0	0
64	1r	1	0	0	0	0
64	1v	4	0	0	0	0
64	1w	15	0	0	0	0
64	1x	16	0	0	1	0
64	1y	1	0	0	0	0
64	20	2	0	0	0	0
64	21	7	0	0	0	0
64	23	2	0	0	1	0
64	25	1	0	0	0	0
64	26	1	0	0	0	0
64	27	4	0	0	0	0
64	28	3	0	0	0	0
64	29	1	0	0	0	0
64	2A	1183	0	0	66	0
64	2B	18	0	0	1	0
64	2D	22	0	0	0	0
64	2E	12	0	0	0	0
64	2F	12	0	0	0	0
64	2N	2	0	0	0	0
64	2O	2	0	0	0	0
64	2P	10	0	0	0	0
64	2Q	1	0	0	0	0
64	2R	4	0	0	0	0
64	2T	6	0	0	0	0
64	2U	2	0	0	0	0
64	2W	1	0	0	0	0
64	2X	2	0	0	0	0
64	2Y	2	0	0	0	0
64	2a	265	0	0	16	0
64	2c	2	0	0	0	0
64	2d	3	0	0	0	0
64	2e	1	0	0	0	0
64	2g	1	0	0	0	0
64	2j	2	0	0	1	0
64	2l	6	0	0	0	0
64	2n	1	0	0	1	0
64	2p	1	0	0	0	0
64	2r	1	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
64	2t	5	0	0	0	0
64	2w	2	0	0	0	0
64	2x	7	0	0	0	0
64	2y	3	0	0	0	0
All	All	300455	0	196744	3290	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

The worst 5 of 3290 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)
59:1A:4118:A1AEZ:NBJ	59:1A:4118:A1AEZ:OBR	1.56	1.34
1:1A:1082:U:H3	1:1A:1086:A:N6	1.35	1.25
1:1A:1082:U:O4	1:1A:1086:A:N1	1.96	0.99
1:2A:2298:A:H62	1:2A:2318:G:H8	1.14	0.95
1:1A:1054:A:H61	1:1A:1105:U:H3	1.15	0.92

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	1D	273/276 (99%)	258 (94%)	15 (6%)	0	100 100
3	2D	273/276 (99%)	261 (96%)	12 (4%)	0	100 100
4	1E	202/206 (98%)	192 (95%)	9 (4%)	1 (0%)	24 37
4	2E	202/206 (98%)	188 (93%)	13 (6%)	1 (0%)	24 37
5	1F	201/210 (96%)	194 (96%)	5 (2%)	2 (1%)	12 20
5	2F	201/210 (96%)	192 (96%)	6 (3%)	3 (2%)	8 12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
6	1G	179/182 (98%)	170 (95%)	6 (3%)	3 (2%)	7 10
6	2G	179/182 (98%)	157 (88%)	16 (9%)	6 (3%)	3 2
7	1H	172/180 (96%)	162 (94%)	9 (5%)	1 (1%)	21 32
7	2H	172/180 (96%)	154 (90%)	17 (10%)	1 (1%)	21 32
8	1I	144/148 (97%)	121 (84%)	23 (16%)	0	100 100
8	2I	144/148 (97%)	118 (82%)	25 (17%)	1 (1%)	18 28
9	1N	138/140 (99%)	132 (96%)	6 (4%)	0	100 100
9	2N	138/140 (99%)	128 (93%)	9 (6%)	1 (1%)	18 28
10	1O	120/122 (98%)	114 (95%)	6 (5%)	0	100 100
10	2O	120/122 (98%)	112 (93%)	8 (7%)	0	100 100
11	1P	147/150 (98%)	131 (89%)	15 (10%)	1 (1%)	18 28
11	2P	147/150 (98%)	133 (90%)	10 (7%)	4 (3%)	4 4
12	1Q	139/141 (99%)	134 (96%)	5 (4%)	0	100 100
12	2Q	139/141 (99%)	127 (91%)	11 (8%)	1 (1%)	18 28
13	1R	116/118 (98%)	112 (97%)	4 (3%)	0	100 100
13	2R	116/118 (98%)	112 (97%)	4 (3%)	0	100 100
14	1S	108/112 (96%)	105 (97%)	3 (3%)	0	100 100
14	2S	108/112 (96%)	103 (95%)	3 (3%)	2 (2%)	6 8
15	1T	129/146 (88%)	124 (96%)	3 (2%)	2 (2%)	7 11
15	2T	129/146 (88%)	119 (92%)	10 (8%)	0	100 100
16	1U	114/118 (97%)	114 (100%)	0	0	100 100
16	2U	114/118 (97%)	114 (100%)	0	0	100 100
17	1V	99/101 (98%)	93 (94%)	4 (4%)	2 (2%)	6 7
17	2V	99/101 (98%)	91 (92%)	6 (6%)	2 (2%)	6 7
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 18
19	2X	93/96 (97%)	87 (94%)	5 (5%)	1 (1%)	11 18
20	1Y	105/110 (96%)	99 (94%)	5 (5%)	1 (1%)	12 20
20	2Y	105/110 (96%)	100 (95%)	5 (5%)	0	100 100
21	1Z	148/206 (72%)	133 (90%)	14 (10%)	1 (1%)	18 28

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
21	2Z	156/206 (76%)	134 (86%)	18 (12%)	4 (3%)	4 4
22	10	81/85 (95%)	79 (98%)	2 (2%)	0	100 100
22	20	81/85 (95%)	77 (95%)	4 (5%)	0	100 100
23	11	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	11 18
23	21	95/98 (97%)	92 (97%)	3 (3%)	0	100 100
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%)	56 (98%)	1 (2%)	0	100 100
25	23	57/60 (95%)	53 (93%)	4 (7%)	0	100 100
26	14	67/71 (94%)	53 (79%)	10 (15%)	4 (6%)	1 0
26	24	67/71 (94%)	52 (78%)	11 (16%)	4 (6%)	1 0
27	15	57/60 (95%)	56 (98%)	1 (2%)	0	100 100
27	25	57/60 (95%)	56 (98%)	1 (2%)	0	100 100
28	16	51/54 (94%)	49 (96%)	2 (4%)	0	100 100
28	26	51/54 (94%)	48 (94%)	3 (6%)	0	100 100
29	17	46/49 (94%)	46 (100%)	0	0	100 100
29	27	46/49 (94%)	46 (100%)	0	0	100 100
30	18	62/65 (95%)	62 (100%)	0	0	100 100
30	28	62/65 (95%)	61 (98%)	1 (2%)	0	100 100
31	19	35/37 (95%)	35 (100%)	0	0	100 100
31	29	35/37 (95%)	35 (100%)	0	0	100 100
33	1b	229/256 (90%)	195 (85%)	27 (12%)	7 (3%)	3 3
33	2b	229/256 (90%)	191 (83%)	31 (14%)	7 (3%)	3 3
34	1c	204/239 (85%)	191 (94%)	13 (6%)	0	100 100
34	2c	204/239 (85%)	182 (89%)	18 (9%)	4 (2%)	6 7
35	1d	206/209 (99%)	196 (95%)	9 (4%)	1 (0%)	24 37
35	2d	206/209 (99%)	195 (95%)	11 (5%)	0	100 100
36	1e	146/162 (90%)	128 (88%)	15 (10%)	3 (2%)	5 7
36	2e	146/162 (90%)	134 (92%)	11 (8%)	1 (1%)	18 28
37	1f	98/101 (97%)	93 (95%)	5 (5%)	0	100 100
37	2f	98/101 (97%)	95 (97%)	3 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
38	1g	153/156 (98%)	140 (92%)	11 (7%)	2 (1%)	9 14
38	2g	153/156 (98%)	136 (89%)	14 (9%)	3 (2%)	6 7
39	1h	135/138 (98%)	129 (96%)	5 (4%)	1 (1%)	18 28
39	2h	135/138 (98%)	127 (94%)	8 (6%)	0	100 100
40	1i	125/128 (98%)	112 (90%)	12 (10%)	1 (1%)	16 25
40	2i	125/128 (98%)	109 (87%)	14 (11%)	2 (2%)	7 11
41	1j	95/105 (90%)	83 (87%)	10 (10%)	2 (2%)	5 7
41	2j	94/105 (90%)	82 (87%)	9 (10%)	3 (3%)	3 3
42	1k	112/129 (87%)	103 (92%)	8 (7%)	1 (1%)	14 22
42	2k	112/129 (87%)	105 (94%)	5 (4%)	2 (2%)	6 9
43	1l	119/132 (90%)	112 (94%)	7 (6%)	0	100 100
43	2l	119/132 (90%)	111 (93%)	7 (6%)	1 (1%)	16 25
44	1m	121/126 (96%)	106 (88%)	13 (11%)	2 (2%)	7 10
44	2m	120/126 (95%)	107 (89%)	12 (10%)	1 (1%)	16 25
45	1n	58/61 (95%)	56 (97%)	2 (3%)	0	100 100
45	2n	58/61 (95%)	53 (91%)	4 (7%)	1 (2%)	7 10
46	1o	86/89 (97%)	81 (94%)	5 (6%)	0	100 100
46	2o	86/89 (97%)	82 (95%)	4 (5%)	0	100 100
47	1p	80/88 (91%)	74 (92%)	6 (8%)	0	100 100
47	2p	80/88 (91%)	75 (94%)	5 (6%)	0	100 100
48	1q	97/105 (92%)	91 (94%)	5 (5%)	1 (1%)	12 20
48	2q	97/105 (92%)	91 (94%)	5 (5%)	1 (1%)	12 20
49	1r	66/88 (75%)	60 (91%)	6 (9%)	0	100 100
49	2r	66/88 (75%)	62 (94%)	4 (6%)	0	100 100
50	1s	81/93 (87%)	71 (88%)	9 (11%)	1 (1%)	10 16
50	2s	81/93 (87%)	68 (84%)	13 (16%)	0	100 100
51	1t	94/106 (89%)	84 (89%)	6 (6%)	4 (4%)	2 1
51	2t	94/106 (89%)	85 (90%)	6 (6%)	3 (3%)	3 3
52	1u	21/27 (78%)	19 (90%)	2 (10%)	0	100 100
52	2u	21/27 (78%)	19 (90%)	2 (10%)	0	100 100
All	All	11370/12128 (94%)	10541 (93%)	723 (6%)	106 (1%)	14 22

5 of 106 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	1F	130	ALA
21	1Z	53	ILE
23	11	3	LYS
33	1b	22	LYS
33	1b	126	GLU

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%)	202 (94%)	13 (6%)	17 31
3	2D	215/218 (99%)	209 (97%)	6 (3%)	38 60
4	1E	164/166 (99%)	157 (96%)	7 (4%)	26 44
4	2E	164/166 (99%)	156 (95%)	8 (5%)	22 39
5	1F	160/166 (96%)	143 (89%)	17 (11%)	6 10
5	2F	159/166 (96%)	149 (94%)	10 (6%)	16 29
6	1G	143/156 (92%)	129 (90%)	14 (10%)	7 12
6	2G	143/156 (92%)	126 (88%)	17 (12%)	5 7
7	1H	144/148 (97%)	134 (93%)	10 (7%)	14 24
7	2H	144/148 (97%)	125 (87%)	19 (13%)	4 5
8	1I	113/124 (91%)	94 (83%)	19 (17%)	2 3
8	2I	105/124 (85%)	92 (88%)	13 (12%)	4 6
9	1N	118/119 (99%)	109 (92%)	9 (8%)	12 21
9	2N	118/119 (99%)	108 (92%)	10 (8%)	10 16
10	1O	100/100 (100%)	99 (99%)	1 (1%)	68 84
10	2O	100/100 (100%)	94 (94%)	6 (6%)	17 31
11	1P	115/116 (99%)	106 (92%)	9 (8%)	11 20
11	2P	115/116 (99%)	106 (92%)	9 (8%)	11 20
12	1Q	111/111 (100%)	103 (93%)	8 (7%)	13 23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
12	2Q	111/111 (100%)	105 (95%)	6 (5%)	20 35
13	1R	101/101 (100%)	94 (93%)	7 (7%)	14 24
13	2R	101/101 (100%)	97 (96%)	4 (4%)	28 47
14	1S	86/88 (98%)	79 (92%)	7 (8%)	11 18
14	2S	85/88 (97%)	79 (93%)	6 (7%)	13 23
15	1T	115/127 (91%)	107 (93%)	8 (7%)	14 24
15	2T	113/127 (89%)	107 (95%)	6 (5%)	20 36
16	1U	93/94 (99%)	86 (92%)	7 (8%)	12 21
16	2U	93/94 (99%)	90 (97%)	3 (3%)	34 56
17	1V	80/82 (98%)	77 (96%)	3 (4%)	29 49
17	2V	80/82 (98%)	73 (91%)	7 (9%)	9 15
18	1W	90/92 (98%)	85 (94%)	5 (6%)	19 33
18	2W	90/92 (98%)	86 (96%)	4 (4%)	25 43
19	1X	77/78 (99%)	73 (95%)	4 (5%)	21 36
19	2X	77/78 (99%)	74 (96%)	3 (4%)	28 48
20	1Y	85/91 (93%)	75 (88%)	10 (12%)	5 7
20	2Y	85/91 (93%)	79 (93%)	6 (7%)	13 23
21	1Z	135/179 (75%)	123 (91%)	12 (9%)	9 15
21	2Z	137/179 (76%)	121 (88%)	16 (12%)	5 7
22	10	65/67 (97%)	65 (100%)	0	100 100
22	20	65/67 (97%)	63 (97%)	2 (3%)	35 57
23	11	80/83 (96%)	77 (96%)	3 (4%)	29 49
23	21	80/83 (96%)	78 (98%)	2 (2%)	42 64
24	12	65/67 (97%)	61 (94%)	4 (6%)	16 29
24	22	65/67 (97%)	59 (91%)	6 (9%)	8 14
25	13	51/52 (98%)	48 (94%)	3 (6%)	18 31
25	23	50/52 (96%)	47 (94%)	3 (6%)	17 31
26	14	59/63 (94%)	55 (93%)	4 (7%)	14 25
26	24	53/63 (84%)	41 (77%)	12 (23%)	1 1
27	15	50/52 (96%)	48 (96%)	2 (4%)	28 47
27	25	50/52 (96%)	47 (94%)	3 (6%)	17 31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
28	16	51/52 (98%)	49 (96%)	2 (4%)	28 48
28	26	50/52 (96%)	43 (86%)	7 (14%)	3 4
29	17	41/42 (98%)	38 (93%)	3 (7%)	13 22
29	27	41/42 (98%)	38 (93%)	3 (7%)	13 22
30	18	54/55 (98%)	52 (96%)	2 (4%)	30 51
30	28	54/55 (98%)	52 (96%)	2 (4%)	30 51
31	19	34/34 (100%)	33 (97%)	1 (3%)	37 60
31	29	34/34 (100%)	33 (97%)	1 (3%)	37 60
33	1b	192/220 (87%)	168 (88%)	24 (12%)	4 6
33	2b	187/220 (85%)	164 (88%)	23 (12%)	4 6
34	1c	142/188 (76%)	129 (91%)	13 (9%)	8 14
34	2c	140/188 (74%)	126 (90%)	14 (10%)	7 11
35	1d	169/181 (93%)	147 (87%)	22 (13%)	4 5
35	2d	173/181 (96%)	157 (91%)	16 (9%)	8 14
36	1e	113/123 (92%)	101 (89%)	12 (11%)	6 10
36	2e	114/123 (93%)	102 (90%)	12 (10%)	6 10
37	1f	84/90 (93%)	78 (93%)	6 (7%)	13 23
37	2f	85/90 (94%)	76 (89%)	9 (11%)	6 10
38	1g	119/127 (94%)	106 (89%)	13 (11%)	6 9
38	2g	120/127 (94%)	109 (91%)	11 (9%)	8 14
39	1h	114/119 (96%)	106 (93%)	8 (7%)	14 24
39	2h	114/119 (96%)	106 (93%)	8 (7%)	14 24
40	1i	90/99 (91%)	80 (89%)	10 (11%)	6 9
40	2i	89/99 (90%)	78 (88%)	11 (12%)	4 6
41	1j	66/92 (72%)	55 (83%)	11 (17%)	2 3
41	2j	69/92 (75%)	59 (86%)	10 (14%)	3 4
42	1k	82/99 (83%)	74 (90%)	8 (10%)	7 12
42	2k	83/99 (84%)	79 (95%)	4 (5%)	23 40
43	1l	96/108 (89%)	92 (96%)	4 (4%)	26 45
43	2l	96/108 (89%)	90 (94%)	6 (6%)	16 29
44	1m	93/101 (92%)	82 (88%)	11 (12%)	5 7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
44	2m	92/101 (91%)	84 (91%)	8 (9%)	9 16
45	1n	49/50 (98%)	46 (94%)	3 (6%)	17 30
45	2n	49/50 (98%)	46 (94%)	3 (6%)	17 30
46	1o	78/80 (98%)	74 (95%)	4 (5%)	21 37
46	2o	78/80 (98%)	71 (91%)	7 (9%)	9 15
47	1p	69/74 (93%)	61 (88%)	8 (12%)	5 8
47	2p	68/74 (92%)	63 (93%)	5 (7%)	13 22
48	1q	94/97 (97%)	87 (93%)	7 (7%)	13 22
48	2q	94/97 (97%)	89 (95%)	5 (5%)	20 36
49	1r	59/77 (77%)	53 (90%)	6 (10%)	7 11
49	2r	59/77 (77%)	53 (90%)	6 (10%)	7 11
50	1s	69/80 (86%)	62 (90%)	7 (10%)	7 11
50	2s	67/80 (84%)	53 (79%)	14 (21%)	1 1
51	1t	70/82 (85%)	67 (96%)	3 (4%)	26 44
51	2t	70/82 (85%)	67 (96%)	3 (4%)	26 44
52	1u	18/22 (82%)	16 (89%)	2 (11%)	6 9
52	2u	18/22 (82%)	16 (89%)	2 (11%)	6 9
All	All	9303/10064 (92%)	8550 (92%)	753 (8%)	11 18

5 of 753 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	2O	91	LEU
30	28	14	VAL
12	2Q	22	LYS
10	2O	69	ILE
21	2Z	33	LEU

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

Mol	Chain	Res	Type
36	2e	73	ASN
50	2s	83	HIS
37	2f	100	ASN
41	2j	62	HIS

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Mol	Chain	Res	Type
38	1g	13	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2864/2915 (98%)	405 (14%)	30 (1%)
1	2A	2791/2915 (95%)	444 (15%)	26 (0%)
2	1B	119/121 (98%)	11 (9%)	0
2	2B	118/121 (97%)	21 (17%)	0
32	1a	1497/1521 (98%)	230 (15%)	0
32	2a	1501/1521 (98%)	253 (16%)	0
53	1v	12/24 (50%)	3 (25%)	0
53	2v	12/24 (50%)	3 (25%)	0
54	1w	71/76 (93%)	21 (29%)	0
54	2w	68/76 (89%)	22 (32%)	0
55	1x	75/77 (97%)	5 (6%)	0
55	2x	75/77 (97%)	5 (6%)	0
56	1y	72/76 (94%)	33 (45%)	0
56	2y	70/76 (92%)	25 (35%)	0
All	All	9345/9620 (97%)	1481 (15%)	56 (0%)

5 of 1481 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	12	U
1	1A	15	G
1	1A	34	C
1	1A	45	C
1	1A	55	G

5 of 56 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	2629	A
1	2A	2689	U
1	2A	528	A
1	2A	2439	A
1	2A	1992	G

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

88 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
32	PSU	2a	516	32	18,21,22	1.35	2 (11%)	21,30,33	2.03	3 (14%)
1	PSU	2A	2605	1	18,21,22	1.30	2 (11%)	21,30,33	2.04	3 (14%)
55	8AN	1x	76	57,63,55	21,24,25	1.51	4 (19%)	26,35,38	2.61	11 (42%)
1	5MC	2A	1942	1	19,22,23	1.59	3 (15%)	26,32,35	1.08	2 (7%)
56	MIA	2y	37	56	21,24,32	1.65	3 (14%)	30,35,47	2.02	7 (23%)
32	5MC	1a	1400	32	19,22,23	1.55	3 (15%)	26,32,35	1.16	3 (11%)
32	PSU	1a	516	32	18,21,22	1.36	2 (11%)	21,30,33	1.93	5 (23%)
1	PSU	2A	1911	1	18,21,22	1.38	2 (11%)	21,30,33	2.12	4 (19%)
54	PSU	1w	39	54	18,21,22	1.34	2 (11%)	21,30,33	2.08	4 (19%)
32	MA6	2a	1518	32	23,26,27	0.43	0	33,38,41	2.05	9 (27%)
43	0TD	2l	92	43	8,9,10	4.59	2 (25%)	6,11,13	2.49	1 (16%)
1	5MC	1A	1962	57,1	19,22,23	1.65	3 (15%)	26,32,35	1.15	3 (11%)
54	PSU	2w	39	54	18,21,22	1.38	2 (11%)	21,30,33	1.91	3 (14%)
1	OMG	1A	2251	57,1,55	23,26,27	1.23	3 (13%)	32,38,41	1.99	5 (15%)
54	PSU	1w	55	54	18,21,22	1.37	2 (11%)	21,30,33	2.05	3 (14%)
32	MA6	1a	1518	32	23,26,27	0.42	0	33,38,41	2.00	9 (27%)
32	2MG	1a	1207	32	23,26,27	1.24	3 (13%)	33,38,41	2.15	6 (18%)
55	8AN	2x	76	57,63,55	21,24,25	1.41	3 (14%)	26,35,38	2.28	10 (38%)
32	M2G	2a	966	32	24,27,28	1.26	3 (12%)	33,40,43	1.82	5 (15%)
32	5MC	1a	967	32	19,22,23	1.73	3 (15%)	26,32,35	1.19	3 (11%)
1	PSU	1A	2605	57,1	18,21,22	1.40	3 (16%)	21,30,33	2.06	5 (23%)
1	2MA	1A	2503	57,1	22,25,26	1.53	4 (18%)	32,37,40	2.26	6 (18%)
54	PSU	1w	32	54	18,21,22	1.39	3 (16%)	21,30,33	1.82	3 (14%)
1	OMC	2A	1920	1	19,22,23	0.82	0	25,31,34	0.96	1 (4%)
56	5MU	1y	54	56	19,22,23	1.49	4 (21%)	27,32,35	1.82	6 (22%)
32	5MC	1a	1404	32	19,22,23	1.70	3 (15%)	26,32,35	1.22	4 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
54	MIA	2w	37	54	24,27,32	2.05	6 (25%)	32,39,47	2.67	12 (37%)
54	PSU	2w	32	54	18,21,22	1.39	2 (11%)	21,30,33	1.84	3 (14%)
43	0TD	1l	92	43	8,9,10	4.68	1 (12%)	6,11,13	1.36	1 (16%)
56	PSU	1y	32	56	18,21,22	1.36	2 (11%)	21,30,33	1.95	3 (14%)
56	G7M	1y	46	56	23,26,27	1.53	4 (17%)	34,39,42	1.74	4 (11%)
32	MA6	1a	1519	32	23,26,27	0.43	0	33,38,41	2.04	9 (27%)
32	UR3	2a	1498	32	19,22,23	1.02	2 (10%)	26,32,35	1.73	3 (11%)
56	4SU	1y	8	56	18,21,22	1.78	6 (33%)	25,30,33	1.83	5 (20%)
32	M2G	1a	966	32	24,27,28	1.32	3 (12%)	33,40,43	1.89	6 (18%)
55	PSU	2x	55	55	18,21,22	1.37	2 (11%)	21,30,33	1.93	5 (23%)
55	5MC	2x	32	55	19,22,23	1.63	3 (15%)	26,32,35	1.27	3 (11%)
32	4OC	2a	1402	32	20,23,24	0.78	0	25,32,35	0.99	1 (4%)
32	5MC	2a	1407	32	19,22,23	1.66	3 (15%)	26,32,35	1.20	3 (11%)
54	G7M	2w	46	54	23,26,27	1.49	4 (17%)	34,39,42	1.73	6 (17%)
1	PSU	2A	1917	1	18,21,22	1.35	2 (11%)	21,30,33	2.05	4 (19%)
32	G7M	2a	527	57,32	23,26,27	1.48	4 (17%)	34,39,42	1.72	5 (14%)
1	OMG	2A	2251	57,1,55	23,26,27	1.22	3 (13%)	32,38,41	1.94	6 (18%)
1	OMU	1A	2552	57,1	19,22,23	1.11	2 (10%)	25,31,34	1.94	5 (20%)
56	PSU	2y	39	56	18,21,22	1.44	2 (11%)	21,30,33	1.68	3 (14%)
1	5MU	2A	1939	57,1	19,22,23	1.44	6 (31%)	27,32,35	2.28	6 (22%)
56	PSU	2y	32	56	18,21,22	1.36	2 (11%)	21,30,33	1.99	3 (14%)
54	5MU	1w	54	54	19,22,23	1.48	5 (26%)	27,32,35	1.88	6 (22%)
56	G7M	2y	46	56	23,26,27	1.63	5 (21%)	34,39,42	1.98	5 (14%)
56	PSU	1y	39	56	18,21,22	1.43	2 (11%)	21,30,33	1.86	4 (19%)
1	OMU	2A	2552	57,1	19,22,23	1.07	1 (5%)	25,31,34	1.90	5 (20%)
54	4SU	2w	8	54	18,21,22	1.70	3 (16%)	25,30,33	2.50	5 (20%)
1	2MA	2A	2503	57,1	22,25,26	1.51	4 (18%)	32,37,40	2.43	8 (25%)
54	MIA	1w	37	54	28,31,32	2.25	6 (21%)	38,44,47	2.80	13 (34%)
54	8AN	1w	76	62,1,54	21,24,25	1.45	3 (14%)	26,35,38	2.14	9 (34%)
55	4SU	1x	8	55	18,21,22	2.25	6 (33%)	25,30,33	1.70	7 (28%)
54	4SU	1w	8	54	18,21,22	1.80	4 (22%)	25,30,33	1.96	4 (16%)
32	5MC	1a	1407	32	19,22,23	1.52	3 (15%)	26,32,35	1.13	3 (11%)
1	5MU	1A	1915	1	19,22,23	1.35	5 (26%)	27,32,35	2.22	8 (29%)
1	5MC	1A	1942	1	19,22,23	1.86	3 (15%)	26,32,35	1.23	3 (11%)
56	PSU	1y	55	56	18,21,22	1.38	2 (11%)	21,30,33	2.08	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
54	8AN	2w	76	62,1,54	21,24,25	1.49	4 (19%)	26,35,38	2.13	9 (34%)
1	5MU	2A	1915	1	19,22,23	1.44	4 (21%)	27,32,35	2.11	6 (22%)
32	2MG	2a	1207	32	23,26,27	1.24	2 (8%)	33,38,41	2.29	7 (21%)
1	PSU	1A	1911	1	18,21,22	1.40	2 (11%)	21,30,33	2.03	5 (23%)
54	PSU	2w	55	54	18,21,22	1.38	2 (11%)	21,30,33	2.03	3 (14%)
55	5MU	2x	54	55	19,22,23	1.42	5 (26%)	27,32,35	2.14	6 (22%)
32	5MC	2a	967	32	19,22,23	1.66	3 (15%)	26,32,35	1.11	2 (7%)
32	MA6	2a	1519	32	23,26,27	0.44	0	33,38,41	2.15	8 (24%)
1	PSU	1A	1917	1	18,21,22	1.32	2 (11%)	21,30,33	2.03	4 (19%)
1	5MC	2A	1962	1	19,22,23	1.69	3 (15%)	26,32,35	1.13	2 (7%)
1	5MU	1A	1939	57,1	19,22,23	1.55	6 (31%)	27,32,35	1.98	7 (25%)
32	5MC	2a	1404	32	19,22,23	1.73	3 (15%)	26,32,35	1.12	2 (7%)
32	G7M	1a	527	57,32	23,26,27	1.55	4 (17%)	34,39,42	1.67	5 (14%)
54	5MU	2w	54	54	19,22,23	1.36	5 (26%)	27,32,35	1.86	7 (25%)
54	G7M	1w	46	54	23,26,27	1.55	4 (17%)	34,39,42	1.63	4 (11%)
56	5MU	2y	54	56	19,22,23	1.44	4 (21%)	27,32,35	1.77	5 (18%)
55	4SU	2x	8	57,55	18,21,22	2.10	6 (33%)	25,30,33	1.38	6 (24%)
55	5MC	1x	32	57,55	19,22,23	1.70	3 (15%)	26,32,35	1.23	3 (11%)
32	UR3	1a	1498	32	19,22,23	0.94	0	26,32,35	1.83	3 (11%)
56	MIA	1y	37	56	21,24,32	1.64	4 (19%)	30,35,47	2.02	7 (23%)
56	PSU	2y	55	56	18,21,22	1.43	3 (16%)	21,30,33	2.01	4 (19%)
32	4OC	1a	1402	32	20,23,24	0.74	0	25,32,35	1.00	1 (4%)
56	4SU	2y	8	56	18,21,22	1.72	4 (22%)	25,30,33	2.38	5 (20%)
55	PSU	1x	55	55	18,21,22	1.35	2 (11%)	21,30,33	2.00	4 (19%)
32	5MC	2a	1400	32	19,22,23	1.71	3 (15%)	26,32,35	1.20	3 (11%)
1	OMC	1A	1920	1	19,22,23	0.78	0	25,31,34	0.91	1 (4%)
55	5MU	1x	54	57,55	19,22,23	1.43	5 (26%)	27,32,35	1.98	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
32	PSU	2a	516	32	-	0/7/25/26	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	8AN	1x	76	57,63,55	-	3/7/25/26	0/3/3/3
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
56	MIA	2y	37	56	-	3/7/25/34	0/3/3/3
32	5MC	1a	1400	32	-	0/7/25/26	0/2/2/2
32	PSU	1a	516	32	-	0/7/25/26	0/2/2/2
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
54	PSU	1w	39	54	-	0/7/25/26	0/2/2/2
32	MA6	2a	1518	32	-	0/11/29/30	0/3/3/3
43	0TD	2l	92	43	-	2/7/12/14	-
1	5MC	1A	1962	57,1	-	0/7/25/26	0/2/2/2
54	PSU	2w	39	54	-	0/7/25/26	0/2/2/2
1	OMG	1A	2251	57,1,55	-	0/9/27/28	0/3/3/3
54	PSU	1w	55	54	-	0/7/25/26	0/2/2/2
32	MA6	1a	1518	32	-	0/11/29/30	0/3/3/3
32	2MG	1a	1207	32	-	0/9/27/28	0/3/3/3
55	8AN	2x	76	57,63,55	-	3/7/25/26	0/3/3/3
32	M2G	2a	966	32	-	0/11/29/30	0/3/3/3
32	5MC	1a	967	32	-	0/7/25/26	0/2/2/2
1	PSU	1A	2605	57,1	-	0/7/25/26	0/2/2/2
1	2MA	1A	2503	57,1	-	1/7/25/26	0/3/3/3
54	PSU	1w	32	54	-	0/7/25/26	0/2/2/2
1	OMC	2A	1920	1	-	0/9/27/28	0/2/2/2
56	5MU	1y	54	56	-	0/7/25/26	0/2/2/2
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
54	MIA	2w	37	54	-	2/11/29/34	0/3/3/3
54	PSU	2w	32	54	-	0/7/25/26	0/2/2/2
43	0TD	1l	92	43	-	2/7/12/14	-
56	PSU	1y	32	56	-	0/7/25/26	0/2/2/2
56	G7M	1y	46	56	-	1/7/25/26	0/3/3/3
32	MA6	1a	1519	32	-	3/11/29/30	0/3/3/3
32	UR3	2a	1498	32	-	0/7/25/26	0/2/2/2
56	4SU	1y	8	56	-	3/7/25/26	0/2/2/2
32	M2G	1a	966	32	-	0/11/29/30	0/3/3/3
55	PSU	2x	55	55	-	0/7/25/26	0/2/2/2
55	5MC	2x	32	55	-	0/7/25/26	0/2/2/2
32	4OC	2a	1402	32	-	1/9/29/30	0/2/2/2
32	5MC	2a	1407	32	-	0/7/25/26	0/2/2/2
54	G7M	2w	46	54	-	3/7/25/26	0/3/3/3
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
32	G7M	2a	527	57,32	-	3/7/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMG	2A	2251	57,1,55	-	0/9/27/28	0/3/3/3
1	OMU	1A	2552	57,1	-	0/9/27/28	0/2/2/2
56	PSU	2y	39	56	-	0/7/25/26	0/2/2/2
1	5MU	2A	1939	57,1	-	0/7/25/26	0/2/2/2
56	PSU	2y	32	56	-	0/7/25/26	0/2/2/2
54	5MU	1w	54	54	-	0/7/25/26	0/2/2/2
56	G7M	2y	46	56	-	2/7/25/26	0/3/3/3
56	PSU	1y	39	56	-	0/7/25/26	0/2/2/2
1	OMU	2A	2552	57,1	-	0/9/27/28	0/2/2/2
54	4SU	2w	8	54	-	0/7/25/26	0/2/2/2
1	2MA	2A	2503	57,1	-	2/7/25/26	0/3/3/3
54	MIA	1w	37	54	-	1/15/33/34	0/3/3/3
54	8AN	1w	76	62,1,54	-	0/7/25/26	0/3/3/3
55	4SU	1x	8	55	-	0/7/25/26	0/2/2/2
54	4SU	1w	8	54	-	0/7/25/26	0/2/2/2
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
1	5MU	1A	1915	1	-	1/7/25/26	0/2/2/2
1	5MC	1A	1942	1	-	0/7/25/26	0/2/2/2
56	PSU	1y	55	56	-	1/7/25/26	0/2/2/2
54	8AN	2w	76	62,1,54	-	0/7/25/26	0/3/3/3
1	5MU	2A	1915	1	-	0/7/25/26	0/2/2/2
32	2MG	2a	1207	32	-	0/9/27/28	0/3/3/3
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
54	PSU	2w	55	54	-	0/7/25/26	0/2/2/2
55	5MU	2x	54	55	-	0/7/25/26	0/2/2/2
32	5MC	2a	967	32	-	0/7/25/26	0/2/2/2
32	MA6	2a	1519	32	-	3/11/29/30	0/3/3/3
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
1	5MC	2A	1962	1	-	0/7/25/26	0/2/2/2
1	5MU	1A	1939	57,1	-	0/7/25/26	0/2/2/2
32	5MC	2a	1404	32	-	0/7/25/26	0/2/2/2
32	G7M	1a	527	57,32	-	3/7/25/26	0/3/3/3
54	5MU	2w	54	54	-	0/7/25/26	0/2/2/2
54	G7M	1w	46	54	-	1/7/25/26	0/3/3/3
56	5MU	2y	54	56	-	0/7/25/26	0/2/2/2
55	4SU	2x	8	57,55	-	0/7/25/26	0/2/2/2
55	5MC	1x	32	57,55	-	0/7/25/26	0/2/2/2
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
56	MIA	1y	37	56	-	2/7/25/34	0/3/3/3
56	PSU	2y	55	56	-	2/7/25/26	0/2/2/2
32	4OC	1a	1402	32	-	1/9/29/30	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	4SU	2y	8	56	-	1/7/25/26	0/2/2/2
55	PSU	1x	55	55	-	0/7/25/26	0/2/2/2
32	5MC	2a	1400	32	-	0/7/25/26	0/2/2/2
1	OMC	1A	1920	1	-	1/9/27/28	0/2/2/2
55	5MU	1x	54	57,55	-	0/7/25/26	0/2/2/2

The worst 5 of 258 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	1l	92	0TD	CB-SB	-12.72	1.69	1.82
43	2l	92	0TD	CB-SB	-12.44	1.69	1.82
1	1A	1942	5MC	C5-C4	7.05	1.49	1.44
54	1w	37	MIA	C13-C14	6.81	1.52	1.32
32	1a	967	5MC	C5-C4	6.47	1.49	1.44

The worst 5 of 429 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	2w	37	MIA	C5-C4-N3	-9.25	117.44	127.18
54	1w	37	MIA	C12-C13-C14	-9.04	110.78	127.01
1	2A	2503	2MA	C5-C4-N3	-8.48	118.24	127.18
1	1A	2503	2MA	C5-C4-N3	-8.18	118.56	127.18
54	1w	37	MIA	C5-C4-N3	-8.09	118.66	127.18

There are no chirality outliers.

5 of 51 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
54	1w	37	MIA	C12-C13-C14-C16
56	1y	46	G7M	C4'-C5'-O5'-P
55	2x	76	8AN	O4'-C4'-C5'-O5'
55	2x	76	8AN	C3'-C4'-C5'-O5'
56	2y	55	PSU	C2'-C1'-C5-C4

There are no ring outliers.

28 monomers are involved in 40 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
55	1x	76	8AN	1	0
56	2y	37	MIA	1	0
32	2a	1518	MA6	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	1a	1518	MA6	1	0
55	2x	76	8AN	2	0
32	1a	967	5MC	1	0
43	1l	92	0TD	2	0
56	1y	46	G7M	2	0
32	1a	1519	MA6	1	0
56	1y	8	4SU	1	0
32	1a	966	M2G	1	0
32	2a	1402	4OC	1	0
54	2w	46	G7M	1	0
1	2A	2251	OMG	1	0
54	1w	54	5MU	1	0
56	2y	46	G7M	3	0
56	1y	39	PSU	1	0
55	1x	8	4SU	2	0
54	1w	8	4SU	1	0
56	1y	55	PSU	1	0
54	2w	76	8AN	1	0
1	2A	1915	5MU	1	0
32	2a	967	5MC	1	0
32	2a	1519	MA6	2	0
56	1y	37	MIA	2	0
56	2y	55	PSU	5	0
32	1a	1402	4OC	1	0
56	2y	8	4SU	4	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2777 ligands modelled in this entry, 2769 are monoatomic - leaving 8 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	$\#\|Z\|>2$
61	SF4	2d	302	35	0,12,12	-	-	-		
62	PHE	2w	108	54	10,11,12	1.56	1 (10%)	8,13,15	0.52	0
63	FME	1x	115	55	8,9,10	0.50	0	8,9,11	1.50	2 (25%)
62	PHE	1w	110	54	10,11,12	1.48	1 (10%)	8,13,15	0.54	0
63	FME	2x	108	55	8,9,10	0.44	0	8,9,11	1.32	2 (25%)
59	A1AEZ	1A	4118	57	90,91,91	2.45	18 (20%)	126,132,132	2.05	31 (24%)
61	SF4	1d	501	35	0,12,12	-	-	-		
59	A1AEZ	2A	3843	57	90,91,91	2.39	16 (17%)	126,132,132	2.22	32 (25%)

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
63	FME	1x	115	55	-	2/7/9/11	-
62	PHE	2w	108	54	-	2/5/6/8	0/1/1/1
61	SF4	2d	302	35	-	-	0/6/5/5
62	PHE	1w	110	54	-	0/5/6/8	0/1/1/1
63	FME	2x	108	55	-	0/7/9/11	-
59	A1AEZ	1A	4118	57	-	18/98/132/132	0/7/7/7
61	SF4	1d	501	35	-	-	0/6/5/5
59	A1AEZ	2A	3843	57	-	16/98/132/132	0/7/7/7

The worst 5 of 36 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	2A	3843	A1AEZ	CAG-CAF	-12.87	1.41	1.53
59	1A	4118	A1AEZ	CAG-CAF	-11.84	1.42	1.53
59	2A	3843	A1AEZ	CBU-CBT	8.71	1.30	1.19
59	1A	4118	A1AEZ	OBR-NBJ	8.19	1.56	1.42
59	1A	4118	A1AEZ	CBU-CBT	7.52	1.29	1.19

The worst 5 of 67 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
59	2A	3843	A1AEZ	CAB-CAF-NBJ	-11.32	117.86	126.21
59	2A	3843	A1AEZ	CCT-NCY-CCZ	9.62	129.90	119.88
59	1A	4118	A1AEZ	CCT-NCY-CCZ	9.59	129.87	119.88
59	1A	4118	A1AEZ	CAB-CAF-NBJ	-9.02	119.56	126.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
59	2A	3843	A1AEZ	CCZ-NCY-CCX	-5.92	111.06	119.74

There are no chirality outliers.

5 of 38 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
59	1A	4118	A1AEZ	OBR-CBS-CBT-CBU
59	1A	4118	A1AEZ	CBT-CBS-OBR-NBJ
59	1A	4118	A1AEZ	CDB-CCZ-NCY-CCT
59	1A	4118	A1AEZ	CDB-CCZ-NCY-CCX
59	2A	3843	A1AEZ	OBR-CBS-CBT-CBU

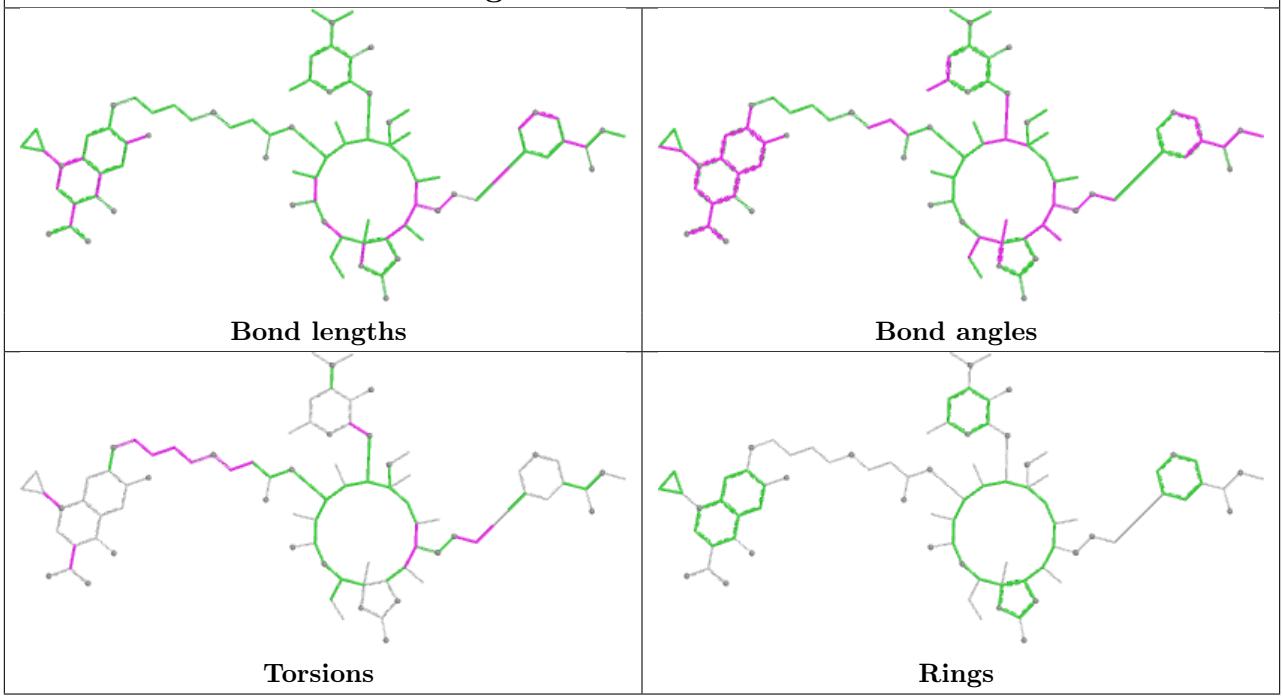
There are no ring outliers.

3 monomers are involved in 4 short contacts:

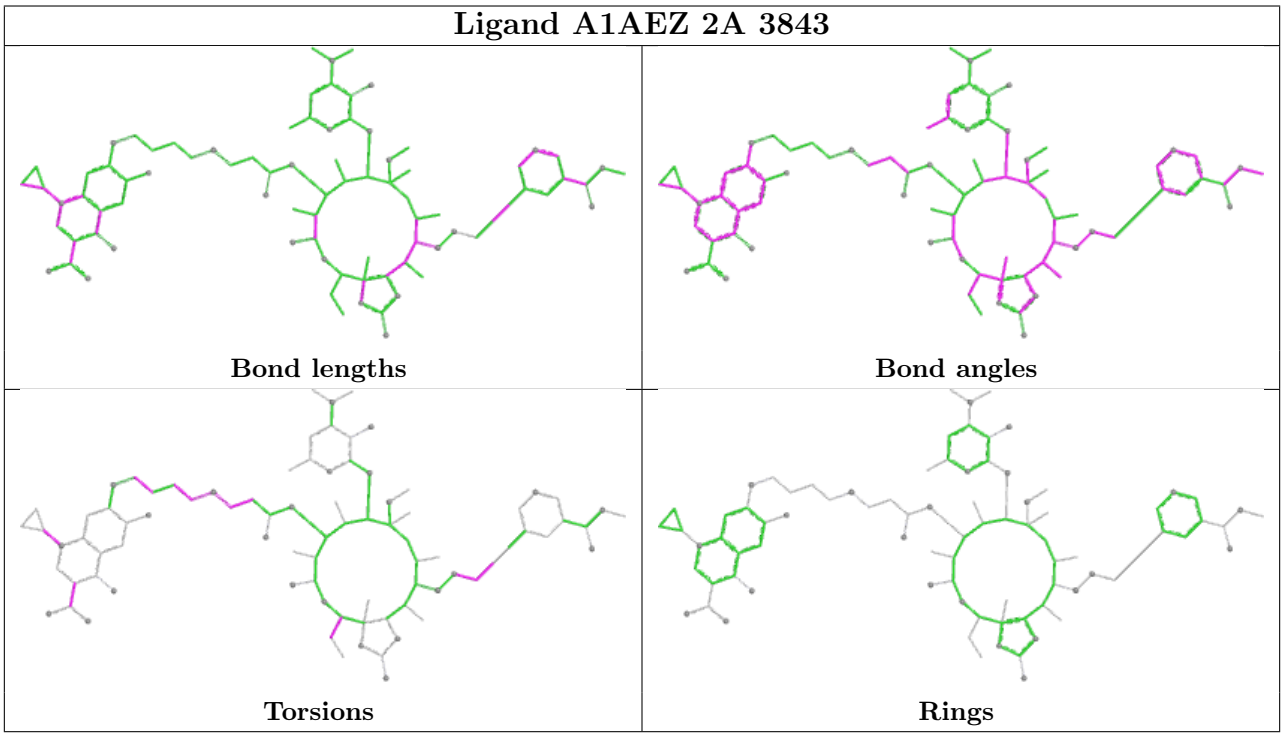
Mol	Chain	Res	Type	Clashes	Symm-Clashes
62	2w	108	PHE	1	0
59	1A	4118	A1AEZ	2	0
59	2A	3843	A1AEZ	1	0

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 A1AEZ 1A 4118



Ligand A1AEZ 2A 3843



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues

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%)	-0.55	174 (6%) 27 23	16, 32, 83, 94	0
1	2A	2789/2915 (95%)	-0.08	147 (5%) 32 28	29, 50, 81, 93	0
2	1B	120/121 (99%)	-0.42	0 100 100	26, 44, 57, 75	0
2	2B	120/121 (99%)	0.47	3 (2%) 58 54	52, 64, 71, 81	0
3	1D	275/276 (99%)	-0.25	3 (1%) 78 74	17, 33, 46, 68	0
3	2D	275/276 (99%)	0.15	4 (1%) 72 68	27, 43, 54, 72	0
4	1E	204/206 (99%)	-0.21	2 (0%) 79 76	17, 35, 55, 63	0
4	2E	204/206 (99%)	0.37	5 (2%) 58 54	30, 52, 63, 71	0
5	1F	203/210 (96%)	-0.13	2 (0%) 79 76	16, 38, 60, 72	0
5	2F	203/210 (96%)	0.47	3 (1%) 72 68	30, 58, 70, 77	0
6	1G	181/182 (99%)	0.42	7 (3%) 43 39	36, 51, 64, 76	0
6	2G	181/182 (99%)	0.97	13 (7%) 21 18	53, 65, 73, 77	0
7	1H	174/180 (96%)	0.28	5 (2%) 53 50	35, 47, 59, 64	0
7	2H	174/180 (96%)	1.52	47 (27%) 1 1	62, 72, 78, 82	0
8	1I	146/148 (98%)	0.83	6 (4%) 41 37	42, 63, 71, 75	0
8	2I	146/148 (98%)	1.01	10 (6%) 23 20	49, 63, 72, 75	0
9	1N	140/140 (100%)	-0.17	2 (1%) 73 69	22, 35, 53, 61	0
9	2N	140/140 (100%)	0.71	4 (2%) 53 50	41, 56, 68, 74	0
10	1O	122/122 (100%)	-0.12	2 (1%) 70 66	23, 36, 52, 57	0
10	2O	122/122 (100%)	0.36	0 100 100	42, 52, 62, 65	0
11	1P	149/150 (99%)	0.04	2 (1%) 75 71	16, 41, 59, 64	0
11	2P	149/150 (99%)	0.62	5 (3%) 48 44	32, 58, 70, 77	0
12	1Q	141/141 (100%)	-0.17	0 100 100	21, 36, 50, 64	0
12	2Q	141/141 (100%)	0.86	9 (6%) 25 22	40, 56, 66, 69	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	1R	118/118 (100%)	-0.39	0 100 100	23, 30, 44, 51	0
13	2R	118/118 (100%)	0.16	1 (0%) 82 80	34, 46, 55, 63	0
14	1S	110/112 (98%)	0.11	0 100 100	31, 43, 55, 59	0
14	2S	110/112 (98%)	0.93	3 (2%) 56 52	52, 61, 68, 74	0
15	1T	131/146 (89%)	0.07	2 (1%) 72 68	29, 40, 60, 69	0
15	2T	131/146 (89%)	0.46	2 (1%) 72 68	43, 54, 66, 70	0
16	1U	116/118 (98%)	-0.46	0 100 100	18, 27, 43, 57	0
16	2U	116/118 (98%)	0.54	3 (2%) 57 53	37, 52, 64, 69	0
17	1V	101/101 (100%)	-0.28	1 (0%) 79 76	18, 34, 50, 58	0
17	2V	101/101 (100%)	0.71	0 100 100	38, 60, 66, 71	0
18	1W	112/113 (99%)	-0.41	1 (0%) 81 78	20, 28, 46, 72	0
18	2W	112/113 (99%)	0.10	1 (0%) 81 78	36, 43, 58, 76	0
19	1X	95/96 (98%)	-0.12	2 (2%) 63 59	23, 34, 59, 73	0
19	2X	95/96 (98%)	0.58	3 (3%) 50 46	39, 51, 66, 76	0
20	1Y	107/110 (97%)	0.22	2 (1%) 66 62	33, 44, 58, 66	0
20	2Y	107/110 (97%)	1.19	12 (11%) 10 7	51, 62, 71, 76	0
21	1Z	154/206 (74%)	0.90	20 (12%) 7 5	34, 56, 72, 78	0
21	2Z	160/206 (77%)	1.48	38 (23%) 2 1	56, 69, 77, 83	0
22	10	83/85 (97%)	-0.13	1 (1%) 76 73	24, 32, 43, 61	0
22	20	83/85 (97%)	0.59	1 (1%) 76 73	38, 52, 60, 74	0
23	11	97/98 (98%)	0.16	1 (1%) 79 76	26, 41, 63, 66	0
23	21	97/98 (98%)	0.43	2 (2%) 63 59	33, 49, 64, 68	0
24	12	70/72 (97%)	0.09	0 100 100	29, 42, 54, 62	0
24	22	70/72 (97%)	0.66	2 (2%) 53 50	49, 60, 68, 72	0
25	13	59/60 (98%)	-0.29	0 100 100	19, 30, 55, 70	0
25	23	59/60 (98%)	0.47	2 (3%) 48 44	47, 55, 65, 74	0
26	14	69/71 (97%)	1.04	14 (20%) 3 2	43, 65, 76, 79	0
26	24	69/71 (97%)	1.50	18 (26%) 1 1	62, 71, 79, 81	0
27	15	59/60 (98%)	-0.39	1 (1%) 69 65	17, 30, 50, 58	0
27	25	59/60 (98%)	0.12	2 (3%) 48 44	30, 46, 60, 72	0
28	16	53/54 (98%)	-0.17	1 (1%) 66 62	28, 38, 49, 55	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
28	26	53/54 (98%)	0.52	0 100 100	44, 52, 60, 62	0
29	17	48/49 (97%)	-0.27	3 (6%) 26 22	17, 24, 50, 57	0
29	27	48/49 (97%)	0.07	4 (8%) 17 14	27, 36, 61, 65	0
30	18	64/65 (98%)	-0.45	0 100 100	22, 29, 36, 53	0
30	28	64/65 (98%)	0.44	0 100 100	41, 47, 53, 59	0
31	19	37/37 (100%)	-0.19	0 100 100	24, 35, 44, 54	0
31	29	37/37 (100%)	0.96	2 (5%) 31 28	50, 59, 68, 71	0
32	1a	1488/1521 (97%)	0.21	67 (4%) 38 34	31, 57, 80, 94	0
32	2a	1491/1521 (98%)	0.48	70 (4%) 36 32	42, 65, 81, 92	0
33	1b	231/256 (90%)	1.33	51 (22%) 2 2	55, 66, 75, 79	0
33	2b	231/256 (90%)	1.52	56 (24%) 2 1	60, 71, 76, 81	0
34	1c	206/239 (86%)	0.91	14 (6%) 23 20	50, 62, 70, 75	0
34	2c	206/239 (86%)	1.56	47 (22%) 2 1	62, 70, 76, 78	0
35	1d	208/209 (99%)	1.04	25 (12%) 9 6	49, 61, 69, 72	0
35	2d	208/209 (99%)	0.79	8 (3%) 44 40	50, 60, 67, 73	0
36	1e	148/162 (91%)	0.65	3 (2%) 65 60	44, 55, 64, 71	0
36	2e	148/162 (91%)	0.98	7 (4%) 36 32	53, 64, 70, 76	0
37	1f	100/101 (99%)	0.65	0 100 100	47, 58, 66, 69	0
37	2f	100/101 (99%)	0.66	2 (2%) 65 60	49, 58, 66, 72	0
38	1g	155/156 (99%)	0.83	13 (8%) 17 14	53, 62, 73, 77	0
38	2g	155/156 (99%)	1.31	21 (13%) 7 5	61, 68, 76, 82	0
39	1h	137/138 (99%)	0.51	2 (1%) 72 68	47, 57, 62, 68	0
39	2h	137/138 (99%)	0.94	6 (4%) 39 34	56, 64, 69, 72	0
40	1i	127/128 (99%)	1.34	30 (23%) 2 1	48, 66, 73, 74	0
40	2i	127/128 (99%)	1.73	36 (28%) 1 1	60, 71, 76, 79	0
41	1j	97/105 (92%)	1.36	13 (13%) 7 5	51, 66, 76, 77	0
41	2j	96/105 (91%)	2.14	48 (50%) 0 0	63, 72, 78, 80	0
42	1k	114/129 (88%)	0.60	4 (3%) 47 43	37, 58, 67, 69	0
42	2k	114/129 (88%)	0.79	5 (4%) 39 34	46, 63, 71, 73	0
43	1l	121/132 (91%)	0.20	3 (2%) 58 54	37, 46, 56, 65	0
43	2l	121/132 (91%)	0.61	2 (1%) 69 65	50, 56, 63, 70	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
44	1m	123/126 (97%)	0.86	12 (9%) 13 10	48, 60, 68, 73	0
44	2m	122/126 (96%)	1.72	35 (28%) 1 1	60, 69, 73, 78	0
45	1n	60/61 (98%)	0.92	2 (3%) 49 45	53, 58, 65, 66	0
45	2n	60/61 (98%)	2.06	29 (48%) 0 0	63, 70, 74, 76	0
46	1o	88/89 (98%)	0.62	4 (4%) 38 34	40, 56, 63, 69	0
46	2o	88/89 (98%)	0.70	3 (3%) 48 44	50, 60, 68, 73	0
47	1p	82/88 (93%)	1.38	12 (14%) 6 4	49, 60, 67, 74	0
47	2p	82/88 (93%)	1.03	6 (7%) 21 17	53, 60, 68, 70	0
48	1q	99/105 (94%)	0.84	5 (5%) 33 30	47, 58, 66, 70	0
48	2q	99/105 (94%)	0.72	4 (4%) 42 38	55, 62, 70, 73	0
49	1r	68/88 (77%)	0.61	5 (7%) 20 17	49, 59, 67, 71	0
49	2r	68/88 (77%)	0.63	2 (2%) 53 50	52, 60, 69, 72	0
50	1s	83/93 (89%)	0.92	5 (6%) 27 24	53, 61, 70, 74	0
50	2s	83/93 (89%)	1.65	25 (30%) 1 1	63, 71, 75, 79	0
51	1t	96/106 (90%)	1.01	8 (8%) 17 14	51, 61, 68, 71	0
51	2t	96/106 (90%)	1.07	10 (10%) 11 9	53, 60, 70, 72	0
52	1u	23/27 (85%)	1.17	2 (8%) 16 13	54, 57, 64, 64	0
52	2u	23/27 (85%)	1.94	11 (47%) 0 0	63, 67, 71, 76	0
53	1v	13/24 (54%)	0.82	3 (23%) 2 1	42, 47, 81, 87	0
53	2v	13/24 (54%)	1.21	3 (23%) 2 1	55, 60, 84, 89	0
54	1w	66/76 (86%)	0.86	7 (10%) 11 8	23, 69, 77, 85	0
54	2w	64/76 (84%)	1.09	8 (12%) 8 6	39, 77, 83, 86	0
55	1x	72/77 (93%)	0.12	3 (4%) 40 36	22, 54, 71, 77	0
55	2x	72/77 (93%)	0.33	1 (1%) 73 69	35, 64, 75, 83	0
56	1y	67/76 (88%)	2.30	46 (68%) 0 0	56, 86, 89, 90	0
56	2y	66/76 (86%)	2.28	46 (69%) 0 0	65, 87, 90, 91	0
All	All	20873/21748 (95%)	0.34	1430 (6%) 23 19	16, 55, 76, 94	0

The worst 5 of 1430 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
44	2m	123	ALA	12.0
45	1n	2	ALA	7.5

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Mol	Chain	Res	Type	RSRZ
44	2m	122	LYS	7.4
44	2m	124	PRO	7.2
1	1A	2174	C	6.5

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	PSU	1y	55	20/21	0.41	0.19	84,88,95,104	0
56	MIA	2y	37	22/30	0.43	0.18	78,86,97,113	0
56	G7M	2y	46	24/25	0.45	0.18	78,86,88,102	0
56	5MU	1y	54	21/22	0.47	0.18	79,85,91,102	0
56	G7M	1y	46	24/25	0.50	0.20	78,84,88,98	0
56	4SU	2y	8	20/21	0.51	0.19	83,92,98,108	0
56	MIA	1y	37	22/30	0.52	0.19	79,83,92,104	0
56	PSU	2y	55	20/21	0.52	0.16	78,83,93,106	0
56	PSU	2y	39	20/21	0.53	0.18	78,83,94,102	0
56	5MU	2y	54	21/22	0.55	0.18	72,81,94,108	0
56	4SU	1y	8	20/21	0.62	0.16	80,87,95,105	0
56	PSU	2y	32	20/21	0.68	0.15	74,80,88,108	0
56	PSU	1y	39	20/21	0.68	0.17	75,83,89,91	0
56	PSU	1y	32	20/21	0.69	0.16	76,83,91,102	0
54	G7M	2w	46	24/25	0.70	0.16	73,80,92,107	0
54	G7M	1w	46	24/25	0.70	0.17	62,70,91,106	0
54	PSU	2w	55	20/21	0.84	0.12	67,71,77,81	0
54	MIA	2w	37	25/30	0.87	0.14	55,63,68,93	0
54	4SU	2w	8	20/21	0.87	0.13	72,77,85,92	0
55	4SU	2x	8	20/21	0.89	0.14	62,68,71,75	0
32	2MG	2a	1207	24/25	0.89	0.12	61,70,73,77	0
55	PSU	2x	55	20/21	0.90	0.10	62,65,71,74	0
54	4SU	1w	8	20/21	0.90	0.13	63,67,72,75	0
54	5MU	2w	54	21/22	0.90	0.11	57,62,68,70	0
55	5MU	2x	54	21/22	0.90	0.12	63,67,71,72	0
55	5MU	1x	54	21/22	0.91	0.11	54,60,68,73	0
32	G7M	2a	527	24/25	0.91	0.13	51,57,62,63	0
55	PSU	1x	55	20/21	0.91	0.10	47,57,71,71	0
43	0TD	2l	92	10/11	0.91	0.12	55,57,63,70	0
55	5MC	2x	32	21/22	0.91	0.14	58,63,65,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MIA	1w	37	29/30	0.91	0.14	32,46,60,87	0
43	0TD	1l	92	10/11	0.91	0.11	43,47,50,67	0
54	PSU	1w	55	20/21	0.92	0.10	48,57,66,67	0
1	5MU	2A	1915	21/22	0.92	0.11	50,56,59,59	0
54	PSU	2w	32	20/21	0.92	0.10	59,67,76,76	0
32	5MC	2a	1400	21/22	0.93	0.13	56,59,65,69	0
32	5MC	2a	1404	21/22	0.93	0.11	44,50,53,54	0
54	PSU	1w	32	20/21	0.93	0.10	46,53,59,60	0
32	M2G	2a	966	25/26	0.93	0.13	51,59,70,72	0
32	2MG	1a	1207	24/25	0.93	0.10	49,56,61,63	0
32	4OC	2a	1402	22/23	0.94	0.11	49,54,56,59	0
1	PSU	2A	1917	20/21	0.94	0.09	47,54,59,62	0
32	5MC	2a	967	21/22	0.94	0.12	52,59,66,68	0
32	PSU	2a	516	20/21	0.94	0.10	54,61,66,67	0
55	4SU	1x	8	20/21	0.94	0.10	50,56,62,63	0
32	M2G	1a	966	25/26	0.95	0.10	39,45,50,54	0
54	PSU	2w	39	20/21	0.95	0.09	59,67,72,72	0
1	PSU	2A	1911	20/21	0.95	0.08	48,50,54,56	0
55	5MC	1x	32	21/22	0.95	0.10	43,48,54,59	0
1	5MU	1A	1915	21/22	0.96	0.09	40,46,50,52	0
32	5MC	1a	967	21/22	0.96	0.10	42,47,53,55	0
54	PSU	1w	39	20/21	0.96	0.08	47,53,59,65	0
32	5MC	2a	1407	21/22	0.96	0.09	36,46,56,56	0
32	UR3	2a	1498	21/22	0.96	0.10	44,49,52,53	0
55	8AN	2x	76	22/23	0.96	0.09	32,37,42,50	0
1	5MC	2A	1942	21/22	0.96	0.08	42,49,54,56	0
1	5MC	2A	1962	21/22	0.96	0.08	30,42,48,55	0
1	5MC	1A	1942	21/22	0.96	0.08	26,32,35,45	0
32	5MC	1a	1407	21/22	0.96	0.09	30,37,40,42	0
32	MA6	1a	1519	24/25	0.96	0.09	32,36,41,50	0
32	PSU	1a	516	20/21	0.96	0.08	43,49,54,55	0
32	G7M	1a	527	24/25	0.96	0.08	37,43,48,50	0
32	4OC	1a	1402	22/23	0.97	0.08	35,40,44,47	0
55	8AN	1x	76	22/23	0.97	0.07	16,21,28,34	0
54	8AN	2w	76	22/23	0.97	0.07	28,34,37,38	0
32	5MC	1a	1404	21/22	0.97	0.08	29,36,40,42	0
1	OMC	2A	1920	21/22	0.97	0.08	43,51,54,59	0
1	5MU	2A	1939	21/22	0.97	0.08	30,35,39,40	0
1	OMC	1A	1920	21/22	0.97	0.07	31,40,43,45	0
32	MA6	2a	1518	24/25	0.97	0.09	39,50,55,56	0
32	MA6	2a	1519	24/25	0.97	0.09	41,50,54,57	0
54	5MU	1w	54	21/22	0.97	0.07	37,49,52,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	OMU	2A	2552	21/22	0.97	0.08	31,37,44,50	0
1	PSU	1A	1911	20/21	0.97	0.07	32,40,45,47	0
1	5MC	1A	1962	21/22	0.97	0.07	25,30,34,36	0
1	PSU	1A	1917	20/21	0.97	0.08	34,43,46,50	0
32	5MC	1a	1400	21/22	0.97	0.08	37,43,47,51	0
1	PSU	1A	2605	20/21	0.98	0.06	17,23,26,27	0
32	UR3	1a	1498	21/22	0.98	0.07	31,36,39,41	0
1	5MU	1A	1939	21/22	0.98	0.06	17,22,26,30	0
1	OMG	2A	2251	24/25	0.98	0.06	31,34,37,39	0
1	2MA	2A	2503	23/24	0.98	0.07	25,33,38,38	0
54	8AN	1w	76	22/23	0.98	0.07	14,20,23,24	0
1	PSU	2A	2605	20/21	0.98	0.06	28,32,36,36	0
1	2MA	1A	2503	23/24	0.98	0.06	13,17,20,23	0
1	OMU	1A	2552	21/22	0.99	0.05	20,23,27,27	0
1	OMG	1A	2251	24/25	0.99	0.06	16,23,25,26	0
32	MA6	1a	1518	24/25	0.99	0.06	30,35,40,41	0

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	10	107	1/1	0.47	0.41	70,70,70,70	0
57	MG	1U	211	1/1	0.49	0.64	69,69,69,69	0
57	MG	1a	1778	1/1	0.49	0.22	77,77,77,77	0
57	MG	2a	1772	1/1	0.57	0.39	77,77,77,77	0
57	MG	1A	4048	1/1	0.58	0.27	73,73,73,73	0
57	MG	1A	3990	1/1	0.59	0.26	50,50,50,50	0
57	MG	1A	3968	1/1	0.59	0.15	73,73,73,73	0
57	MG	1B	229	1/1	0.60	0.21	66,66,66,66	0
57	MG	2A	3734	1/1	0.61	0.20	54,54,54,54	0
57	MG	1w	108	1/1	0.64	0.29	71,71,71,71	0
57	MG	2A	3718	1/1	0.65	0.18	65,65,65,65	0
57	MG	1A	4055	1/1	0.65	0.24	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3574	1/1	0.65	0.13	27,27,27,27	0
57	MG	2v	102	1/1	0.65	0.42	79,79,79,79	0
57	MG	1A	3992	1/1	0.66	0.19	52,52,52,52	0
57	MG	2B	213	1/1	0.66	0.35	72,72,72,72	0
57	MG	2A	3285	1/1	0.66	0.34	68,68,68,68	0
57	MG	1A	4119	1/1	0.66	0.15	43,43,43,43	0
57	MG	2A	3723	1/1	0.67	0.21	82,82,82,82	0
57	MG	1A	3961	1/1	0.67	0.21	46,46,46,46	0
57	MG	1A	3476	1/1	0.67	0.38	69,69,69,69	0
57	MG	2A	3562	1/1	0.67	0.26	66,66,66,66	0
57	MG	1B	230	1/1	0.67	0.21	77,77,77,77	0
57	MG	1A	3850	1/1	0.68	0.23	41,41,41,41	0
57	MG	2A	3593	1/1	0.68	0.26	68,68,68,68	0
57	MG	2A	3656	1/1	0.68	0.18	67,67,67,67	0
57	MG	2A	3683	1/1	0.69	0.18	39,39,39,39	0
57	MG	1A	3889	1/1	0.69	0.14	29,29,29,29	0
57	MG	2A	3805	1/1	0.69	0.21	65,65,65,65	0
57	MG	2A	3689	1/1	0.70	0.17	48,48,48,48	0
57	MG	2A	3616	1/1	0.70	0.25	64,64,64,64	0
57	MG	2A	3737	1/1	0.70	0.20	52,52,52,52	0
57	MG	2A	3777	1/1	0.70	0.24	66,66,66,66	0
57	MG	1A	3764	1/1	0.71	0.16	56,56,56,56	0
57	MG	1A	3491	1/1	0.71	0.18	72,72,72,72	0
57	MG	2A	3182	1/1	0.71	0.17	69,69,69,69	0
57	MG	2A	3280	1/1	0.71	0.34	68,68,68,68	0
57	MG	1A	3754	1/1	0.72	0.24	80,80,80,80	0
57	MG	2a	1605	1/1	0.72	0.26	65,65,65,65	0
57	MG	1a	1822	1/1	0.72	0.20	64,64,64,64	0
57	MG	2A	3518	1/1	0.72	0.15	56,56,56,56	0
57	MG	1A	3669	1/1	0.73	0.16	27,27,27,27	0
57	MG	1a	1814	1/1	0.73	0.27	69,69,69,69	0
57	MG	1E	312	1/1	0.74	0.19	65,65,65,65	0
57	MG	1A	4030	1/1	0.74	0.13	44,44,44,44	0
57	MG	1A	3500	1/1	0.74	0.16	58,58,58,58	0
57	MG	2a	1756	1/1	0.74	0.21	68,68,68,68	0
57	MG	2A	3551	1/1	0.74	0.15	40,40,40,40	0
57	MG	2a	1796	1/1	0.74	0.30	66,66,66,66	0
57	MG	1E	310	1/1	0.74	0.10	25,25,25,25	0
57	MG	1A	3824	1/1	0.75	0.18	56,56,56,56	0
57	MG	2a	1626	1/1	0.75	0.34	74,74,74,74	0
57	MG	1a	1725	1/1	0.75	0.23	56,56,56,56	0
57	MG	1A	3392	1/1	0.75	0.30	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3838	1/1	0.75	0.16	64,64,64,64	0
57	MG	2A	3572	1/1	0.75	0.22	43,43,43,43	0
57	MG	2A	3579	1/1	0.76	0.16	45,45,45,45	0
57	MG	2a	1641	1/1	0.76	0.28	63,63,63,63	0
57	MG	1A	3672	1/1	0.76	0.18	45,45,45,45	0
57	MG	2A	3306	1/1	0.76	0.41	69,69,69,69	0
57	MG	2A	3565	1/1	0.76	0.21	53,53,53,53	0
57	MG	2A	3082	1/1	0.76	0.20	72,72,72,72	0
57	MG	1A	4102	1/1	0.77	0.26	59,59,59,59	0
57	MG	1A	3917	1/1	0.77	0.22	67,67,67,67	0
57	MG	1B	215	1/1	0.77	0.15	54,54,54,54	0
57	MG	2A	3299	1/1	0.77	0.18	57,57,57,57	0
57	MG	2A	3729	1/1	0.77	0.14	61,61,61,61	0
57	MG	1A	3996	1/1	0.77	0.30	55,55,55,55	0
57	MG	1x	111	1/1	0.77	0.27	62,62,62,62	0
57	MG	2A	3622	1/1	0.77	0.28	72,72,72,72	0
57	MG	1A	4001	1/1	0.77	0.17	47,47,47,47	0
57	MG	1a	1741	1/1	0.78	0.13	74,74,74,74	0
57	MG	2A	3316	1/1	0.78	0.20	60,60,60,60	0
57	MG	1A	3847	1/1	0.78	0.15	27,27,27,27	0
57	MG	1a	1790	1/1	0.78	0.14	62,62,62,62	0
57	MG	1A	3547	1/1	0.78	0.29	60,60,60,60	0
57	MG	2A	3743	1/1	0.78	0.11	66,66,66,66	0
57	MG	2A	3744	1/1	0.78	0.22	50,50,50,50	0
57	MG	2A	3762	1/1	0.78	0.14	41,41,41,41	0
57	MG	2A	3563	1/1	0.78	0.23	56,56,56,56	0
57	MG	1A	3879	1/1	0.78	0.12	21,21,21,21	0
57	MG	2A	3811	1/1	0.78	0.21	62,62,62,62	0
57	MG	1A	3734	1/1	0.78	0.08	15,15,15,15	0
57	MG	1B	231	1/1	0.78	0.13	65,65,65,65	0
57	MG	1A	4007	1/1	0.78	0.13	34,34,34,34	0
57	MG	2A	3602	1/1	0.78	0.18	65,65,65,65	0
57	MG	2A	3167	1/1	0.78	0.14	47,47,47,47	0
57	MG	2a	1705	1/1	0.78	0.22	67,67,67,67	0
57	MG	1A	3573	1/1	0.78	0.14	51,51,51,51	0
57	MG	2a	1765	1/1	0.78	0.31	63,63,63,63	0
57	MG	1A	3384	1/1	0.78	0.18	56,56,56,56	0
57	MG	1A	3967	1/1	0.78	0.10	57,57,57,57	0
57	MG	1A	3505	1/1	0.78	0.22	58,58,58,58	0
57	MG	2A	3614	1/1	0.79	0.18	62,62,62,62	0
57	MG	1A	3701	1/1	0.79	0.11	63,63,63,63	0
57	MG	2a	1610	1/1	0.79	0.31	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	3158	1/1	0.79	0.11	73,73,73,73	0
57	MG	2a	1633	1/1	0.79	0.26	62,62,62,62	0
57	MG	1A	3554	1/1	0.79	0.20	61,61,61,61	0
57	MG	2a	1689	1/1	0.79	0.29	68,68,68,68	0
57	MG	1A	3584	1/1	0.79	0.16	60,60,60,60	0
57	MG	2A	3309	1/1	0.79	0.19	69,69,69,69	0
57	MG	2A	3783	1/1	0.79	0.17	58,58,58,58	0
57	MG	2a	1770	1/1	0.79	0.18	63,63,63,63	0
57	MG	2A	3311	1/1	0.79	0.23	67,67,67,67	0
57	MG	2A	3199	1/1	0.79	0.36	70,70,70,70	0
57	MG	2f	202	1/1	0.79	0.17	71,71,71,71	0
57	MG	2A	3266	1/1	0.79	0.29	71,71,71,71	0
57	MG	2A	3519	1/1	0.80	0.25	66,66,66,66	0
57	MG	2A	3541	1/1	0.80	0.27	55,55,55,55	0
57	MG	1O	206	1/1	0.80	0.28	61,61,61,61	0
57	MG	2A	3552	1/1	0.80	0.14	45,45,45,45	0
57	MG	1A	3419	1/1	0.80	0.27	68,68,68,68	0
57	MG	1A	3378	1/1	0.80	0.39	71,71,71,71	0
57	MG	1a	1710	1/1	0.80	0.22	67,67,67,67	0
57	MG	1A	3832	1/1	0.80	0.12	45,45,45,45	0
57	MG	2A	3822	1/1	0.80	0.17	59,59,59,59	0
57	MG	1A	3981	1/1	0.80	0.16	59,59,59,59	0
57	MG	1A	3697	1/1	0.80	0.18	58,58,58,58	0
57	MG	2D	304	1/1	0.80	0.30	74,74,74,74	0
57	MG	1a	1779	1/1	0.80	0.26	60,60,60,60	0
57	MG	2A	3291	1/1	0.80	0.18	67,67,67,67	0
57	MG	1A	3504	1/1	0.80	0.26	61,61,61,61	0
57	MG	1A	3731	1/1	0.80	0.14	38,38,38,38	0
57	MG	2A	3627	1/1	0.80	0.20	43,43,43,43	0
57	MG	1a	1815	1/1	0.80	0.31	77,77,77,77	0
57	MG	2A	3668	1/1	0.80	0.18	59,59,59,59	0
57	MG	2A	3681	1/1	0.80	0.21	68,68,68,68	0
57	MG	1A	3629	1/1	0.80	0.13	32,32,32,32	0
57	MG	1A	3654	1/1	0.80	0.13	22,22,22,22	0
57	MG	2A	3388	1/1	0.80	0.19	61,61,61,61	0
57	MG	2a	1780	1/1	0.80	0.29	59,59,59,59	0
57	MG	2a	1785	1/1	0.80	0.27	64,64,64,64	0
57	MG	2A	3471	1/1	0.80	0.17	58,58,58,58	0
57	MG	2a	1814	1/1	0.80	0.29	62,62,62,62	0
57	MG	2A	3513	1/1	0.80	0.21	50,50,50,50	0
57	MG	2j	201	1/1	0.80	0.16	65,65,65,65	0
57	MG	1A	3940	1/1	0.80	0.14	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1x	112	1/1	0.81	0.16	61,61,61,61	0
57	MG	2A	3056	1/1	0.81	0.17	65,65,65,65	0
57	MG	2A	3749	1/1	0.81	0.17	56,56,56,56	0
57	MG	2A	3536	1/1	0.81	0.23	64,64,64,64	0
57	MG	1A	4095	1/1	0.81	0.12	56,56,56,56	0
57	MG	1a	1643	1/1	0.81	0.23	62,62,62,62	0
57	MG	1a	1659	1/1	0.81	0.30	66,66,66,66	0
57	MG	1a	1702	1/1	0.81	0.21	54,54,54,54	0
57	MG	2A	3192	1/1	0.81	0.16	60,60,60,60	0
57	MG	1A	3796	1/1	0.81	0.20	64,64,64,64	0
57	MG	2A	3844	1/1	0.81	0.27	67,67,67,67	0
57	MG	2A	3242	1/1	0.81	0.17	56,56,56,56	0
57	MG	2A	3264	1/1	0.81	0.24	58,58,58,58	0
57	MG	2U	202	1/1	0.81	0.12	60,60,60,60	0
57	MG	2a	1601	1/1	0.81	0.16	71,71,71,71	0
57	MG	2a	1604	1/1	0.81	0.27	71,71,71,71	0
57	MG	2A	3580	1/1	0.81	0.15	46,46,46,46	0
57	MG	1A	3802	1/1	0.81	0.18	61,61,61,61	0
57	MG	2a	1611	1/1	0.81	0.19	62,62,62,62	0
57	MG	2A	3600	1/1	0.81	0.12	59,59,59,59	0
57	MG	2A	3268	1/1	0.81	0.17	68,68,68,68	0
57	MG	1A	3818	1/1	0.81	0.14	59,59,59,59	0
57	MG	1B	222	1/1	0.81	0.21	57,57,57,57	0
57	MG	1A	3400	1/1	0.81	0.25	61,61,61,61	0
57	MG	1A	3957	1/1	0.81	0.12	59,59,59,59	0
57	MG	1A	3602	1/1	0.81	0.12	39,39,39,39	0
57	MG	1A	3677	1/1	0.81	0.25	55,55,55,55	0
57	MG	1a	1819	1/1	0.81	0.17	53,53,53,53	0
57	MG	1A	3782	1/1	0.81	0.11	47,47,47,47	0
57	MG	1v	101	1/1	0.81	0.36	74,74,74,74	0
57	MG	1A	3969	1/1	0.81	0.16	50,50,50,50	0
57	MG	2A	3481	1/1	0.81	0.11	34,34,34,34	0
57	MG	2A	3493	1/1	0.81	0.14	70,70,70,70	0
57	MG	1A	4076	1/1	0.81	0.12	56,56,56,56	0
57	MG	2A	3517	1/1	0.81	0.16	45,45,45,45	0
57	MG	2A	3750	1/1	0.82	0.13	40,40,40,40	0
57	MG	1a	1807	1/1	0.82	0.23	65,65,65,65	0
57	MG	2A	3227	1/1	0.82	0.15	54,54,54,54	0
57	MG	2A	3234	1/1	0.82	0.35	63,63,63,63	0
57	MG	2A	3801	1/1	0.82	0.17	52,52,52,52	0
57	MG	2A	3554	1/1	0.82	0.18	46,46,46,46	0
57	MG	1A	4002	1/1	0.82	0.10	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	3653	1/1	0.82	0.14	27,27,27,27	0
57	MG	1A	4024	1/1	0.82	0.15	58,58,58,58	0
57	MG	1a	1680	1/1	0.82	0.17	66,66,66,66	0
57	MG	1A	3613	1/1	0.82	0.14	55,55,55,55	0
57	MG	1a	1706	1/1	0.82	0.22	70,70,70,70	0
57	MG	1A	4043	1/1	0.82	0.19	38,38,38,38	0
57	MG	2Z	301	1/1	0.82	0.12	69,69,69,69	0
57	MG	2A	3296	1/1	0.82	0.22	56,56,56,56	0
57	MG	1A	3441	1/1	0.82	0.22	68,68,68,68	0
57	MG	2A	3033	1/1	0.82	0.18	61,61,61,61	0
57	MG	2A	3615	1/1	0.82	0.19	60,60,60,60	0
57	MG	2A	3039	1/1	0.82	0.20	67,67,67,67	0
57	MG	2a	1612	1/1	0.82	0.24	67,67,67,67	0
57	MG	2a	1617	1/1	0.82	0.15	57,57,57,57	0
57	MG	1a	1727	1/1	0.82	0.20	56,56,56,56	0
57	MG	2A	3313	1/1	0.82	0.30	74,74,74,74	0
57	MG	2A	3059	1/1	0.82	0.31	64,64,64,64	0
57	MG	2a	1688	1/1	0.82	0.27	64,64,64,64	0
57	MG	2A	3667	1/1	0.82	0.12	45,45,45,45	0
57	MG	2A	3351	1/1	0.82	0.26	52,52,52,52	0
57	MG	2a	1721	1/1	0.82	0.20	68,68,68,68	0
57	MG	2a	1754	1/1	0.82	0.15	69,69,69,69	0
57	MG	1A	3711	1/1	0.82	0.16	55,55,55,55	0
57	MG	2A	3399	1/1	0.82	0.14	64,64,64,64	0
57	MG	2A	3462	1/1	0.82	0.20	63,63,63,63	0
57	MG	2A	3089	1/1	0.82	0.21	69,69,69,69	0
57	MG	2A	3151	1/1	0.82	0.21	59,59,59,59	0
57	MG	2a	1784	1/1	0.82	0.21	72,72,72,72	0
57	MG	1A	3795	1/1	0.82	0.18	50,50,50,50	0
57	MG	2a	1787	1/1	0.82	0.26	64,64,64,64	0
57	MG	2a	1792	1/1	0.82	0.25	62,62,62,62	0
57	MG	1A	3644	1/1	0.82	0.09	28,28,28,28	0
57	MG	1A	3871	1/1	0.82	0.14	50,50,50,50	0
57	MG	2A	3191	1/1	0.82	0.23	63,63,63,63	0
57	MG	1a	1806	1/1	0.82	0.22	62,62,62,62	0
57	MG	2A	3198	1/1	0.82	0.13	69,69,69,69	0
57	MG	2y	102	1/1	0.82	0.21	77,77,77,77	0
57	MG	1A	4050	1/1	0.83	0.16	52,52,52,52	0
57	MG	1A	3766	1/1	0.83	0.16	54,54,54,54	0
57	MG	1a	1766	1/1	0.83	0.17	60,60,60,60	0
57	MG	2A	3695	1/1	0.83	0.17	59,59,59,59	0
57	MG	2A	3221	1/1	0.83	0.23	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	3332	1/1	0.83	0.17	55,55,55,55	0
57	MG	2A	3728	1/1	0.83	0.13	44,44,44,44	0
57	MG	1A	3993	1/1	0.83	0.13	55,55,55,55	0
57	MG	2a	1630	1/1	0.83	0.21	67,67,67,67	0
57	MG	2a	1631	1/1	0.83	0.33	65,65,65,65	0
57	MG	2A	3385	1/1	0.83	0.26	56,56,56,56	0
57	MG	1A	3953	1/1	0.83	0.11	34,34,34,34	0
57	MG	1A	3375	1/1	0.83	0.20	55,55,55,55	0
57	MG	2A	3401	1/1	0.83	0.15	65,65,65,65	0
57	MG	2a	1701	1/1	0.83	0.27	65,65,65,65	0
57	MG	2A	3746	1/1	0.83	0.14	41,41,41,41	0
57	MG	2A	3583	1/1	0.83	0.14	60,60,60,60	0
57	MG	2A	3412	1/1	0.83	0.23	64,64,64,64	0
57	MG	2A	3458	1/1	0.83	0.17	57,57,57,57	0
57	MG	1A	3025	1/1	0.83	0.19	51,51,51,51	0
57	MG	1A	3752	1/1	0.83	0.08	40,40,40,40	0
57	MG	1A	3327	1/1	0.83	0.20	59,59,59,59	0
57	MG	1A	3763	1/1	0.83	0.10	41,41,41,41	0
57	MG	2A	3618	1/1	0.83	0.18	64,64,64,64	0
57	MG	1A	3649	1/1	0.83	0.18	64,64,64,64	0
57	MG	1A	3924	1/1	0.83	0.10	30,30,30,30	0
57	MG	2A	3842	1/1	0.83	0.15	61,61,61,61	0
57	MG	2A	3632	1/1	0.83	0.18	56,56,56,56	0
57	MG	2a	1811	1/1	0.83	0.13	65,65,65,65	0
57	MG	2B	209	1/1	0.83	0.26	73,73,73,73	0
57	MG	2A	3653	1/1	0.83	0.17	59,59,59,59	0
57	MG	1E	309	1/1	0.83	0.14	59,59,59,59	0
57	MG	2A	3189	1/1	0.83	0.30	63,63,63,63	0
57	MG	1w	107	1/1	0.83	0.17	66,66,66,66	0
57	MG	1A	3809	1/1	0.84	0.15	47,47,47,47	0
57	MG	1a	1604	1/1	0.84	0.23	55,55,55,55	0
57	MG	1a	1639	1/1	0.84	0.26	64,64,64,64	0
57	MG	2T	204	1/1	0.84	0.14	69,69,69,69	0
57	MG	2A	3195	1/1	0.84	0.18	65,65,65,65	0
57	MG	2A	3428	1/1	0.84	0.28	66,66,66,66	0
57	MG	1a	1816	1/1	0.84	0.24	62,62,62,62	0
57	MG	2A	3652	1/1	0.84	0.14	52,52,52,52	0
57	MG	1A	3911	1/1	0.84	0.10	51,51,51,51	0
57	MG	1A	3817	1/1	0.84	0.15	57,57,57,57	0
57	MG	1h	201	1/1	0.84	0.12	63,63,63,63	0
57	MG	1A	3923	1/1	0.84	0.09	45,45,45,45	0
57	MG	2A	3674	1/1	0.84	0.17	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2a	1619	1/1	0.84	0.32	62,62,62,62	0
57	MG	2A	3496	1/1	0.84	0.18	41,41,41,41	0
57	MG	1a	1688	1/1	0.84	0.27	58,58,58,58	0
57	MG	2A	3248	1/1	0.84	0.25	70,70,70,70	0
57	MG	1A	3676	1/1	0.84	0.12	53,53,53,53	0
57	MG	2A	3700	1/1	0.84	0.19	47,47,47,47	0
57	MG	2a	1683	1/1	0.84	0.33	61,61,61,61	0
57	MG	1A	3624	1/1	0.84	0.09	23,23,23,23	0
57	MG	2A	3521	1/1	0.84	0.12	62,62,62,62	0
57	MG	1A	3949	1/1	0.84	0.13	34,34,34,34	0
57	MG	2A	3540	1/1	0.84	0.17	64,64,64,64	0
57	MG	2A	3731	1/1	0.84	0.16	58,58,58,58	0
57	MG	2a	1725	1/1	0.84	0.18	64,64,64,64	0
57	MG	2a	1727	1/1	0.84	0.15	65,65,65,65	0
57	MG	1A	3438	1/1	0.84	0.14	60,60,60,60	0
57	MG	1A	3956	1/1	0.84	0.12	60,60,60,60	0
57	MG	1D	313	1/1	0.84	0.21	41,41,41,41	0
57	MG	1a	1751	1/1	0.84	0.14	47,47,47,47	0
57	MG	1A	3514	1/1	0.84	0.14	61,61,61,61	0
57	MG	2A	3088	1/1	0.84	0.18	62,62,62,62	0
57	MG	1A	3761	1/1	0.84	0.10	17,17,17,17	0
57	MG	1A	3855	1/1	0.84	0.11	29,29,29,29	0
57	MG	1A	3799	1/1	0.84	0.10	35,35,35,35	0
57	MG	2A	3162	1/1	0.84	0.21	67,67,67,67	0
57	MG	2A	3331	1/1	0.84	0.28	59,59,59,59	0
57	MG	2a	1808	1/1	0.84	0.20	60,60,60,60	0
57	MG	2A	3589	1/1	0.84	0.21	55,55,55,55	0
57	MG	2A	3590	1/1	0.84	0.26	68,68,68,68	0
57	MG	1a	1794	1/1	0.84	0.18	59,59,59,59	0
57	MG	2A	3168	1/1	0.84	0.29	62,62,62,62	0
57	MG	2m	201	1/1	0.84	0.26	68,68,68,68	0
57	MG	2A	3354	1/1	0.84	0.12	68,68,68,68	0
57	MG	1A	3304	1/1	0.84	0.17	57,57,57,57	0
57	MG	2A	3794	1/1	0.85	0.22	64,64,64,64	0
57	MG	2A	3799	1/1	0.85	0.14	74,74,74,74	0
57	MG	2A	3270	1/1	0.85	0.23	62,62,62,62	0
57	MG	2A	3025	1/1	0.85	0.15	56,56,56,56	0
57	MG	2A	3809	1/1	0.85	0.13	51,51,51,51	0
57	MG	1A	3565	1/1	0.85	0.15	57,57,57,57	0
57	MG	1A	3791	1/1	0.85	0.17	50,50,50,50	0
57	MG	2A	3825	1/1	0.85	0.16	56,56,56,56	0
57	MG	2A	3292	1/1	0.85	0.25	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	3839	1/1	0.85	0.13	53,53,53,53	0
57	MG	1a	1711	1/1	0.85	0.18	59,59,59,59	0
57	MG	1a	1712	1/1	0.85	0.20	60,60,60,60	0
57	MG	2B	203	1/1	0.85	0.16	54,54,54,54	0
57	MG	1A	3831	1/1	0.85	0.17	48,48,48,48	0
57	MG	2A	3584	1/1	0.85	0.22	50,50,50,50	0
57	MG	2A	3083	1/1	0.85	0.17	66,66,66,66	0
57	MG	2Q	203	1/1	0.85	0.37	67,67,67,67	0
57	MG	1A	3683	1/1	0.85	0.12	46,46,46,46	0
57	MG	1a	1739	1/1	0.85	0.11	59,59,59,59	0
57	MG	2A	3092	1/1	0.85	0.20	59,59,59,59	0
57	MG	2A	3324	1/1	0.85	0.18	63,63,63,63	0
57	MG	2A	3117	1/1	0.85	0.14	55,55,55,55	0
57	MG	1A	3936	1/1	0.85	0.12	65,65,65,65	0
57	MG	2A	3335	1/1	0.85	0.24	54,54,54,54	0
57	MG	2A	3617	1/1	0.85	0.27	68,68,68,68	0
57	MG	1A	3840	1/1	0.85	0.13	35,35,35,35	0
57	MG	1A	3426	1/1	0.85	0.11	54,54,54,54	0
57	MG	2A	3624	1/1	0.85	0.18	56,56,56,56	0
57	MG	2a	1624	1/1	0.85	0.15	80,80,80,80	0
57	MG	2A	3358	1/1	0.85	0.12	57,57,57,57	0
57	MG	2A	3370	1/1	0.85	0.25	57,57,57,57	0
57	MG	2A	3376	1/1	0.85	0.27	58,58,58,58	0
57	MG	2A	3164	1/1	0.85	0.12	58,58,58,58	0
57	MG	2A	3387	1/1	0.85	0.22	53,53,53,53	0
57	MG	1A	3432	1/1	0.85	0.22	59,59,59,59	0
57	MG	1A	4021	1/1	0.85	0.16	33,33,33,33	0
57	MG	1A	3703	1/1	0.85	0.13	48,48,48,48	0
57	MG	2a	1697	1/1	0.85	0.20	64,64,64,64	0
57	MG	2A	3188	1/1	0.85	0.52	70,70,70,70	0
57	MG	2A	3414	1/1	0.85	0.21	54,54,54,54	0
57	MG	2a	1706	1/1	0.85	0.11	68,68,68,68	0
57	MG	1A	3858	1/1	0.85	0.11	21,21,21,21	0
57	MG	2A	3190	1/1	0.85	0.22	53,53,53,53	0
57	MG	1A	4038	1/1	0.85	0.13	51,51,51,51	0
57	MG	1A	4039	1/1	0.85	0.15	38,38,38,38	0
57	MG	2A	3476	1/1	0.85	0.17	57,57,57,57	0
57	MG	1A	3960	1/1	0.85	0.12	47,47,47,47	0
57	MG	2a	1766	1/1	0.85	0.25	64,64,64,64	0
57	MG	1A	4046	1/1	0.85	0.22	52,52,52,52	0
57	MG	2a	1771	1/1	0.85	0.15	57,57,57,57	0
57	MG	1a	1605	1/1	0.85	0.22	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	1773	1/1	0.85	0.20	64,64,64,64	0
57	MG	1A	3386	1/1	0.85	0.20	59,59,59,59	0
57	MG	1A	3810	1/1	0.85	0.12	52,52,52,52	0
57	MG	2A	3228	1/1	0.85	0.24	58,58,58,58	0
57	MG	2A	3233	1/1	0.85	0.23	66,66,66,66	0
57	MG	1A	3886	1/1	0.85	0.11	42,42,42,42	0
57	MG	1a	1661	1/1	0.85	0.33	67,67,67,67	0
57	MG	2a	1802	1/1	0.85	0.23	56,56,56,56	0
57	MG	1a	1666	1/1	0.85	0.21	73,73,73,73	0
57	MG	2A	3756	1/1	0.85	0.13	65,65,65,65	0
57	MG	2A	3761	1/1	0.85	0.15	53,53,53,53	0
57	MG	2a	1819	1/1	0.85	0.28	67,67,67,67	0
57	MG	1A	3227	1/1	0.85	0.12	56,56,56,56	0
57	MG	2A	3776	1/1	0.85	0.16	47,47,47,47	0
57	MG	2l	202	1/1	0.85	0.18	59,59,59,59	0
57	MG	1A	4091	1/1	0.85	0.20	65,65,65,65	0
57	MG	2A	3779	1/1	0.85	0.12	56,56,56,56	0
57	MG	1A	3973	1/1	0.85	0.12	31,31,31,31	0
57	MG	2A	3218	1/1	0.86	0.33	49,49,49,49	0
57	MG	2A	3077	1/1	0.86	0.18	55,55,55,55	0
57	MG	2a	1616	1/1	0.86	0.12	65,65,65,65	0
57	MG	1a	1799	1/1	0.86	0.11	57,57,57,57	0
57	MG	1D	302	1/1	0.86	0.18	60,60,60,60	0
57	MG	2a	1621	1/1	0.86	0.18	58,58,58,58	0
57	MG	2a	1622	1/1	0.86	0.14	54,54,54,54	0
57	MG	2a	1623	1/1	0.86	0.18	59,59,59,59	0
57	MG	1A	3092	1/1	0.86	0.15	59,59,59,59	0
57	MG	1A	3154	1/1	0.86	0.19	57,57,57,57	0
57	MG	1A	3443	1/1	0.86	0.15	52,52,52,52	0
57	MG	2A	3093	1/1	0.86	0.23	66,66,66,66	0
57	MG	2a	1632	1/1	0.86	0.22	67,67,67,67	0
57	MG	2A	3393	1/1	0.86	0.32	68,68,68,68	0
57	MG	2a	1640	1/1	0.86	0.34	63,63,63,63	0
57	MG	2A	3398	1/1	0.86	0.20	58,58,58,58	0
57	MG	2a	1646	1/1	0.86	0.17	65,65,65,65	0
57	MG	2a	1682	1/1	0.86	0.45	67,67,67,67	0
57	MG	2A	3260	1/1	0.86	0.23	62,62,62,62	0
57	MG	1A	3185	1/1	0.86	0.16	46,46,46,46	0
57	MG	2A	3404	1/1	0.86	0.14	63,63,63,63	0
57	MG	2A	3766	1/1	0.86	0.14	39,39,39,39	0
57	MG	2A	3770	1/1	0.86	0.10	65,65,65,65	0
57	MG	1G	205	1/1	0.86	0.17	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3610	1/1	0.86	0.17	48,48,48,48	0
57	MG	1A	3719	1/1	0.86	0.16	60,60,60,60	0
57	MG	1A	4014	1/1	0.86	0.12	46,46,46,46	0
57	MG	2A	3440	1/1	0.86	0.18	50,50,50,50	0
57	MG	2a	1728	1/1	0.86	0.16	63,63,63,63	0
57	MG	2a	1733	1/1	0.86	0.18	56,56,56,56	0
57	MG	1l	201	1/1	0.86	0.12	68,68,68,68	0
57	MG	1A	3725	1/1	0.86	0.12	21,21,21,21	0
57	MG	1A	3188	1/1	0.86	0.16	60,60,60,60	0
57	MG	2A	3808	1/1	0.86	0.20	62,62,62,62	0
57	MG	2A	3475	1/1	0.86	0.12	43,43,43,43	0
57	MG	2A	3174	1/1	0.86	0.19	54,54,54,54	0
57	MG	2A	3480	1/1	0.86	0.23	59,59,59,59	0
57	MG	2A	3293	1/1	0.86	0.22	60,60,60,60	0
57	MG	1A	4029	1/1	0.86	0.17	53,53,53,53	0
57	MG	1x	101	1/1	0.86	0.29	60,60,60,60	0
57	MG	2A	3661	1/1	0.86	0.12	46,46,46,46	0
57	MG	1A	3379	1/1	0.86	0.11	47,47,47,47	0
57	MG	2a	1789	1/1	0.86	0.27	69,69,69,69	0
57	MG	2a	1790	1/1	0.86	0.18	55,55,55,55	0
57	MG	1A	3047	1/1	0.86	0.15	48,48,48,48	0
57	MG	1a	1647	1/1	0.86	0.21	62,62,62,62	0
57	MG	2a	1801	1/1	0.86	0.22	59,59,59,59	0
57	MG	2B	211	1/1	0.86	0.23	61,61,61,61	0
57	MG	2a	1806	1/1	0.86	0.23	63,63,63,63	0
57	MG	2A	3679	1/1	0.86	0.12	63,63,63,63	0
57	MG	2A	3680	1/1	0.86	0.14	57,57,57,57	0
57	MG	1A	3686	1/1	0.86	0.14	59,59,59,59	0
57	MG	2A	3682	1/1	0.86	0.22	61,61,61,61	0
57	MG	1a	1789	1/1	0.86	0.17	66,66,66,66	0
57	MG	2A	3321	1/1	0.86	0.26	65,65,65,65	0
57	MG	1A	3689	1/1	0.86	0.21	64,64,64,64	0
57	MG	2l	204	1/1	0.86	0.14	59,59,59,59	0
57	MG	1A	4044	1/1	0.86	0.19	44,44,44,44	0
57	MG	2v	101	1/1	0.86	0.17	57,57,57,57	0
57	MG	2A	3201	1/1	0.86	0.29	66,66,66,66	0
57	MG	2x	104	1/1	0.86	0.22	60,60,60,60	0
57	MG	2A	3209	1/1	0.86	0.31	60,60,60,60	0
57	MG	1A	3786	1/1	0.87	0.10	23,23,23,23	0
57	MG	2A	3713	1/1	0.87	0.11	55,55,55,55	0
57	MG	2A	3537	1/1	0.87	0.21	59,59,59,59	0
57	MG	2A	3538	1/1	0.87	0.10	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	1b	301	1/1	0.87	0.12	61,61,61,61	0
57	MG	1a	1670	1/1	0.87	0.19	64,64,64,64	0
57	MG	1A	3713	1/1	0.87	0.11	34,34,34,34	0
57	MG	2a	1629	1/1	0.87	0.27	56,56,56,56	0
57	MG	2A	3732	1/1	0.87	0.14	72,72,72,72	0
57	MG	1A	3263	1/1	0.87	0.14	53,53,53,53	0
57	MG	2A	3334	1/1	0.87	0.23	71,71,71,71	0
57	MG	2A	3558	1/1	0.87	0.19	54,54,54,54	0
57	MG	2a	1634	1/1	0.87	0.26	60,60,60,60	0
57	MG	1A	3607	1/1	0.87	0.20	61,61,61,61	0
57	MG	1B	232	1/1	0.87	0.15	61,61,61,61	0
57	MG	1A	3026	1/1	0.87	0.19	73,73,73,73	0
57	MG	2a	1666	1/1	0.87	0.26	59,59,59,59	0
57	MG	1x	108	1/1	0.87	0.32	66,66,66,66	0
57	MG	2A	3367	1/1	0.87	0.21	54,54,54,54	0
57	MG	2a	1687	1/1	0.87	0.17	64,64,64,64	0
57	MG	1A	3880	1/1	0.87	0.12	39,39,39,39	0
57	MG	1A	3733	1/1	0.87	0.09	29,29,29,29	0
57	MG	2A	3210	1/1	0.87	0.15	61,61,61,61	0
57	MG	2A	3006	1/1	0.87	0.14	50,50,50,50	0
57	MG	1A	3408	1/1	0.87	0.10	61,61,61,61	0
57	MG	1A	3907	1/1	0.87	0.09	56,56,56,56	0
57	MG	2a	1708	1/1	0.87	0.22	67,67,67,67	0
57	MG	1A	3454	1/1	0.87	0.15	48,48,48,48	0
57	MG	2A	3230	1/1	0.87	0.13	61,61,61,61	0
57	MG	1A	3630	1/1	0.87	0.07	27,27,27,27	0
57	MG	2A	3057	1/1	0.87	0.20	58,58,58,58	0
57	MG	2a	1729	1/1	0.87	0.11	62,62,62,62	0
57	MG	2A	3409	1/1	0.87	0.21	64,64,64,64	0
57	MG	1U	202	1/1	0.87	0.25	45,45,45,45	0
57	MG	1A	3633	1/1	0.87	0.09	35,35,35,35	0
57	MG	2A	3417	1/1	0.87	0.28	69,69,69,69	0
57	MG	1Z	304	1/1	0.87	0.11	53,53,53,53	0
57	MG	1A	3307	1/1	0.87	0.13	50,50,50,50	0
57	MG	2A	3446	1/1	0.87	0.11	53,53,53,53	0
57	MG	1a	1785	1/1	0.87	0.13	54,54,54,54	0
57	MG	2A	3633	1/1	0.87	0.15	53,53,53,53	0
57	MG	2A	3634	1/1	0.87	0.31	63,63,63,63	0
57	MG	2A	3640	1/1	0.87	0.09	27,27,27,27	0
57	MG	1A	3312	1/1	0.87	0.15	57,57,57,57	0
57	MG	1A	3430	1/1	0.87	0.17	52,52,52,52	0
57	MG	1a	1606	1/1	0.87	0.11	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	2A	3096	1/1	0.87	0.24	64,64,64,64	0
57	MG	2B	217	1/1	0.87	0.12	69,69,69,69	0
57	MG	2A	3097	1/1	0.87	0.21	63,63,63,63	0
57	MG	2Q	202	1/1	0.87	0.16	55,55,55,55	0
57	MG	1a	1797	1/1	0.87	0.19	57,57,57,57	0
57	MG	2A	3670	1/1	0.87	0.16	52,52,52,52	0
57	MG	2A	3673	1/1	0.87	0.16	53,53,53,53	0
57	MG	1a	1611	1/1	0.87	0.26	59,59,59,59	0
57	MG	21	101	1/1	0.87	0.18	62,62,62,62	0
57	MG	1A	4003	1/1	0.87	0.17	42,42,42,42	0
57	MG	2a	1820	1/1	0.87	0.16	70,70,70,70	0
57	MG	2a	1825	1/1	0.87	0.17	69,69,69,69	0
57	MG	2a	1602	1/1	0.87	0.28	59,59,59,59	0
57	MG	2a	1603	1/1	0.87	0.22	61,61,61,61	0
57	MG	1A	4104	1/1	0.87	0.12	75,75,75,75	0
57	MG	1A	3780	1/1	0.87	0.23	57,57,57,57	0
57	MG	2a	1606	1/1	0.87	0.29	64,64,64,64	0
57	MG	2t	201	1/1	0.87	0.15	52,52,52,52	0
57	MG	1a	1650	1/1	0.87	0.28	63,63,63,63	0
57	MG	1B	202	1/1	0.87	0.28	56,56,56,56	0
57	MG	1A	3151	1/1	0.87	0.24	53,53,53,53	0
57	MG	2A	3523	1/1	0.87	0.14	47,47,47,47	0
57	MG	1A	3808	1/1	0.88	0.09	55,55,55,55	0
57	MG	1A	4066	1/1	0.88	0.16	53,53,53,53	0
57	MG	2A	3836	1/1	0.88	0.10	54,54,54,54	0
57	MG	2A	3245	1/1	0.88	0.11	56,56,56,56	0
57	MG	1A	4073	1/1	0.88	0.14	49,49,49,49	0
57	MG	1a	1619	1/1	0.88	0.12	58,58,58,58	0
57	MG	1a	1631	1/1	0.88	0.23	60,60,60,60	0
57	MG	1a	1633	1/1	0.88	0.17	56,56,56,56	0
57	MG	2A	3267	1/1	0.88	0.10	67,67,67,67	0
57	MG	1A	3909	1/1	0.88	0.08	48,48,48,48	0
57	MG	1A	4089	1/1	0.88	0.11	51,51,51,51	0
57	MG	2A	3273	1/1	0.88	0.20	55,55,55,55	0
57	MG	2A	3276	1/1	0.88	0.28	54,54,54,54	0
57	MG	2A	3278	1/1	0.88	0.20	55,55,55,55	0
57	MG	1x	103	1/1	0.88	0.13	58,58,58,58	0
57	MG	1A	3453	1/1	0.88	0.24	59,59,59,59	0
57	MG	1A	3735	1/1	0.88	0.10	52,52,52,52	0
57	MG	2X	101	1/1	0.88	0.18	56,56,56,56	0
57	MG	2A	3582	1/1	0.88	0.15	42,42,42,42	0
57	MG	1a	1656	1/1	0.88	0.27	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	3999	1/1	0.88	0.08	45,45,45,45	0
57	MG	2A	3011	1/1	0.88	0.22	66,66,66,66	0
57	MG	2A	3298	1/1	0.88	0.34	71,71,71,71	0
57	MG	2A	3592	1/1	0.88	0.13	54,54,54,54	0
57	MG	2A	3017	1/1	0.88	0.21	64,64,64,64	0
57	MG	2A	3305	1/1	0.88	0.14	73,73,73,73	0
57	MG	2a	1607	1/1	0.88	0.31	67,67,67,67	0
57	MG	1A	4000	1/1	0.88	0.11	43,43,43,43	0
57	MG	2A	3604	1/1	0.88	0.11	47,47,47,47	0
57	MG	1a	1662	1/1	0.88	0.17	61,61,61,61	0
57	MG	1A	4112	1/1	0.88	0.16	64,64,64,64	0
57	MG	1a	1668	1/1	0.88	0.34	68,68,68,68	0
57	MG	2A	3315	1/1	0.88	0.10	73,73,73,73	0
57	MG	1A	4113	1/1	0.88	0.18	45,45,45,45	0
57	MG	1a	1679	1/1	0.88	0.12	53,53,53,53	0
57	MG	2A	3065	1/1	0.88	0.13	49,49,49,49	0
57	MG	2A	3326	1/1	0.88	0.26	64,64,64,64	0
57	MG	2A	3329	1/1	0.88	0.25	62,62,62,62	0
57	MG	1A	3423	1/1	0.88	0.17	51,51,51,51	0
57	MG	1a	1683	1/1	0.88	0.17	60,60,60,60	0
57	MG	1A	3365	1/1	0.88	0.23	35,35,35,35	0
57	MG	1a	1693	1/1	0.88	0.29	58,58,58,58	0
57	MG	2A	3649	1/1	0.88	0.19	60,60,60,60	0
57	MG	2A	3650	1/1	0.88	0.15	51,51,51,51	0
57	MG	1B	213	1/1	0.88	0.26	65,65,65,65	0
57	MG	2A	3352	1/1	0.88	0.21	66,66,66,66	0
57	MG	1A	3927	1/1	0.88	0.16	43,43,43,43	0
57	MG	2a	1660	1/1	0.88	0.39	65,65,65,65	0
57	MG	2A	3659	1/1	0.88	0.13	60,60,60,60	0
57	MG	2A	3355	1/1	0.88	0.11	63,63,63,63	0
57	MG	2A	3662	1/1	0.88	0.10	57,57,57,57	0
57	MG	2a	1684	1/1	0.88	0.20	53,53,53,53	0
57	MG	1A	4004	1/1	0.88	0.10	54,54,54,54	0
57	MG	1A	3389	1/1	0.88	0.15	51,51,51,51	0
57	MG	1A	4008	1/1	0.88	0.10	21,21,21,21	0
57	MG	2A	3373	1/1	0.88	0.22	54,54,54,54	0
57	MG	2A	3375	1/1	0.88	0.35	54,54,54,54	0
57	MG	1a	1721	1/1	0.88	0.19	65,65,65,65	0
57	MG	2A	3382	1/1	0.88	0.26	54,54,54,54	0
57	MG	1A	3051	1/1	0.88	0.10	49,49,49,49	0
57	MG	2a	1712	1/1	0.88	0.22	72,72,72,72	0
57	MG	2A	3155	1/1	0.88	0.24	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2a	1722	1/1	0.88	0.36	64,64,64,64	0
57	MG	1A	3248	1/1	0.88	0.10	51,51,51,51	0
57	MG	1a	1729	1/1	0.88	0.20	62,62,62,62	0
57	MG	2A	3395	1/1	0.88	0.19	48,48,48,48	0
57	MG	2A	3696	1/1	0.88	0.23	70,70,70,70	0
57	MG	2a	1732	1/1	0.88	0.09	72,72,72,72	0
57	MG	1a	1735	1/1	0.88	0.17	52,52,52,52	0
57	MG	1a	1738	1/1	0.88	0.16	69,69,69,69	0
57	MG	1B	237	1/1	0.88	0.09	39,39,39,39	0
57	MG	2A	3721	1/1	0.88	0.14	58,58,58,58	0
57	MG	2A	3722	1/1	0.88	0.17	41,41,41,41	0
57	MG	1A	4023	1/1	0.88	0.10	36,36,36,36	0
57	MG	2A	3179	1/1	0.88	0.19	62,62,62,62	0
57	MG	2A	3181	1/1	0.88	0.38	64,64,64,64	0
57	MG	2A	3730	1/1	0.88	0.14	61,61,61,61	0
57	MG	2a	1779	1/1	0.88	0.16	63,63,63,63	0
57	MG	1A	3709	1/1	0.88	0.26	54,54,54,54	0
57	MG	2A	3415	1/1	0.88	0.22	63,63,63,63	0
57	MG	1E	306	1/1	0.88	0.20	53,53,53,53	0
57	MG	1A	3146	1/1	0.88	0.12	58,58,58,58	0
57	MG	2a	1788	1/1	0.88	0.31	54,54,54,54	0
57	MG	2A	3741	1/1	0.88	0.12	58,58,58,58	0
57	MG	2A	3429	1/1	0.88	0.28	58,58,58,58	0
57	MG	1A	3665	1/1	0.88	0.10	28,28,28,28	0
57	MG	1A	3716	1/1	0.88	0.16	47,47,47,47	0
57	MG	2a	1800	1/1	0.88	0.20	71,71,71,71	0
57	MG	2A	3448	1/1	0.88	0.12	34,34,34,34	0
57	MG	1G	204	1/1	0.88	0.10	65,65,65,65	0
57	MG	2A	3193	1/1	0.88	0.14	61,61,61,61	0
57	MG	1A	3718	1/1	0.88	0.10	28,28,28,28	0
57	MG	2a	1810	1/1	0.88	0.23	57,57,57,57	0
57	MG	1A	4040	1/1	0.88	0.09	24,24,24,24	0
57	MG	1A	3282	1/1	0.88	0.10	58,58,58,58	0
57	MG	1A	3445	1/1	0.88	0.19	59,59,59,59	0
57	MG	1a	1805	1/1	0.88	0.12	58,58,58,58	0
57	MG	1Z	302	1/1	0.88	0.08	57,57,57,57	0
57	MG	1A	3626	1/1	0.88	0.12	55,55,55,55	0
57	MG	2A	3503	1/1	0.88	0.11	59,59,59,59	0
57	MG	2A	3791	1/1	0.88	0.13	66,66,66,66	0
57	MG	2A	3508	1/1	0.88	0.09	34,34,34,34	0
57	MG	2A	3509	1/1	0.88	0.25	56,56,56,56	0
57	MG	1A	3800	1/1	0.88	0.10	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	17	105	1/1	0.88	0.23	38,38,38,38	0
57	MG	18	105	1/1	0.88	0.14	63,63,63,63	0
57	MG	2w	103	1/1	0.88	0.10	65,65,65,65	0
57	MG	2w	106	1/1	0.88	0.15	65,65,65,65	0
57	MG	2w	107	1/1	0.88	0.33	70,70,70,70	0
57	MG	1a	1817	1/1	0.88	0.22	62,62,62,62	0
57	MG	1A	3627	1/1	0.88	0.09	42,42,42,42	0
57	MG	1A	3813	1/1	0.89	0.11	55,55,55,55	0
57	MG	1A	4015	1/1	0.89	0.15	59,59,59,59	0
57	MG	1A	3931	1/1	0.89	0.17	50,50,50,50	0
57	MG	25	101	1/1	0.89	0.19	57,57,57,57	0
57	MG	2A	3383	1/1	0.89	0.24	55,55,55,55	0
57	MG	1A	3182	1/1	0.89	0.11	51,51,51,51	0
57	MG	2A	3208	1/1	0.89	0.34	58,58,58,58	0
57	MG	1A	3938	1/1	0.89	0.15	65,65,65,65	0
57	MG	2A	3390	1/1	0.89	0.29	58,58,58,58	0
57	MG	2A	3636	1/1	0.89	0.14	68,68,68,68	0
57	MG	1A	3329	1/1	0.89	0.12	49,49,49,49	0
57	MG	2A	3641	1/1	0.89	0.16	60,60,60,60	0
57	MG	2A	3643	1/1	0.89	0.30	67,67,67,67	0
57	MG	1A	3946	1/1	0.89	0.13	59,59,59,59	0
57	MG	1A	3589	1/1	0.89	0.14	46,46,46,46	0
57	MG	1x	109	1/1	0.89	0.26	61,61,61,61	0
57	MG	1A	3452	1/1	0.89	0.13	49,49,49,49	0
57	MG	1A	3333	1/1	0.89	0.16	46,46,46,46	0
57	MG	2A	3407	1/1	0.89	0.10	57,57,57,57	0
57	MG	2A	3232	1/1	0.89	0.27	59,59,59,59	0
57	MG	2A	3411	1/1	0.89	0.17	64,64,64,64	0
57	MG	2A	3666	1/1	0.89	0.16	53,53,53,53	0
57	MG	1a	1707	1/1	0.89	0.21	48,48,48,48	0
57	MG	1A	3405	1/1	0.89	0.28	49,49,49,49	0
57	MG	1E	314	1/1	0.89	0.14	55,55,55,55	0
57	MG	1A	3406	1/1	0.89	0.24	51,51,51,51	0
57	MG	2A	3425	1/1	0.89	0.23	59,59,59,59	0
57	MG	2A	3427	1/1	0.89	0.12	59,59,59,59	0
57	MG	1A	3342	1/1	0.89	0.22	47,47,47,47	0
57	MG	2A	3255	1/1	0.89	0.15	62,62,62,62	0
57	MG	2A	3256	1/1	0.89	0.20	58,58,58,58	0
57	MG	2a	1654	1/1	0.89	0.24	64,64,64,64	0
57	MG	1A	3851	1/1	0.89	0.08	20,20,20,20	0
57	MG	2a	1661	1/1	0.89	0.21	57,57,57,57	0
57	MG	1A	3773	1/1	0.89	0.13	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	1677	1/1	0.89	0.21	60,60,60,60	0
57	MG	1A	3038	1/1	0.89	0.26	55,55,55,55	0
57	MG	1A	3082	1/1	0.89	0.17	52,52,52,52	0
57	MG	1a	1737	1/1	0.89	0.10	61,61,61,61	0
57	MG	2A	3474	1/1	0.89	0.23	58,58,58,58	0
57	MG	1A	4069	1/1	0.89	0.09	43,43,43,43	0
57	MG	2A	3271	1/1	0.89	0.27	63,63,63,63	0
57	MG	1A	3203	1/1	0.89	0.18	45,45,45,45	0
57	MG	2a	1698	1/1	0.89	0.25	64,64,64,64	0
57	MG	2a	1699	1/1	0.89	0.12	67,67,67,67	0
57	MG	14	101	1/1	0.89	0.27	68,68,68,68	0
57	MG	2A	3277	1/1	0.89	0.20	68,68,68,68	0
57	MG	15	107	1/1	0.89	0.09	53,53,53,53	0
57	MG	1A	3989	1/1	0.89	0.11	58,58,58,58	0
57	MG	2a	1710	1/1	0.89	0.37	68,68,68,68	0
57	MG	2A	3282	1/1	0.89	0.12	47,47,47,47	0
57	MG	2a	1716	1/1	0.89	0.19	71,71,71,71	0
57	MG	1A	4080	1/1	0.89	0.09	33,33,33,33	0
57	MG	2A	3288	1/1	0.89	0.17	55,55,55,55	0
57	MG	2a	1724	1/1	0.89	0.27	66,66,66,66	0
57	MG	1A	4083	1/1	0.89	0.11	48,48,48,48	0
57	MG	2A	3094	1/1	0.89	0.23	53,53,53,53	0
57	MG	1A	4086	1/1	0.89	0.16	57,57,57,57	0
57	MG	1a	1786	1/1	0.89	0.12	47,47,47,47	0
57	MG	2A	3106	1/1	0.89	0.20	52,52,52,52	0
57	MG	1a	1787	1/1	0.89	0.18	56,56,56,56	0
57	MG	2a	1741	1/1	0.89	0.17	69,69,69,69	0
57	MG	2A	3135	1/1	0.89	0.34	61,61,61,61	0
57	MG	1A	3211	1/1	0.89	0.25	59,59,59,59	0
57	MG	2A	3154	1/1	0.89	0.33	70,70,70,70	0
57	MG	1A	3884	1/1	0.89	0.08	67,67,67,67	0
57	MG	2A	3542	1/1	0.89	0.16	51,51,51,51	0
57	MG	2A	3544	1/1	0.89	0.19	55,55,55,55	0
57	MG	2A	3772	1/1	0.89	0.13	62,62,62,62	0
57	MG	1A	3526	1/1	0.89	0.15	52,52,52,52	0
57	MG	1a	1796	1/1	0.89	0.11	56,56,56,56	0
57	MG	1a	1628	1/1	0.89	0.25	60,60,60,60	0
57	MG	2A	3557	1/1	0.89	0.19	59,59,59,59	0
57	MG	1A	4098	1/1	0.89	0.13	40,40,40,40	0
57	MG	1a	1802	1/1	0.89	0.11	63,63,63,63	0
57	MG	2A	3796	1/1	0.89	0.21	69,69,69,69	0
57	MG	2A	3797	1/1	0.89	0.15	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3325	1/1	0.89	0.17	52,52,52,52	0
57	MG	2A	3171	1/1	0.89	0.23	52,52,52,52	0
57	MG	2A	3568	1/1	0.89	0.08	36,36,36,36	0
57	MG	2A	3172	1/1	0.89	0.12	42,42,42,42	0
57	MG	2A	3574	1/1	0.89	0.09	34,34,34,34	0
57	MG	1A	3157	1/1	0.89	0.15	52,52,52,52	0
57	MG	2a	1804	1/1	0.89	0.20	52,52,52,52	0
57	MG	1A	3552	1/1	0.89	0.12	35,35,35,35	0
57	MG	2A	3180	1/1	0.89	0.14	60,60,60,60	0
57	MG	1A	3317	1/1	0.89	0.15	56,56,56,56	0
57	MG	2A	3338	1/1	0.89	0.31	61,61,61,61	0
57	MG	2A	3586	1/1	0.89	0.27	63,63,63,63	0
57	MG	2a	1815	1/1	0.89	0.24	62,62,62,62	0
57	MG	2a	1818	1/1	0.89	0.12	61,61,61,61	0
57	MG	2A	3840	1/1	0.89	0.10	59,59,59,59	0
57	MG	2A	3343	1/1	0.89	0.16	64,64,64,64	0
57	MG	2a	1824	1/1	0.89	0.25	65,65,65,65	0
57	MG	1a	1646	1/1	0.89	0.31	59,59,59,59	0
57	MG	2B	201	1/1	0.89	0.17	66,66,66,66	0
57	MG	2A	3185	1/1	0.89	0.14	55,55,55,55	0
57	MG	1A	3729	1/1	0.89	0.10	25,25,25,25	0
57	MG	2A	3599	1/1	0.89	0.15	58,58,58,58	0
57	MG	1A	3916	1/1	0.89	0.10	46,46,46,46	0
57	MG	2A	3357	1/1	0.89	0.15	54,54,54,54	0
57	MG	1A	3730	1/1	0.89	0.13	27,27,27,27	0
57	MG	2E	305	1/1	0.89	0.10	34,34,34,34	0
57	MG	2F	307	1/1	0.89	0.29	48,48,48,48	0
57	MG	2A	3364	1/1	0.89	0.23	43,43,43,43	0
57	MG	1A	3922	1/1	0.89	0.08	28,28,28,28	0
57	MG	1A	3440	1/1	0.89	0.21	59,59,59,59	0
57	MG	1A	3388	1/1	0.89	0.20	54,54,54,54	0
57	MG	2A	3133	1/1	0.90	0.32	67,67,67,67	0
57	MG	2A	3328	1/1	0.90	0.31	64,64,64,64	0
57	MG	2D	309	1/1	0.90	0.10	46,46,46,46	0
57	MG	1A	3205	1/1	0.90	0.11	44,44,44,44	0
57	MG	1A	3908	1/1	0.90	0.10	46,46,46,46	0
57	MG	2F	308	1/1	0.90	0.17	55,55,55,55	0
57	MG	2P	201	1/1	0.90	0.17	56,56,56,56	0
57	MG	1O	201	1/1	0.90	0.10	52,52,52,52	0
57	MG	2A	3333	1/1	0.90	0.30	62,62,62,62	0
57	MG	2R	201	1/1	0.90	0.10	57,57,57,57	0
57	MG	2T	202	1/1	0.90	0.16	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	1750	1/1	0.90	0.11	57,57,57,57	0
57	MG	1O	202	1/1	0.90	0.27	49,49,49,49	0
57	MG	1a	1759	1/1	0.90	0.14	73,73,73,73	0
57	MG	1A	3660	1/1	0.90	0.09	31,31,31,31	0
57	MG	2A	3345	1/1	0.90	0.13	66,66,66,66	0
57	MG	2A	3347	1/1	0.90	0.29	61,61,61,61	0
57	MG	25	103	1/1	0.90	0.17	50,50,50,50	0
57	MG	28	102	1/1	0.90	0.22	48,48,48,48	0
57	MG	1T	202	1/1	0.90	0.20	48,48,48,48	0
57	MG	1A	3559	1/1	0.90	0.26	56,56,56,56	0
57	MG	1A	3913	1/1	0.90	0.08	55,55,55,55	0
57	MG	1A	3667	1/1	0.90	0.14	44,44,44,44	0
57	MG	1A	3561	1/1	0.90	0.20	43,43,43,43	0
57	MG	10	102	1/1	0.90	0.21	39,39,39,39	0
57	MG	1A	3670	1/1	0.90	0.10	39,39,39,39	0
57	MG	2A	3626	1/1	0.90	0.10	41,41,41,41	0
57	MG	2A	3366	1/1	0.90	0.20	37,37,37,37	0
57	MG	2A	3630	1/1	0.90	0.12	63,63,63,63	0
57	MG	1A	3562	1/1	0.90	0.18	59,59,59,59	0
57	MG	2A	3368	1/1	0.90	0.22	47,47,47,47	0
57	MG	1A	3166	1/1	0.90	0.16	43,43,43,43	0
57	MG	2A	3371	1/1	0.90	0.15	58,58,58,58	0
57	MG	2A	3639	1/1	0.90	0.15	65,65,65,65	0
57	MG	1A	3569	1/1	0.90	0.10	49,49,49,49	0
57	MG	2A	3374	1/1	0.90	0.19	58,58,58,58	0
57	MG	2A	3642	1/1	0.90	0.11	51,51,51,51	0
57	MG	1a	1798	1/1	0.90	0.10	62,62,62,62	0
57	MG	1A	3325	1/1	0.90	0.11	55,55,55,55	0
57	MG	1A	4053	1/1	0.90	0.09	48,48,48,48	0
57	MG	1A	3180	1/1	0.90	0.09	34,34,34,34	0
57	MG	1A	4057	1/1	0.90	0.14	59,59,59,59	0
57	MG	1A	3015	1/1	0.90	0.19	46,46,46,46	0
57	MG	1a	1809	1/1	0.90	0.23	56,56,56,56	0
57	MG	2A	3389	1/1	0.90	0.30	59,59,59,59	0
57	MG	2a	1642	1/1	0.90	0.27	65,65,65,65	0
57	MG	2A	3197	1/1	0.90	0.18	53,53,53,53	0
57	MG	2a	1651	1/1	0.90	0.17	63,63,63,63	0
57	MG	1a	1614	1/1	0.90	0.28	55,55,55,55	0
57	MG	1A	3939	1/1	0.90	0.11	42,42,42,42	0
57	MG	1A	3690	1/1	0.90	0.15	47,47,47,47	0
57	MG	2A	3207	1/1	0.90	0.19	60,60,60,60	0
57	MG	2a	1673	1/1	0.90	0.20	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	3672	1/1	0.90	0.19	62,62,62,62	0
57	MG	1A	3696	1/1	0.90	0.10	63,63,63,63	0
57	MG	1A	3803	1/1	0.90	0.16	44,44,44,44	0
57	MG	1a	1638	1/1	0.90	0.18	53,53,53,53	0
57	MG	2a	1685	1/1	0.90	0.20	62,62,62,62	0
57	MG	2A	3212	1/1	0.90	0.20	67,67,67,67	0
57	MG	1A	3807	1/1	0.90	0.12	69,69,69,69	0
57	MG	1f	201	1/1	0.90	0.16	42,42,42,42	0
57	MG	2a	1690	1/1	0.90	0.13	64,64,64,64	0
57	MG	2a	1693	1/1	0.90	0.13	54,54,54,54	0
57	MG	1A	3090	1/1	0.90	0.18	63,63,63,63	0
57	MG	2A	3685	1/1	0.90	0.10	52,52,52,52	0
57	MG	2A	3688	1/1	0.90	0.34	42,42,42,42	0
57	MG	1A	3458	1/1	0.90	0.17	57,57,57,57	0
57	MG	2A	3691	1/1	0.90	0.15	63,63,63,63	0
57	MG	1A	3604	1/1	0.90	0.08	20,20,20,20	0
57	MG	1A	3811	1/1	0.90	0.10	51,51,51,51	0
57	MG	1a	1655	1/1	0.90	0.25	58,58,58,58	0
57	MG	1A	3606	1/1	0.90	0.14	49,49,49,49	0
57	MG	2A	3235	1/1	0.90	0.15	59,59,59,59	0
57	MG	1A	3468	1/1	0.90	0.08	40,40,40,40	0
57	MG	1x	107	1/1	0.90	0.23	63,63,63,63	0
57	MG	2a	1723	1/1	0.90	0.17	59,59,59,59	0
57	MG	1A	3270	1/1	0.90	0.20	59,59,59,59	0
57	MG	2A	3725	1/1	0.90	0.20	50,50,50,50	0
57	MG	2A	3450	1/1	0.90	0.15	64,64,64,64	0
57	MG	2A	3454	1/1	0.90	0.21	51,51,51,51	0
57	MG	2A	3250	1/1	0.90	0.20	65,65,65,65	0
57	MG	2A	3253	1/1	0.90	0.15	60,60,60,60	0
57	MG	2A	3254	1/1	0.90	0.16	56,56,56,56	0
57	MG	1A	3819	1/1	0.90	0.08	18,18,18,18	0
57	MG	2a	1748	1/1	0.90	0.10	63,63,63,63	0
57	MG	1A	3976	1/1	0.90	0.08	38,38,38,38	0
57	MG	1A	3353	1/1	0.90	0.29	62,62,62,62	0
57	MG	2a	1764	1/1	0.90	0.17	49,49,49,49	0
57	MG	2A	3263	1/1	0.90	0.17	55,55,55,55	0
57	MG	1A	3493	1/1	0.90	0.12	64,64,64,64	0
57	MG	2A	3483	1/1	0.90	0.11	42,42,42,42	0
57	MG	1a	1671	1/1	0.90	0.28	66,66,66,66	0
57	MG	1A	3002	1/1	0.90	0.17	53,53,53,53	0
57	MG	2A	3499	1/1	0.90	0.16	46,46,46,46	0
57	MG	2a	1778	1/1	0.90	0.10	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3018	1/1	0.90	0.11	41,41,41,41	0
57	MG	2A	3023	1/1	0.90	0.21	54,54,54,54	0
57	MG	2A	3763	1/1	0.90	0.10	51,51,51,51	0
57	MG	1A	3721	1/1	0.90	0.12	40,40,40,40	0
57	MG	1A	3722	1/1	0.90	0.09	14,14,14,14	0
57	MG	2A	3036	1/1	0.90	0.29	57,57,57,57	0
57	MG	1a	1684	1/1	0.90	0.31	58,58,58,58	0
57	MG	2A	3040	1/1	0.90	0.14	46,46,46,46	0
57	MG	2A	3048	1/1	0.90	0.20	60,60,60,60	0
57	MG	2A	3782	1/1	0.90	0.08	54,54,54,54	0
57	MG	2a	1798	1/1	0.90	0.28	61,61,61,61	0
57	MG	2a	1799	1/1	0.90	0.13	63,63,63,63	0
57	MG	2A	3055	1/1	0.90	0.21	70,70,70,70	0
57	MG	2A	3786	1/1	0.90	0.12	55,55,55,55	0
57	MG	2A	3530	1/1	0.90	0.26	54,54,54,54	0
57	MG	2a	1803	1/1	0.90	0.14	69,69,69,69	0
57	MG	2A	3284	1/1	0.90	0.14	58,58,58,58	0
57	MG	1B	226	1/1	0.90	0.11	41,41,41,41	0
57	MG	1A	3723	1/1	0.90	0.09	38,38,38,38	0
57	MG	1a	1697	1/1	0.90	0.09	56,56,56,56	0
57	MG	1A	3283	1/1	0.90	0.19	49,49,49,49	0
57	MG	1A	3289	1/1	0.90	0.15	53,53,53,53	0
57	MG	2A	3080	1/1	0.90	0.15	58,58,58,58	0
57	MG	1A	3194	1/1	0.90	0.14	49,49,49,49	0
57	MG	1A	3122	1/1	0.90	0.12	33,33,33,33	0
57	MG	2A	3820	1/1	0.90	0.10	60,60,60,60	0
57	MG	2A	3303	1/1	0.90	0.17	58,58,58,58	0
57	MG	2A	3823	1/1	0.90	0.17	57,57,57,57	0
57	MG	1A	3873	1/1	0.90	0.17	57,57,57,57	0
57	MG	1A	3645	1/1	0.90	0.24	59,59,59,59	0
57	MG	1a	1719	1/1	0.90	0.19	55,55,55,55	0
57	MG	1A	3647	1/1	0.90	0.09	39,39,39,39	0
57	MG	1A	3439	1/1	0.90	0.25	66,66,66,66	0
57	MG	1A	3652	1/1	0.90	0.13	33,33,33,33	0
57	MG	1A	3311	1/1	0.90	0.17	41,41,41,41	0
57	MG	2A	3318	1/1	0.90	0.14	64,64,64,64	0
57	MG	1A	3906	1/1	0.90	0.09	24,24,24,24	0
57	MG	1F	311	1/1	0.90	0.12	56,56,56,56	0
57	MG	2B	210	1/1	0.90	0.27	66,66,66,66	0
57	MG	2A	3581	1/1	0.90	0.10	43,43,43,43	0
57	MG	2A	3128	1/1	0.90	0.18	59,59,59,59	0
57	MG	2A	3827	1/1	0.91	0.10	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	13	104	1/1	0.91	0.09	45,45,45,45	0
57	MG	1A	4017	1/1	0.91	0.13	63,63,63,63	0
57	MG	2A	3529	1/1	0.91	0.12	51,51,51,51	0
57	MG	1A	4019	1/1	0.91	0.08	52,52,52,52	0
57	MG	2A	3261	1/1	0.91	0.21	54,54,54,54	0
57	MG	16	101	1/1	0.91	0.09	54,54,54,54	0
57	MG	1A	3496	1/1	0.91	0.22	57,57,57,57	0
57	MG	2A	3539	1/1	0.91	0.14	59,59,59,59	0
57	MG	1A	3765	1/1	0.91	0.09	48,48,48,48	0
57	MG	1A	3883	1/1	0.91	0.09	29,29,29,29	0
57	MG	1A	3429	1/1	0.91	0.26	38,38,38,38	0
57	MG	2A	3269	1/1	0.91	0.18	58,58,58,58	0
57	MG	2A	3547	1/1	0.91	0.10	51,51,51,51	0
57	MG	2A	3549	1/1	0.91	0.17	57,57,57,57	0
57	MG	1A	3501	1/1	0.91	0.24	44,44,44,44	0
57	MG	1A	3777	1/1	0.91	0.14	56,56,56,56	0
57	MG	1A	3900	1/1	0.91	0.10	42,42,42,42	0
57	MG	2A	3556	1/1	0.91	0.11	42,42,42,42	0
57	MG	1A	3905	1/1	0.91	0.10	24,24,24,24	0
57	MG	1a	1621	1/1	0.91	0.08	40,40,40,40	0
57	MG	1x	113	1/1	0.91	0.12	55,55,55,55	0
57	MG	2A	3002	1/1	0.91	0.17	49,49,49,49	0
57	MG	2A	3281	1/1	0.91	0.13	58,58,58,58	0
57	MG	1a	1625	1/1	0.91	0.21	60,60,60,60	0
57	MG	1A	3302	1/1	0.91	0.16	47,47,47,47	0
57	MG	1A	3237	1/1	0.91	0.11	44,44,44,44	0
57	MG	1A	3693	1/1	0.91	0.08	42,42,42,42	0
57	MG	1A	3239	1/1	0.91	0.20	66,66,66,66	0
57	MG	1A	3794	1/1	0.91	0.26	58,58,58,58	0
57	MG	1A	4051	1/1	0.91	0.10	47,47,47,47	0
57	MG	25	104	1/1	0.91	0.20	66,66,66,66	0
57	MG	27	101	1/1	0.91	0.13	53,53,53,53	0
57	MG	2A	3035	1/1	0.91	0.25	63,63,63,63	0
57	MG	1A	3515	1/1	0.91	0.13	56,56,56,56	0
57	MG	2A	3037	1/1	0.91	0.15	58,58,58,58	0
57	MG	1A	3914	1/1	0.91	0.13	50,50,50,50	0
57	MG	1A	3241	1/1	0.91	0.10	43,43,43,43	0
57	MG	1a	1653	1/1	0.91	0.11	60,60,60,60	0
57	MG	2A	3051	1/1	0.91	0.20	62,62,62,62	0
57	MG	2A	3310	1/1	0.91	0.21	63,63,63,63	0
57	MG	1A	3797	1/1	0.91	0.09	54,54,54,54	0
57	MG	1A	3918	1/1	0.91	0.12	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1a	1657	1/1	0.91	0.28	54,54,54,54	0
57	MG	2a	1613	1/1	0.91	0.17	55,55,55,55	0
57	MG	2A	3607	1/1	0.91	0.12	55,55,55,55	0
57	MG	1A	3921	1/1	0.91	0.06	39,39,39,39	0
57	MG	2A	3060	1/1	0.91	0.08	40,40,40,40	0
57	MG	1A	3527	1/1	0.91	0.27	49,49,49,49	0
57	MG	1A	4079	1/1	0.91	0.22	53,53,53,53	0
57	MG	1A	3632	1/1	0.91	0.12	31,31,31,31	0
57	MG	1a	1667	1/1	0.91	0.19	66,66,66,66	0
57	MG	1A	3801	1/1	0.91	0.12	60,60,60,60	0
57	MG	2A	3087	1/1	0.91	0.12	38,38,38,38	0
57	MG	1A	3058	1/1	0.91	0.10	43,43,43,43	0
57	MG	1A	3712	1/1	0.91	0.14	42,42,42,42	0
57	MG	1A	3805	1/1	0.91	0.17	51,51,51,51	0
57	MG	1A	3637	1/1	0.91	0.05	18,18,18,18	0
57	MG	1a	1681	1/1	0.91	0.10	58,58,58,58	0
57	MG	2a	1637	1/1	0.91	0.17	53,53,53,53	0
57	MG	2a	1638	1/1	0.91	0.18	52,52,52,52	0
57	MG	1A	3715	1/1	0.91	0.09	35,35,35,35	0
57	MG	2A	3341	1/1	0.91	0.29	50,50,50,50	0
57	MG	2A	3637	1/1	0.91	0.16	56,56,56,56	0
57	MG	1A	3642	1/1	0.91	0.14	46,46,46,46	0
57	MG	2a	1647	1/1	0.91	0.18	64,64,64,64	0
57	MG	2a	1649	1/1	0.91	0.18	54,54,54,54	0
57	MG	1A	3005	1/1	0.91	0.12	43,43,43,43	0
57	MG	2A	3346	1/1	0.91	0.23	67,67,67,67	0
57	MG	2A	3110	1/1	0.91	0.24	58,58,58,58	0
57	MG	2A	3348	1/1	0.91	0.12	54,54,54,54	0
57	MG	2A	3116	1/1	0.91	0.20	53,53,53,53	0
57	MG	1A	4111	1/1	0.91	0.17	42,42,42,42	0
57	MG	2a	1675	1/1	0.91	0.31	56,56,56,56	0
57	MG	2A	3651	1/1	0.91	0.14	48,48,48,48	0
57	MG	2A	3353	1/1	0.91	0.12	55,55,55,55	0
57	MG	2A	3125	1/1	0.91	0.20	48,48,48,48	0
57	MG	2A	3655	1/1	0.91	0.10	48,48,48,48	0
57	MG	1A	3083	1/1	0.91	0.12	51,51,51,51	0
57	MG	2A	3130	1/1	0.91	0.17	54,54,54,54	0
57	MG	1A	3951	1/1	0.91	0.10	22,22,22,22	0
57	MG	2A	3361	1/1	0.91	0.21	61,61,61,61	0
57	MG	2A	3362	1/1	0.91	0.11	56,56,56,56	0
57	MG	2a	1691	1/1	0.91	0.10	58,58,58,58	0
57	MG	1A	4116	1/1	0.91	0.10	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3812	1/1	0.91	0.15	50,50,50,50	0
57	MG	1A	3281	1/1	0.91	0.12	54,54,54,54	0
57	MG	1B	212	1/1	0.91	0.30	59,59,59,59	0
57	MG	1A	3126	1/1	0.91	0.12	50,50,50,50	0
57	MG	1A	3223	1/1	0.91	0.20	51,51,51,51	0
57	MG	2A	3675	1/1	0.91	0.08	60,60,60,60	0
57	MG	2A	3676	1/1	0.91	0.15	44,44,44,44	0
57	MG	1B	221	1/1	0.91	0.11	52,52,52,52	0
57	MG	1A	3284	1/1	0.91	0.27	55,55,55,55	0
57	MG	2a	1713	1/1	0.91	0.31	53,53,53,53	0
57	MG	1B	224	1/1	0.91	0.12	53,53,53,53	0
57	MG	2a	1718	1/1	0.91	0.36	57,57,57,57	0
57	MG	1A	3566	1/1	0.91	0.16	43,43,43,43	0
57	MG	1B	227	1/1	0.91	0.08	37,37,37,37	0
57	MG	1A	3828	1/1	0.91	0.08	40,40,40,40	0
57	MG	2A	3178	1/1	0.91	0.10	64,64,64,64	0
57	MG	1A	3659	1/1	0.91	0.09	38,38,38,38	0
57	MG	1A	3970	1/1	0.91	0.06	27,27,27,27	0
57	MG	1A	3350	1/1	0.91	0.12	64,64,64,64	0
57	MG	1a	1742	1/1	0.91	0.13	53,53,53,53	0
57	MG	2A	3392	1/1	0.91	0.13	47,47,47,47	0
57	MG	1a	1746	1/1	0.91	0.10	64,64,64,64	0
57	MG	2a	1736	1/1	0.91	0.11	56,56,56,56	0
57	MG	2A	3394	1/1	0.91	0.13	47,47,47,47	0
57	MG	2A	3187	1/1	0.91	0.18	59,59,59,59	0
57	MG	2a	1749	1/1	0.91	0.12	64,64,64,64	0
57	MG	1B	234	1/1	0.91	0.13	66,66,66,66	0
57	MG	1A	3975	1/1	0.91	0.08	43,43,43,43	0
57	MG	1A	3412	1/1	0.91	0.14	44,44,44,44	0
57	MG	1a	1765	1/1	0.91	0.12	67,67,67,67	0
57	MG	1A	3979	1/1	0.91	0.12	43,43,43,43	0
57	MG	1a	1768	1/1	0.91	0.09	72,72,72,72	0
57	MG	1a	1776	1/1	0.91	0.31	48,48,48,48	0
57	MG	1A	3842	1/1	0.91	0.16	30,30,30,30	0
57	MG	1A	3982	1/1	0.91	0.08	55,55,55,55	0
57	MG	2A	3735	1/1	0.91	0.11	63,63,63,63	0
57	MG	1A	3986	1/1	0.91	0.09	57,57,57,57	0
57	MG	2A	3740	1/1	0.91	0.07	44,44,44,44	0
57	MG	1A	3844	1/1	0.91	0.08	27,27,27,27	0
57	MG	2A	3204	1/1	0.91	0.15	44,44,44,44	0
57	MG	2A	3205	1/1	0.91	0.12	47,47,47,47	0
57	MG	2A	3745	1/1	0.91	0.08	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	3845	1/1	0.91	0.06	35,35,35,35	0
57	MG	1A	3846	1/1	0.91	0.10	38,38,38,38	0
57	MG	2a	1791	1/1	0.91	0.26	56,56,56,56	0
57	MG	2A	3430	1/1	0.91	0.14	58,58,58,58	0
57	MG	1A	3158	1/1	0.91	0.10	38,38,38,38	0
57	MG	2A	3759	1/1	0.91	0.08	55,55,55,55	0
57	MG	2A	3760	1/1	0.91	0.12	60,60,60,60	0
57	MG	1A	3488	1/1	0.91	0.10	42,42,42,42	0
57	MG	1A	3743	1/1	0.91	0.11	25,25,25,25	0
57	MG	2A	3214	1/1	0.91	0.14	53,53,53,53	0
57	MG	1A	3364	1/1	0.91	0.10	66,66,66,66	0
57	MG	2A	3457	1/1	0.91	0.14	60,60,60,60	0
57	MG	2A	3220	1/1	0.91	0.14	49,49,49,49	0
57	MG	2A	3773	1/1	0.91	0.09	25,25,25,25	0
57	MG	2a	1809	1/1	0.91	0.23	68,68,68,68	0
57	MG	1O	205	1/1	0.91	0.11	45,45,45,45	0
57	MG	2A	3224	1/1	0.91	0.15	43,43,43,43	0
57	MG	1A	3856	1/1	0.91	0.12	20,20,20,20	0
57	MG	1Q	204	1/1	0.91	0.14	64,64,64,64	0
57	MG	1R	205	1/1	0.91	0.12	43,43,43,43	0
57	MG	1S	202	1/1	0.91	0.11	49,49,49,49	0
57	MG	1A	3596	1/1	0.91	0.10	21,21,21,21	0
57	MG	2a	1821	1/1	0.91	0.17	58,58,58,58	0
57	MG	2a	1822	1/1	0.91	0.12	61,61,61,61	0
57	MG	2a	1823	1/1	0.91	0.14	48,48,48,48	0
57	MG	1A	3864	1/1	0.91	0.09	42,42,42,42	0
57	MG	1A	3868	1/1	0.91	0.12	42,42,42,42	0
57	MG	2a	1826	1/1	0.91	0.09	62,62,62,62	0
57	MG	2A	3239	1/1	0.91	0.15	60,60,60,60	0
57	MG	2A	3498	1/1	0.91	0.08	34,34,34,34	0
57	MG	1V	204	1/1	0.91	0.19	49,49,49,49	0
57	MG	1A	3870	1/1	0.91	0.17	52,52,52,52	0
57	MG	2A	3247	1/1	0.91	0.11	57,57,57,57	0
57	MG	1A	3675	1/1	0.91	0.20	53,53,53,53	0
57	MG	2A	3511	1/1	0.91	0.09	38,38,38,38	0
57	MG	1A	3295	1/1	0.91	0.13	44,44,44,44	0
57	MG	2w	101	1/1	0.91	0.19	61,61,61,61	0
57	MG	2A	3251	1/1	0.91	0.13	50,50,50,50	0
57	MG	1O	103	1/1	0.91	0.11	42,42,42,42	0
57	MG	2A	3824	1/1	0.91	0.17	59,59,59,59	0
57	MG	2x	101	1/1	0.91	0.20	59,59,59,59	0
57	MG	1A	3876	1/1	0.91	0.15	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3826	1/1	0.91	0.14	67,67,67,67	0
57	MG	1A	3772	1/1	0.92	0.13	49,49,49,49	0
57	MG	1A	3656	1/1	0.92	0.08	52,52,52,52	0
57	MG	1A	3776	1/1	0.92	0.10	59,59,59,59	0
57	MG	2A	3512	1/1	0.92	0.13	64,64,64,64	0
57	MG	1x	106	1/1	0.92	0.20	62,62,62,62	0
57	MG	1A	3529	1/1	0.92	0.12	54,54,54,54	0
57	MG	2A	3833	1/1	0.92	0.08	49,49,49,49	0
57	MG	1A	3778	1/1	0.92	0.15	58,58,58,58	0
57	MG	2A	3837	1/1	0.92	0.20	56,56,56,56	0
57	MG	1A	4049	1/1	0.92	0.23	67,67,67,67	0
57	MG	1A	3546	1/1	0.92	0.13	44,44,44,44	0
57	MG	2A	3522	1/1	0.92	0.26	58,58,58,58	0
57	MG	1A	3912	1/1	0.92	0.09	67,67,67,67	0
57	MG	2A	3524	1/1	0.92	0.14	53,53,53,53	0
57	MG	1A	3663	1/1	0.92	0.24	53,53,53,53	0
57	MG	2A	3001	1/1	0.92	0.12	54,54,54,54	0
57	MG	2B	205	1/1	0.92	0.12	61,61,61,61	0
57	MG	1A	3276	1/1	0.92	0.32	50,50,50,50	0
57	MG	1A	4056	1/1	0.92	0.10	45,45,45,45	0
57	MG	1a	1634	1/1	0.92	0.20	60,60,60,60	0
57	MG	1a	1635	1/1	0.92	0.26	56,56,56,56	0
57	MG	2B	215	1/1	0.92	0.13	63,63,63,63	0
57	MG	2A	3272	1/1	0.92	0.23	56,56,56,56	0
57	MG	1A	3280	1/1	0.92	0.34	53,53,53,53	0
57	MG	1A	4058	1/1	0.92	0.11	43,43,43,43	0
57	MG	1A	3370	1/1	0.92	0.12	58,58,58,58	0
57	MG	2F	305	1/1	0.92	0.11	47,47,47,47	0
57	MG	2A	3027	1/1	0.92	0.15	49,49,49,49	0
57	MG	1A	3308	1/1	0.92	0.10	54,54,54,54	0
57	MG	2G	201	1/1	0.92	0.14	58,58,58,58	0
57	MG	2N	201	1/1	0.92	0.14	64,64,64,64	0
57	MG	1A	4072	1/1	0.92	0.12	34,34,34,34	0
57	MG	1A	3560	1/1	0.92	0.18	58,58,58,58	0
57	MG	2A	3283	1/1	0.92	0.17	53,53,53,53	0
57	MG	1A	3674	1/1	0.92	0.10	51,51,51,51	0
57	MG	2A	3038	1/1	0.92	0.10	48,48,48,48	0
57	MG	2A	3286	1/1	0.92	0.19	64,64,64,64	0
57	MG	2A	3559	1/1	0.92	0.17	56,56,56,56	0
57	MG	2V	202	1/1	0.92	0.13	52,52,52,52	0
57	MG	1A	3376	1/1	0.92	0.18	43,43,43,43	0
57	MG	2A	3289	1/1	0.92	0.22	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	20	101	1/1	0.92	0.21	57,57,57,57	0
57	MG	1A	3085	1/1	0.92	0.11	51,51,51,51	0
57	MG	2A	3566	1/1	0.92	0.15	42,42,42,42	0
57	MG	25	102	1/1	0.92	0.14	46,46,46,46	0
57	MG	2A	3046	1/1	0.92	0.22	66,66,66,66	0
57	MG	1A	3119	1/1	0.92	0.17	47,47,47,47	0
57	MG	2A	3295	1/1	0.92	0.10	53,53,53,53	0
57	MG	1A	4084	1/1	0.92	0.11	45,45,45,45	0
57	MG	1A	3928	1/1	0.92	0.09	23,23,23,23	0
57	MG	1A	3929	1/1	0.92	0.10	44,44,44,44	0
57	MG	2A	3302	1/1	0.92	0.11	57,57,57,57	0
57	MG	1A	3380	1/1	0.92	0.09	45,45,45,45	0
57	MG	1A	3934	1/1	0.92	0.17	55,55,55,55	0
57	MG	2A	3585	1/1	0.92	0.10	58,58,58,58	0
57	MG	1A	4097	1/1	0.92	0.15	57,57,57,57	0
57	MG	1A	3444	1/1	0.92	0.12	45,45,45,45	0
57	MG	2A	3066	1/1	0.92	0.17	68,68,68,68	0
57	MG	1A	3937	1/1	0.92	0.07	62,62,62,62	0
57	MG	1a	1672	1/1	0.92	0.28	57,57,57,57	0
57	MG	1a	1675	1/1	0.92	0.18	62,62,62,62	0
57	MG	1A	3313	1/1	0.92	0.22	60,60,60,60	0
57	MG	2A	3086	1/1	0.92	0.12	42,42,42,42	0
57	MG	1A	4108	1/1	0.92	0.09	53,53,53,53	0
57	MG	2A	3605	1/1	0.92	0.12	52,52,52,52	0
57	MG	2A	3606	1/1	0.92	0.10	45,45,45,45	0
57	MG	1A	3385	1/1	0.92	0.07	44,44,44,44	0
57	MG	2A	3609	1/1	0.92	0.11	47,47,47,47	0
57	MG	1A	3575	1/1	0.92	0.10	48,48,48,48	0
57	MG	1A	3945	1/1	0.92	0.12	57,57,57,57	0
57	MG	1a	1687	1/1	0.92	0.14	47,47,47,47	0
57	MG	1A	3578	1/1	0.92	0.10	43,43,43,43	0
57	MG	1a	1690	1/1	0.92	0.29	57,57,57,57	0
57	MG	1A	3246	1/1	0.92	0.15	37,37,37,37	0
57	MG	2a	1636	1/1	0.92	0.15	56,56,56,56	0
57	MG	1a	1695	1/1	0.92	0.14	49,49,49,49	0
57	MG	2A	3107	1/1	0.92	0.18	62,62,62,62	0
57	MG	2a	1639	1/1	0.92	0.20	63,63,63,63	0
57	MG	2A	3625	1/1	0.92	0.10	47,47,47,47	0
57	MG	1A	3588	1/1	0.92	0.11	49,49,49,49	0
57	MG	2A	3336	1/1	0.92	0.17	48,48,48,48	0
57	MG	2A	3111	1/1	0.92	0.22	63,63,63,63	0
57	MG	2A	3340	1/1	0.92	0.18	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3322	1/1	0.92	0.15	66,66,66,66	0
57	MG	1A	3954	1/1	0.92	0.20	47,47,47,47	0
57	MG	2A	3344	1/1	0.92	0.12	65,65,65,65	0
57	MG	2A	3120	1/1	0.92	0.13	61,61,61,61	0
57	MG	1A	3705	1/1	0.92	0.10	19,19,19,19	0
57	MG	1A	3456	1/1	0.92	0.11	44,44,44,44	0
57	MG	2a	1671	1/1	0.92	0.21	47,47,47,47	0
57	MG	2a	1672	1/1	0.92	0.26	57,57,57,57	0
57	MG	1A	3710	1/1	0.92	0.08	57,57,57,57	0
57	MG	2A	3132	1/1	0.92	0.26	53,53,53,53	0
57	MG	2a	1676	1/1	0.92	0.08	66,66,66,66	0
57	MG	1A	3597	1/1	0.92	0.10	54,54,54,54	0
57	MG	2A	3647	1/1	0.92	0.13	30,30,30,30	0
57	MG	1a	1715	1/1	0.92	0.07	46,46,46,46	0
57	MG	2A	3138	1/1	0.92	0.17	45,45,45,45	0
57	MG	2A	3141	1/1	0.92	0.16	59,59,59,59	0
57	MG	2A	3149	1/1	0.92	0.15	63,63,63,63	0
57	MG	1A	3225	1/1	0.92	0.15	50,50,50,50	0
57	MG	1a	1720	1/1	0.92	0.08	54,54,54,54	0
57	MG	1A	3827	1/1	0.92	0.12	53,53,53,53	0
57	MG	2A	3657	1/1	0.92	0.12	43,43,43,43	0
57	MG	2a	1692	1/1	0.92	0.12	58,58,58,58	0
57	MG	1a	1724	1/1	0.92	0.10	50,50,50,50	0
57	MG	2a	1696	1/1	0.92	0.20	57,57,57,57	0
57	MG	2A	3365	1/1	0.92	0.20	46,46,46,46	0
57	MG	1A	3464	1/1	0.92	0.23	54,54,54,54	0
57	MG	1A	3714	1/1	0.92	0.10	52,52,52,52	0
57	MG	2a	1700	1/1	0.92	0.33	62,62,62,62	0
57	MG	1A	3286	1/1	0.92	0.36	64,64,64,64	0
57	MG	2A	3369	1/1	0.92	0.15	35,35,35,35	0
57	MG	1a	1732	1/1	0.92	0.14	63,63,63,63	0
57	MG	1A	3472	1/1	0.92	0.11	61,61,61,61	0
57	MG	1B	233	1/1	0.92	0.10	45,45,45,45	0
57	MG	1A	3474	1/1	0.92	0.10	48,48,48,48	0
57	MG	1A	3619	1/1	0.92	0.13	50,50,50,50	0
57	MG	1A	3720	1/1	0.92	0.11	44,44,44,44	0
57	MG	2a	1717	1/1	0.92	0.19	49,49,49,49	0
57	MG	2A	3380	1/1	0.92	0.26	53,53,53,53	0
57	MG	2a	1719	1/1	0.92	0.22	62,62,62,62	0
57	MG	1A	3622	1/1	0.92	0.07	25,25,25,25	0
57	MG	1A	3121	1/1	0.92	0.14	63,63,63,63	0
57	MG	2A	3384	1/1	0.92	0.12	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	1747	1/1	0.92	0.10	40,40,40,40	0
57	MG	2A	3183	1/1	0.92	0.14	59,59,59,59	0
57	MG	1A	3625	1/1	0.92	0.06	18,18,18,18	0
57	MG	1A	3481	1/1	0.92	0.16	56,56,56,56	0
57	MG	1a	1752	1/1	0.92	0.13	50,50,50,50	0
57	MG	2A	3693	1/1	0.92	0.08	48,48,48,48	0
57	MG	1A	3728	1/1	0.92	0.08	31,31,31,31	0
57	MG	1A	3292	1/1	0.92	0.10	57,57,57,57	0
57	MG	1E	315	1/1	0.92	0.09	34,34,34,34	0
57	MG	2a	1747	1/1	0.92	0.11	65,65,65,65	0
57	MG	2A	3704	1/1	0.92	0.12	57,57,57,57	0
57	MG	1A	3857	1/1	0.92	0.08	30,30,30,30	0
57	MG	2a	1753	1/1	0.92	0.18	62,62,62,62	0
57	MG	2A	3716	1/1	0.92	0.09	56,56,56,56	0
57	MG	2A	3397	1/1	0.92	0.24	36,36,36,36	0
57	MG	2a	1762	1/1	0.92	0.18	46,46,46,46	0
57	MG	2A	3719	1/1	0.92	0.07	35,35,35,35	0
57	MG	1A	3336	1/1	0.92	0.14	50,50,50,50	0
57	MG	1A	3861	1/1	0.92	0.13	29,29,29,29	0
57	MG	2a	1767	1/1	0.92	0.12	57,57,57,57	0
57	MG	1N	201	1/1	0.92	0.15	39,39,39,39	0
57	MG	2A	3724	1/1	0.92	0.12	44,44,44,44	0
57	MG	1A	3862	1/1	0.92	0.09	48,48,48,48	0
57	MG	1A	3340	1/1	0.92	0.11	47,47,47,47	0
57	MG	2a	1775	1/1	0.92	0.23	55,55,55,55	0
57	MG	2a	1776	1/1	0.92	0.26	55,55,55,55	0
57	MG	2A	3200	1/1	0.92	0.12	64,64,64,64	0
57	MG	1O	203	1/1	0.92	0.15	52,52,52,52	0
57	MG	2A	3202	1/1	0.92	0.19	58,58,58,58	0
57	MG	1A	3269	1/1	0.92	0.21	48,48,48,48	0
57	MG	1A	3417	1/1	0.92	0.11	53,53,53,53	0
57	MG	1A	3346	1/1	0.92	0.12	40,40,40,40	0
57	MG	2A	3736	1/1	0.92	0.09	73,73,73,73	0
57	MG	2A	3421	1/1	0.92	0.20	56,56,56,56	0
57	MG	2A	3738	1/1	0.92	0.10	55,55,55,55	0
57	MG	2A	3422	1/1	0.92	0.10	58,58,58,58	0
57	MG	1A	3420	1/1	0.92	0.14	56,56,56,56	0
57	MG	2A	3426	1/1	0.92	0.09	41,41,41,41	0
57	MG	1A	4009	1/1	0.92	0.06	30,30,30,30	0
57	MG	1A	4010	1/1	0.92	0.07	41,41,41,41	0
57	MG	1A	3421	1/1	0.92	0.14	40,40,40,40	0
57	MG	1A	3512	1/1	0.92	0.12	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3435	1/1	0.92	0.09	43,43,43,43	0
57	MG	2A	3751	1/1	0.92	0.12	42,42,42,42	0
57	MG	2A	3437	1/1	0.92	0.19	54,54,54,54	0
57	MG	1A	4016	1/1	0.92	0.06	11,11,11,11	0
57	MG	1V	207	1/1	0.92	0.09	46,46,46,46	0
57	MG	1A	3756	1/1	0.92	0.11	46,46,46,46	0
57	MG	2A	3449	1/1	0.92	0.20	52,52,52,52	0
57	MG	1A	4018	1/1	0.92	0.13	53,53,53,53	0
57	MG	2A	3451	1/1	0.92	0.12	35,35,35,35	0
57	MG	2A	3452	1/1	0.92	0.13	40,40,40,40	0
57	MG	1A	3300	1/1	0.92	0.07	36,36,36,36	0
57	MG	1A	3425	1/1	0.92	0.11	54,54,54,54	0
57	MG	1A	3518	1/1	0.92	0.14	51,51,51,51	0
57	MG	2A	3231	1/1	0.92	0.12	57,57,57,57	0
57	MG	2A	3467	1/1	0.92	0.10	34,34,34,34	0
57	MG	2A	3469	1/1	0.92	0.07	33,33,33,33	0
57	MG	11	105	1/1	0.92	0.10	47,47,47,47	0
57	MG	1A	3887	1/1	0.92	0.09	48,48,48,48	0
57	MG	2A	3789	1/1	0.92	0.11	60,60,60,60	0
57	MG	2a	1828	1/1	0.92	0.15	63,63,63,63	0
57	MG	2e	201	1/1	0.92	0.07	56,56,56,56	0
57	MG	1A	3888	1/1	0.92	0.08	52,52,52,52	0
57	MG	15	105	1/1	0.92	0.16	30,30,30,30	0
57	MG	2A	3795	1/1	0.92	0.10	49,49,49,49	0
57	MG	2A	3236	1/1	0.92	0.11	67,67,67,67	0
57	MG	2A	3237	1/1	0.92	0.11	66,66,66,66	0
57	MG	1A	3206	1/1	0.92	0.15	59,59,59,59	0
57	MG	1f	202	1/1	0.92	0.09	65,65,65,65	0
57	MG	1A	4034	1/1	0.92	0.09	49,49,49,49	0
57	MG	2A	3806	1/1	0.92	0.14	65,65,65,65	0
57	MG	2w	102	1/1	0.92	0.11	74,74,74,74	0
57	MG	1A	3893	1/1	0.92	0.07	35,35,35,35	0
57	MG	18	104	1/1	0.92	0.12	45,45,45,45	0
57	MG	2A	3500	1/1	0.92	0.13	59,59,59,59	0
57	MG	2A	3815	1/1	0.92	0.09	63,63,63,63	0
57	MG	2A	3816	1/1	0.92	0.09	61,61,61,61	0
57	MG	1A	3427	1/1	0.92	0.12	44,44,44,44	0
57	MG	2A	3812	1/1	0.93	0.16	58,58,58,58	0
57	MG	1A	3471	1/1	0.93	0.08	51,51,51,51	0
57	MG	1A	3285	1/1	0.93	0.16	50,50,50,50	0
57	MG	2A	3818	1/1	0.93	0.12	72,72,72,72	0
57	MG	1A	3473	1/1	0.93	0.09	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3506	1/1	0.93	0.13	28,28,28,28	0
57	MG	2A	3507	1/1	0.93	0.10	38,38,38,38	0
57	MG	1A	3698	1/1	0.93	0.08	47,47,47,47	0
57	MG	1A	3331	1/1	0.93	0.09	48,48,48,48	0
57	MG	1A	3133	1/1	0.93	0.08	49,49,49,49	0
57	MG	1A	4085	1/1	0.93	0.10	48,48,48,48	0
57	MG	2A	3829	1/1	0.93	0.07	53,53,53,53	0
57	MG	2A	3832	1/1	0.93	0.09	57,57,57,57	0
57	MG	1A	3601	1/1	0.93	0.13	48,48,48,48	0
57	MG	1A	3944	1/1	0.93	0.08	55,55,55,55	0
57	MG	1A	3409	1/1	0.93	0.10	39,39,39,39	0
57	MG	1A	3816	1/1	0.93	0.17	42,42,42,42	0
57	MG	2A	3013	1/1	0.93	0.18	52,52,52,52	0
57	MG	1A	4096	1/1	0.93	0.12	58,58,58,58	0
57	MG	1A	3603	1/1	0.93	0.10	45,45,45,45	0
57	MG	2A	3020	1/1	0.93	0.13	40,40,40,40	0
57	MG	1A	3950	1/1	0.93	0.13	34,34,34,34	0
57	MG	1A	4099	1/1	0.93	0.08	44,44,44,44	0
57	MG	2B	204	1/1	0.93	0.17	49,49,49,49	0
57	MG	1A	3483	1/1	0.93	0.24	34,34,34,34	0
57	MG	2B	206	1/1	0.93	0.10	50,50,50,50	0
57	MG	2B	208	1/1	0.93	0.09	71,71,71,71	0
57	MG	2A	3031	1/1	0.93	0.14	49,49,49,49	0
57	MG	2A	3274	1/1	0.93	0.21	64,64,64,64	0
57	MG	1A	3134	1/1	0.93	0.10	33,33,33,33	0
57	MG	2B	212	1/1	0.93	0.09	64,64,64,64	0
57	MG	1A	3822	1/1	0.93	0.11	47,47,47,47	0
57	MG	2B	214	1/1	0.93	0.19	54,54,54,54	0
57	MG	1A	3955	1/1	0.93	0.09	40,40,40,40	0
57	MG	1A	3490	1/1	0.93	0.10	46,46,46,46	0
57	MG	2B	218	1/1	0.93	0.26	67,67,67,67	0
57	MG	1A	3610	1/1	0.93	0.08	26,26,26,26	0
57	MG	1A	3242	1/1	0.93	0.10	53,53,53,53	0
57	MG	2E	302	1/1	0.93	0.07	51,51,51,51	0
57	MG	1A	4117	1/1	0.93	0.25	50,50,50,50	0
57	MG	2E	306	1/1	0.93	0.15	57,57,57,57	0
57	MG	2A	3550	1/1	0.93	0.08	26,26,26,26	0
57	MG	2A	3041	1/1	0.93	0.26	51,51,51,51	0
57	MG	2A	3045	1/1	0.93	0.08	50,50,50,50	0
57	MG	2A	3553	1/1	0.93	0.12	49,49,49,49	0
57	MG	1A	3204	1/1	0.93	0.10	36,36,36,36	0
57	MG	2A	3555	1/1	0.93	0.11	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1a	1674	1/1	0.93	0.22	44,44,44,44	0
57	MG	1A	3343	1/1	0.93	0.08	44,44,44,44	0
57	MG	2A	3052	1/1	0.93	0.14	49,49,49,49	0
57	MG	2T	201	1/1	0.93	0.07	52,52,52,52	0
57	MG	1a	1676	1/1	0.93	0.18	49,49,49,49	0
57	MG	2A	3560	1/1	0.93	0.09	33,33,33,33	0
57	MG	1a	1677	1/1	0.93	0.21	46,46,46,46	0
57	MG	1B	207	1/1	0.93	0.12	50,50,50,50	0
57	MG	2W	201	1/1	0.93	0.09	50,50,50,50	0
57	MG	1A	3833	1/1	0.93	0.10	27,27,27,27	0
57	MG	1A	3345	1/1	0.93	0.07	35,35,35,35	0
57	MG	1A	3298	1/1	0.93	0.33	53,53,53,53	0
57	MG	2A	3570	1/1	0.93	0.16	54,54,54,54	0
57	MG	21	102	1/1	0.93	0.18	49,49,49,49	0
57	MG	21	103	1/1	0.93	0.11	49,49,49,49	0
57	MG	2A	3300	1/1	0.93	0.10	63,63,63,63	0
57	MG	1B	216	1/1	0.93	0.07	60,60,60,60	0
57	MG	2A	3067	1/1	0.93	0.10	41,41,41,41	0
57	MG	2A	3072	1/1	0.93	0.10	44,44,44,44	0
57	MG	2A	3074	1/1	0.93	0.19	56,56,56,56	0
57	MG	2A	3308	1/1	0.93	0.10	54,54,54,54	0
57	MG	2A	3075	1/1	0.93	0.12	48,48,48,48	0
57	MG	1A	3502	1/1	0.93	0.20	44,44,44,44	0
57	MG	1A	3503	1/1	0.93	0.25	46,46,46,46	0
57	MG	2A	3312	1/1	0.93	0.21	64,64,64,64	0
57	MG	1B	223	1/1	0.93	0.11	41,41,41,41	0
57	MG	1A	3349	1/1	0.93	0.15	35,35,35,35	0
57	MG	2A	3591	1/1	0.93	0.24	51,51,51,51	0
57	MG	2a	1608	1/1	0.93	0.32	66,66,66,66	0
57	MG	2a	1609	1/1	0.93	0.21	62,62,62,62	0
57	MG	1B	225	1/1	0.93	0.07	43,43,43,43	0
57	MG	1A	3171	1/1	0.93	0.10	42,42,42,42	0
57	MG	1a	1698	1/1	0.93	0.08	55,55,55,55	0
57	MG	2A	3322	1/1	0.93	0.16	50,50,50,50	0
57	MG	2a	1614	1/1	0.93	0.14	60,60,60,60	0
57	MG	2a	1615	1/1	0.93	0.13	69,69,69,69	0
57	MG	2A	3323	1/1	0.93	0.14	58,58,58,58	0
57	MG	1a	1700	1/1	0.93	0.18	38,38,38,38	0
57	MG	1A	3848	1/1	0.93	0.06	24,24,24,24	0
57	MG	1a	1703	1/1	0.93	0.08	44,44,44,44	0
57	MG	1a	1704	1/1	0.93	0.14	51,51,51,51	0
57	MG	1a	1705	1/1	0.93	0.12	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3727	1/1	0.93	0.05	22,22,22,22	0
57	MG	2A	3611	1/1	0.93	0.12	60,60,60,60	0
57	MG	2A	3613	1/1	0.93	0.11	41,41,41,41	0
57	MG	2A	3098	1/1	0.93	0.12	45,45,45,45	0
57	MG	2A	3101	1/1	0.93	0.08	63,63,63,63	0
57	MG	2A	3104	1/1	0.93	0.14	49,49,49,49	0
57	MG	1A	3301	1/1	0.93	0.11	51,51,51,51	0
57	MG	1A	3175	1/1	0.93	0.09	41,41,41,41	0
57	MG	2A	3621	1/1	0.93	0.17	44,44,44,44	0
57	MG	1A	3264	1/1	0.93	0.07	37,37,37,37	0
57	MG	1A	3431	1/1	0.93	0.16	58,58,58,58	0
57	MG	2A	3115	1/1	0.93	0.08	58,58,58,58	0
57	MG	1A	3643	1/1	0.93	0.11	46,46,46,46	0
57	MG	1a	1716	1/1	0.93	0.24	61,61,61,61	0
57	MG	1A	3859	1/1	0.93	0.16	63,63,63,63	0
57	MG	2a	1645	1/1	0.93	0.07	63,63,63,63	0
57	MG	1A	3998	1/1	0.93	0.06	31,31,31,31	0
57	MG	1A	3522	1/1	0.93	0.30	41,41,41,41	0
57	MG	1A	3523	1/1	0.93	0.13	41,41,41,41	0
57	MG	1A	3736	1/1	0.93	0.08	15,15,15,15	0
57	MG	2a	1653	1/1	0.93	0.36	65,65,65,65	0
57	MG	1a	1726	1/1	0.93	0.10	52,52,52,52	0
57	MG	2A	3134	1/1	0.93	0.20	58,58,58,58	0
57	MG	1A	3865	1/1	0.93	0.09	50,50,50,50	0
57	MG	1A	3741	1/1	0.93	0.07	27,27,27,27	0
57	MG	2a	1669	1/1	0.93	0.14	58,58,58,58	0
57	MG	2a	1670	1/1	0.93	0.17	54,54,54,54	0
57	MG	1E	313	1/1	0.93	0.12	36,36,36,36	0
57	MG	2A	3144	1/1	0.93	0.12	46,46,46,46	0
57	MG	2A	3644	1/1	0.93	0.11	49,49,49,49	0
57	MG	1A	3369	1/1	0.93	0.08	40,40,40,40	0
57	MG	1A	4005	1/1	0.93	0.08	39,39,39,39	0
57	MG	1A	3433	1/1	0.93	0.12	33,33,33,33	0
57	MG	2a	1679	1/1	0.93	0.35	58,58,58,58	0
57	MG	1A	3305	1/1	0.93	0.18	51,51,51,51	0
57	MG	2A	3156	1/1	0.93	0.12	41,41,41,41	0
57	MG	1A	3755	1/1	0.93	0.15	53,53,53,53	0
57	MG	1A	3014	1/1	0.93	0.10	37,37,37,37	0
57	MG	1A	3760	1/1	0.93	0.16	29,29,29,29	0
57	MG	1A	3095	1/1	0.93	0.24	46,46,46,46	0
57	MG	1A	3762	1/1	0.93	0.09	37,37,37,37	0
57	MG	2A	3170	1/1	0.93	0.10	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3655	1/1	0.93	0.10	26,26,26,26	0
57	MG	1A	3551	1/1	0.93	0.21	35,35,35,35	0
57	MG	1A	3657	1/1	0.93	0.13	28,28,28,28	0
57	MG	2a	1694	1/1	0.93	0.18	57,57,57,57	0
57	MG	2a	1695	1/1	0.93	0.22	52,52,52,52	0
57	MG	2A	3378	1/1	0.93	0.31	58,58,58,58	0
57	MG	2A	3669	1/1	0.93	0.15	51,51,51,51	0
57	MG	2A	3175	1/1	0.93	0.10	46,46,46,46	0
57	MG	2A	3176	1/1	0.93	0.14	52,52,52,52	0
57	MG	1R	201	1/1	0.93	0.09	43,43,43,43	0
57	MG	1A	3658	1/1	0.93	0.13	39,39,39,39	0
57	MG	2a	1703	1/1	0.93	0.30	57,57,57,57	0
57	MG	2a	1704	1/1	0.93	0.18	62,62,62,62	0
57	MG	1R	206	1/1	0.93	0.15	41,41,41,41	0
57	MG	1a	1771	1/1	0.93	0.08	51,51,51,51	0
57	MG	2A	3677	1/1	0.93	0.09	57,57,57,57	0
57	MG	1a	1775	1/1	0.93	0.20	47,47,47,47	0
57	MG	1A	3310	1/1	0.93	0.18	44,44,44,44	0
57	MG	1A	3895	1/1	0.93	0.07	38,38,38,38	0
57	MG	2A	3186	1/1	0.93	0.15	56,56,56,56	0
57	MG	1A	4028	1/1	0.93	0.11	27,27,27,27	0
57	MG	2A	3684	1/1	0.93	0.10	53,53,53,53	0
57	MG	1a	1780	1/1	0.93	0.16	58,58,58,58	0
57	MG	2a	1720	1/1	0.93	0.28	67,67,67,67	0
57	MG	2A	3686	1/1	0.93	0.10	36,36,36,36	0
57	MG	1U	203	1/1	0.93	0.12	47,47,47,47	0
57	MG	1A	3224	1/1	0.93	0.09	47,47,47,47	0
57	MG	2A	3690	1/1	0.93	0.14	60,60,60,60	0
57	MG	1A	3904	1/1	0.93	0.07	45,45,45,45	0
57	MG	2a	1726	1/1	0.93	0.15	66,66,66,66	0
57	MG	1A	3661	1/1	0.93	0.08	22,22,22,22	0
57	MG	2A	3694	1/1	0.93	0.20	57,57,57,57	0
57	MG	1W	202	1/1	0.93	0.08	44,44,44,44	0
57	MG	1A	3556	1/1	0.93	0.19	43,43,43,43	0
57	MG	2A	3697	1/1	0.93	0.10	48,48,48,48	0
57	MG	2A	3699	1/1	0.93	0.12	39,39,39,39	0
57	MG	2a	1738	1/1	0.93	0.12	63,63,63,63	0
57	MG	2a	1739	1/1	0.93	0.09	82,82,82,82	0
57	MG	2A	3406	1/1	0.93	0.23	55,55,55,55	0
57	MG	2a	1744	1/1	0.93	0.06	46,46,46,46	0
57	MG	2A	3702	1/1	0.93	0.17	58,58,58,58	0
57	MG	1A	3277	1/1	0.93	0.19	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3779	1/1	0.93	0.07	25,25,25,25	0
57	MG	2a	1751	1/1	0.93	0.10	42,42,42,42	0
57	MG	2A	3715	1/1	0.93	0.08	32,32,32,32	0
57	MG	1A	3382	1/1	0.93	0.27	56,56,56,56	0
57	MG	1A	3450	1/1	0.93	0.15	35,35,35,35	0
57	MG	2A	3413	1/1	0.93	0.24	47,47,47,47	0
57	MG	2a	1763	1/1	0.93	0.07	49,49,49,49	0
57	MG	1a	1801	1/1	0.93	0.13	57,57,57,57	0
57	MG	1A	3113	1/1	0.93	0.18	41,41,41,41	0
57	MG	1a	1804	1/1	0.93	0.13	54,54,54,54	0
57	MG	2A	3418	1/1	0.93	0.18	51,51,51,51	0
57	MG	2a	1768	1/1	0.93	0.27	67,67,67,67	0
57	MG	2A	3419	1/1	0.93	0.23	64,64,64,64	0
57	MG	2A	3420	1/1	0.93	0.07	36,36,36,36	0
57	MG	1A	4047	1/1	0.93	0.10	42,42,42,42	0
57	MG	2A	3206	1/1	0.93	0.09	49,49,49,49	0
57	MG	2A	3424	1/1	0.93	0.07	50,50,50,50	0
57	MG	1A	3187	1/1	0.93	0.10	46,46,46,46	0
57	MG	2A	3733	1/1	0.93	0.09	68,68,68,68	0
57	MG	1A	3793	1/1	0.93	0.15	36,36,36,36	0
57	MG	1a	1808	1/1	0.93	0.28	56,56,56,56	0
57	MG	1A	3229	1/1	0.93	0.14	59,59,59,59	0
57	MG	1A	3323	1/1	0.93	0.13	39,39,39,39	0
57	MG	2a	1786	1/1	0.93	0.13	67,67,67,67	0
57	MG	1A	4052	1/1	0.93	0.09	55,55,55,55	0
57	MG	2A	3431	1/1	0.93	0.12	35,35,35,35	0
57	MG	2A	3215	1/1	0.93	0.12	43,43,43,43	0
57	MG	2A	3742	1/1	0.93	0.09	48,48,48,48	0
57	MG	2A	3436	1/1	0.93	0.10	50,50,50,50	0
57	MG	2A	3216	1/1	0.93	0.20	51,51,51,51	0
57	MG	18	101	1/1	0.93	0.29	45,45,45,45	0
57	MG	2A	3442	1/1	0.93	0.19	53,53,53,53	0
57	MG	2A	3748	1/1	0.93	0.10	32,32,32,32	0
57	MG	2A	3445	1/1	0.93	0.13	60,60,60,60	0
57	MG	1A	3570	1/1	0.93	0.10	26,26,26,26	0
57	MG	1A	4054	1/1	0.93	0.13	51,51,51,51	0
57	MG	2A	3752	1/1	0.93	0.14	45,45,45,45	0
57	MG	2A	3222	1/1	0.93	0.08	63,63,63,63	0
57	MG	1a	1821	1/1	0.93	0.15	62,62,62,62	0
57	MG	1A	3233	1/1	0.93	0.14	61,61,61,61	0
57	MG	1A	3463	1/1	0.93	0.09	44,44,44,44	0
57	MG	2A	3229	1/1	0.93	0.20	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3326	1/1	0.93	0.12	39,39,39,39	0
57	MG	1A	3688	1/1	0.93	0.10	45,45,45,45	0
57	MG	2A	3768	1/1	0.93	0.23	67,67,67,67	0
57	MG	2a	1816	1/1	0.93	0.11	65,65,65,65	0
57	MG	2A	3769	1/1	0.93	0.11	54,54,54,54	0
57	MG	2A	3459	1/1	0.93	0.12	46,46,46,46	0
57	MG	1A	4061	1/1	0.93	0.05	26,26,26,26	0
57	MG	2A	3463	1/1	0.93	0.07	42,42,42,42	0
57	MG	2A	3774	1/1	0.93	0.09	70,70,70,70	0
57	MG	2A	3464	1/1	0.93	0.10	53,53,53,53	0
57	MG	2A	3466	1/1	0.93	0.09	49,49,49,49	0
57	MG	1a	1615	1/1	0.93	0.10	54,54,54,54	0
57	MG	1t	201	1/1	0.93	0.12	51,51,51,51	0
57	MG	1A	3114	1/1	0.93	0.16	50,50,50,50	0
57	MG	2a	1830	1/1	0.93	0.12	55,55,55,55	0
57	MG	2A	3472	1/1	0.93	0.07	25,25,25,25	0
57	MG	2A	3787	1/1	0.93	0.08	59,59,59,59	0
57	MG	2A	3473	1/1	0.93	0.12	66,66,66,66	0
57	MG	1w	102	1/1	0.93	0.11	75,75,75,75	0
57	MG	2A	3792	1/1	0.93	0.19	60,60,60,60	0
57	MG	1a	1620	1/1	0.93	0.10	49,49,49,49	0
57	MG	2A	3238	1/1	0.93	0.18	52,52,52,52	0
57	MG	1A	3581	1/1	0.93	0.15	14,14,14,14	0
57	MG	1w	109	1/1	0.93	0.09	67,67,67,67	0
57	MG	2A	3798	1/1	0.93	0.21	46,46,46,46	0
57	MG	2A	3243	1/1	0.93	0.12	50,50,50,50	0
57	MG	2A	3485	1/1	0.93	0.08	43,43,43,43	0
57	MG	2A	3486	1/1	0.93	0.11	45,45,45,45	0
57	MG	2A	3488	1/1	0.93	0.09	34,34,34,34	0
57	MG	2A	3244	1/1	0.93	0.12	59,59,59,59	0
57	MG	2x	103	1/1	0.93	0.13	62,62,62,62	0
57	MG	1a	1623	1/1	0.93	0.24	54,54,54,54	0
57	MG	2x	107	1/1	0.93	0.12	38,38,38,38	0
57	MG	1A	3804	1/1	0.93	0.05	29,29,29,29	0
57	MG	1A	3268	1/1	0.94	0.07	34,34,34,34	0
57	MG	1A	3852	1/1	0.94	0.12	50,50,50,50	0
57	MG	2U	201	1/1	0.94	0.21	43,43,43,43	0
57	MG	1B	201	1/1	0.94	0.18	51,51,51,51	0
57	MG	1A	3854	1/1	0.94	0.13	26,26,26,26	0
57	MG	2A	3203	1/1	0.94	0.13	41,41,41,41	0
57	MG	1x	104	1/1	0.94	0.19	58,58,58,58	0
57	MG	1A	3373	1/1	0.94	0.09	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3635	1/1	0.94	0.09	53,53,53,53	0
57	MG	1a	1658	1/1	0.94	0.29	60,60,60,60	0
57	MG	1B	209	1/1	0.94	0.10	43,43,43,43	0
57	MG	1a	1660	1/1	0.94	0.24	54,54,54,54	0
57	MG	1A	3064	1/1	0.94	0.12	51,51,51,51	0
57	MG	1A	3745	1/1	0.94	0.08	42,42,42,42	0
57	MG	2A	3211	1/1	0.94	0.27	37,37,37,37	0
57	MG	1a	1665	1/1	0.94	0.13	41,41,41,41	0
57	MG	1A	3074	1/1	0.94	0.22	40,40,40,40	0
57	MG	27	102	1/1	0.94	0.12	53,53,53,53	0
57	MG	2A	3645	1/1	0.94	0.10	52,52,52,52	0
57	MG	2A	3400	1/1	0.94	0.25	50,50,50,50	0
57	MG	1A	3753	1/1	0.94	0.04	14,14,14,14	0
57	MG	2A	3003	1/1	0.94	0.16	55,55,55,55	0
57	MG	1B	219	1/1	0.94	0.21	41,41,41,41	0
57	MG	1A	3377	1/1	0.94	0.12	42,42,42,42	0
57	MG	2A	3012	1/1	0.94	0.18	45,45,45,45	0
57	MG	1A	3534	1/1	0.94	0.23	53,53,53,53	0
57	MG	1A	3544	1/1	0.94	0.12	65,65,65,65	0
57	MG	2A	3225	1/1	0.94	0.17	56,56,56,56	0
57	MG	1A	3759	1/1	0.94	0.05	15,15,15,15	0
57	MG	2A	3019	1/1	0.94	0.12	50,50,50,50	0
57	MG	1A	3866	1/1	0.94	0.13	49,49,49,49	0
57	MG	1A	3271	1/1	0.94	0.12	49,49,49,49	0
57	MG	1A	3080	1/1	0.94	0.09	39,39,39,39	0
57	MG	1A	3212	1/1	0.94	0.11	47,47,47,47	0
57	MG	2A	3030	1/1	0.94	0.09	56,56,56,56	0
57	MG	1A	3320	1/1	0.94	0.09	59,59,59,59	0
57	MG	2A	3671	1/1	0.94	0.11	35,35,35,35	0
57	MG	2a	1620	1/1	0.94	0.16	61,61,61,61	0
57	MG	1A	3553	1/1	0.94	0.07	32,32,32,32	0
57	MG	1A	3878	1/1	0.94	0.06	33,33,33,33	0
57	MG	1A	3222	1/1	0.94	0.09	37,37,37,37	0
57	MG	1A	3167	1/1	0.94	0.11	59,59,59,59	0
57	MG	1A	3881	1/1	0.94	0.10	33,33,33,33	0
57	MG	2a	1627	1/1	0.94	0.25	47,47,47,47	0
57	MG	2A	3240	1/1	0.94	0.13	44,44,44,44	0
57	MG	1A	3558	1/1	0.94	0.24	51,51,51,51	0
57	MG	1D	303	1/1	0.94	0.16	48,48,48,48	0
57	MG	2A	3433	1/1	0.94	0.18	39,39,39,39	0
57	MG	2A	3434	1/1	0.94	0.15	42,42,42,42	0
57	MG	1D	312	1/1	0.94	0.09	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3042	1/1	0.94	0.16	45,45,45,45	0
57	MG	1A	3169	1/1	0.94	0.11	40,40,40,40	0
57	MG	2A	3438	1/1	0.94	0.18	46,46,46,46	0
57	MG	2A	3687	1/1	0.94	0.16	53,53,53,53	0
57	MG	1D	314	1/1	0.94	0.23	34,34,34,34	0
57	MG	1A	3387	1/1	0.94	0.14	48,48,48,48	0
57	MG	1A	3023	1/1	0.94	0.13	45,45,45,45	0
57	MG	2a	1644	1/1	0.94	0.19	63,63,63,63	0
57	MG	2A	3252	1/1	0.94	0.13	58,58,58,58	0
57	MG	2A	3692	1/1	0.94	0.13	54,54,54,54	0
57	MG	2A	3447	1/1	0.94	0.09	45,45,45,45	0
57	MG	2a	1648	1/1	0.94	0.11	68,68,68,68	0
57	MG	1A	3024	1/1	0.94	0.17	34,34,34,34	0
57	MG	2A	3053	1/1	0.94	0.15	50,50,50,50	0
57	MG	2A	3054	1/1	0.94	0.10	42,42,42,42	0
57	MG	1A	3459	1/1	0.94	0.17	50,50,50,50	0
57	MG	2a	1655	1/1	0.94	0.16	47,47,47,47	0
57	MG	2a	1658	1/1	0.94	0.26	56,56,56,56	0
57	MG	2A	3257	1/1	0.94	0.08	47,47,47,47	0
57	MG	2A	3258	1/1	0.94	0.13	51,51,51,51	0
57	MG	2a	1662	1/1	0.94	0.21	58,58,58,58	0
57	MG	2a	1663	1/1	0.94	0.09	55,55,55,55	0
57	MG	2A	3701	1/1	0.94	0.14	53,53,53,53	0
57	MG	2a	1667	1/1	0.94	0.23	52,52,52,52	0
57	MG	2a	1668	1/1	0.94	0.22	52,52,52,52	0
57	MG	2A	3259	1/1	0.94	0.21	64,64,64,64	0
57	MG	1A	3890	1/1	0.94	0.09	37,37,37,37	0
57	MG	2A	3712	1/1	0.94	0.08	47,47,47,47	0
57	MG	1A	3328	1/1	0.94	0.12	51,51,51,51	0
57	MG	2A	3714	1/1	0.94	0.08	59,59,59,59	0
57	MG	2A	3460	1/1	0.94	0.08	54,54,54,54	0
57	MG	2A	3262	1/1	0.94	0.12	57,57,57,57	0
57	MG	2A	3058	1/1	0.94	0.21	51,51,51,51	0
57	MG	1A	4020	1/1	0.94	0.14	54,54,54,54	0
57	MG	2a	1680	1/1	0.94	0.19	54,54,54,54	0
57	MG	2a	1681	1/1	0.94	0.18	64,64,64,64	0
57	MG	1F	308	1/1	0.94	0.08	38,38,38,38	0
57	MG	1F	310	1/1	0.94	0.15	28,28,28,28	0
57	MG	1A	3396	1/1	0.94	0.08	42,42,42,42	0
57	MG	2A	3470	1/1	0.94	0.14	57,57,57,57	0
57	MG	1G	202	1/1	0.94	0.12	51,51,51,51	0
57	MG	1A	3465	1/1	0.94	0.21	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	3787	1/1	0.94	0.07	31,31,31,31	0
57	MG	1I	201	1/1	0.94	0.07	55,55,55,55	0
57	MG	1A	3399	1/1	0.94	0.08	45,45,45,45	0
57	MG	1A	3470	1/1	0.94	0.11	54,54,54,54	0
57	MG	2A	3081	1/1	0.94	0.13	56,56,56,56	0
57	MG	1A	3001	1/1	0.94	0.15	38,38,38,38	0
57	MG	2A	3482	1/1	0.94	0.06	43,43,43,43	0
57	MG	1A	4031	1/1	0.94	0.09	15,15,15,15	0
57	MG	1O	204	1/1	0.94	0.20	63,63,63,63	0
57	MG	1A	3402	1/1	0.94	0.11	45,45,45,45	0
57	MG	1a	1730	1/1	0.94	0.15	56,56,56,56	0
57	MG	2A	3489	1/1	0.94	0.13	47,47,47,47	0
57	MG	1A	4035	1/1	0.94	0.08	47,47,47,47	0
57	MG	2A	3494	1/1	0.94	0.13	35,35,35,35	0
57	MG	1A	4037	1/1	0.94	0.12	45,45,45,45	0
57	MG	1A	3132	1/1	0.94	0.10	41,41,41,41	0
57	MG	1A	3692	1/1	0.94	0.10	52,52,52,52	0
57	MG	2a	1707	1/1	0.94	0.16	50,50,50,50	0
57	MG	2A	3287	1/1	0.94	0.26	48,48,48,48	0
57	MG	1A	3287	1/1	0.94	0.05	32,32,32,32	0
57	MG	2a	1711	1/1	0.94	0.19	52,52,52,52	0
57	MG	1S	201	1/1	0.94	0.16	40,40,40,40	0
57	MG	1A	3587	1/1	0.94	0.12	35,35,35,35	0
57	MG	2a	1715	1/1	0.94	0.25	61,61,61,61	0
57	MG	1S	203	1/1	0.94	0.06	53,53,53,53	0
57	MG	1A	3086	1/1	0.94	0.18	36,36,36,36	0
57	MG	2A	3510	1/1	0.94	0.18	54,54,54,54	0
57	MG	1A	3915	1/1	0.94	0.06	46,46,46,46	0
57	MG	1A	3477	1/1	0.94	0.15	20,20,20,20	0
57	MG	2A	3109	1/1	0.94	0.08	42,42,42,42	0
57	MG	2A	3515	1/1	0.94	0.10	36,36,36,36	0
57	MG	2A	3764	1/1	0.94	0.07	37,37,37,37	0
57	MG	1U	205	1/1	0.94	0.14	51,51,51,51	0
57	MG	1a	1753	1/1	0.94	0.10	58,58,58,58	0
57	MG	2A	3301	1/1	0.94	0.25	52,52,52,52	0
57	MG	2A	3520	1/1	0.94	0.07	30,30,30,30	0
57	MG	2A	3112	1/1	0.94	0.29	61,61,61,61	0
57	MG	2A	3113	1/1	0.94	0.21	47,47,47,47	0
57	MG	1A	3480	1/1	0.94	0.10	55,55,55,55	0
57	MG	1A	3019	1/1	0.94	0.10	46,46,46,46	0
57	MG	2a	1734	1/1	0.94	0.09	70,70,70,70	0
57	MG	2A	3307	1/1	0.94	0.14	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	3411	1/1	0.94	0.14	52,52,52,52	0
57	MG	2A	3535	1/1	0.94	0.09	53,53,53,53	0
57	MG	2A	3119	1/1	0.94	0.12	43,43,43,43	0
57	MG	1A	3706	1/1	0.94	0.08	29,29,29,29	0
57	MG	1A	3708	1/1	0.94	0.05	11,11,11,11	0
57	MG	2A	3788	1/1	0.94	0.10	45,45,45,45	0
57	MG	2A	3126	1/1	0.94	0.22	40,40,40,40	0
57	MG	2A	3790	1/1	0.94	0.14	55,55,55,55	0
57	MG	1a	1772	1/1	0.94	0.08	49,49,49,49	0
57	MG	1Z	303	1/1	0.94	0.17	44,44,44,44	0
57	MG	2A	3793	1/1	0.94	0.09	61,61,61,61	0
57	MG	2a	1758	1/1	0.94	0.12	59,59,59,59	0
57	MG	2a	1759	1/1	0.94	0.17	53,53,53,53	0
57	MG	1A	3484	1/1	0.94	0.24	34,34,34,34	0
57	MG	1A	3341	1/1	0.94	0.14	46,46,46,46	0
57	MG	2A	3545	1/1	0.94	0.15	56,56,56,56	0
57	MG	2A	3546	1/1	0.94	0.12	40,40,40,40	0
57	MG	2A	3320	1/1	0.94	0.25	53,53,53,53	0
57	MG	2A	3548	1/1	0.94	0.12	60,60,60,60	0
57	MG	2A	3800	1/1	0.94	0.13	46,46,46,46	0
57	MG	2a	1769	1/1	0.94	0.23	50,50,50,50	0
57	MG	1A	3489	1/1	0.94	0.11	57,57,57,57	0
57	MG	2A	3802	1/1	0.94	0.12	59,59,59,59	0
57	MG	2A	3803	1/1	0.94	0.07	57,57,57,57	0
57	MG	2A	3804	1/1	0.94	0.08	65,65,65,65	0
57	MG	10	105	1/1	0.94	0.17	51,51,51,51	0
57	MG	1A	3144	1/1	0.94	0.06	33,33,33,33	0
57	MG	2a	1777	1/1	0.94	0.17	58,58,58,58	0
57	MG	2A	3807	1/1	0.94	0.14	50,50,50,50	0
57	MG	1A	3296	1/1	0.94	0.16	48,48,48,48	0
57	MG	2A	3142	1/1	0.94	0.12	54,54,54,54	0
57	MG	2a	1782	1/1	0.94	0.20	55,55,55,55	0
57	MG	2a	1783	1/1	0.94	0.18	63,63,63,63	0
57	MG	1A	3492	1/1	0.94	0.17	67,67,67,67	0
57	MG	2A	3148	1/1	0.94	0.10	54,54,54,54	0
57	MG	1A	3935	1/1	0.94	0.07	58,58,58,58	0
57	MG	1A	4065	1/1	0.94	0.09	17,17,17,17	0
57	MG	1A	3193	1/1	0.94	0.09	37,37,37,37	0
57	MG	1A	3618	1/1	0.94	0.09	36,36,36,36	0
57	MG	2A	3821	1/1	0.94	0.11	54,54,54,54	0
57	MG	1A	3494	1/1	0.94	0.08	45,45,45,45	0
57	MG	1A	3299	1/1	0.94	0.17	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3159	1/1	0.94	0.08	54,54,54,54	0
57	MG	2a	1797	1/1	0.94	0.11	57,57,57,57	0
57	MG	2A	3160	1/1	0.94	0.18	64,64,64,64	0
57	MG	1A	3422	1/1	0.94	0.14	52,52,52,52	0
57	MG	2A	3567	1/1	0.94	0.10	48,48,48,48	0
57	MG	1A	3245	1/1	0.94	0.25	50,50,50,50	0
57	MG	2A	3342	1/1	0.94	0.28	63,63,63,63	0
57	MG	2A	3165	1/1	0.94	0.09	58,58,58,58	0
57	MG	1a	1602	1/1	0.94	0.23	54,54,54,54	0
57	MG	2a	1805	1/1	0.94	0.16	61,61,61,61	0
57	MG	1A	3424	1/1	0.94	0.13	43,43,43,43	0
57	MG	1A	3829	1/1	0.94	0.15	56,56,56,56	0
57	MG	1A	3948	1/1	0.94	0.10	22,22,22,22	0
57	MG	1A	3059	1/1	0.94	0.30	53,53,53,53	0
57	MG	2A	3350	1/1	0.94	0.13	58,58,58,58	0
57	MG	1A	3198	1/1	0.94	0.12	31,31,31,31	0
57	MG	1A	3358	1/1	0.94	0.08	49,49,49,49	0
57	MG	1A	3834	1/1	0.94	0.17	27,27,27,27	0
57	MG	2a	1817	1/1	0.94	0.14	58,58,58,58	0
57	MG	2A	3587	1/1	0.94	0.22	39,39,39,39	0
57	MG	2A	3588	1/1	0.94	0.12	41,41,41,41	0
57	MG	1A	3836	1/1	0.94	0.13	29,29,29,29	0
57	MG	1A	3428	1/1	0.94	0.17	54,54,54,54	0
57	MG	1A	3513	1/1	0.94	0.06	51,51,51,51	0
57	MG	1a	1818	1/1	0.94	0.17	53,53,53,53	0
57	MG	2A	3359	1/1	0.94	0.13	43,43,43,43	0
57	MG	2A	3596	1/1	0.94	0.11	55,55,55,55	0
57	MG	2A	3360	1/1	0.94	0.09	63,63,63,63	0
57	MG	1A	3843	1/1	0.94	0.10	56,56,56,56	0
57	MG	2A	3601	1/1	0.94	0.17	53,53,53,53	0
57	MG	1A	3958	1/1	0.94	0.14	47,47,47,47	0
57	MG	2A	3184	1/1	0.94	0.27	52,52,52,52	0
57	MG	1A	3251	1/1	0.94	0.11	41,41,41,41	0
57	MG	1A	4103	1/1	0.94	0.10	50,50,50,50	0
57	MG	2l	203	1/1	0.94	0.09	58,58,58,58	0
57	MG	2E	301	1/1	0.94	0.17	59,59,59,59	0
57	MG	1A	3638	1/1	0.94	0.12	24,24,24,24	0
57	MG	2q	201	1/1	0.94	0.09	67,67,67,67	0
57	MG	2q	202	1/1	0.94	0.07	69,69,69,69	0
57	MG	2r	101	1/1	0.94	0.09	64,64,64,64	0
57	MG	1A	4107	1/1	0.94	0.13	53,53,53,53	0
57	MG	1A	3962	1/1	0.94	0.07	11,11,11,11	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3732	1/1	0.94	0.10	23,23,23,23	0
57	MG	1A	3060	1/1	0.94	0.23	43,43,43,43	0
57	MG	1a	1645	1/1	0.94	0.20	52,52,52,52	0
57	MG	1A	3096	1/1	0.94	0.12	28,28,28,28	0
57	MG	2A	3194	1/1	0.94	0.10	50,50,50,50	0
57	MG	1w	105	1/1	0.94	0.14	72,72,72,72	0
57	MG	1w	106	1/1	0.94	0.10	66,66,66,66	0
57	MG	2A	3379	1/1	0.94	0.14	49,49,49,49	0
57	MG	1A	3521	1/1	0.94	0.13	33,33,33,33	0
57	MG	2x	105	1/1	0.94	0.13	58,58,58,58	0
57	MG	2R	203	1/1	0.94	0.12	48,48,48,48	0
57	MG	2y	101	1/1	0.94	0.15	70,70,70,70	0
57	MG	2A	3381	1/1	0.94	0.15	61,61,61,61	0
58	K	2A	3402	1/1	0.94	0.07	49,49,49,49	0
59	A1AEZ	2A	3843	85/85	0.94	0.11	30,40,54,61	0
60	ZN	24	501	1/1	0.94	0.11	104,104,104,104	0
57	MG	2A	3543	1/1	0.95	0.17	57,57,57,57	0
57	MG	1x	105	1/1	0.95	0.16	50,50,50,50	0
57	MG	1A	3901	1/1	0.95	0.08	33,33,33,33	0
57	MG	1A	3902	1/1	0.95	0.05	56,56,56,56	0
57	MG	17	104	1/1	0.95	0.16	47,47,47,47	0
57	MG	1A	3903	1/1	0.95	0.12	46,46,46,46	0
57	MG	1x	110	1/1	0.95	0.11	23,23,23,23	0
57	MG	1A	3163	1/1	0.95	0.11	20,20,20,20	0
57	MG	2D	308	1/1	0.95	0.15	56,56,56,56	0
57	MG	1A	3662	1/1	0.95	0.06	16,16,16,16	0
57	MG	2A	3275	1/1	0.95	0.09	57,57,57,57	0
57	MG	1A	3339	1/1	0.95	0.14	46,46,46,46	0
57	MG	1x	114	1/1	0.95	0.17	54,54,54,54	0
57	MG	1a	1601	1/1	0.95	0.14	52,52,52,52	0
57	MG	2E	307	1/1	0.95	0.13	47,47,47,47	0
57	MG	2E	308	1/1	0.95	0.12	35,35,35,35	0
57	MG	2F	303	1/1	0.95	0.08	56,56,56,56	0
57	MG	2F	304	1/1	0.95	0.08	43,43,43,43	0
57	MG	2A	3279	1/1	0.95	0.30	52,52,52,52	0
57	MG	1A	3401	1/1	0.95	0.10	47,47,47,47	0
57	MG	1a	1603	1/1	0.95	0.07	38,38,38,38	0
57	MG	1A	3199	1/1	0.95	0.11	45,45,45,45	0
57	MG	2A	3007	1/1	0.95	0.08	38,38,38,38	0
57	MG	2O	201	1/1	0.95	0.20	68,68,68,68	0
57	MG	1A	3200	1/1	0.95	0.09	39,39,39,39	0
57	MG	1A	3165	1/1	0.95	0.09	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1a	1607	1/1	0.95	0.07	45,45,45,45	0
57	MG	1a	1610	1/1	0.95	0.26	47,47,47,47	0
57	MG	2R	202	1/1	0.95	0.24	50,50,50,50	0
57	MG	1A	3788	1/1	0.95	0.09	35,35,35,35	0
57	MG	1a	1612	1/1	0.95	0.09	53,53,53,53	0
57	MG	2A	3290	1/1	0.95	0.12	57,57,57,57	0
57	MG	1a	1613	1/1	0.95	0.06	54,54,54,54	0
57	MG	1A	4059	1/1	0.95	0.07	44,44,44,44	0
57	MG	2A	3575	1/1	0.95	0.09	37,37,37,37	0
57	MG	2A	3576	1/1	0.95	0.10	41,41,41,41	0
57	MG	2A	3577	1/1	0.95	0.13	47,47,47,47	0
57	MG	2A	3578	1/1	0.95	0.12	55,55,55,55	0
57	MG	2A	3024	1/1	0.95	0.19	44,44,44,44	0
57	MG	1A	3789	1/1	0.95	0.07	31,31,31,31	0
57	MG	2A	3026	1/1	0.95	0.12	37,37,37,37	0
57	MG	1A	4064	1/1	0.95	0.07	25,25,25,25	0
57	MG	1A	3790	1/1	0.95	0.06	34,34,34,34	0
57	MG	1A	3671	1/1	0.95	0.07	27,27,27,27	0
57	MG	1a	1622	1/1	0.95	0.21	54,54,54,54	0
57	MG	1A	4067	1/1	0.95	0.06	17,17,17,17	0
57	MG	1a	1624	1/1	0.95	0.11	49,49,49,49	0
57	MG	1A	3792	1/1	0.95	0.09	36,36,36,36	0
57	MG	1a	1626	1/1	0.95	0.17	58,58,58,58	0
57	MG	1A	4071	1/1	0.95	0.07	28,28,28,28	0
57	MG	1a	1629	1/1	0.95	0.21	67,67,67,67	0
57	MG	1A	3407	1/1	0.95	0.08	55,55,55,55	0
57	MG	1a	1632	1/1	0.95	0.28	58,58,58,58	0
57	MG	1A	3673	1/1	0.95	0.11	50,50,50,50	0
57	MG	2A	3598	1/1	0.95	0.11	46,46,46,46	0
57	MG	1A	3919	1/1	0.95	0.07	39,39,39,39	0
57	MG	2A	3047	1/1	0.95	0.08	47,47,47,47	0
57	MG	1A	3920	1/1	0.95	0.11	47,47,47,47	0
57	MG	1a	1637	1/1	0.95	0.12	50,50,50,50	0
57	MG	2A	3603	1/1	0.95	0.06	28,28,28,28	0
57	MG	2A	3317	1/1	0.95	0.14	61,61,61,61	0
57	MG	1A	3567	1/1	0.95	0.09	20,20,20,20	0
57	MG	2A	3319	1/1	0.95	0.13	54,54,54,54	0
57	MG	1A	4081	1/1	0.95	0.09	16,16,16,16	0
57	MG	1a	1640	1/1	0.95	0.07	45,45,45,45	0
57	MG	1A	3568	1/1	0.95	0.08	31,31,31,31	0
57	MG	1A	3297	1/1	0.95	0.14	42,42,42,42	0
57	MG	2a	1618	1/1	0.95	0.14	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3247	1/1	0.95	0.09	41,41,41,41	0
57	MG	1A	3681	1/1	0.95	0.08	42,42,42,42	0
57	MG	1A	4087	1/1	0.95	0.08	50,50,50,50	0
57	MG	2A	3327	1/1	0.95	0.12	57,57,57,57	0
57	MG	1a	1651	1/1	0.95	0.20	60,60,60,60	0
57	MG	2A	3064	1/1	0.95	0.08	43,43,43,43	0
57	MG	2a	1625	1/1	0.95	0.09	76,76,76,76	0
57	MG	2A	3330	1/1	0.95	0.37	49,49,49,49	0
57	MG	1A	3682	1/1	0.95	0.17	41,41,41,41	0
57	MG	1a	1654	1/1	0.95	0.13	51,51,51,51	0
57	MG	1A	3572	1/1	0.95	0.10	30,30,30,30	0
57	MG	2A	3068	1/1	0.95	0.21	38,38,38,38	0
57	MG	2A	3069	1/1	0.95	0.06	46,46,46,46	0
57	MG	2A	3628	1/1	0.95	0.08	63,63,63,63	0
57	MG	1A	4092	1/1	0.95	0.07	37,37,37,37	0
57	MG	2a	1635	1/1	0.95	0.11	56,56,56,56	0
57	MG	1A	3930	1/1	0.95	0.11	52,52,52,52	0
57	MG	1A	3684	1/1	0.95	0.13	39,39,39,39	0
57	MG	1A	3933	1/1	0.95	0.15	58,58,58,58	0
57	MG	1A	3475	1/1	0.95	0.11	37,37,37,37	0
57	MG	1A	3687	1/1	0.95	0.07	42,42,42,42	0
57	MG	1A	4100	1/1	0.95	0.14	49,49,49,49	0
57	MG	1A	3806	1/1	0.95	0.10	24,24,24,24	0
57	MG	2a	1643	1/1	0.95	0.09	61,61,61,61	0
57	MG	1A	3130	1/1	0.95	0.14	40,40,40,40	0
57	MG	1A	3250	1/1	0.95	0.06	37,37,37,37	0
57	MG	1A	3576	1/1	0.95	0.07	32,32,32,32	0
57	MG	1A	3413	1/1	0.95	0.16	39,39,39,39	0
57	MG	2A	3091	1/1	0.95	0.08	43,43,43,43	0
57	MG	1A	4110	1/1	0.95	0.17	36,36,36,36	0
57	MG	1A	3943	1/1	0.95	0.06	55,55,55,55	0
57	MG	1A	3579	1/1	0.95	0.07	22,22,22,22	0
57	MG	1A	3414	1/1	0.95	0.08	42,42,42,42	0
57	MG	2A	3356	1/1	0.95	0.15	58,58,58,58	0
57	MG	2a	1656	1/1	0.95	0.16	48,48,48,48	0
57	MG	2a	1657	1/1	0.95	0.16	41,41,41,41	0
57	MG	1A	3110	1/1	0.95	0.13	47,47,47,47	0
57	MG	1A	3947	1/1	0.95	0.15	46,46,46,46	0
57	MG	1A	3815	1/1	0.95	0.09	16,16,16,16	0
57	MG	2A	3102	1/1	0.95	0.14	48,48,48,48	0
57	MG	2A	3103	1/1	0.95	0.14	34,34,34,34	0
57	MG	2a	1664	1/1	0.95	0.10	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2a	1665	1/1	0.95	0.10	47,47,47,47	0
57	MG	1A	3586	1/1	0.95	0.10	25,25,25,25	0
57	MG	2A	3363	1/1	0.95	0.13	38,38,38,38	0
57	MG	2A	3105	1/1	0.95	0.10	46,46,46,46	0
57	MG	2A	3665	1/1	0.95	0.16	58,58,58,58	0
57	MG	1A	3699	1/1	0.95	0.07	47,47,47,47	0
57	MG	1a	1682	1/1	0.95	0.21	52,52,52,52	0
57	MG	2A	3108	1/1	0.95	0.08	26,26,26,26	0
57	MG	1B	206	1/1	0.95	0.10	41,41,41,41	0
57	MG	1A	3700	1/1	0.95	0.07	36,36,36,36	0
57	MG	1a	1686	1/1	0.95	0.13	44,44,44,44	0
57	MG	1B	208	1/1	0.95	0.18	60,60,60,60	0
57	MG	2A	3372	1/1	0.95	0.36	56,56,56,56	0
57	MG	1A	3952	1/1	0.95	0.10	26,26,26,26	0
57	MG	1B	210	1/1	0.95	0.11	49,49,49,49	0
57	MG	1a	1692	1/1	0.95	0.17	52,52,52,52	0
57	MG	1A	3351	1/1	0.95	0.08	36,36,36,36	0
57	MG	2A	3118	1/1	0.95	0.12	41,41,41,41	0
57	MG	1a	1694	1/1	0.95	0.10	57,57,57,57	0
57	MG	2a	1686	1/1	0.95	0.10	55,55,55,55	0
57	MG	1A	3820	1/1	0.95	0.11	22,22,22,22	0
57	MG	2A	3121	1/1	0.95	0.06	60,60,60,60	0
57	MG	1A	3821	1/1	0.95	0.05	25,25,25,25	0
57	MG	1A	3702	1/1	0.95	0.06	46,46,46,46	0
57	MG	1A	3486	1/1	0.95	0.15	44,44,44,44	0
57	MG	2A	3129	1/1	0.95	0.16	37,37,37,37	0
57	MG	1A	3010	1/1	0.95	0.14	37,37,37,37	0
57	MG	1A	3594	1/1	0.95	0.09	23,23,23,23	0
57	MG	1A	3303	1/1	0.95	0.20	47,47,47,47	0
57	MG	1A	3830	1/1	0.95	0.06	17,17,17,17	0
57	MG	2A	3391	1/1	0.95	0.21	45,45,45,45	0
57	MG	1A	3964	1/1	0.95	0.10	20,20,20,20	0
57	MG	2A	3136	1/1	0.95	0.18	37,37,37,37	0
57	MG	1A	3362	1/1	0.95	0.09	53,53,53,53	0
57	MG	2A	3139	1/1	0.95	0.13	41,41,41,41	0
57	MG	2a	1702	1/1	0.95	0.14	44,44,44,44	0
57	MG	1A	3600	1/1	0.95	0.09	52,52,52,52	0
57	MG	1B	228	1/1	0.95	0.05	32,32,32,32	0
57	MG	1A	3363	1/1	0.95	0.22	49,49,49,49	0
57	MG	1a	1713	1/1	0.95	0.06	53,53,53,53	0
57	MG	1A	3091	1/1	0.95	0.07	39,39,39,39	0
57	MG	1A	3972	1/1	0.95	0.04	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	2A	3405	1/1	0.95	0.13	53,53,53,53	0
57	MG	2A	3705	1/1	0.95	0.10	43,43,43,43	0
57	MG	2A	3706	1/1	0.95	0.18	66,66,66,66	0
57	MG	2A	3708	1/1	0.95	0.07	61,61,61,61	0
57	MG	1a	1718	1/1	0.95	0.07	42,42,42,42	0
57	MG	1A	3265	1/1	0.95	0.15	52,52,52,52	0
57	MG	2A	3408	1/1	0.95	0.24	41,41,41,41	0
57	MG	1A	3266	1/1	0.95	0.10	47,47,47,47	0
57	MG	1A	3141	1/1	0.95	0.10	37,37,37,37	0
57	MG	1B	235	1/1	0.95	0.19	65,65,65,65	0
57	MG	1B	236	1/1	0.95	0.07	35,35,35,35	0
57	MG	1A	3977	1/1	0.95	0.08	41,41,41,41	0
57	MG	1A	3372	1/1	0.95	0.07	44,44,44,44	0
57	MG	1a	1728	1/1	0.95	0.07	55,55,55,55	0
57	MG	1A	3179	1/1	0.95	0.13	29,29,29,29	0
57	MG	1D	304	1/1	0.95	0.10	32,32,32,32	0
57	MG	2A	3726	1/1	0.95	0.11	34,34,34,34	0
57	MG	2A	3727	1/1	0.95	0.10	37,37,37,37	0
57	MG	1A	3611	1/1	0.95	0.09	30,30,30,30	0
57	MG	1a	1733	1/1	0.95	0.14	43,43,43,43	0
57	MG	1A	3984	1/1	0.95	0.07	48,48,48,48	0
57	MG	1a	1736	1/1	0.95	0.07	60,60,60,60	0
57	MG	1A	3985	1/1	0.95	0.07	55,55,55,55	0
57	MG	1A	3142	1/1	0.95	0.06	32,32,32,32	0
57	MG	1A	3616	1/1	0.95	0.09	34,34,34,34	0
57	MG	1A	3118	1/1	0.95	0.17	34,34,34,34	0
57	MG	2a	1742	1/1	0.95	0.08	69,69,69,69	0
57	MG	1A	3849	1/1	0.95	0.09	30,30,30,30	0
57	MG	1a	1743	1/1	0.95	0.06	52,52,52,52	0
57	MG	1a	1744	1/1	0.95	0.06	46,46,46,46	0
57	MG	1A	3272	1/1	0.95	0.09	51,51,51,51	0
57	MG	1A	3620	1/1	0.95	0.12	46,46,46,46	0
57	MG	1A	3726	1/1	0.95	0.07	31,31,31,31	0
57	MG	1A	3853	1/1	0.95	0.06	39,39,39,39	0
57	MG	2a	1755	1/1	0.95	0.10	68,68,68,68	0
57	MG	1F	309	1/1	0.95	0.10	50,50,50,50	0
57	MG	2a	1757	1/1	0.95	0.06	60,60,60,60	0
57	MG	1A	3042	1/1	0.95	0.11	33,33,33,33	0
57	MG	1A	3623	1/1	0.95	0.06	21,21,21,21	0
57	MG	2a	1760	1/1	0.95	0.13	54,54,54,54	0
57	MG	2a	1761	1/1	0.95	0.26	60,60,60,60	0
57	MG	1A	3506	1/1	0.95	0.32	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3444	1/1	0.95	0.08	36,36,36,36	0
57	MG	1G	203	1/1	0.95	0.07	55,55,55,55	0
57	MG	1A	3508	1/1	0.95	0.16	44,44,44,44	0
57	MG	1A	3510	1/1	0.95	0.23	54,54,54,54	0
57	MG	2A	3753	1/1	0.95	0.07	39,39,39,39	0
57	MG	1A	3434	1/1	0.95	0.19	33,33,33,33	0
57	MG	1a	1774	1/1	0.95	0.06	50,50,50,50	0
57	MG	1A	3436	1/1	0.95	0.07	48,48,48,48	0
57	MG	1N	204	1/1	0.95	0.13	43,43,43,43	0
57	MG	1a	1777	1/1	0.95	0.20	59,59,59,59	0
57	MG	1A	3437	1/1	0.95	0.09	44,44,44,44	0
57	MG	2a	1774	1/1	0.95	0.15	61,61,61,61	0
57	MG	1A	3863	1/1	0.95	0.10	25,25,25,25	0
57	MG	1A	3120	1/1	0.95	0.08	38,38,38,38	0
57	MG	1a	1781	1/1	0.95	0.16	58,58,58,58	0
57	MG	1a	1782	1/1	0.95	0.07	45,45,45,45	0
57	MG	2A	3461	1/1	0.95	0.08	39,39,39,39	0
57	MG	1a	1784	1/1	0.95	0.21	61,61,61,61	0
57	MG	2a	1781	1/1	0.95	0.20	58,58,58,58	0
57	MG	1A	4012	1/1	0.95	0.10	43,43,43,43	0
57	MG	1A	4013	1/1	0.95	0.08	24,24,24,24	0
57	MG	1A	3321	1/1	0.95	0.11	47,47,47,47	0
57	MG	1a	1788	1/1	0.95	0.12	45,45,45,45	0
57	MG	2A	3778	1/1	0.95	0.07	33,33,33,33	0
57	MG	1P	205	1/1	0.95	0.05	33,33,33,33	0
57	MG	2A	3781	1/1	0.95	0.09	39,39,39,39	0
57	MG	1A	3044	1/1	0.95	0.08	31,31,31,31	0
57	MG	1a	1791	1/1	0.95	0.11	59,59,59,59	0
57	MG	2A	3784	1/1	0.95	0.10	39,39,39,39	0
57	MG	1a	1792	1/1	0.95	0.08	45,45,45,45	0
57	MG	2a	1794	1/1	0.95	0.08	58,58,58,58	0
57	MG	1Q	205	1/1	0.95	0.11	53,53,53,53	0
57	MG	1a	1795	1/1	0.95	0.07	43,43,43,43	0
57	MG	1A	3230	1/1	0.95	0.17	43,43,43,43	0
57	MG	1A	3869	1/1	0.95	0.24	22,22,22,22	0
57	MG	2A	3477	1/1	0.95	0.16	56,56,56,56	0
57	MG	2A	3479	1/1	0.95	0.08	41,41,41,41	0
57	MG	1A	3442	1/1	0.95	0.11	55,55,55,55	0
57	MG	1A	3232	1/1	0.95	0.07	54,54,54,54	0
57	MG	1a	1800	1/1	0.95	0.07	70,70,70,70	0
57	MG	1A	3089	1/1	0.95	0.10	46,46,46,46	0
57	MG	2A	3484	1/1	0.95	0.06	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3234	1/1	0.95	0.12	27,27,27,27	0
57	MG	1A	3533	1/1	0.95	0.07	46,46,46,46	0
57	MG	1A	3447	1/1	0.95	0.11	49,49,49,49	0
57	MG	1A	3758	1/1	0.95	0.06	15,15,15,15	0
57	MG	2a	1812	1/1	0.95	0.21	48,48,48,48	0
57	MG	2a	1813	1/1	0.95	0.17	55,55,55,55	0
57	MG	1U	204	1/1	0.95	0.20	32,32,32,32	0
57	MG	1A	3650	1/1	0.95	0.06	25,25,25,25	0
57	MG	2A	3495	1/1	0.95	0.11	34,34,34,34	0
57	MG	1U	207	1/1	0.95	0.14	30,30,30,30	0
57	MG	1a	1811	1/1	0.95	0.06	44,44,44,44	0
57	MG	1A	3651	1/1	0.95	0.07	25,25,25,25	0
57	MG	1A	3540	1/1	0.95	0.08	24,24,24,24	0
57	MG	2A	3502	1/1	0.95	0.07	35,35,35,35	0
57	MG	1V	206	1/1	0.95	0.11	51,51,51,51	0
57	MG	1A	3106	1/1	0.95	0.20	36,36,36,36	0
57	MG	2A	3814	1/1	0.95	0.19	53,53,53,53	0
57	MG	1W	201	1/1	0.95	0.23	47,47,47,47	0
57	MG	1A	3238	1/1	0.95	0.09	56,56,56,56	0
57	MG	1X	102	1/1	0.95	0.12	40,40,40,40	0
57	MG	1Z	301	1/1	0.95	0.07	50,50,50,50	0
57	MG	1A	4036	1/1	0.95	0.09	30,30,30,30	0
57	MG	1e	202	1/1	0.95	0.11	50,50,50,50	0
57	MG	2g	201	1/1	0.95	0.13	66,66,66,66	0
57	MG	2A	3246	1/1	0.95	0.25	53,53,53,53	0
57	MG	2A	3514	1/1	0.95	0.09	35,35,35,35	0
57	MG	1A	3391	1/1	0.95	0.08	45,45,45,45	0
57	MG	1A	3197	1/1	0.95	0.10	45,45,45,45	0
57	MG	2A	3249	1/1	0.95	0.12	51,51,51,51	0
57	MG	2A	3828	1/1	0.95	0.07	62,62,62,62	0
57	MG	1A	3395	1/1	0.95	0.18	40,40,40,40	0
57	MG	2A	3830	1/1	0.95	0.10	38,38,38,38	0
57	MG	1k	201	1/1	0.95	0.12	44,44,44,44	0
57	MG	1A	3288	1/1	0.95	0.16	47,47,47,47	0
57	MG	1n	101	1/1	0.95	0.08	39,39,39,39	0
57	MG	1A	4042	1/1	0.95	0.12	40,40,40,40	0
57	MG	1A	3398	1/1	0.95	0.11	60,60,60,60	0
57	MG	10	108	1/1	0.95	0.17	62,62,62,62	0
57	MG	2w	104	1/1	0.95	0.09	48,48,48,48	0
57	MG	1w	104	1/1	0.95	0.10	59,59,59,59	0
57	MG	2A	3533	1/1	0.95	0.10	54,54,54,54	0
57	MG	2A	3534	1/1	0.95	0.10	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	10	109	1/1	0.95	0.07	39,39,39,39	0
57	MG	2B	202	1/1	0.95	0.15	64,64,64,64	0
57	MG	11	103	1/1	0.95	0.07	31,31,31,31	0
57	MG	1A	3898	1/1	0.95	0.04	34,34,34,34	0
57	MG	12	102	1/1	0.95	0.09	42,42,42,42	0
57	MG	1A	4045	1/1	0.95	0.14	46,46,46,46	0
57	MG	1A	3899	1/1	0.95	0.11	33,33,33,33	0
59	A1AEZ	1A	4118	85/85	0.95	0.09	10,28,38,42	0
57	MG	15	103	1/1	0.95	0.17	33,33,33,33	0
57	MG	1A	3462	1/1	0.95	0.07	44,44,44,44	0
62	PHE	2w	108	11/12	0.95	0.11	31,35,38,42	0
63	FME	1x	115	10/11	0.95	0.15	17,19,23,28	10
57	MG	1A	3680	1/1	0.96	0.07	28,28,28,28	0
57	MG	1a	1669	1/1	0.96	0.05	48,48,48,48	0
57	MG	1A	3314	1/1	0.96	0.10	40,40,40,40	0
57	MG	1A	4022	1/1	0.96	0.06	16,16,16,16	0
57	MG	1A	3189	1/1	0.96	0.09	43,43,43,43	0
57	MG	1a	1673	1/1	0.96	0.06	55,55,55,55	0
57	MG	1A	3590	1/1	0.96	0.05	18,18,18,18	0
57	MG	1A	3592	1/1	0.96	0.07	28,28,28,28	0
57	MG	1A	3593	1/1	0.96	0.06	35,35,35,35	0
57	MG	1A	3275	1/1	0.96	0.04	19,19,19,19	0
57	MG	2A	3022	1/1	0.96	0.22	45,45,45,45	0
57	MG	1A	3045	1/1	0.96	0.14	30,30,30,30	0
57	MG	1A	3381	1/1	0.96	0.11	37,37,37,37	0
57	MG	1A	3599	1/1	0.96	0.07	17,17,17,17	0
57	MG	1A	3691	1/1	0.96	0.16	57,57,57,57	0
57	MG	1A	3039	1/1	0.96	0.06	31,31,31,31	0
57	MG	2A	3029	1/1	0.96	0.07	25,25,25,25	0
57	MG	1A	3383	1/1	0.96	0.15	37,37,37,37	0
57	MG	2A	3456	1/1	0.96	0.08	39,39,39,39	0
57	MG	1A	3694	1/1	0.96	0.05	24,24,24,24	0
57	MG	1A	3279	1/1	0.96	0.16	47,47,47,47	0
57	MG	2A	3034	1/1	0.96	0.08	44,44,44,44	0
57	MG	2A	3698	1/1	0.96	0.08	30,30,30,30	0
57	MG	1A	3324	1/1	0.96	0.08	49,49,49,49	0
57	MG	1a	1689	1/1	0.96	0.15	37,37,37,37	0
57	MG	1N	202	1/1	0.96	0.09	43,43,43,43	0
57	MG	1a	1691	1/1	0.96	0.22	63,63,63,63	0
57	MG	1A	3511	1/1	0.96	0.06	38,38,38,38	0
57	MG	1A	3195	1/1	0.96	0.15	39,39,39,39	0
57	MG	1A	3104	1/1	0.96	0.11	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3609	1/1	0.96	0.06	28,28,28,28	0
57	MG	2A	3710	1/1	0.96	0.05	49,49,49,49	0
57	MG	2A	3711	1/1	0.96	0.08	50,50,50,50	0
57	MG	2A	3044	1/1	0.96	0.20	58,58,58,58	0
57	MG	1a	1696	1/1	0.96	0.09	46,46,46,46	0
57	MG	1A	3105	1/1	0.96	0.07	34,34,34,34	0
57	MG	1A	3127	1/1	0.96	0.11	25,25,25,25	0
57	MG	2a	1650	1/1	0.96	0.18	37,37,37,37	0
57	MG	1a	1699	1/1	0.96	0.07	30,30,30,30	0
57	MG	2a	1652	1/1	0.96	0.07	58,58,58,58	0
57	MG	2A	3049	1/1	0.96	0.08	43,43,43,43	0
57	MG	2A	3050	1/1	0.96	0.18	59,59,59,59	0
57	MG	1A	3240	1/1	0.96	0.10	44,44,44,44	0
57	MG	2A	3478	1/1	0.96	0.10	41,41,41,41	0
57	MG	1a	1701	1/1	0.96	0.08	38,38,38,38	0
57	MG	1A	3614	1/1	0.96	0.09	56,56,56,56	0
57	MG	1A	3925	1/1	0.96	0.04	43,43,43,43	0
57	MG	1A	3615	1/1	0.96	0.07	32,32,32,32	0
57	MG	1Q	206	1/1	0.96	0.09	35,35,35,35	0
57	MG	1A	3814	1/1	0.96	0.10	35,35,35,35	0
57	MG	1R	203	1/1	0.96	0.28	44,44,44,44	0
57	MG	1a	1709	1/1	0.96	0.09	40,40,40,40	0
57	MG	2A	3487	1/1	0.96	0.08	38,38,38,38	0
57	MG	1R	204	1/1	0.96	0.07	25,25,25,25	0
57	MG	2A	3062	1/1	0.96	0.09	48,48,48,48	0
57	MG	2A	3063	1/1	0.96	0.17	44,44,44,44	0
57	MG	1A	3448	1/1	0.96	0.09	36,36,36,36	0
57	MG	1A	3330	1/1	0.96	0.12	51,51,51,51	0
57	MG	1A	3034	1/1	0.96	0.09	34,34,34,34	0
57	MG	1A	3932	1/1	0.96	0.12	45,45,45,45	0
57	MG	2a	1674	1/1	0.96	0.14	48,48,48,48	0
57	MG	1A	3107	1/1	0.96	0.17	39,39,39,39	0
57	MG	1T	201	1/1	0.96	0.11	50,50,50,50	0
57	MG	2A	3501	1/1	0.96	0.09	52,52,52,52	0
57	MG	2a	1678	1/1	0.96	0.20	38,38,38,38	0
57	MG	2A	3071	1/1	0.96	0.10	39,39,39,39	0
57	MG	1A	3621	1/1	0.96	0.07	22,22,22,22	0
57	MG	2A	3505	1/1	0.96	0.09	37,37,37,37	0
57	MG	2A	3073	1/1	0.96	0.09	44,44,44,44	0
57	MG	1A	3334	1/1	0.96	0.11	54,54,54,54	0
57	MG	1A	4062	1/1	0.96	0.08	30,30,30,30	0
57	MG	1A	3243	1/1	0.96	0.11	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3079	1/1	0.96	0.08	41,41,41,41	0
57	MG	1A	3530	1/1	0.96	0.09	29,29,29,29	0
57	MG	1U	206	1/1	0.96	0.15	40,40,40,40	0
57	MG	2A	3754	1/1	0.96	0.08	34,34,34,34	0
57	MG	1A	3457	1/1	0.96	0.12	46,46,46,46	0
57	MG	2A	3758	1/1	0.96	0.09	47,47,47,47	0
57	MG	1A	3825	1/1	0.96	0.08	43,43,43,43	0
57	MG	2A	3085	1/1	0.96	0.15	48,48,48,48	0
57	MG	2A	3297	1/1	0.96	0.06	39,39,39,39	0
57	MG	1A	3244	1/1	0.96	0.12	39,39,39,39	0
57	MG	1A	3941	1/1	0.96	0.06	53,53,53,53	0
57	MG	1A	3535	1/1	0.96	0.11	38,38,38,38	0
57	MG	2A	3765	1/1	0.96	0.08	53,53,53,53	0
57	MG	1A	3538	1/1	0.96	0.32	36,36,36,36	0
57	MG	2A	3090	1/1	0.96	0.17	48,48,48,48	0
57	MG	1a	1734	1/1	0.96	0.10	50,50,50,50	0
57	MG	1A	3539	1/1	0.96	0.08	42,42,42,42	0
57	MG	2A	3527	1/1	0.96	0.13	53,53,53,53	0
57	MG	1W	204	1/1	0.96	0.10	37,37,37,37	0
57	MG	1A	4077	1/1	0.96	0.05	51,51,51,51	0
57	MG	1X	105	1/1	0.96	0.12	37,37,37,37	0
57	MG	1X	106	1/1	0.96	0.06	34,34,34,34	0
57	MG	1Y	201	1/1	0.96	0.11	46,46,46,46	0
57	MG	2A	3099	1/1	0.96	0.17	45,45,45,45	0
57	MG	2A	3780	1/1	0.96	0.08	34,34,34,34	0
57	MG	2A	3100	1/1	0.96	0.09	35,35,35,35	0
57	MG	1A	3072	1/1	0.96	0.06	37,37,37,37	0
57	MG	2a	1714	1/1	0.96	0.23	51,51,51,51	0
57	MG	2A	3314	1/1	0.96	0.18	54,54,54,54	0
57	MG	1A	3542	1/1	0.96	0.10	35,35,35,35	0
57	MG	2A	3785	1/1	0.96	0.10	42,42,42,42	0
57	MG	1A	3634	1/1	0.96	0.09	42,42,42,42	0
57	MG	1a	1745	1/1	0.96	0.06	55,55,55,55	0
57	MG	1A	4082	1/1	0.96	0.07	35,35,35,35	0
57	MG	1A	3635	1/1	0.96	0.08	19,19,19,19	0
57	MG	1A	3835	1/1	0.96	0.06	41,41,41,41	0
57	MG	1A	3461	1/1	0.96	0.16	39,39,39,39	0
57	MG	10	106	1/1	0.96	0.08	40,40,40,40	0
57	MG	1A	3837	1/1	0.96	0.12	26,26,26,26	0
57	MG	1a	1757	1/1	0.96	0.06	59,59,59,59	0
57	MG	1A	3111	1/1	0.96	0.05	33,33,33,33	0
57	MG	1a	1764	1/1	0.96	0.06	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	3114	1/1	0.96	0.07	45,45,45,45	0
57	MG	2a	1730	1/1	0.96	0.08	65,65,65,65	0
57	MG	1A	3841	1/1	0.96	0.08	25,25,25,25	0
57	MG	1A	3293	1/1	0.96	0.13	35,35,35,35	0
57	MG	1a	1767	1/1	0.96	0.06	61,61,61,61	0
57	MG	11	104	1/1	0.96	0.06	54,54,54,54	0
57	MG	1A	3172	1/1	0.96	0.14	38,38,38,38	0
57	MG	1A	4094	1/1	0.96	0.13	52,52,52,52	0
57	MG	2a	1740	1/1	0.96	0.08	59,59,59,59	0
57	MG	13	102	1/1	0.96	0.11	37,37,37,37	0
57	MG	13	103	1/1	0.96	0.08	37,37,37,37	0
57	MG	2a	1743	1/1	0.96	0.08	48,48,48,48	0
57	MG	1A	3344	1/1	0.96	0.12	27,27,27,27	0
57	MG	2a	1745	1/1	0.96	0.20	53,53,53,53	0
57	MG	1A	3466	1/1	0.96	0.08	28,28,28,28	0
57	MG	1A	3959	1/1	0.96	0.05	43,43,43,43	0
57	MG	1A	3210	1/1	0.96	0.16	47,47,47,47	0
57	MG	2a	1750	1/1	0.96	0.06	76,76,76,76	0
57	MG	2A	3131	1/1	0.96	0.14	39,39,39,39	0
57	MG	2a	1752	1/1	0.96	0.14	60,60,60,60	0
57	MG	1A	3138	1/1	0.96	0.18	32,32,32,32	0
57	MG	1A	3178	1/1	0.96	0.19	28,28,28,28	0
57	MG	17	101	1/1	0.96	0.06	31,31,31,31	0
57	MG	17	103	1/1	0.96	0.09	33,33,33,33	0
57	MG	1A	3252	1/1	0.96	0.07	38,38,38,38	0
57	MG	2A	3819	1/1	0.96	0.08	70,70,70,70	0
57	MG	1A	3253	1/1	0.96	0.07	34,34,34,34	0
57	MG	2A	3349	1/1	0.96	0.15	43,43,43,43	0
57	MG	1A	3744	1/1	0.96	0.07	42,42,42,42	0
57	MG	2A	3140	1/1	0.96	0.21	50,50,50,50	0
57	MG	1A	4106	1/1	0.96	0.18	30,30,30,30	0
57	MG	1A	3257	1/1	0.96	0.12	30,30,30,30	0
57	MG	19	101	1/1	0.96	0.16	45,45,45,45	0
57	MG	1A	3746	1/1	0.96	0.08	22,22,22,22	0
57	MG	1A	4109	1/1	0.96	0.20	30,30,30,30	0
57	MG	1A	3971	1/1	0.96	0.07	20,20,20,20	0
57	MG	1A	3748	1/1	0.96	0.07	42,42,42,42	0
57	MG	1A	3750	1/1	0.96	0.05	36,36,36,36	0
57	MG	1A	3415	1/1	0.96	0.13	32,32,32,32	0
57	MG	1A	4115	1/1	0.96	0.10	45,45,45,45	0
57	MG	1a	1608	1/1	0.96	0.21	59,59,59,59	0
57	MG	1A	3563	1/1	0.96	0.16	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3564	1/1	0.96	0.27	36,36,36,36	0
57	MG	2A	3163	1/1	0.96	0.21	52,52,52,52	0
57	MG	2A	3594	1/1	0.96	0.09	44,44,44,44	0
57	MG	2A	3595	1/1	0.96	0.13	54,54,54,54	0
57	MG	1A	3978	1/1	0.96	0.05	28,28,28,28	0
57	MG	1A	3416	1/1	0.96	0.25	34,34,34,34	0
57	MG	1A	3258	1/1	0.96	0.24	29,29,29,29	0
57	MG	1B	205	1/1	0.96	0.06	45,45,45,45	0
57	MG	1a	1616	1/1	0.96	0.11	48,48,48,48	0
57	MG	1a	1617	1/1	0.96	0.10	42,42,42,42	0
57	MG	2B	207	1/1	0.96	0.18	50,50,50,50	0
57	MG	1A	3478	1/1	0.96	0.06	45,45,45,45	0
57	MG	2A	3173	1/1	0.96	0.09	32,32,32,32	0
57	MG	1a	1810	1/1	0.96	0.20	56,56,56,56	0
57	MG	1A	3360	1/1	0.96	0.25	32,32,32,32	0
57	MG	1a	1812	1/1	0.96	0.07	71,71,71,71	0
57	MG	2A	3377	1/1	0.96	0.33	59,59,59,59	0
57	MG	1A	3361	1/1	0.96	0.16	55,55,55,55	0
57	MG	2a	1793	1/1	0.96	0.19	53,53,53,53	0
57	MG	1A	3261	1/1	0.96	0.10	42,42,42,42	0
57	MG	2a	1795	1/1	0.96	0.06	53,53,53,53	0
57	MG	2B	216	1/1	0.96	0.10	53,53,53,53	0
57	MG	1A	3988	1/1	0.96	0.12	70,70,70,70	0
57	MG	1A	3214	1/1	0.96	0.10	51,51,51,51	0
57	MG	2D	302	1/1	0.96	0.15	50,50,50,50	0
57	MG	2D	303	1/1	0.96	0.17	46,46,46,46	0
57	MG	1A	3664	1/1	0.96	0.07	27,27,27,27	0
57	MG	1B	214	1/1	0.96	0.07	55,55,55,55	0
57	MG	1a	1820	1/1	0.96	0.15	54,54,54,54	0
57	MG	1A	3991	1/1	0.96	0.05	35,35,35,35	0
57	MG	2A	3619	1/1	0.96	0.11	36,36,36,36	0
57	MG	2E	303	1/1	0.96	0.12	49,49,49,49	0
57	MG	2a	1807	1/1	0.96	0.17	51,51,51,51	0
57	MG	1A	3221	1/1	0.96	0.14	43,43,43,43	0
57	MG	1B	217	1/1	0.96	0.10	45,45,45,45	0
57	MG	2A	3623	1/1	0.96	0.12	53,53,53,53	0
57	MG	1e	201	1/1	0.96	0.14	63,63,63,63	0
57	MG	2F	302	1/1	0.96	0.13	49,49,49,49	0
57	MG	1A	3306	1/1	0.96	0.09	39,39,39,39	0
57	MG	1B	220	1/1	0.96	0.06	34,34,34,34	0
57	MG	1A	3995	1/1	0.96	0.06	45,45,45,45	0
57	MG	1A	3139	1/1	0.96	0.16	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1a	1636	1/1	0.96	0.17	48,48,48,48	0
57	MG	2A	3631	1/1	0.96	0.05	57,57,57,57	0
57	MG	1A	3769	1/1	0.96	0.06	41,41,41,41	0
57	MG	2A	3396	1/1	0.96	0.07	59,59,59,59	0
57	MG	2O	202	1/1	0.96	0.15	54,54,54,54	0
57	MG	1l	202	1/1	0.96	0.05	53,53,53,53	0
57	MG	2Q	201	1/1	0.96	0.10	44,44,44,44	0
57	MG	2A	3196	1/1	0.96	0.06	54,54,54,54	0
57	MG	1A	3875	1/1	0.96	0.11	32,32,32,32	0
57	MG	1A	3112	1/1	0.96	0.28	39,39,39,39	0
57	MG	2A	3638	1/1	0.96	0.05	50,50,50,50	0
57	MG	2a	1829	1/1	0.96	0.10	46,46,46,46	0
57	MG	1A	3371	1/1	0.96	0.07	44,44,44,44	0
57	MG	2a	1831	1/1	0.96	0.06	78,78,78,78	0
57	MG	1w	101	1/1	0.96	0.12	38,38,38,38	0
57	MG	1A	3774	1/1	0.96	0.05	32,32,32,32	0
57	MG	1A	3775	1/1	0.96	0.08	35,35,35,35	0
57	MG	1A	3055	1/1	0.96	0.09	41,41,41,41	0
57	MG	2l	201	1/1	0.96	0.07	61,61,61,61	0
57	MG	1A	3076	1/1	0.96	0.14	19,19,19,19	0
57	MG	1a	1649	1/1	0.96	0.09	47,47,47,47	0
57	MG	2A	3410	1/1	0.96	0.13	44,44,44,44	0
57	MG	2A	3648	1/1	0.96	0.07	33,33,33,33	0
57	MG	1A	4006	1/1	0.96	0.10	25,25,25,25	0
57	MG	1A	3079	1/1	0.96	0.12	29,29,29,29	0
57	MG	1a	1652	1/1	0.96	0.08	48,48,48,48	0
57	MG	1A	3885	1/1	0.96	0.14	39,39,39,39	0
57	MG	1A	3585	1/1	0.96	0.06	28,28,28,28	0
57	MG	23	102	1/1	0.96	0.08	45,45,45,45	0
57	MG	1A	3495	1/1	0.96	0.09	47,47,47,47	0
57	MG	1A	3781	1/1	0.96	0.22	22,22,22,22	0
57	MG	1A	3016	1/1	0.96	0.08	41,41,41,41	0
57	MG	2A	3658	1/1	0.96	0.12	38,38,38,38	0
57	MG	2w	105	1/1	0.96	0.09	55,55,55,55	0
57	MG	1A	3783	1/1	0.96	0.10	32,32,32,32	0
57	MG	1A	3892	1/1	0.96	0.07	29,29,29,29	0
57	MG	28	101	1/1	0.96	0.13	45,45,45,45	0
57	MG	2x	102	1/1	0.96	0.18	58,58,58,58	0
57	MG	1A	3784	1/1	0.96	0.05	19,19,19,19	0
57	MG	2A	3664	1/1	0.96	0.09	50,50,50,50	0
57	MG	2A	3423	1/1	0.96	0.09	32,32,32,32	0
57	MG	1D	310	1/1	0.96	0.06	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3785	1/1	0.96	0.05	24,24,24,24	0
57	MG	1a	1664	1/1	0.96	0.23	51,51,51,51	0
57	MG	2A	3223	1/1	0.96	0.10	48,48,48,48	0
57	MG	1A	3678	1/1	0.96	0.05	14,14,14,14	0
57	MG	1A	3679	1/1	0.96	0.17	51,51,51,51	0
57	MG	2A	3226	1/1	0.96	0.17	47,47,47,47	0
57	MG	1D	315	1/1	0.96	0.17	30,30,30,30	0
57	MG	2A	3432	1/1	0.96	0.09	46,46,46,46	0
63	FME	2x	108	10/11	0.96	0.10	36,41,46,49	0
57	MG	1A	3087	1/1	0.97	0.08	33,33,33,33	0
57	MG	2A	3455	1/1	0.97	0.12	36,36,36,36	0
57	MG	1N	203	1/1	0.97	0.05	28,28,28,28	0
57	MG	2A	3241	1/1	0.97	0.06	58,58,58,58	0
57	MG	1A	3390	1/1	0.97	0.05	45,45,45,45	0
57	MG	2A	3032	1/1	0.97	0.07	24,24,24,24	0
57	MG	1A	3910	1/1	0.97	0.06	45,45,45,45	0
57	MG	1A	3030	1/1	0.97	0.12	25,25,25,25	0
57	MG	2a	1628	1/1	0.97	0.23	45,45,45,45	0
57	MG	1A	3467	1/1	0.97	0.15	25,25,25,25	0
57	MG	1A	3267	1/1	0.97	0.22	31,31,31,31	0
57	MG	1A	3469	1/1	0.97	0.10	30,30,30,30	0
57	MG	1A	3394	1/1	0.97	0.08	31,31,31,31	0
57	MG	1P	203	1/1	0.97	0.12	27,27,27,27	0
57	MG	2A	3468	1/1	0.97	0.05	41,41,41,41	0
57	MG	2A	3707	1/1	0.97	0.10	37,37,37,37	0
57	MG	1A	3032	1/1	0.97	0.19	23,23,23,23	0
57	MG	2A	3709	1/1	0.97	0.10	43,43,43,43	0
57	MG	1Q	201	1/1	0.97	0.12	35,35,35,35	0
57	MG	1A	3008	1/1	0.97	0.04	22,22,22,22	0
57	MG	2A	3043	1/1	0.97	0.07	19,19,19,19	0
57	MG	1A	3397	1/1	0.97	0.08	40,40,40,40	0
57	MG	1A	3218	1/1	0.97	0.07	26,26,26,26	0
57	MG	1A	3220	1/1	0.97	0.18	37,37,37,37	0
57	MG	1R	202	1/1	0.97	0.14	39,39,39,39	0
57	MG	1A	3798	1/1	0.97	0.08	37,37,37,37	0
57	MG	1A	3577	1/1	0.97	0.10	38,38,38,38	0
57	MG	2A	3720	1/1	0.97	0.11	46,46,46,46	0
57	MG	1A	3168	1/1	0.97	0.06	28,28,28,28	0
57	MG	1A	3274	1/1	0.97	0.08	26,26,26,26	0
57	MG	1a	1708	1/1	0.97	0.05	35,35,35,35	0
57	MG	1A	3073	1/1	0.97	0.17	35,35,35,35	0
57	MG	2A	3265	1/1	0.97	0.17	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3926	1/1	0.97	0.08	48,48,48,48	0
57	MG	1A	3403	1/1	0.97	0.13	34,34,34,34	0
57	MG	1A	4060	1/1	0.97	0.08	18,18,18,18	0
57	MG	1A	3123	1/1	0.97	0.05	35,35,35,35	0
57	MG	1a	1714	1/1	0.97	0.09	46,46,46,46	0
57	MG	1A	3093	1/1	0.97	0.07	24,24,24,24	0
57	MG	2A	3491	1/1	0.97	0.09	33,33,33,33	0
57	MG	2A	3492	1/1	0.97	0.11	49,49,49,49	0
57	MG	1A	4063	1/1	0.97	0.06	16,16,16,16	0
57	MG	2A	3061	1/1	0.97	0.08	29,29,29,29	0
57	MG	1a	1717	1/1	0.97	0.16	37,37,37,37	0
57	MG	1A	3173	1/1	0.97	0.09	29,29,29,29	0
57	MG	1A	3485	1/1	0.97	0.20	34,34,34,34	0
57	MG	2A	3739	1/1	0.97	0.04	48,48,48,48	0
57	MG	1A	3337	1/1	0.97	0.08	34,34,34,34	0
57	MG	1A	3695	1/1	0.97	0.05	21,21,21,21	0
57	MG	1U	209	1/1	0.97	0.14	33,33,33,33	0
57	MG	1A	3338	1/1	0.97	0.11	40,40,40,40	0
57	MG	1A	3410	1/1	0.97	0.10	32,32,32,32	0
57	MG	2A	3070	1/1	0.97	0.10	26,26,26,26	0
57	MG	1V	205	1/1	0.97	0.07	29,29,29,29	0
57	MG	2A	3747	1/1	0.97	0.09	40,40,40,40	0
57	MG	1A	3226	1/1	0.97	0.14	38,38,38,38	0
57	MG	1A	3049	1/1	0.97	0.09	42,42,42,42	0
57	MG	1A	3228	1/1	0.97	0.07	50,50,50,50	0
57	MG	1A	3176	1/1	0.97	0.22	33,33,33,33	0
57	MG	2A	3076	1/1	0.97	0.06	40,40,40,40	0
57	MG	1A	4078	1/1	0.97	0.04	50,50,50,50	0
57	MG	2A	3078	1/1	0.97	0.09	51,51,51,51	0
57	MG	2A	3755	1/1	0.97	0.07	37,37,37,37	0
57	MG	1A	3177	1/1	0.97	0.17	25,25,25,25	0
57	MG	1A	3231	1/1	0.97	0.10	24,24,24,24	0
57	MG	2A	3516	1/1	0.97	0.12	27,27,27,27	0
57	MG	1A	3704	1/1	0.97	0.04	50,50,50,50	0
57	MG	2A	3294	1/1	0.97	0.15	59,59,59,59	0
57	MG	1A	3075	1/1	0.97	0.10	34,34,34,34	0
57	MG	1A	3498	1/1	0.97	0.17	32,32,32,32	0
57	MG	1A	3707	1/1	0.97	0.09	18,18,18,18	0
57	MG	1a	1740	1/1	0.97	0.05	68,68,68,68	0
57	MG	1A	3499	1/1	0.97	0.13	37,37,37,37	0
57	MG	1A	3098	1/1	0.97	0.19	35,35,35,35	0
57	MG	2A	3525	1/1	0.97	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	10	101	1/1	0.97	0.14	36,36,36,36	0
57	MG	2A	3771	1/1	0.97	0.06	60,60,60,60	0
57	MG	1A	3347	1/1	0.97	0.06	39,39,39,39	0
57	MG	1A	4088	1/1	0.97	0.06	64,64,64,64	0
57	MG	2A	3304	1/1	0.97	0.05	37,37,37,37	0
57	MG	2A	3775	1/1	0.97	0.06	50,50,50,50	0
57	MG	10	104	1/1	0.97	0.11	37,37,37,37	0
57	MG	1A	3826	1/1	0.97	0.11	51,51,51,51	0
57	MG	1a	1748	1/1	0.97	0.06	57,57,57,57	0
57	MG	2A	3095	1/1	0.97	0.07	31,31,31,31	0
57	MG	1A	3103	1/1	0.97	0.14	27,27,27,27	0
57	MG	1A	3236	1/1	0.97	0.05	31,31,31,31	0
57	MG	1A	4093	1/1	0.97	0.04	57,57,57,57	0
57	MG	1A	3290	1/1	0.97	0.20	34,34,34,34	0
57	MG	1a	1756	1/1	0.97	0.06	54,54,54,54	0
57	MG	11	101	1/1	0.97	0.19	32,32,32,32	0
57	MG	1a	1758	1/1	0.97	0.09	42,42,42,42	0
57	MG	1A	3352	1/1	0.97	0.06	45,45,45,45	0
57	MG	1a	1763	1/1	0.97	0.07	54,54,54,54	0
57	MG	1A	3612	1/1	0.97	0.03	26,26,26,26	0
57	MG	1A	3291	1/1	0.97	0.17	27,27,27,27	0
57	MG	12	101	1/1	0.97	0.05	41,41,41,41	0
57	MG	1A	3717	1/1	0.97	0.04	14,14,14,14	0
57	MG	1A	3507	1/1	0.97	0.09	24,24,24,24	0
57	MG	1A	3354	1/1	0.97	0.14	38,38,38,38	0
57	MG	1A	4101	1/1	0.97	0.32	29,29,29,29	0
57	MG	1a	1773	1/1	0.97	0.05	49,49,49,49	0
57	MG	1A	3509	1/1	0.97	0.07	46,46,46,46	0
57	MG	15	101	1/1	0.97	0.15	25,25,25,25	0
57	MG	15	102	1/1	0.97	0.16	35,35,35,35	0
57	MG	1A	3617	1/1	0.97	0.06	38,38,38,38	0
57	MG	1A	3355	1/1	0.97	0.19	28,28,28,28	0
57	MG	1A	4105	1/1	0.97	0.04	60,60,60,60	0
57	MG	2A	3561	1/1	0.97	0.06	33,33,33,33	0
57	MG	1A	3963	1/1	0.97	0.20	21,21,21,21	0
57	MG	1A	3357	1/1	0.97	0.07	31,31,31,31	0
57	MG	1A	3965	1/1	0.97	0.04	27,27,27,27	0
57	MG	2a	1735	1/1	0.97	0.07	60,60,60,60	0
57	MG	2A	3122	1/1	0.97	0.09	42,42,42,42	0
57	MG	2A	3124	1/1	0.97	0.05	33,33,33,33	0
57	MG	1A	3050	1/1	0.97	0.05	43,43,43,43	0
57	MG	2A	3569	1/1	0.97	0.08	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3339	1/1	0.97	0.10	47,47,47,47	0
57	MG	2A	3813	1/1	0.97	0.07	48,48,48,48	0
57	MG	1A	3359	1/1	0.97	0.24	38,38,38,38	0
57	MG	2A	3127	1/1	0.97	0.12	32,32,32,32	0
57	MG	1A	3183	1/1	0.97	0.09	16,16,16,16	0
57	MG	2A	3817	1/1	0.97	0.07	51,51,51,51	0
57	MG	18	103	1/1	0.97	0.10	37,37,37,37	0
57	MG	1A	3294	1/1	0.97	0.21	35,35,35,35	0
57	MG	1A	3516	1/1	0.97	0.09	33,33,33,33	0
57	MG	1A	4114	1/1	0.97	0.09	28,28,28,28	0
57	MG	1A	3517	1/1	0.97	0.13	26,26,26,26	0
57	MG	1A	3137	1/1	0.97	0.18	37,37,37,37	0
57	MG	1a	1793	1/1	0.97	0.11	55,55,55,55	0
57	MG	1A	3974	1/1	0.97	0.08	28,28,28,28	0
57	MG	2A	3137	1/1	0.97	0.05	35,35,35,35	0
57	MG	1A	3186	1/1	0.97	0.09	32,32,32,32	0
57	MG	1A	3628	1/1	0.97	0.09	33,33,33,33	0
57	MG	1A	3435	1/1	0.97	0.07	41,41,41,41	0
57	MG	1B	203	1/1	0.97	0.10	46,46,46,46	0
57	MG	2A	3831	1/1	0.97	0.07	61,61,61,61	0
57	MG	1B	204	1/1	0.97	0.21	48,48,48,48	0
57	MG	1a	1609	1/1	0.97	0.05	42,42,42,42	0
57	MG	2A	3834	1/1	0.97	0.12	48,48,48,48	0
57	MG	2A	3146	1/1	0.97	0.10	45,45,45,45	0
57	MG	1A	3077	1/1	0.97	0.13	27,27,27,27	0
57	MG	1A	3631	1/1	0.97	0.06	19,19,19,19	0
57	MG	1a	1803	1/1	0.97	0.07	54,54,54,54	0
57	MG	2A	3153	1/1	0.97	0.05	33,33,33,33	0
57	MG	1A	3980	1/1	0.97	0.06	47,47,47,47	0
57	MG	2A	3597	1/1	0.97	0.08	48,48,48,48	0
57	MG	1A	3737	1/1	0.97	0.06	23,23,23,23	0
57	MG	1A	3739	1/1	0.97	0.05	51,51,51,51	0
57	MG	2A	3157	1/1	0.97	0.08	37,37,37,37	0
57	MG	1A	3983	1/1	0.97	0.09	48,48,48,48	0
57	MG	1B	211	1/1	0.97	0.11	44,44,44,44	0
57	MG	1A	3740	1/1	0.97	0.07	34,34,34,34	0
57	MG	2A	3161	1/1	0.97	0.10	53,53,53,53	0
57	MG	1A	3011	1/1	0.97	0.04	25,25,25,25	0
57	MG	1A	3742	1/1	0.97	0.03	16,16,16,16	0
57	MG	1A	3987	1/1	0.97	0.05	35,35,35,35	0
57	MG	2A	3608	1/1	0.97	0.07	36,36,36,36	0
57	MG	1a	1813	1/1	0.97	0.05	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3366	1/1	0.97	0.04	23,23,23,23	0
57	MG	1A	3368	1/1	0.97	0.11	40,40,40,40	0
57	MG	2A	3169	1/1	0.97	0.23	51,51,51,51	0
57	MG	1B	218	1/1	0.97	0.06	41,41,41,41	0
57	MG	1A	3140	1/1	0.97	0.07	31,31,31,31	0
57	MG	1A	3636	1/1	0.97	0.06	22,22,22,22	0
57	MG	1A	3747	1/1	0.97	0.04	53,53,53,53	0
57	MG	1A	3531	1/1	0.97	0.08	18,18,18,18	0
57	MG	1a	1630	1/1	0.97	0.10	39,39,39,39	0
57	MG	2D	305	1/1	0.97	0.05	31,31,31,31	0
57	MG	2D	307	1/1	0.97	0.21	48,48,48,48	0
57	MG	2A	3620	1/1	0.97	0.13	46,46,46,46	0
57	MG	1A	3749	1/1	0.97	0.05	32,32,32,32	0
57	MG	2A	3177	1/1	0.97	0.06	48,48,48,48	0
57	MG	2A	3386	1/1	0.97	0.07	34,34,34,34	0
57	MG	1A	3867	1/1	0.97	0.07	39,39,39,39	0
57	MG	2E	304	1/1	0.97	0.09	36,36,36,36	0
57	MG	1A	3190	1/1	0.97	0.09	36,36,36,36	0
57	MG	1A	3640	1/1	0.97	0.07	21,21,21,21	0
57	MG	1A	3641	1/1	0.97	0.04	24,24,24,24	0
57	MG	1A	3009	1/1	0.97	0.08	26,26,26,26	0
57	MG	2F	301	1/1	0.97	0.07	39,39,39,39	0
57	MG	2A	3629	1/1	0.97	0.05	25,25,25,25	0
57	MG	1A	3872	1/1	0.97	0.06	30,30,30,30	0
57	MG	1j	201	1/1	0.97	0.09	63,63,63,63	0
57	MG	1A	3108	1/1	0.97	0.14	23,23,23,23	0
57	MG	1A	3056	1/1	0.97	0.10	39,39,39,39	0
57	MG	1A	3057	1/1	0.97	0.06	30,30,30,30	0
57	MG	1A	3646	1/1	0.97	0.06	15,15,15,15	0
57	MG	1A	3446	1/1	0.97	0.15	48,48,48,48	0
57	MG	1A	3541	1/1	0.97	0.12	31,31,31,31	0
57	MG	1A	3084	1/1	0.97	0.06	49,49,49,49	0
57	MG	1a	1648	1/1	0.97	0.06	49,49,49,49	0
57	MG	1w	103	1/1	0.97	0.07	53,53,53,53	0
57	MG	1A	3882	1/1	0.97	0.19	51,51,51,51	0
57	MG	1D	301	1/1	0.97	0.11	25,25,25,25	0
57	MG	1A	3543	1/1	0.97	0.07	31,31,31,31	0
57	MG	1A	3152	1/1	0.97	0.07	37,37,37,37	0
57	MG	1A	3449	1/1	0.97	0.14	46,46,46,46	0
57	MG	1D	306	1/1	0.97	0.06	30,30,30,30	0
57	MG	1D	309	1/1	0.97	0.08	39,39,39,39	0
57	MG	2T	203	1/1	0.97	0.17	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1x	102	1/1	0.97	0.26	58,58,58,58	0
57	MG	2a	1827	1/1	0.97	0.04	73,73,73,73	0
57	MG	1A	3153	1/1	0.97	0.12	29,29,29,29	0
57	MG	1D	311	1/1	0.97	0.17	24,24,24,24	0
57	MG	2V	201	1/1	0.97	0.20	45,45,45,45	0
57	MG	1A	3768	1/1	0.97	0.06	16,16,16,16	0
57	MG	2d	301	1/1	0.97	0.12	51,51,51,51	0
57	MG	1A	3548	1/1	0.97	0.09	40,40,40,40	0
57	MG	1A	3771	1/1	0.97	0.22	20,20,20,20	0
57	MG	2X	102	1/1	0.97	0.11	47,47,47,47	0
57	MG	2Y	201	1/1	0.97	0.13	48,48,48,48	0
57	MG	1A	3549	1/1	0.97	0.09	39,39,39,39	0
57	MG	1E	302	1/1	0.97	0.12	36,36,36,36	0
57	MG	1a	1663	1/1	0.97	0.12	49,49,49,49	0
57	MG	1E	305	1/1	0.97	0.12	26,26,26,26	0
57	MG	1A	3550	1/1	0.97	0.12	36,36,36,36	0
57	MG	1A	3201	1/1	0.97	0.06	37,37,37,37	0
57	MG	1A	3040	1/1	0.97	0.07	27,27,27,27	0
57	MG	1E	311	1/1	0.97	0.10	20,20,20,20	0
57	MG	1A	3896	1/1	0.97	0.04	54,54,54,54	0
57	MG	2A	3217	1/1	0.97	0.25	41,41,41,41	0
57	MG	1A	3021	1/1	0.97	0.07	36,36,36,36	0
57	MG	2A	3219	1/1	0.97	0.26	32,32,32,32	0
57	MG	2A	3005	1/1	0.97	0.12	45,45,45,45	0
57	MG	1A	4026	1/1	0.97	0.06	39,39,39,39	0
57	MG	1A	4027	1/1	0.97	0.10	11,11,11,11	0
57	MG	2A	3008	1/1	0.97	0.07	38,38,38,38	0
57	MG	1F	303	1/1	0.97	0.11	31,31,31,31	0
57	MG	1F	304	1/1	0.97	0.06	29,29,29,29	0
57	MG	1A	3455	1/1	0.97	0.13	42,42,42,42	0
57	MG	2A	3014	1/1	0.97	0.08	55,55,55,55	0
57	MG	2A	3015	1/1	0.97	0.10	24,24,24,24	0
57	MG	1A	3259	1/1	0.97	0.21	34,34,34,34	0
57	MG	2A	3443	1/1	0.97	0.08	56,56,56,56	0
57	MG	1A	3557	1/1	0.97	0.19	32,32,32,32	0
57	MG	1a	1678	1/1	0.97	0.05	50,50,50,50	0
57	MG	1A	3260	1/1	0.97	0.16	39,39,39,39	0
57	MG	1A	4032	1/1	0.97	0.07	43,43,43,43	0
57	MG	1A	3117	1/1	0.97	0.13	37,37,37,37	0
57	MG	1A	3316	1/1	0.97	0.15	29,29,29,29	0
60	ZN	2Y	202	1/1	0.97	0.05	87,87,87,87	0
57	MG	1A	3262	1/1	0.97	0.13	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	ZN	29	501	1/1	0.97	0.05	70,70,70,70	0
60	ZN	2n	501	1/1	0.97	0.05	83,83,83,83	0
62	PHE	1w	110	11/12	0.97	0.09	14,19,25,25	0
57	MG	1A	3162	1/1	0.97	0.08	23,23,23,23	0
57	MG	1A	3208	1/1	0.97	0.08	24,24,24,24	0
57	MG	2A	3453	1/1	0.97	0.08	13,13,13,13	0
57	MG	1D	305	1/1	0.98	0.09	17,17,17,17	0
57	MG	17	102	1/1	0.98	0.17	25,25,25,25	0
57	MG	1A	3757	1/1	0.98	0.05	39,39,39,39	0
57	MG	2A	3841	1/1	0.98	0.06	58,58,58,58	0
57	MG	2A	3021	1/1	0.98	0.09	33,33,33,33	0
57	MG	1D	307	1/1	0.98	0.04	29,29,29,29	0
57	MG	1a	1731	1/1	0.98	0.05	43,43,43,43	0
57	MG	1A	3497	1/1	0.98	0.12	37,37,37,37	0
57	MG	1A	3668	1/1	0.98	0.09	29,29,29,29	0
57	MG	2A	3497	1/1	0.98	0.06	36,36,36,36	0
57	MG	18	102	1/1	0.98	0.11	31,31,31,31	0
57	MG	1A	3580	1/1	0.98	0.04	29,29,29,29	0
57	MG	2A	3337	1/1	0.98	0.06	35,35,35,35	0
57	MG	2A	3028	1/1	0.98	0.07	38,38,38,38	0
57	MG	1A	3128	1/1	0.98	0.28	27,27,27,27	0
57	MG	1A	3583	1/1	0.98	0.05	26,26,26,26	0
57	MG	2A	3678	1/1	0.98	0.08	38,38,38,38	0
57	MG	2A	3504	1/1	0.98	0.08	33,33,33,33	0
57	MG	1A	3129	1/1	0.98	0.10	36,36,36,36	0
57	MG	1A	3235	1/1	0.98	0.06	26,26,26,26	0
57	MG	1E	301	1/1	0.98	0.12	25,25,25,25	0
57	MG	1A	3069	1/1	0.98	0.22	43,43,43,43	0
57	MG	1E	303	1/1	0.98	0.07	29,29,29,29	0
57	MG	1A	3181	1/1	0.98	0.09	28,28,28,28	0
57	MG	2D	301	1/1	0.98	0.09	34,34,34,34	0
57	MG	1A	3860	1/1	0.98	0.06	35,35,35,35	0
57	MG	1E	307	1/1	0.98	0.04	35,35,35,35	0
57	MG	1E	308	1/1	0.98	0.05	38,38,38,38	0
57	MG	1A	3767	1/1	0.98	0.04	16,16,16,16	0
57	MG	2D	306	1/1	0.98	0.27	40,40,40,40	0
57	MG	1A	3131	1/1	0.98	0.09	27,27,27,27	0
57	MG	1A	3070	1/1	0.98	0.09	33,33,33,33	0
57	MG	1A	3770	1/1	0.98	0.05	16,16,16,16	0
57	MG	1A	3184	1/1	0.98	0.06	26,26,26,26	0
57	MG	1A	3966	1/1	0.98	0.04	49,49,49,49	0
57	MG	1a	1754	1/1	0.98	0.04	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1a	1755	1/1	0.98	0.05	48,48,48,48	0
57	MG	2a	1731	1/1	0.98	0.06	53,53,53,53	0
57	MG	1A	3071	1/1	0.98	0.10	24,24,24,24	0
57	MG	1F	301	1/1	0.98	0.10	32,32,32,32	0
57	MG	1F	302	1/1	0.98	0.09	23,23,23,23	0
57	MG	1a	1618	1/1	0.98	0.05	37,37,37,37	0
57	MG	2A	3526	1/1	0.98	0.07	36,36,36,36	0
57	MG	1a	1762	1/1	0.98	0.06	56,56,56,56	0
57	MG	2A	3528	1/1	0.98	0.08	59,59,59,59	0
57	MG	1A	4074	1/1	0.98	0.05	29,29,29,29	0
57	MG	1A	4075	1/1	0.98	0.19	29,29,29,29	0
57	MG	1A	3367	1/1	0.98	0.16	32,32,32,32	0
57	MG	1A	3097	1/1	0.98	0.04	24,24,24,24	0
57	MG	1A	3595	1/1	0.98	0.03	23,23,23,23	0
57	MG	2A	3213	1/1	0.98	0.07	45,45,45,45	0
57	MG	2a	1746	1/1	0.98	0.05	53,53,53,53	0
57	MG	1A	3135	1/1	0.98	0.15	25,25,25,25	0
57	MG	1a	1769	1/1	0.98	0.05	61,61,61,61	0
57	MG	1a	1770	1/1	0.98	0.04	63,63,63,63	0
57	MG	1F	312	1/1	0.98	0.09	45,45,45,45	0
57	MG	1A	3020	1/1	0.98	0.06	24,24,24,24	0
57	MG	1A	3598	1/1	0.98	0.06	22,22,22,22	0
57	MG	2A	3717	1/1	0.98	0.09	60,60,60,60	0
57	MG	1A	3099	1/1	0.98	0.21	31,31,31,31	0
57	MG	1A	3100	1/1	0.98	0.19	22,22,22,22	0
57	MG	1A	3191	1/1	0.98	0.14	25,25,25,25	0
57	MG	1A	3877	1/1	0.98	0.08	23,23,23,23	0
57	MG	1A	3192	1/1	0.98	0.04	32,32,32,32	0
57	MG	1A	3249	1/1	0.98	0.12	22,22,22,22	0
57	MG	1A	3309	1/1	0.98	0.04	36,36,36,36	0
57	MG	1A	3605	1/1	0.98	0.06	11,11,11,11	0
57	MG	1A	4090	1/1	0.98	0.05	33,33,33,33	0
57	MG	1A	3101	1/1	0.98	0.04	33,33,33,33	0
57	MG	1A	3033	1/1	0.98	0.05	40,40,40,40	0
57	MG	1A	3608	1/1	0.98	0.09	18,18,18,18	0
57	MG	1a	1641	1/1	0.98	0.11	35,35,35,35	0
57	MG	1a	1642	1/1	0.98	0.10	41,41,41,41	0
57	MG	1A	3520	1/1	0.98	0.13	26,26,26,26	0
57	MG	1a	1644	1/1	0.98	0.04	41,41,41,41	0
57	MG	1P	201	1/1	0.98	0.20	26,26,26,26	0
57	MG	1A	3006	1/1	0.98	0.05	32,32,32,32	0
57	MG	1A	3196	1/1	0.98	0.16	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1P	206	1/1	0.98	0.07	35,35,35,35	0
57	MG	1A	3255	1/1	0.98	0.07	25,25,25,25	0
57	MG	2A	3564	1/1	0.98	0.04	38,38,38,38	0
57	MG	1Q	202	1/1	0.98	0.07	20,20,20,20	0
57	MG	1A	3524	1/1	0.98	0.14	35,35,35,35	0
57	MG	1A	3525	1/1	0.98	0.11	27,27,27,27	0
57	MG	1A	3891	1/1	0.98	0.10	38,38,38,38	0
57	MG	1A	3256	1/1	0.98	0.23	33,33,33,33	0
57	MG	1A	3143	1/1	0.98	0.07	30,30,30,30	0
57	MG	2A	3571	1/1	0.98	0.08	27,27,27,27	0
57	MG	2A	3403	1/1	0.98	0.09	17,17,17,17	0
57	MG	2A	3573	1/1	0.98	0.12	39,39,39,39	0
57	MG	1A	3319	1/1	0.98	0.10	34,34,34,34	0
57	MG	1A	3007	1/1	0.98	0.10	23,23,23,23	0
57	MG	1A	3052	1/1	0.98	0.10	33,33,33,33	0
57	MG	1A	3148	1/1	0.98	0.12	26,26,26,26	0
57	MG	1A	3053	1/1	0.98	0.14	40,40,40,40	0
57	MG	1A	3078	1/1	0.98	0.13	36,36,36,36	0
57	MG	1A	3536	1/1	0.98	0.10	32,32,32,32	0
57	MG	1A	3004	1/1	0.98	0.06	37,37,37,37	0
57	MG	2A	3757	1/1	0.98	0.04	48,48,48,48	0
57	MG	1A	3460	1/1	0.98	0.20	40,40,40,40	0
57	MG	1A	3017	1/1	0.98	0.11	26,26,26,26	0
57	MG	1A	3393	1/1	0.98	0.16	33,33,33,33	0
57	MG	1A	3156	1/1	0.98	0.19	32,32,32,32	0
57	MG	2A	3416	1/1	0.98	0.04	23,23,23,23	0
57	MG	1A	3081	1/1	0.98	0.22	42,42,42,42	0
57	MG	1A	3209	1/1	0.98	0.10	28,28,28,28	0
57	MG	1A	3545	1/1	0.98	0.03	27,27,27,27	0
57	MG	1U	208	1/1	0.98	0.22	34,34,34,34	0
57	MG	1A	4011	1/1	0.98	0.04	31,31,31,31	0
57	MG	1U	210	1/1	0.98	0.14	29,29,29,29	0
57	MG	1A	3041	1/1	0.98	0.16	28,28,28,28	0
57	MG	1V	201	1/1	0.98	0.16	27,27,27,27	0
57	MG	1V	202	1/1	0.98	0.17	28,28,28,28	0
57	MG	1A	3159	1/1	0.98	0.07	31,31,31,31	0
57	MG	1A	3332	1/1	0.98	0.16	30,30,30,30	0
57	MG	1A	3161	1/1	0.98	0.14	29,29,29,29	0
57	MG	1A	3213	1/1	0.98	0.18	42,42,42,42	0
57	MG	1A	3335	1/1	0.98	0.18	34,34,34,34	0
57	MG	1A	3018	1/1	0.98	0.28	46,46,46,46	0
57	MG	1A	3639	1/1	0.98	0.06	18,18,18,18	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3273	1/1	0.98	0.09	32,32,32,32	0
57	MG	1a	1685	1/1	0.98	0.13	37,37,37,37	0
57	MG	1X	103	1/1	0.98	0.09	41,41,41,41	0
57	MG	1m	3001	1/1	0.98	0.08	51,51,51,51	0
57	MG	1X	104	1/1	0.98	0.10	32,32,32,32	0
57	MG	1A	3215	1/1	0.98	0.28	33,33,33,33	0
57	MG	2A	3439	1/1	0.98	0.04	60,60,60,60	0
57	MG	1A	3216	1/1	0.98	0.08	25,25,25,25	0
57	MG	2A	3441	1/1	0.98	0.07	58,58,58,58	0
57	MG	1A	3823	1/1	0.98	0.23	32,32,32,32	0
57	MG	1Y	202	1/1	0.98	0.20	41,41,41,41	0
57	MG	1A	3217	1/1	0.98	0.12	23,23,23,23	0
57	MG	1A	4025	1/1	0.98	0.04	38,38,38,38	0
57	MG	1A	3115	1/1	0.98	0.13	28,28,28,28	0
57	MG	1A	3278	1/1	0.98	0.03	26,26,26,26	0
57	MG	1A	3479	1/1	0.98	0.23	42,42,42,42	0
57	MG	1A	3116	1/1	0.98	0.19	27,27,27,27	0
57	MG	1A	3648	1/1	0.98	0.05	23,23,23,23	0
57	MG	1A	3028	1/1	0.98	0.18	30,30,30,30	0
57	MG	2f	201	1/1	0.98	0.14	42,42,42,42	0
57	MG	1A	3482	1/1	0.98	0.14	29,29,29,29	0
57	MG	1A	3012	1/1	0.98	0.07	21,21,21,21	0
57	MG	1A	3061	1/1	0.98	0.14	33,33,33,33	0
57	MG	1A	3062	1/1	0.98	0.14	46,46,46,46	0
57	MG	1A	3170	1/1	0.98	0.12	38,38,38,38	0
57	MG	2A	3143	1/1	0.98	0.12	44,44,44,44	0
57	MG	2a	1659	1/1	0.98	0.08	42,42,42,42	0
57	MG	1A	3487	1/1	0.98	0.11	25,25,25,25	0
57	MG	2A	3145	1/1	0.98	0.08	31,31,31,31	0
57	MG	11	102	1/1	0.98	0.04	29,29,29,29	0
57	MG	2A	3147	1/1	0.98	0.06	56,56,56,56	0
57	MG	1A	3088	1/1	0.98	0.10	17,17,17,17	0
57	MG	2A	3810	1/1	0.98	0.09	33,33,33,33	0
57	MG	1A	3838	1/1	0.98	0.21	27,27,27,27	0
57	MG	2A	3150	1/1	0.98	0.19	39,39,39,39	0
57	MG	2A	3465	1/1	0.98	0.06	32,32,32,32	0
57	MG	1A	4041	1/1	0.98	0.06	31,31,31,31	0
57	MG	2A	3152	1/1	0.98	0.14	44,44,44,44	0
57	MG	1A	3839	1/1	0.98	0.20	32,32,32,32	0
57	MG	1A	3418	1/1	0.98	0.11	35,35,35,35	0
57	MG	13	101	1/1	0.98	0.06	28,28,28,28	0
57	MG	1A	3571	1/1	0.98	0.04	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3046	1/1	0.98	0.03	10,10,10,10	0
57	MG	1A	3942	1/1	0.98	0.03	34,34,34,34	0
57	MG	2A	3004	1/1	0.98	0.07	31,31,31,31	0
57	MG	1A	3066	1/1	0.98	0.16	27,27,27,27	0
57	MG	2x	106	1/1	0.98	0.04	29,29,29,29	0
57	MG	1A	3751	1/1	0.98	0.04	34,34,34,34	0
57	MG	1A	3174	1/1	0.98	0.13	30,30,30,30	0
57	MG	1A	3125	1/1	0.98	0.06	32,32,32,32	0
57	MG	2A	3010	1/1	0.98	0.06	45,45,45,45	0
57	MG	15	104	1/1	0.98	0.22	32,32,32,32	0
57	MG	2A	3166	1/1	0.98	0.09	30,30,30,30	0
60	ZN	14	102	1/1	0.98	0.07	79,79,79,79	0
57	MG	2A	3654	1/1	0.98	0.04	48,48,48,48	0
57	MG	1A	3067	1/1	0.98	0.05	11,11,11,11	0
60	ZN	25	105	1/1	0.98	0.04	67,67,67,67	0
57	MG	1a	1723	1/1	0.98	0.03	35,35,35,35	0
57	MG	15	106	1/1	0.98	0.13	43,43,43,43	0
61	SF4	2d	302	8/8	0.98	0.05	55,62,70,73	0
57	MG	1A	3356	1/1	0.98	0.24	36,36,36,36	0
57	MG	2A	3835	1/1	0.98	0.05	65,65,65,65	0
57	MG	2A	3016	1/1	0.98	0.10	39,39,39,39	0
57	MG	1A	3068	1/1	0.98	0.03	24,24,24,24	0
57	MG	2a	1709	1/1	0.99	0.18	38,38,38,38	0
57	MG	1A	3003	1/1	0.99	0.11	23,23,23,23	0
57	MG	1A	3532	1/1	0.99	0.13	29,29,29,29	0
57	MG	1A	3063	1/1	0.99	0.05	22,22,22,22	0
57	MG	1A	3027	1/1	0.99	0.12	25,25,25,25	0
57	MG	1P	204	1/1	0.99	0.11	25,25,25,25	0
57	MG	1A	3164	1/1	0.99	0.03	29,29,29,29	0
57	MG	1A	3065	1/1	0.99	0.09	11,11,11,11	0
57	MG	1A	3537	1/1	0.99	0.13	25,25,25,25	0
57	MG	1A	3043	1/1	0.99	0.03	29,29,29,29	0
57	MG	1Q	203	1/1	0.99	0.03	35,35,35,35	0
57	MG	2A	3123	1/1	0.99	0.07	39,39,39,39	0
57	MG	1D	308	1/1	0.99	0.07	33,33,33,33	0
57	MG	1A	3219	1/1	0.99	0.15	27,27,27,27	0
57	MG	1A	3124	1/1	0.99	0.03	37,37,37,37	0
57	MG	1A	3874	1/1	0.99	0.04	32,32,32,32	0
57	MG	1A	3054	1/1	0.99	0.05	16,16,16,16	0
57	MG	2A	3490	1/1	0.99	0.09	27,27,27,27	0
57	MG	2F	306	1/1	0.99	0.17	41,41,41,41	0
57	MG	1A	3109	1/1	0.99	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	3404	1/1	0.99	0.03	35,35,35,35	0
57	MG	1A	3582	1/1	0.99	0.04	30,30,30,30	0
57	MG	1A	4068	1/1	0.99	0.03	22,22,22,22	0
57	MG	2A	3646	1/1	0.99	0.03	28,28,28,28	0
57	MG	1A	3145	1/1	0.99	0.19	27,27,27,27	0
57	MG	1A	4070	1/1	0.99	0.05	11,11,11,11	0
57	MG	1a	1783	1/1	0.99	0.09	27,27,27,27	0
57	MG	1E	304	1/1	0.99	0.08	25,25,25,25	0
57	MG	2a	1737	1/1	0.99	0.03	57,57,57,57	0
57	MG	1A	3094	1/1	0.99	0.07	33,33,33,33	0
57	MG	1A	3374	1/1	0.99	0.07	42,42,42,42	0
57	MG	1U	201	1/1	0.99	0.06	24,24,24,24	0
57	MG	1A	3666	1/1	0.99	0.06	10,10,10,10	0
57	MG	1A	3147	1/1	0.99	0.06	27,27,27,27	0
57	MG	1A	3254	1/1	0.99	0.08	22,22,22,22	0
57	MG	1a	1722	1/1	0.99	0.08	55,55,55,55	0
57	MG	1A	3013	1/1	0.99	0.03	19,19,19,19	0
57	MG	1A	3149	1/1	0.99	0.07	24,24,24,24	0
57	MG	2A	3660	1/1	0.99	0.04	32,32,32,32	0
57	MG	1A	3315	1/1	0.99	0.21	25,25,25,25	0
57	MG	1A	3591	1/1	0.99	0.05	39,39,39,39	0
57	MG	2A	3663	1/1	0.99	0.08	38,38,38,38	0
57	MG	1A	3150	1/1	0.99	0.17	26,26,26,26	0
57	MG	1A	3036	1/1	0.99	0.16	28,28,28,28	0
57	MG	1A	3318	1/1	0.99	0.20	33,33,33,33	0
57	MG	2A	3009	1/1	0.99	0.02	34,34,34,34	0
57	MG	1A	3555	1/1	0.99	0.10	30,30,30,30	0
57	MG	1A	4033	1/1	0.99	0.14	36,36,36,36	0
57	MG	1V	203	1/1	0.99	0.12	24,24,24,24	0
57	MG	1A	3202	1/1	0.99	0.07	37,37,37,37	0
57	MG	23	101	1/1	0.99	0.04	45,45,45,45	0
57	MG	2A	3084	1/1	0.99	0.13	36,36,36,36	0
57	MG	1F	305	1/1	0.99	0.04	34,34,34,34	0
57	MG	1F	306	1/1	0.99	0.06	22,22,22,22	0
57	MG	1F	307	1/1	0.99	0.11	28,28,28,28	0
57	MG	1A	3894	1/1	0.99	0.04	8,8,8,8	0
57	MG	1A	3037	1/1	0.99	0.19	26,26,26,26	0
57	MG	1W	203	1/1	0.99	0.13	35,35,35,35	0
57	MG	1A	3519	1/1	0.99	0.13	29,29,29,29	0
57	MG	1X	101	1/1	0.99	0.16	29,29,29,29	0
57	MG	1A	3897	1/1	0.99	0.09	34,34,34,34	0
57	MG	1A	3451	1/1	0.99	0.10	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1G	201	1/1	0.99	0.10	36,36,36,36	0
57	MG	1A	3029	1/1	0.99	0.07	30,30,30,30	0
57	MG	2A	3531	1/1	0.99	0.08	32,32,32,32	0
57	MG	2A	3532	1/1	0.99	0.06	34,34,34,34	0
57	MG	2A	3767	1/1	0.99	0.06	32,32,32,32	0
57	MG	1A	3724	1/1	0.99	0.07	32,32,32,32	0
57	MG	1A	3048	1/1	0.99	0.07	17,17,17,17	0
57	MG	1A	3994	1/1	0.99	0.04	22,22,22,22	0
57	MG	1a	1749	1/1	0.99	0.04	65,65,65,65	0
58	K	1A	3528	1/1	0.99	0.04	36,36,36,36	0
57	MG	2A	3612	1/1	0.99	0.10	29,29,29,29	0
57	MG	1A	3155	1/1	0.99	0.09	12,12,12,12	0
57	MG	1A	3207	1/1	0.99	0.09	26,26,26,26	0
60	ZN	1Y	203	1/1	0.99	0.02	55,55,55,55	0
57	MG	1A	3997	1/1	0.99	0.05	43,43,43,43	0
60	ZN	15	108	1/1	0.99	0.02	42,42,42,42	0
60	ZN	1n	102	1/1	0.99	0.04	56,56,56,56	0
57	MG	1A	3685	1/1	0.99	0.07	19,19,19,19	0
57	MG	1A	3022	1/1	0.99	0.06	11,11,11,11	0
57	MG	1A	3031	1/1	0.99	0.23	29,29,29,29	0
57	MG	1A	3102	1/1	0.99	0.11	25,25,25,25	0
57	MG	1a	1627	1/1	0.99	0.14	26,26,26,26	0
61	SF4	1d	501	8/8	0.99	0.05	56,57,62,66	0
57	MG	1A	3136	1/1	0.99	0.07	26,26,26,26	0
57	MG	1A	3160	1/1	0.99	0.28	30,30,30,30	0
57	MG	1a	1760	1/1	0.99	0.06	56,56,56,56	0
57	MG	2A	3703	1/1	0.99	0.05	57,57,57,57	0
57	MG	1a	1761	1/1	0.99	0.03	44,44,44,44	0
60	ZN	19	102	1/1	1.00	0.03	34,34,34,34	0
57	MG	1A	3738	1/1	1.00	0.04	30,30,30,30	0
57	MG	1A	3035	1/1	1.00	0.12	17,17,17,17	0
57	MG	1A	3348	1/1	1.00	0.06	16,16,16,16	0
57	MG	1P	202	1/1	1.00	0.17	27,27,27,27	0
60	ZN	26	501	1/1	1.00	0.03	53,53,53,53	0
60	ZN	16	102	1/1	1.00	0.04	39,39,39,39	0

6.5 Other polymers (i)

There are no such residues in this entry.