wwPDB X-ray Structure Validation Summary Report (i)

Aug 6, 2026 – 09:17 AM EDT

PDB ID	:	6CAE / pdb_00006cae
Title	:	Crystal structure of the Thermus thermophilus 70S ribosome in complex with NOSO-95179 antibiotic and bound to mRNA and A-, P- and E-site tRNAs at 2.6A resolution
Authors	:	Pantel, L.; Florin, T.; Dobosz-Bartoszek, M.; Racine, E.; Sarciaux, M.; Serri, M.; Houard, J.; Campagne, J.M.; Marcia de Figueiredo, R.; Midrier, C.; Gaudriault, S.; Givaudan, A.; Lanois, A.; Forst, S.; Aumelas, A.; Cotteaux-Lautard, C.; Bolla, J.M.; Vingsbo Lundberg, C.; Huseby, D.; Hughes, D.; Villain-Guillot, P.; Mankin, A.S.; Polikanov, Y.S.; Gualtieri, M.
Deposited on	:	2018-01-30
Resolution	:	2.60 Å(reported)

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

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

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

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

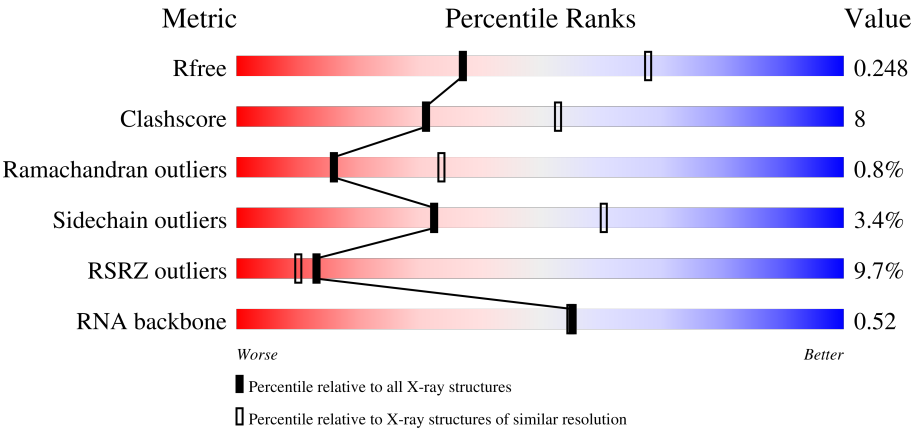
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)
RNA backbone	3983	1014 (2.84-2.36)

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

Mol	Chain	Length	Quality of chain
1	1A	2915	4% 67% 26% 6% •

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Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

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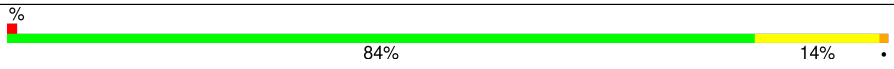
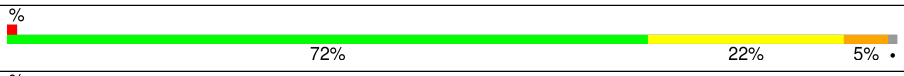
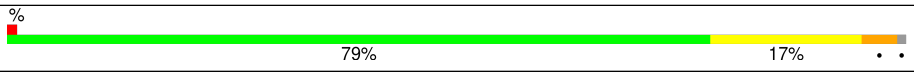
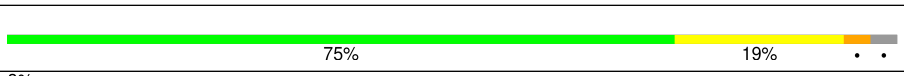
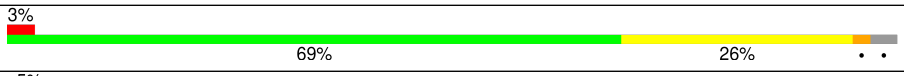
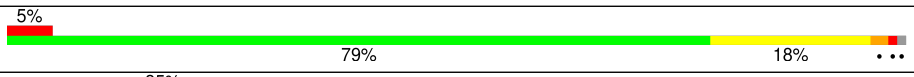
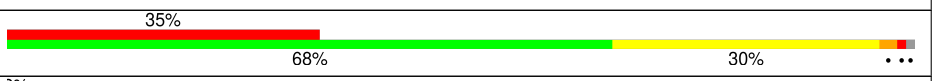
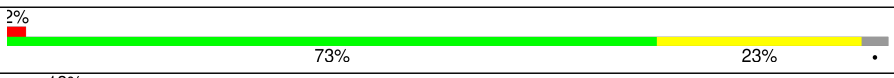
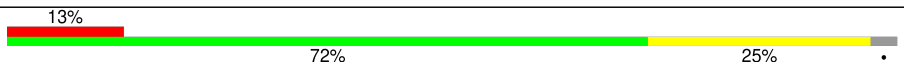
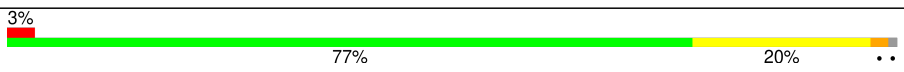
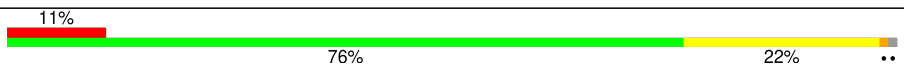
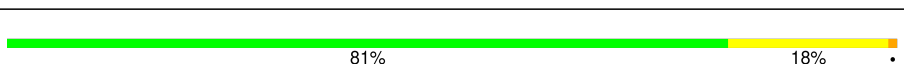
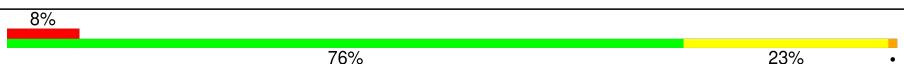
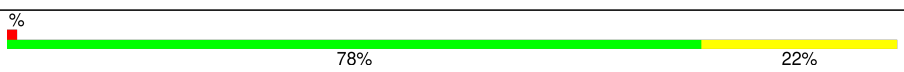
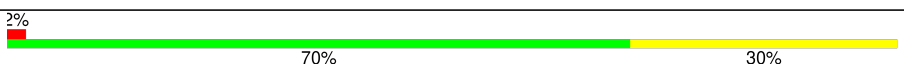
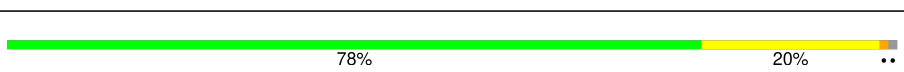
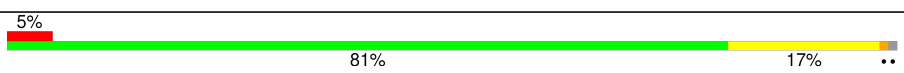
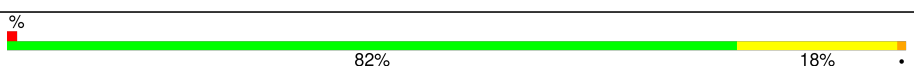
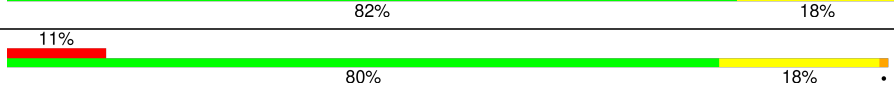
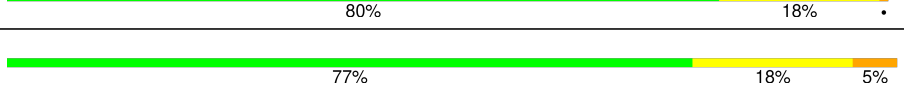
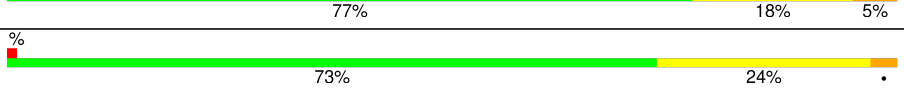
2	1B	121	
2	2B	121	
3	1D	276	
3	2D	276	
4	1E	206	
4	2E	206	
5	1F	210	
5	2F	210	
6	1G	182	
6	2G	182	
7	1H	180	
7	2H	180	
8	1I	148	
8	2I	148	
9	1N	140	
9	2N	140	
10	1O	122	
10	2O	122	
11	1P	150	
11	2P	150	
12	1Q	141	
12	2Q	141	
13	1R	118	
13	2R	118	

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Mol	Chain	Length	Quality of chain
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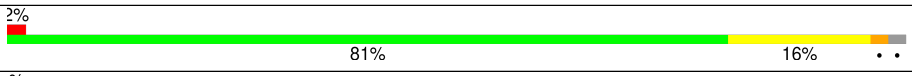
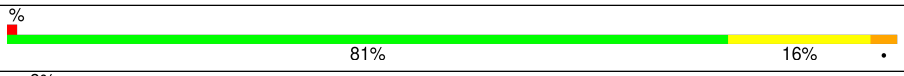
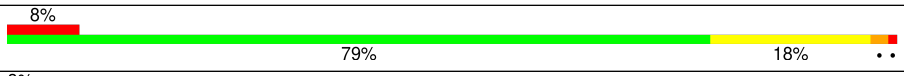
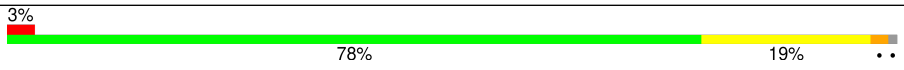
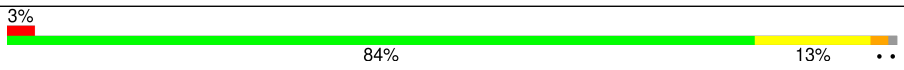
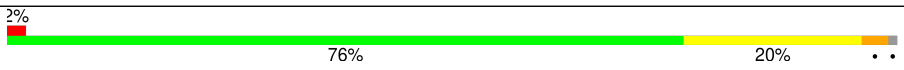
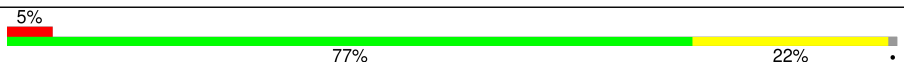
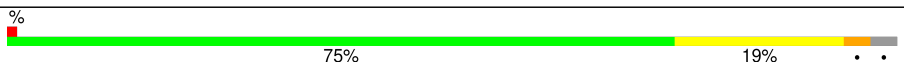
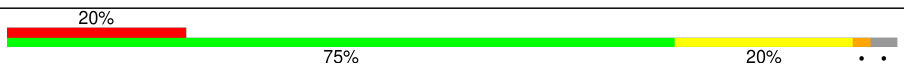
14	2S	112	
15	1T	146	
15	2T	146	
16	1U	118	
16	2U	118	
17	1V	101	
17	2V	101	
18	1W	113	
18	2W	113	
19	1X	96	
19	2X	96	
20	1Y	110	
20	2Y	110	
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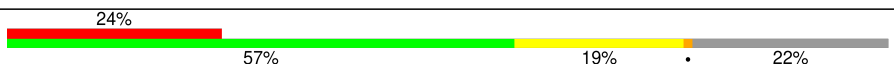
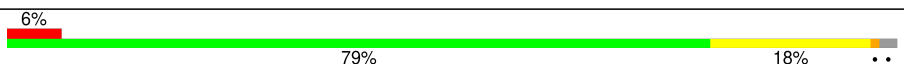
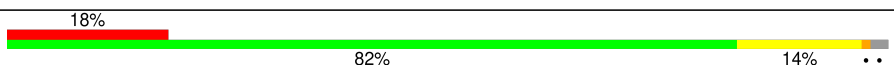
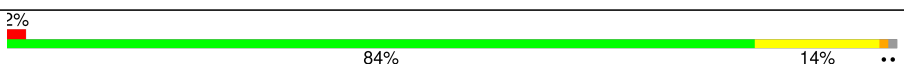
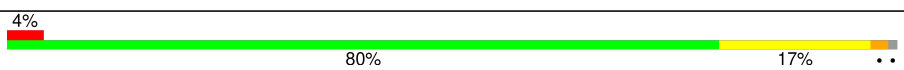
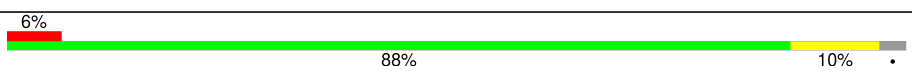
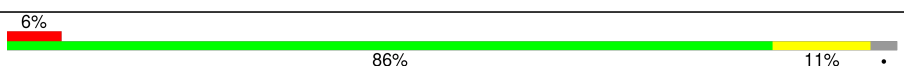
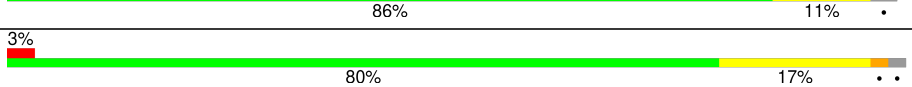
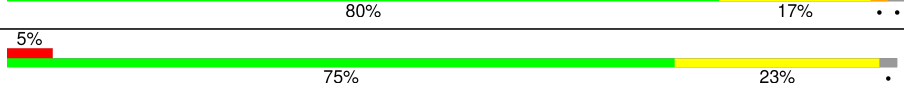
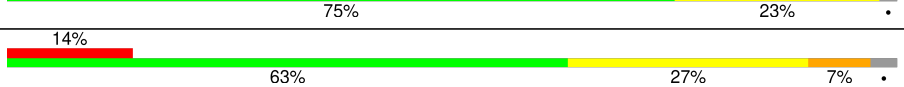
21	2Z	206	
22	10	85	
22	20	85	
23	11	98	
23	21	98	
24	12	72	
24	22	72	
25	13	60	
25	23	60	
26	14	71	

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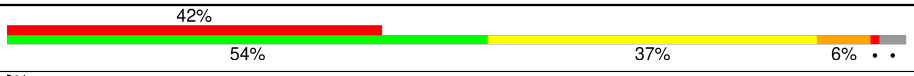
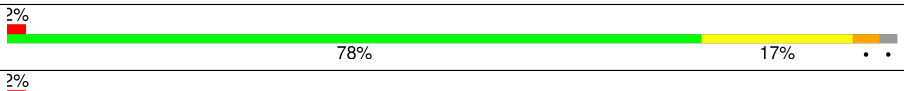
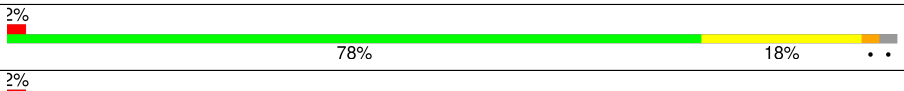
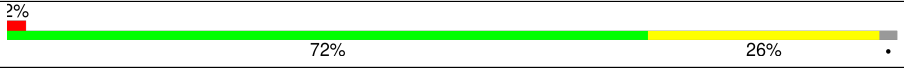
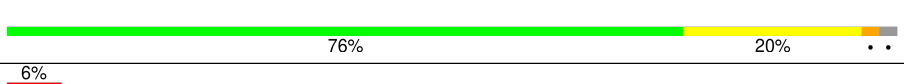
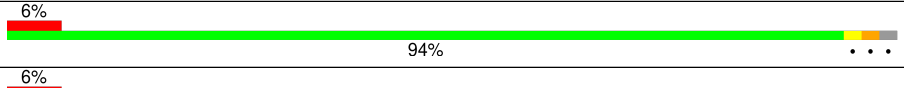
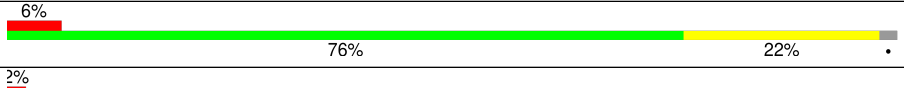
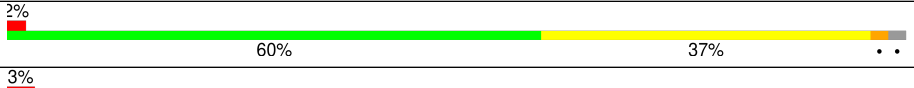
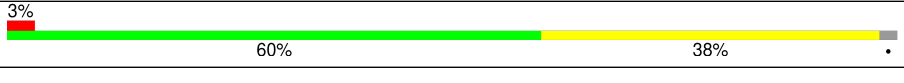
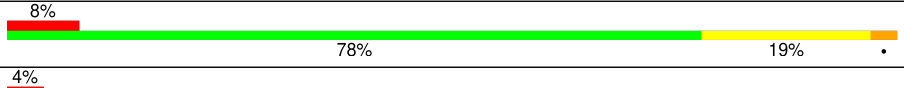
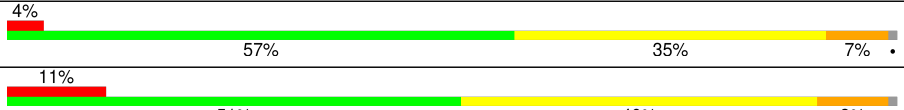
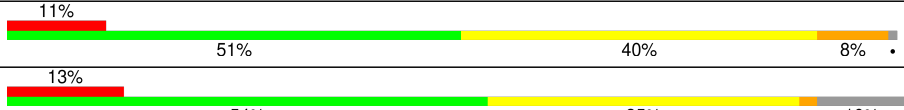
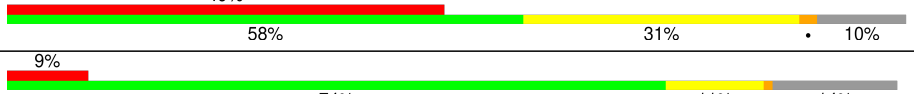
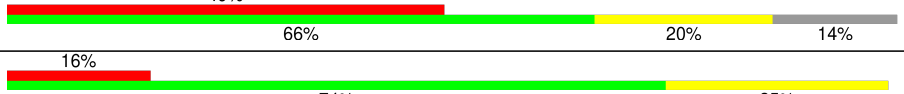
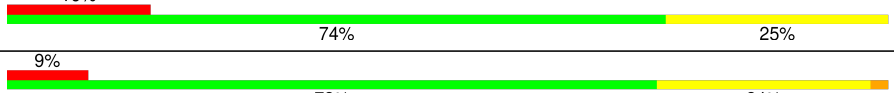
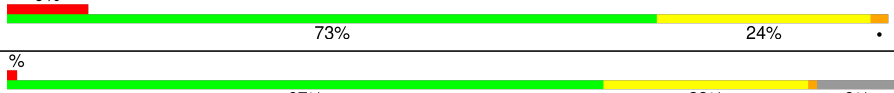
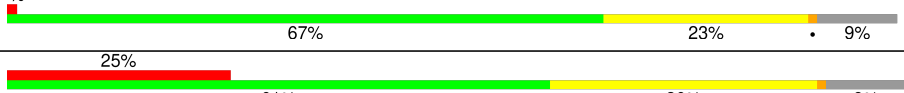
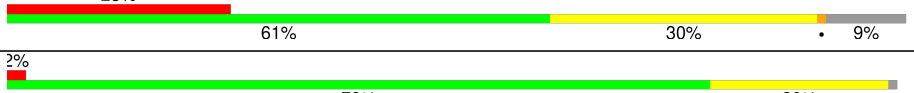
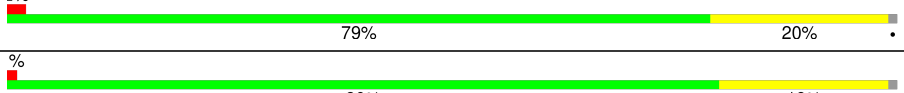
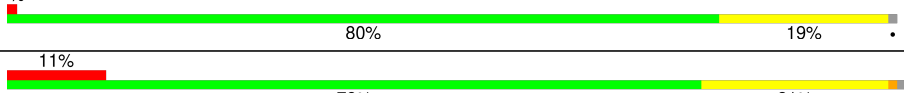
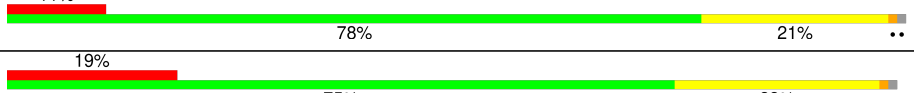
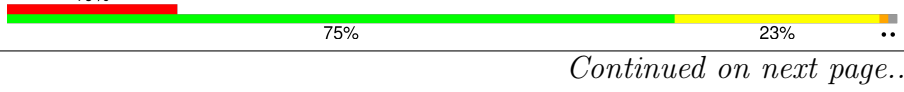
Mol	Chain	Length	Quality of chain
26	24	71	
27	15	60	
27	25	60	
28	16	54	
28	26	54	
29	17	49	
29	27	49	
30	18	65	
30	28	65	
31	19	37	
31	29	37	
32	1a	1521	
32	2a	1521	
33	1b	256	
33	2b	256	
34	1c	239	
34	2c	239	
35	1d	209	
35	2d	209	
36	1e	162	
36	2e	162	
37	1f	101	
37	2f	101	
38	1g	156	
38	2g	156	

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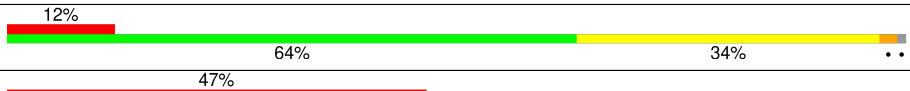
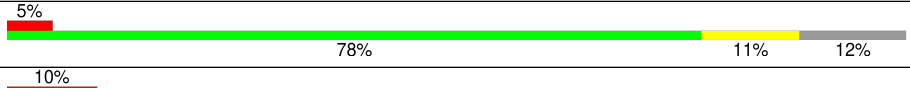
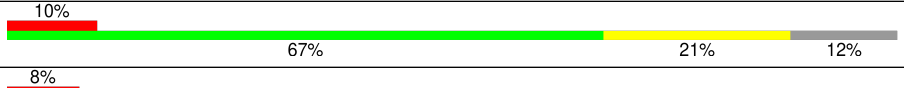
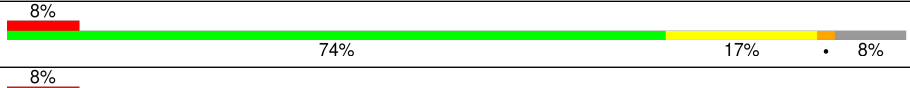
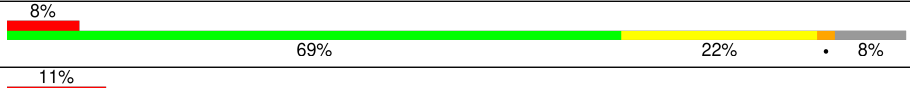
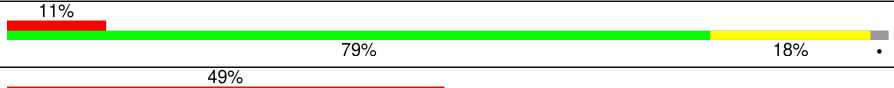
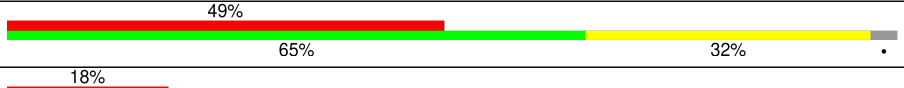
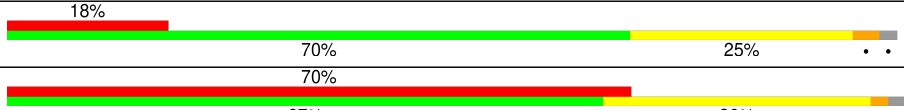
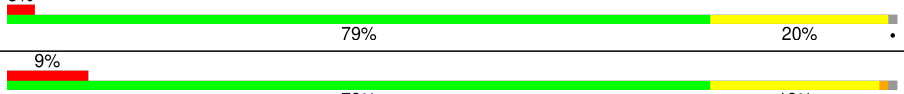
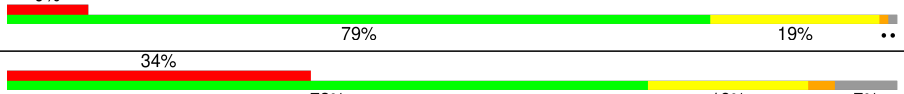
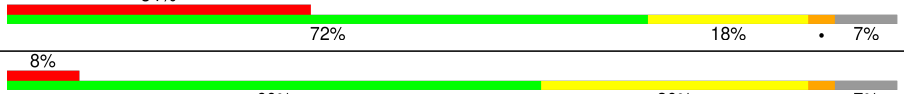
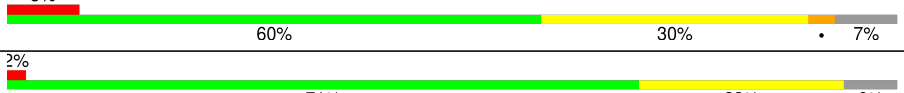
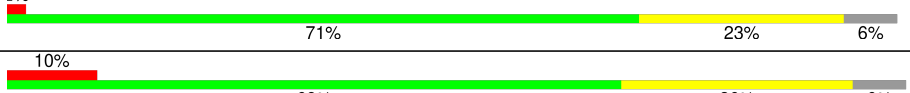
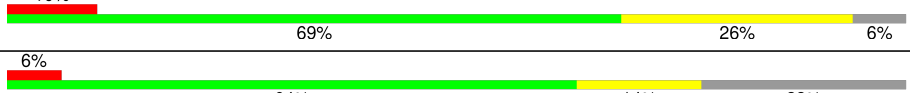
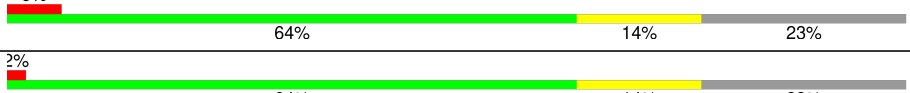
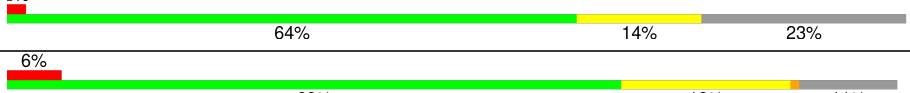
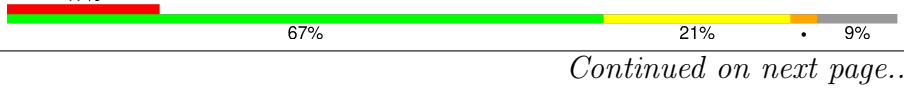
Mol	Chain	Length	Quality of chain
39	1h	138	
39	2h	138	
40	1i	128	
40	2i	128	
41	1j	105	
41	2j	105	
42	1k	129	
42	2k	129	
43	1l	132	
43	2l	132	
44	1m	126	
44	2m	126	
45	1n	61	
45	2n	61	
46	1o	89	
46	2o	89	
47	1p	88	
47	2p	88	
48	1q	105	
48	2q	105	
49	1r	88	
49	2r	88	
50	1s	93	
50	2s	93	
51	1t	106	

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Mol	Chain	Length	Quality of chain
51	2t	106	11% 69% 18% 9%
52	1u	27	7% 59% 26% 15%
52	2u	27	59% 44% 41% 15%
53	1v	27	15% 37% 7% 52%
53	2v	27	22% 37% 7% 52%
54	1w	76	32% 29% 43% 22%
54	1y	76	43% 32% 41% 24%
54	2w	76	33% 33% 46% 16%
54	2y	76	61% 25% 42% 22% 7%
55	1x	77	3% 71% 22% 5%
55	2x	77	6% 53% 38% 8%
56	A	9	11% 44% 44%
56	B	9	56% 33% 22% 11% 11% 22%
56	C	9	67% 56% 44%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	1A	3754	-	-	-	X
57	MG	2X	3002	-	-	-	X
57	MG	2a	1687	-	-	-	X
57	MG	C	8001	-	-	-	X

2 Entry composition (i)

There are 61 unique types of molecules in this entry. The entry contains 301143 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 mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	1v	13	Total	C	N	O	P	0	0	0
			276	124	48	91	13			
53	2v	13	Total	C	N	O	P	0	0	0
			276	124	48	91	13			

- Molecule 54 is a RNA chain called A-site and E-site tRNAs.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
54	1w	73	Total	C	N	O	P	S	0	0	0
			1568	700	282	512	73	1			
54	1y	74	Total	C	N	O	P	S	0	0	0
			1591	710	287	519	74	1			
54	2w	73	Total	C	N	O	P	S	0	0	0
			1568	700	282	512	73	1			
54	2y	73	Total	C	N	O	P	S	0	0	0
			1568	700	282	512	73	1			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
55	1x	76	Total	C	N	O	P	S	0	0	0
			1625	725	294	529	76	1			
55	2x	76	Total	C	N	O	P	S	0	0	0
			1625	725	294	529	76	1			

- Molecule 56 is a protein called NOSO-95179 antibiotic.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
56	A	9	Total	C	N	O	0	0	0
			72	43	18	11			
56	B	7	Total	C	N	O	0	0	0
			55	33	14	8			
56	C	9	Total	C	N	O	0	0	0
			72	43	18	11			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	1A	1149	Total	Mg	0	0
			1149	1149		
57	1B	36	Total	Mg	0	0
			36	36		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	1D	9	Total Mg 9 9	0	0
57	1E	10	Total Mg 10 10	0	0
57	1F	8	Total Mg 8 8	0	0
57	1G	5	Total Mg 5 5	0	0
57	1I	1	Total Mg 1 1	0	0
57	1N	7	Total Mg 7 7	0	0
57	1O	4	Total Mg 4 4	0	0
57	1P	4	Total Mg 4 4	0	0
57	1Q	5	Total Mg 5 5	0	0
57	1R	3	Total Mg 3 3	0	0
57	1S	3	Total Mg 3 3	0	0
57	1T	2	Total Mg 2 2	0	0
57	1U	6	Total Mg 6 6	0	0
57	1V	2	Total Mg 2 2	0	0
57	1W	5	Total Mg 5 5	0	0
57	1X	6	Total Mg 6 6	0	0
57	1Y	3	Total Mg 3 3	0	0
57	1Z	4	Total Mg 4 4	0	0
57	10	6	Total Mg 6 6	0	0
57	11	2	Total Mg 2 2	0	0
57	12	2	Total Mg 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	13	2	Total Mg 2 2	0	0
57	15	2	Total Mg 2 2	0	0
57	16	1	Total Mg 1 1	0	0
57	17	2	Total Mg 2 2	0	0
57	18	4	Total Mg 4 4	0	0
57	19	1	Total Mg 1 1	0	0
57	1a	314	Total Mg 314 314	0	0
57	1b	2	Total Mg 2 2	0	0
57	1d	2	Total Mg 2 2	0	0
57	1e	2	Total Mg 2 2	0	0
57	1f	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	1r	1	Total Mg 1 1	0	0
57	1s	1	Total Mg 1 1	0	0
57	1t	1	Total Mg 1 1	0	0
57	1v	1	Total Mg 1 1	0	0
57	1w	8	Total Mg 8 8	0	0
57	1x	14	Total Mg 14 14	0	0
57	1y	6	Total Mg 6 6	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	2A	861	Total Mg 861 861	0	0
57	2B	21	Total Mg 21 21	0	0
57	2D	4	Total Mg 4 4	0	0
57	2E	10	Total Mg 10 10	0	0
57	2F	3	Total Mg 3 3	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	2Q	3	Total Mg 3 3	0	0
57	2R	2	Total Mg 2 2	0	0
57	2T	4	Total Mg 4 4	0	0
57	2U	4	Total Mg 4 4	0	0
57	2V	2	Total Mg 2 2	0	0
57	2W	2	Total Mg 2 2	0	0
57	2X	3	Total Mg 3 3	0	0
57	2Z	1	Total Mg 1 1	0	0
57	20	2	Total Mg 2 2	0	0
57	21	2	Total Mg 2 2	0	0
57	23	2	Total Mg 2 2	0	0
57	25	3	Total Mg 3 3	0	0
57	26	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	28	3	Total Mg 3 3	0	0
57	29	1	Total Mg 1 1	0	0
57	2a	202	Total Mg 202 202	0	0
57	2d	1	Total Mg 1 1	0	0
57	2e	2	Total Mg 2 2	0	0
57	2f	2	Total Mg 2 2	0	0
57	2g	1	Total Mg 1 1	0	0
57	2i	1	Total Mg 1 1	0	0
57	2j	2	Total Mg 2 2	0	0
57	2l	3	Total Mg 3 3	0	0
57	2n	1	Total Mg 1 1	0	0
57	2q	3	Total Mg 3 3	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	2x	6	Total Mg 6 6	0	0
57	2y	7	Total Mg 7 7	0	0
57	C	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

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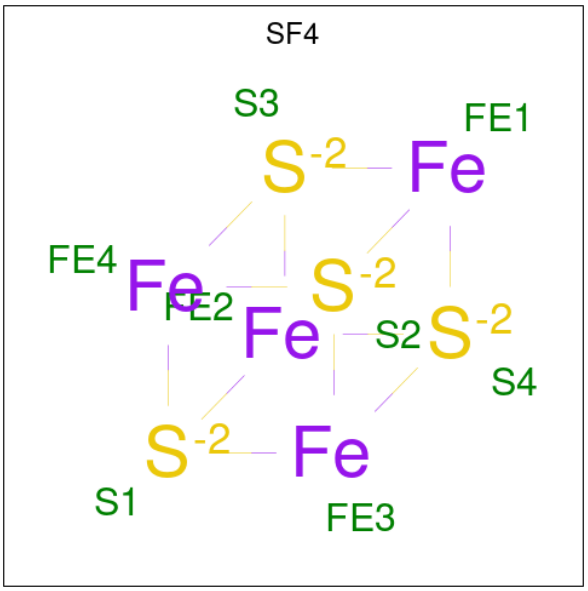
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	2A	1	Total K 1 1	0	0

- Molecule 59 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	1Y	1	Total Zn 1 1	0	0
59	14	1	Total Zn 1 1	0	0
59	15	1	Total Zn 1 1	0	0
59	16	1	Total Zn 1 1	0	0
59	19	1	Total Zn 1 1	0	0
59	1n	1	Total Zn 1 1	0	0
59	2Y	1	Total Zn 1 1	0	0
59	24	1	Total Zn 1 1	0	0
59	25	1	Total Zn 1 1	0	0
59	26	1	Total Zn 1 1	0	0
59	29	1	Total Zn 1 1	0	0
59	2n	1	Total Zn 1 1	0	0

- Molecule 60 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	1d	1	Total Fe S 8 4 4	0	0
60	2d	1	Total Fe S 8 4 4	0	0

- Molecule 61 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1A	2172	Total O 2172 2172	0	0
61	1B	71	Total O 71 71	0	0
61	1D	28	Total O 28 28	0	0
61	1E	29	Total O 29 29	0	0
61	1F	18	Total O 18 18	0	0
61	1G	7	Total O 7 7	0	0
61	1H	2	Total O 2 2	0	0
61	1I	2	Total O 2 2	0	0
61	1N	5	Total O 5 5	0	0
61	1O	8	Total O 8 8	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1P	23	Total O 23 23	0	0
61	1Q	11	Total O 11 11	0	0
61	1R	18	Total O 18 18	0	0
61	1S	3	Total O 3 3	0	0
61	1T	10	Total O 10 10	0	0
61	1U	11	Total O 11 11	0	0
61	1V	8	Total O 8 8	0	0
61	1W	7	Total O 7 7	0	0
61	1X	7	Total O 7 7	0	0
61	1Y	4	Total O 4 4	0	0
61	1Z	1	Total O 1 1	0	0
61	10	11	Total O 11 11	0	0
61	11	9	Total O 9 9	0	0
61	12	5	Total O 5 5	0	0
61	13	6	Total O 6 6	0	0
61	15	5	Total O 5 5	0	0
61	16	4	Total O 4 4	0	0
61	17	7	Total O 7 7	0	0
61	18	12	Total O 12 12	0	0
61	19	1	Total O 1 1	0	0
61	1a	686	Total O 686 686	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1b	1	Total O 1 1	0	0
61	1d	3	Total O 3 3	0	0
61	1f	1	Total O 1 1	0	0
61	1g	1	Total O 1 1	0	0
61	1i	1	Total O 1 1	0	0
61	1l	10	Total O 10 10	0	0
61	1m	1	Total O 1 1	0	0
61	1o	2	Total O 2 2	0	0
61	1p	3	Total O 3 3	0	0
61	1q	5	Total O 5 5	0	0
61	1u	1	Total O 1 1	0	0
61	1v	6	Total O 6 6	0	0
61	1w	7	Total O 7 7	0	0
61	1x	17	Total O 17 17	0	0
61	1y	4	Total O 4 4	0	0
61	2A	1348	Total O 1348 1348	0	0
61	2B	27	Total O 27 27	0	0
61	2D	26	Total O 26 26	0	0
61	2E	12	Total O 12 12	0	0
61	2F	17	Total O 17 17	0	0
61	2I	4	Total O 4 4	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	2N	2	Total O 2 2	0	0
61	2O	2	Total O 2 2	0	0
61	2P	14	Total O 14 14	0	0
61	2Q	2	Total O 2 2	0	0
61	2R	3	Total O 3 3	0	0
61	2T	6	Total O 6 6	0	0
61	2U	4	Total O 4 4	0	0
61	2V	1	Total O 1 1	0	0
61	2W	5	Total O 5 5	0	0
61	2X	6	Total O 6 6	0	0
61	2Y	1	Total O 1 1	0	0
61	2Z	2	Total O 2 2	0	0
61	20	5	Total O 5 5	0	0
61	21	12	Total O 12 12	0	0
61	22	1	Total O 1 1	0	0
61	23	1	Total O 1 1	0	0
61	25	4	Total O 4 4	0	0
61	26	1	Total O 1 1	0	0
61	27	3	Total O 3 3	0	0
61	28	5	Total O 5 5	0	0
61	29	1	Total O 1 1	0	0

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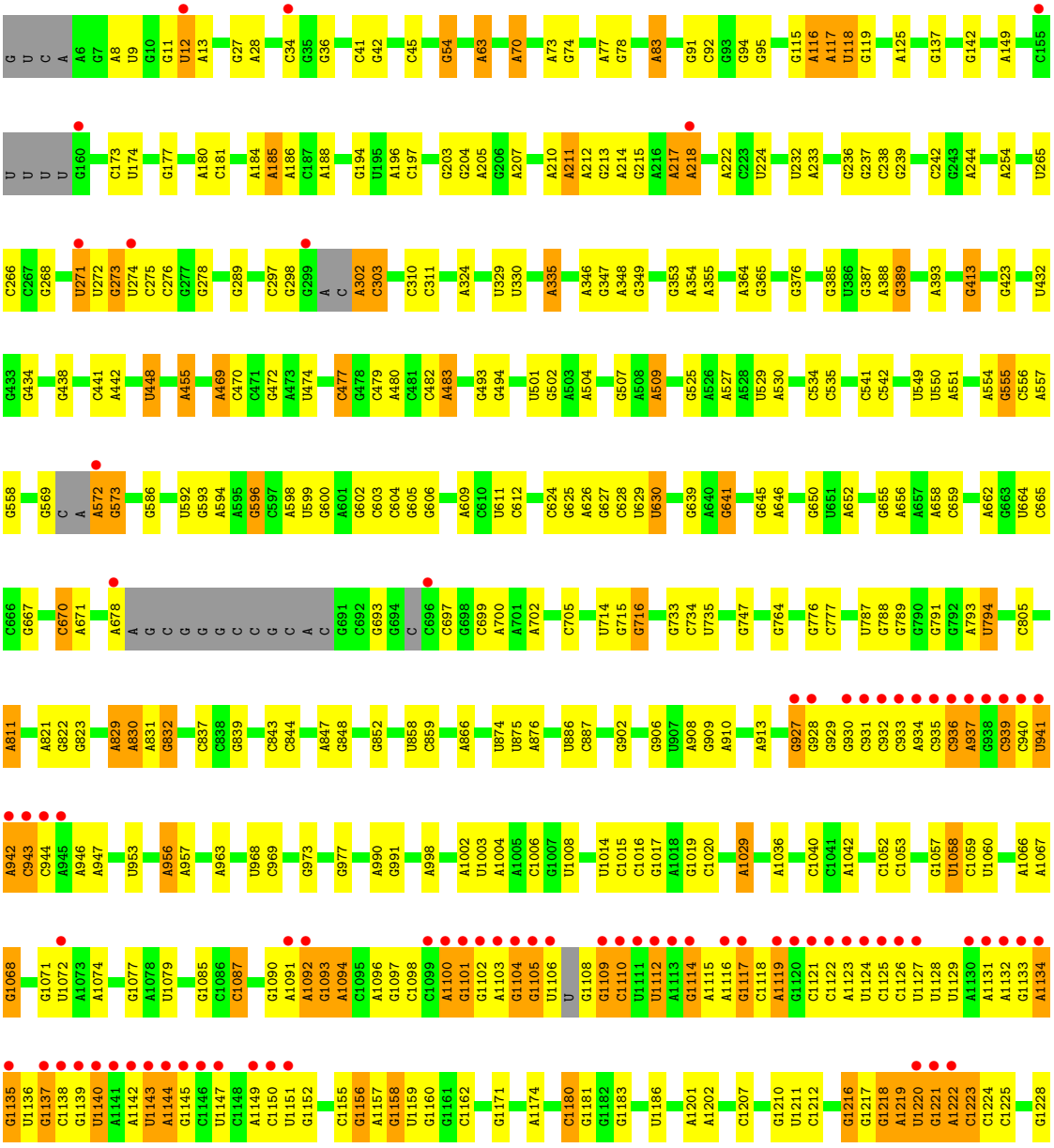
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	2a	270	Total O 270 270	0	0
61	2d	1	Total O 1 1	0	0
61	2g	1	Total O 1 1	0	0
61	2j	4	Total O 4 4	0	0
61	2l	5	Total O 5 5	0	0
61	2m	1	Total O 1 1	0	0
61	2o	1	Total O 1 1	0	0
61	2p	2	Total O 2 2	0	0
61	2q	1	Total O 1 1	0	0
61	2r	1	Total O 1 1	0	0
61	2t	2	Total O 2 2	0	0
61	2v	4	Total O 4 4	0	0
61	2w	4	Total O 4 4	0	0
61	2x	7	Total O 7 7	0	0
61	2y	19	Total O 19 19	0	0
61	C	4	Total O 4 4	0	0

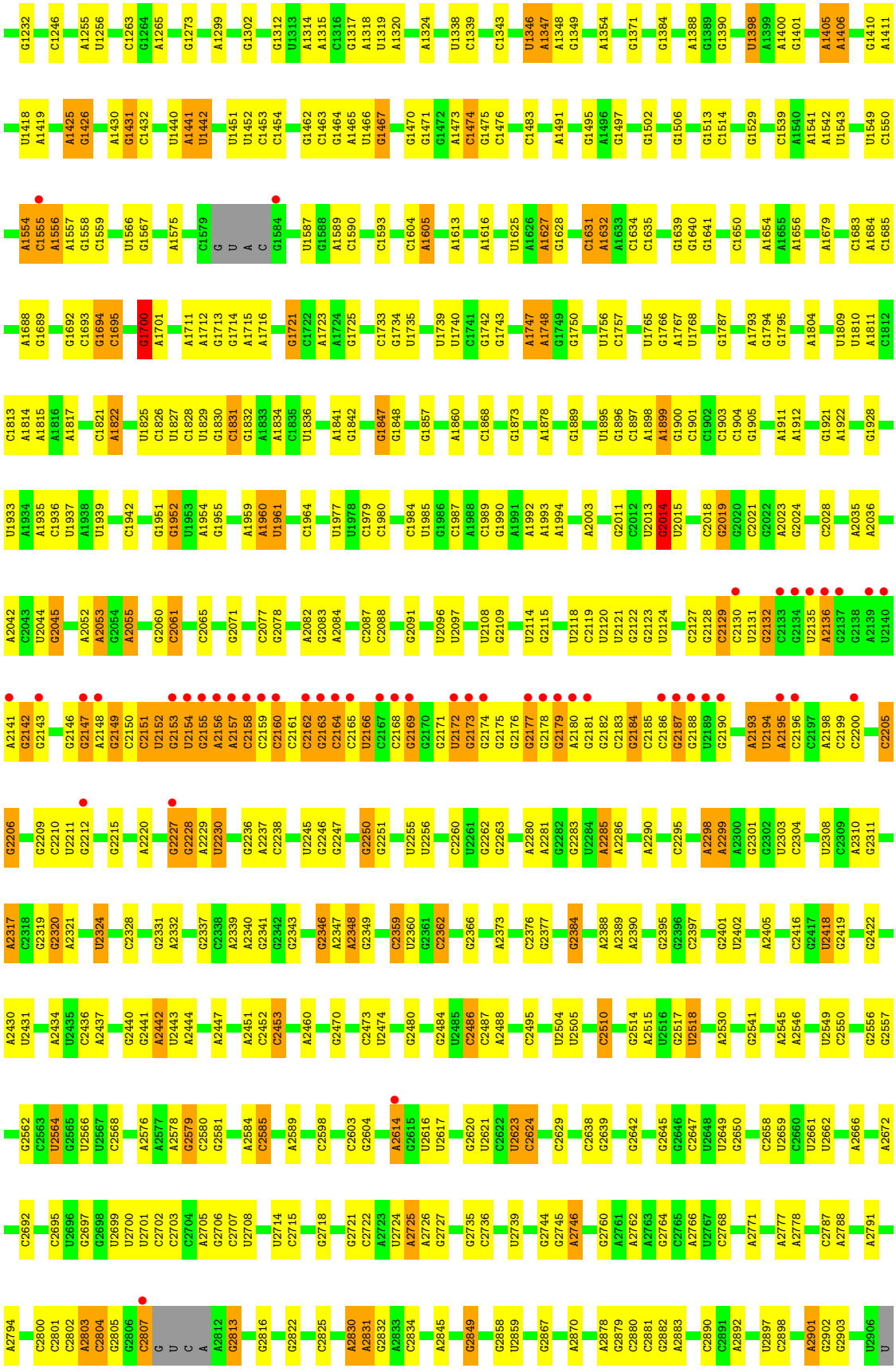
3 Residue-property plots (i)

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

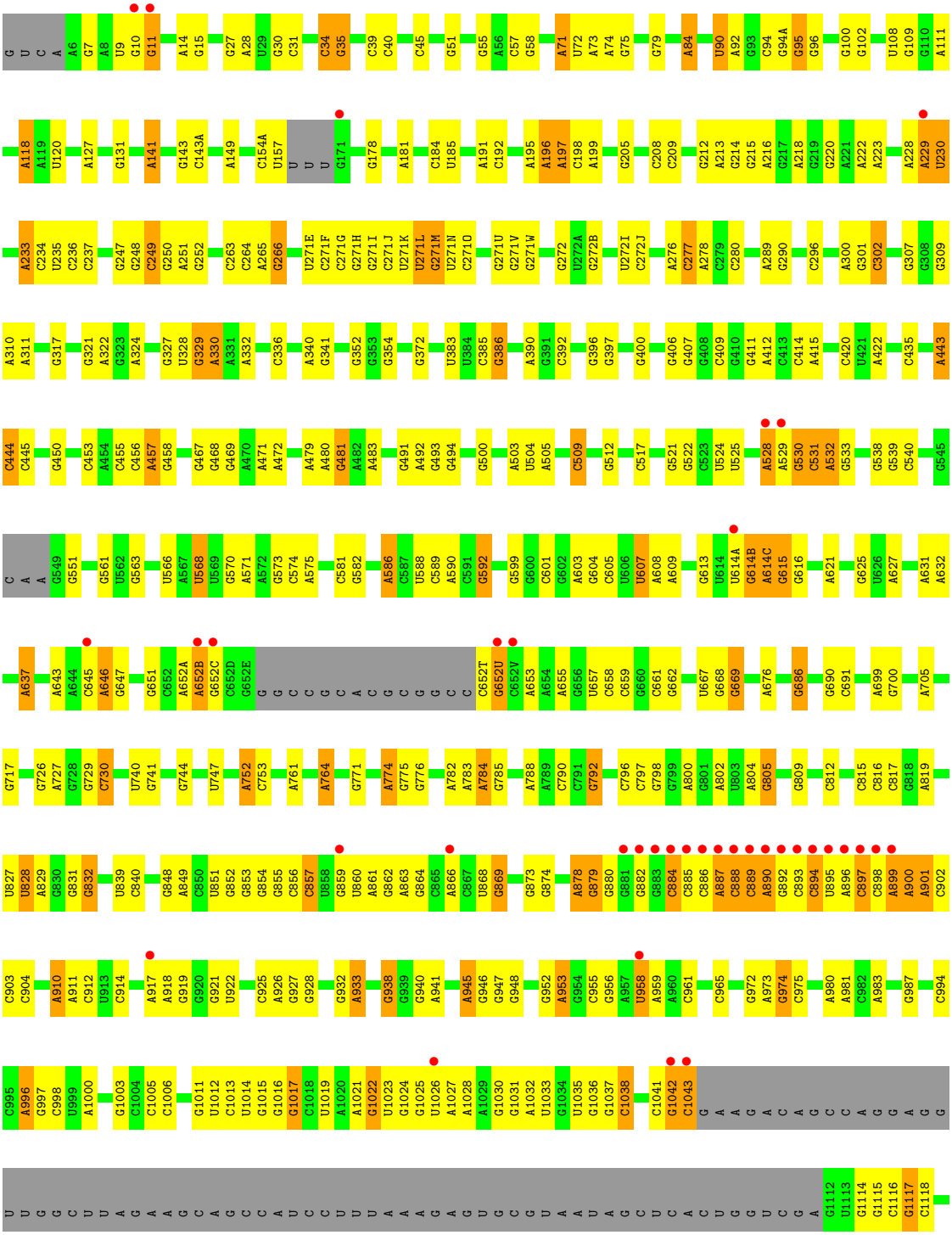
Chain 1A:

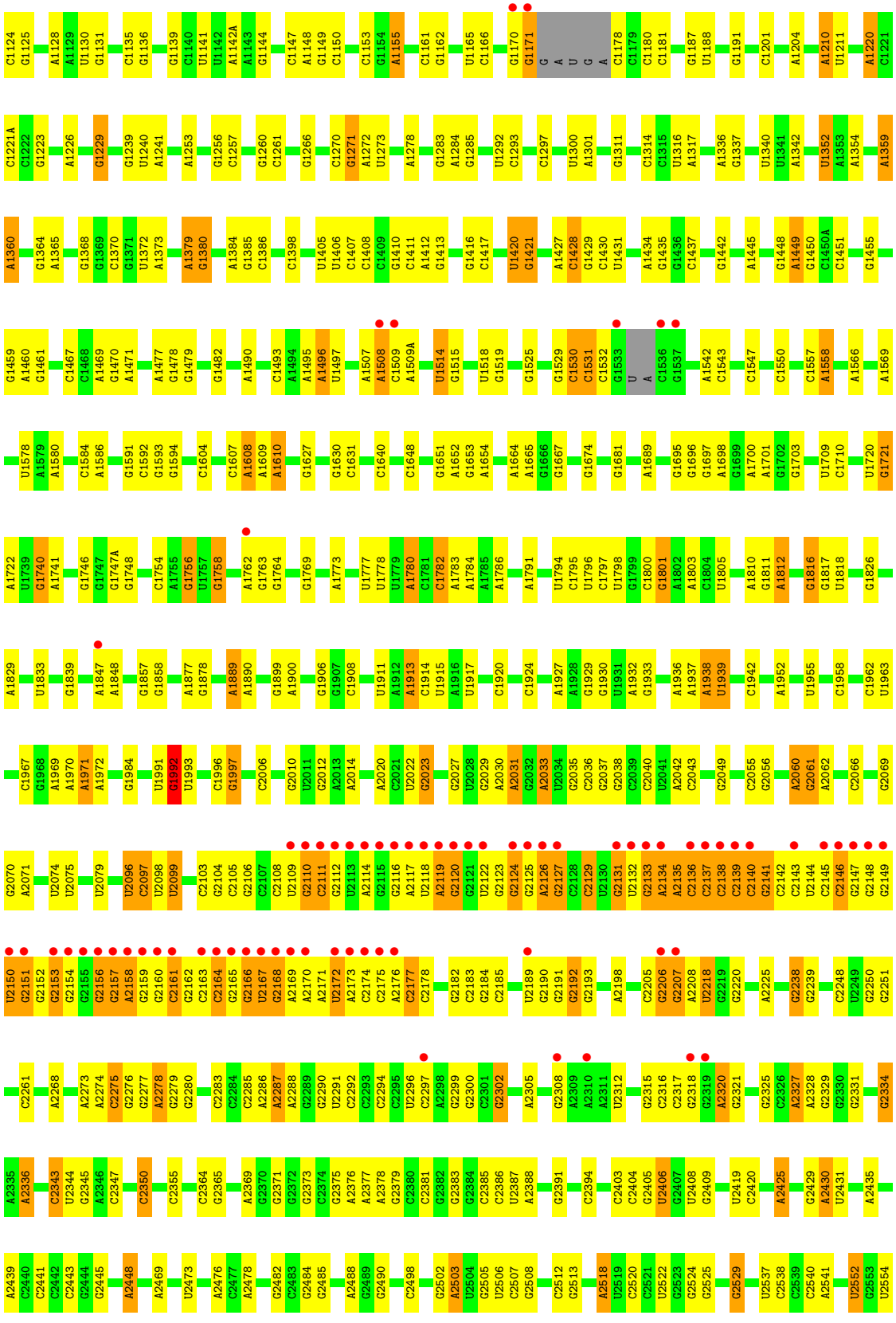




- Molecule 1: 23S Ribosomal RNA

Chain 2A:

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C1221A C1222 G1223 A1226 G1229 G1239 U1240 A1241 A1253 G1256 C1257 G1260 C1261 G1266 C1270 G1271 A1272 U1273 A1278 G1283 A1284 G1285 U1292 C1293 C1297 U1300 A1301 G1311 C1314 C1315 U1316 A1317 A1336 G1337 U1340 U1341 A1342 U1352 A1353 A1354 A1359
A1360 G1364 A1365 G1368 G1369 C1370 G1371 U1372 A1373 A1379 G1380 A1384 G1385 C1386 C1398 U1405 U1406 C1407 C1408 C1409 G1410 C1411 A1412 G1413 G1416 C1417 U1420 G1421 A1427 C1428 G1429 C1430 U1431 A1434 G1435 G1436 C1437 G1442 A1445 G1448 A1449 G1450 C1450A C1451 G1455
G1459 A1460 C1461 C1467 C1468 A1469 G1470 A1471 A1477 G1478 G1479 G1482 A1490 C1493 A1494 A1495 A1496 U1497 A1507 A1508 C1509 A1509A U1514 G1515 U1518 G1519 G1525 G1529 C1530 C1531 C1532 G1533 U A C1536 G1537 A1542 C1543 C1547 C1550 C1557 A1558 A1566 A1569
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U2150 G2151 G2152 G2153 G2154 G2155 G2156 G2157 A2158 G2159 G2160 C2161 G2162 C2163 C2164 G2165 G2166 U2167 G2168 A2169 A2170 A2171 U2172 A2173 C2174 C2175 A2176 C2177 C2178 G2182 C2183 C2184 C2185 U2189 G2190 G2191 G2192 G2193 A2198 C2205 G2206 G2207 A2208 U2218 G2219 G2220 A2225 G2238 G2239 C2248 U2249 G2250 G2251
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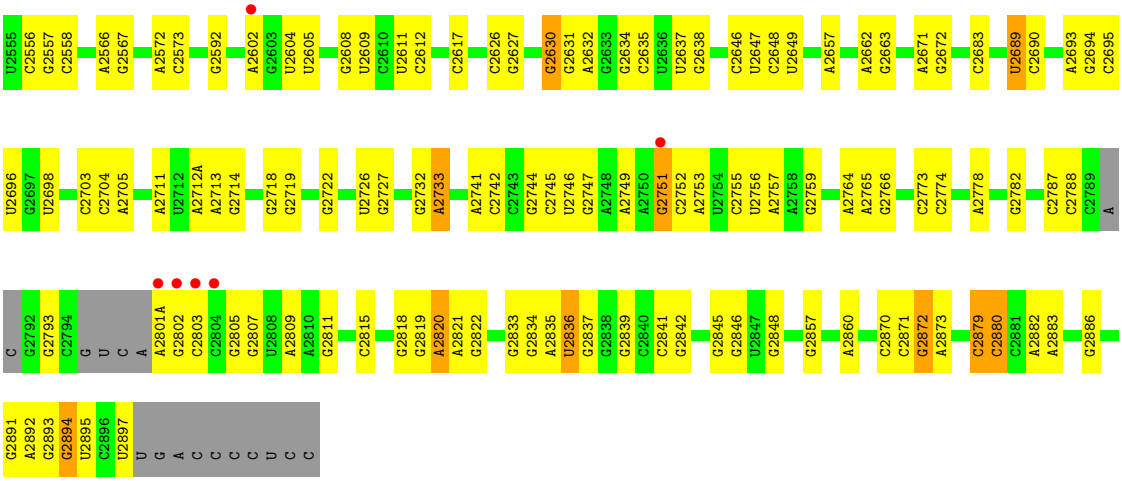
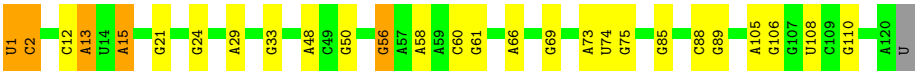
A2439 C2440 C2441 C2442 C2443 G2444 G2445 A2448 A2469 U2473 A2476 C2477 A2478 G2482 C2483 G2484 G2485 A2488 G2489 G2490 C2498 G2502 A2503 U2504 G2505 U2506 C2507 G2508 C2512 G2513 A2518 U2519 C2520 C2521 U2522 G2523 G2524 G2525 G2529 U2537 C2538 C2539 C2540 A2541 U2552 G2553 U2554



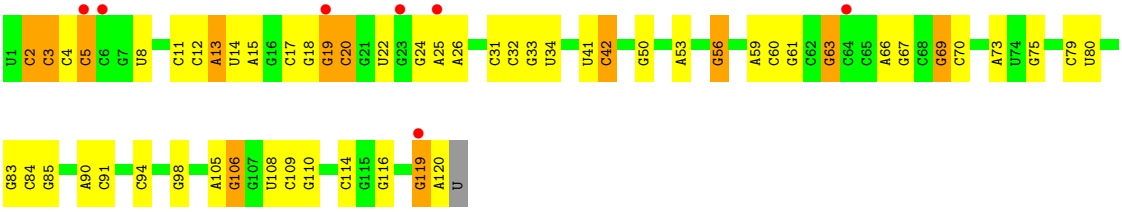
• Molecule 2: 5S Ribosomal RNA

Chain 1B:



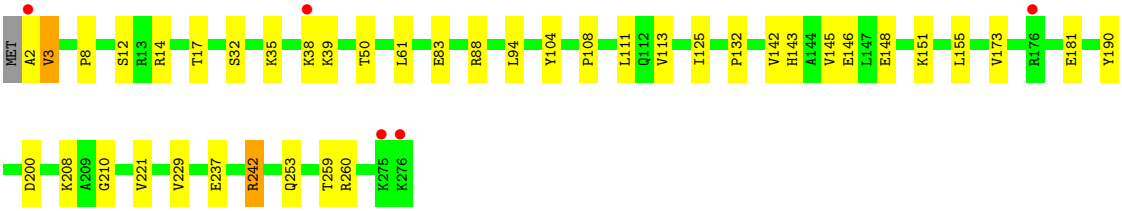
• Molecule 2: 5S Ribosomal RNA

Chain 2B:



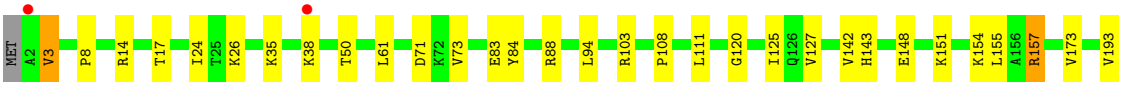
• Molecule 3: 50S ribosomal protein L2

Chain 1D:



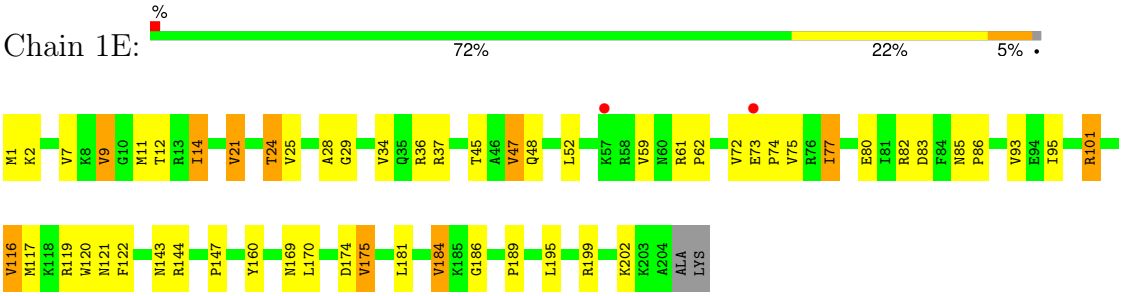
• Molecule 3: 50S ribosomal protein L2

Chain 2D:



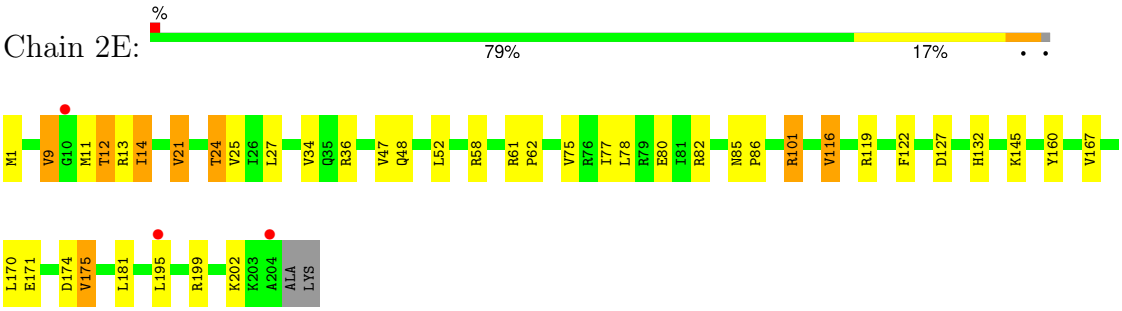
• Molecule 4: 50S ribosomal protein L3

Chain 1E:



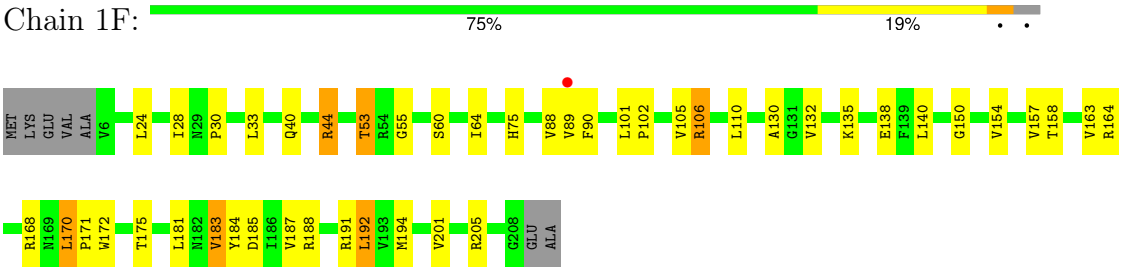
• Molecule 4: 50S ribosomal protein L3

Chain 2E:



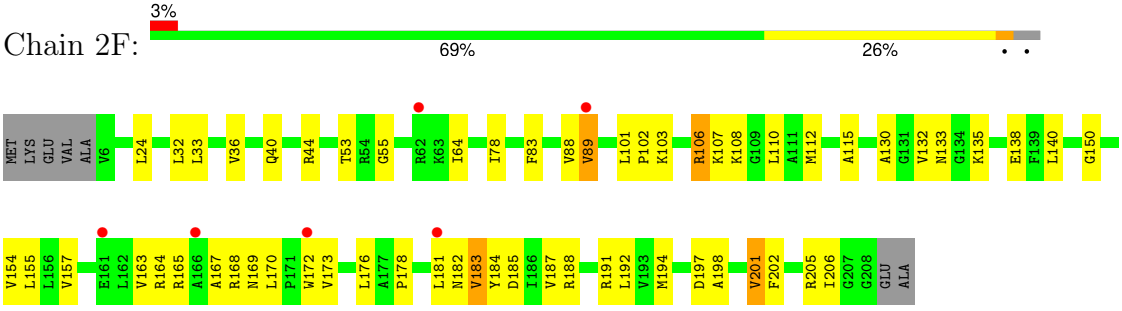
• Molecule 5: 50S ribosomal protein L4

Chain 1F:



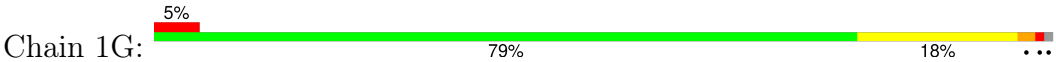
• Molecule 5: 50S ribosomal protein L4

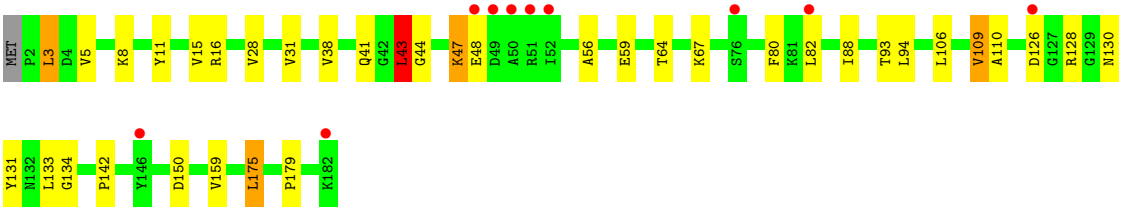
Chain 2F:



• Molecule 6: 50S ribosomal protein L5

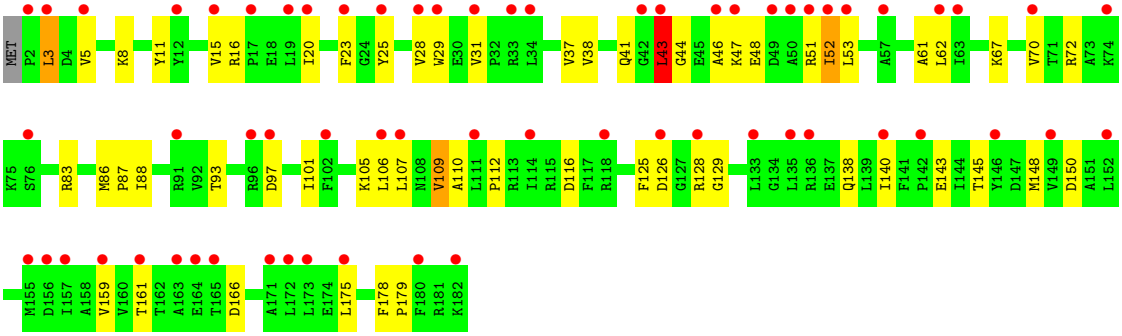
Chain 1G:





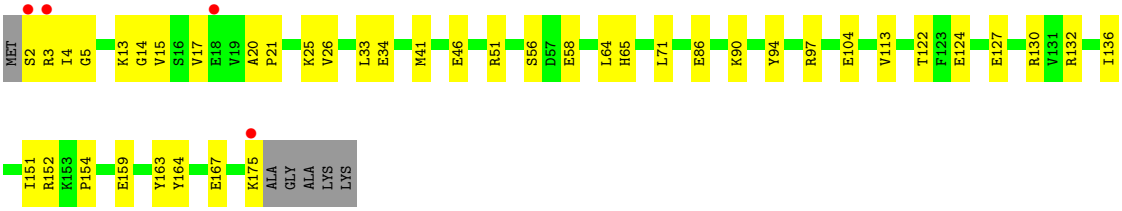
• Molecule 6: 50S ribosomal protein L5

Chain 2G:



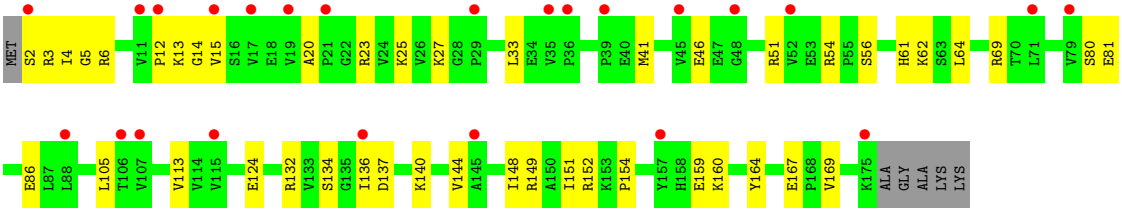
• Molecule 7: 50S ribosomal protein L6

Chain 1H:



• Molecule 7: 50S ribosomal protein L6

Chain 2H:

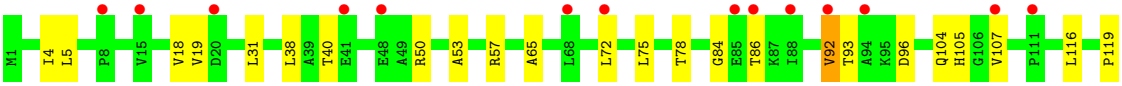


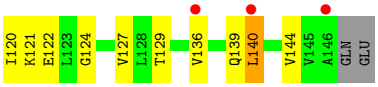
• Molecule 8: 50S ribosomal protein L9

Chain 1I:

• Molecule 8: 50S ribosomal protein L9

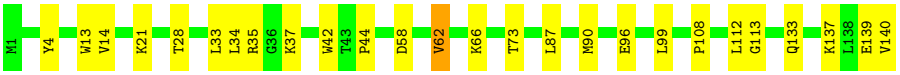
Chain 2I:





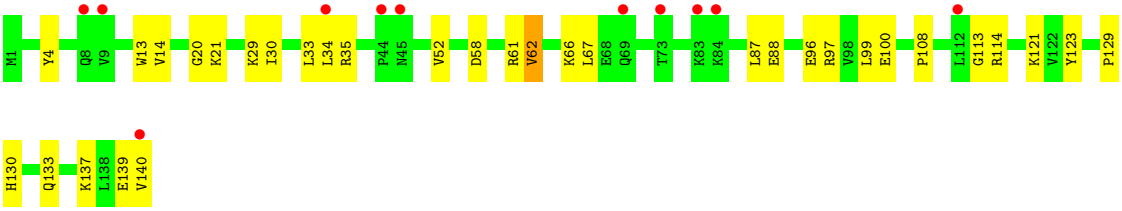
• Molecule 9: 50S ribosomal protein L13

Chain 1N:



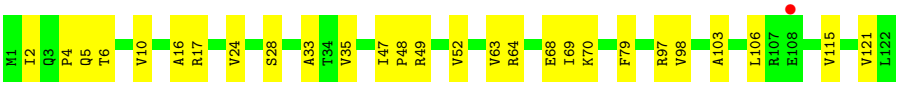
• Molecule 9: 50S ribosomal protein L13

Chain 2N:



• Molecule 10: 50S ribosomal protein L14

Chain 1O:

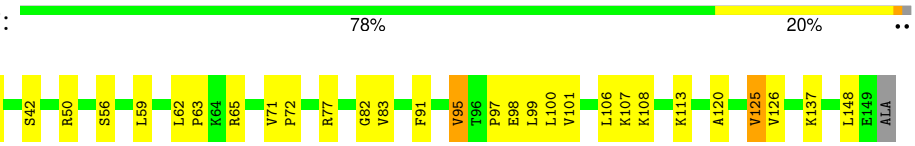


• Molecule 10: 50S ribosomal protein L14

Chain 2O:

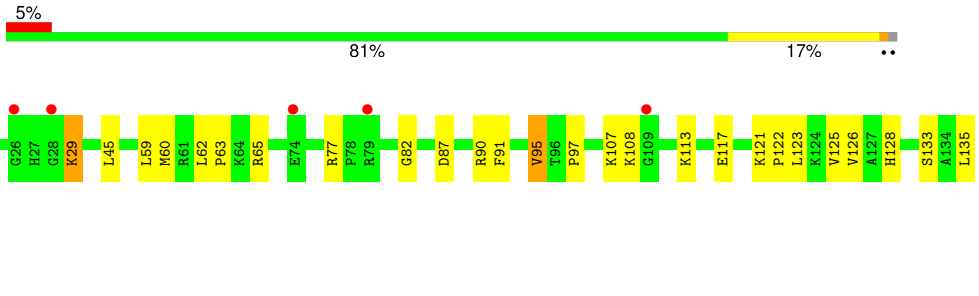
• Molecule 11: 50S ribosomal protein L15

Chain 1P:



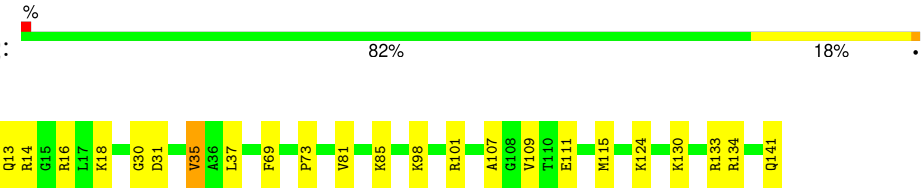
• Molecule 11: 50S ribosomal protein L15

Chain 2P:



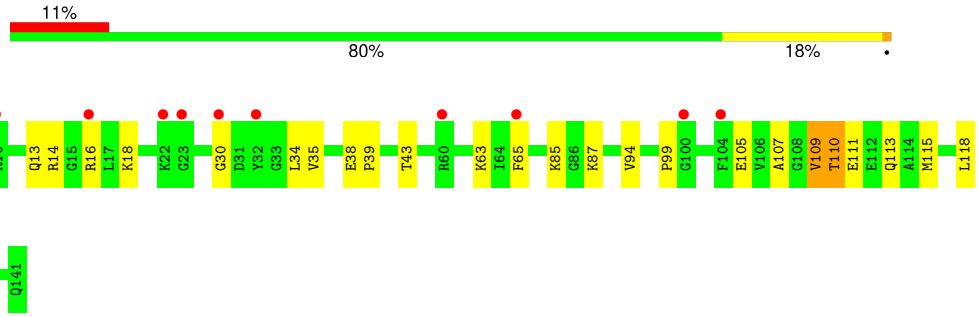
• Molecule 12: 50S ribosomal protein L16

Chain 1Q:



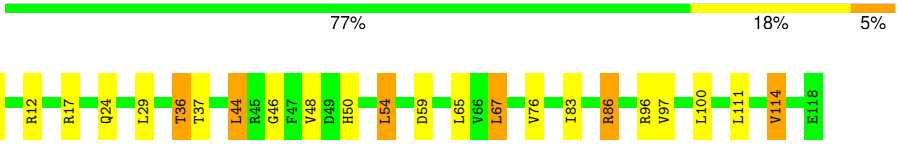
• Molecule 12: 50S ribosomal protein L16

Chain 2Q:



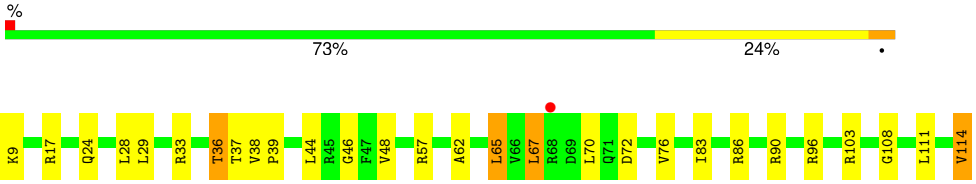
• Molecule 13: 50S ribosomal protein L17

Chain 1R:



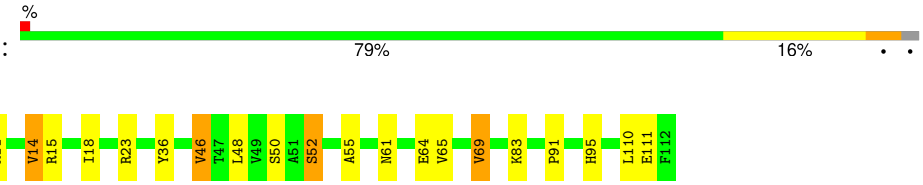
• Molecule 13: 50S ribosomal protein L17

Chain 2R:



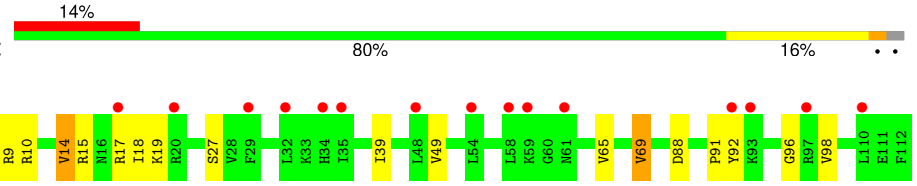
• Molecule 14: 50S ribosomal protein L18

Chain 1S:



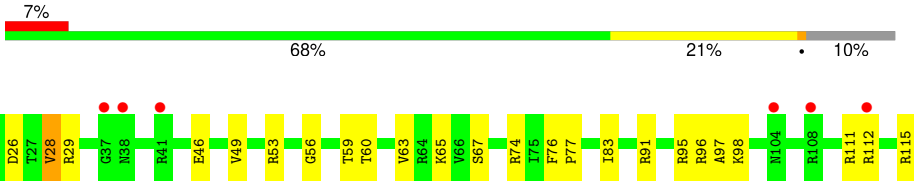
• Molecule 14: 50S ribosomal protein L18

Chain 2S:



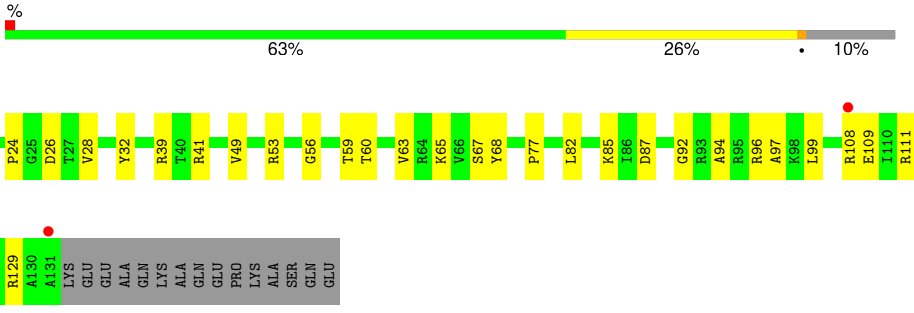
• Molecule 15: 50S ribosomal protein L19

Chain 1T:



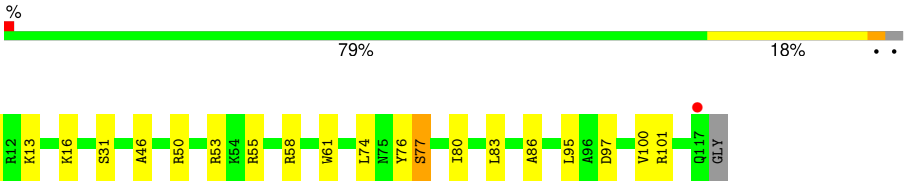
• Molecule 15: 50S ribosomal protein L19

Chain 2T:



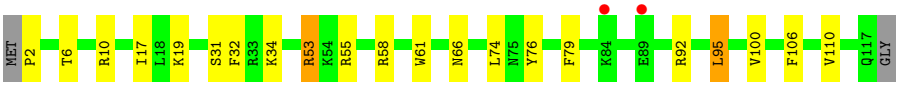
• Molecule 16: 50S ribosomal protein L20

Chain 1U:

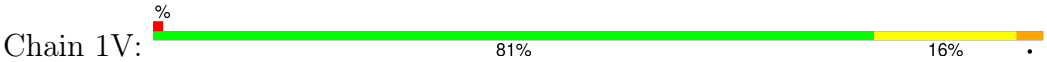


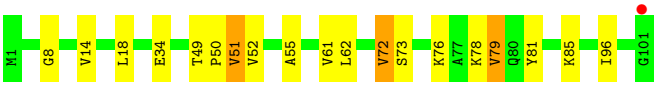
• Molecule 16: 50S ribosomal protein L20

Chain 2U:

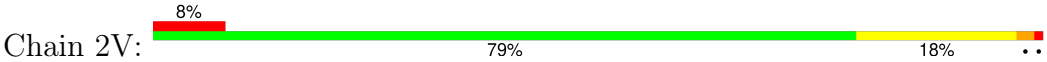


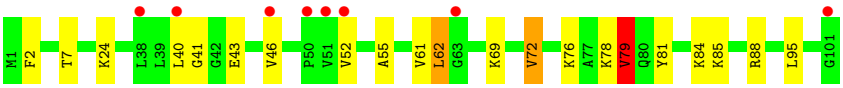
• Molecule 17: 50S ribosomal protein L21



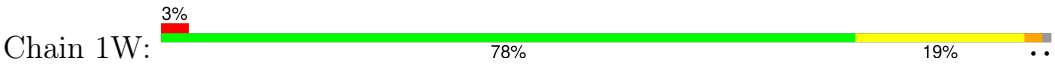


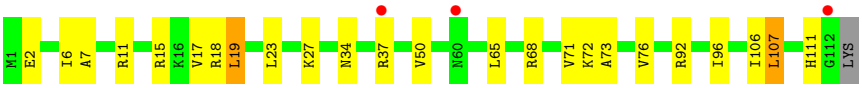
• Molecule 17: 50S ribosomal protein L21



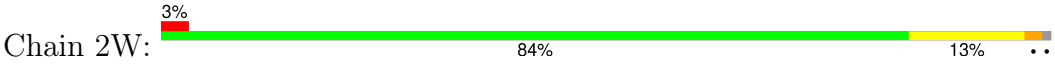


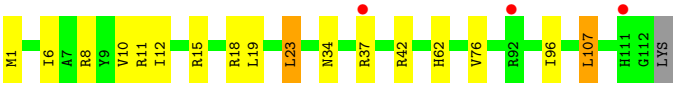
• Molecule 18: 50S ribosomal protein L22



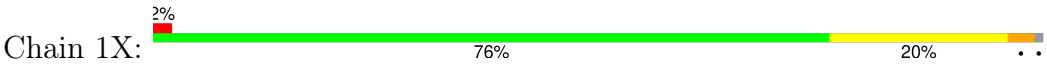


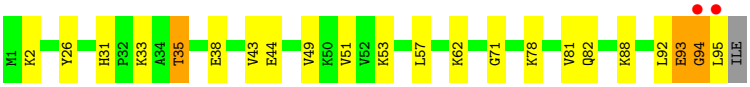
• Molecule 18: 50S ribosomal protein L22



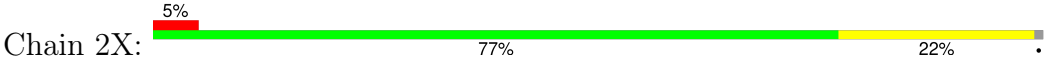


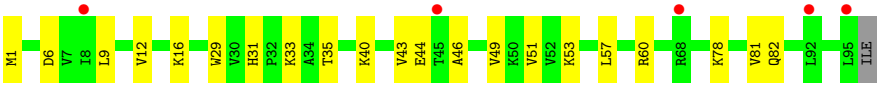
• Molecule 19: 50S ribosomal protein L23





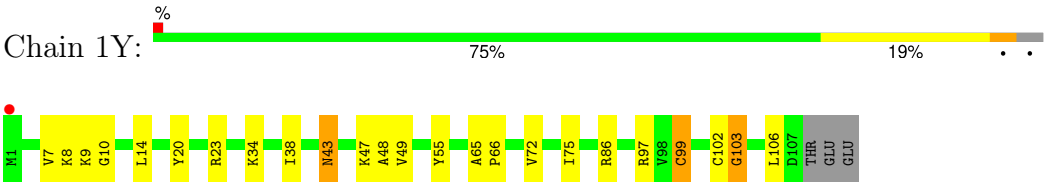
• Molecule 19: 50S ribosomal protein L23





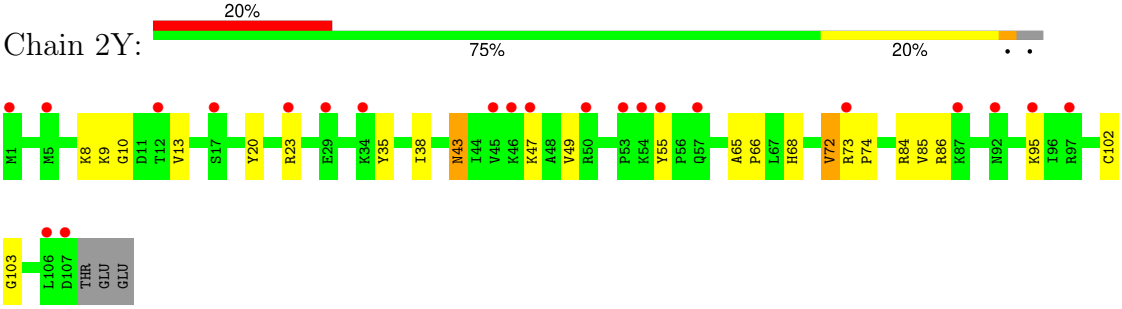
• Molecule 20: 50S ribosomal protein L24

Chain 1Y:



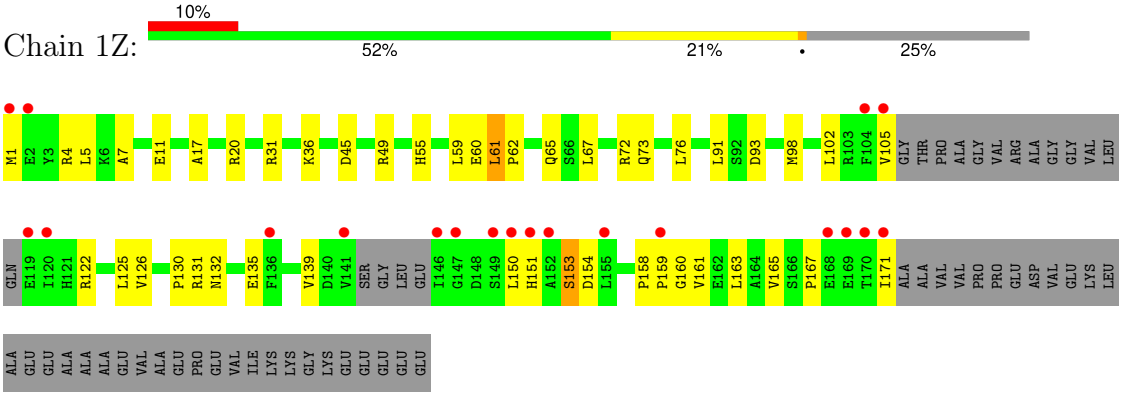
• Molecule 20: 50S ribosomal protein L24

Chain 2Y:



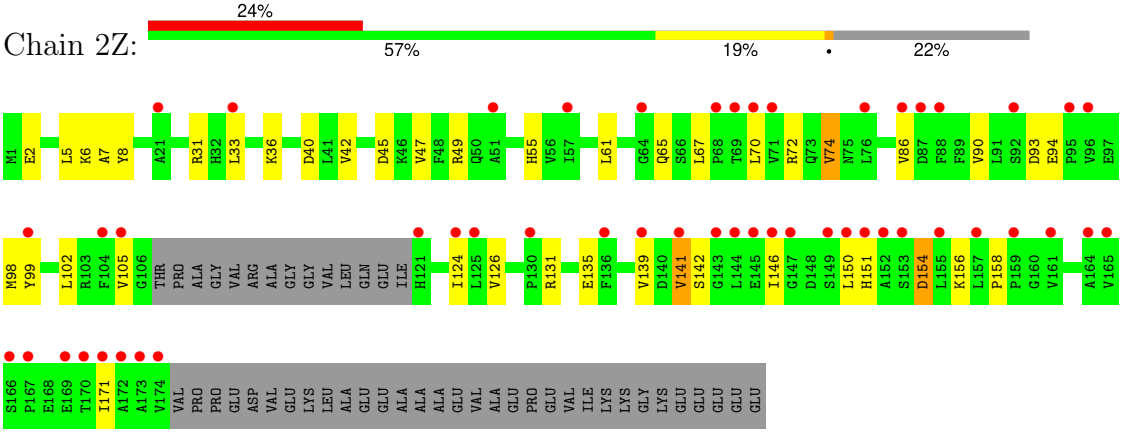
• Molecule 21: 50S ribosomal protein L25

Chain 1Z:



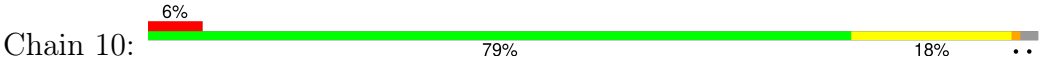
• Molecule 21: 50S ribosomal protein L25

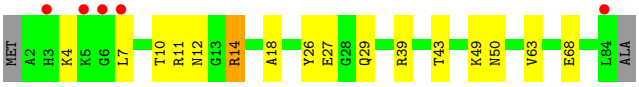
Chain 2Z:



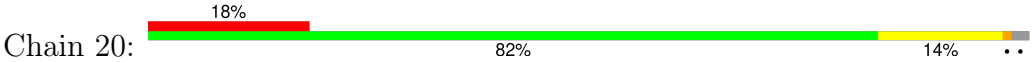
• Molecule 22: 50S ribosomal protein L27

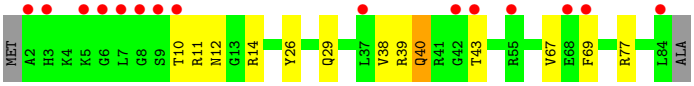
Chain 10:



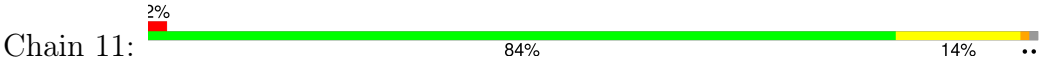


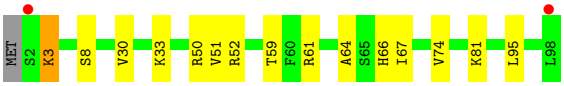
• Molecule 22: 50S ribosomal protein L27



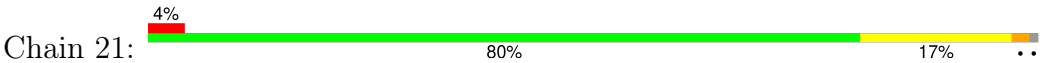


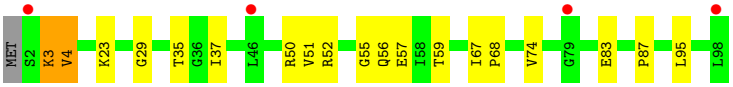
• Molecule 23: 50S ribosomal protein L28



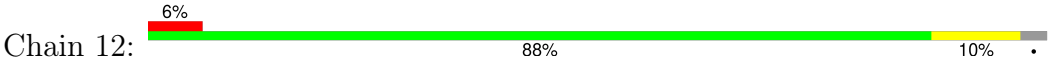


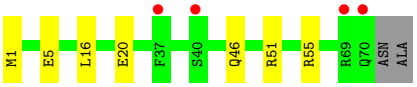
• Molecule 23: 50S ribosomal protein L28



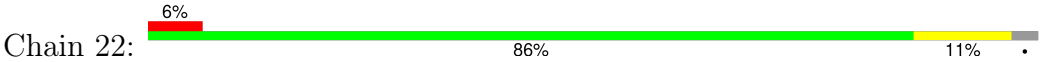


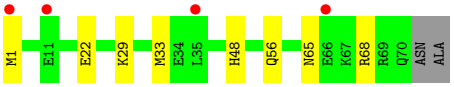
• Molecule 24: 50S ribosomal protein L29



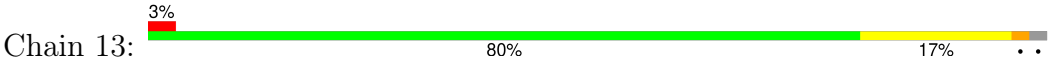


• Molecule 24: 50S ribosomal protein L29





• Molecule 25: 50S ribosomal protein L30

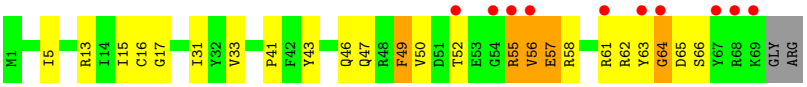


• Molecule 25: 50S ribosomal protein L30

Chain 23:

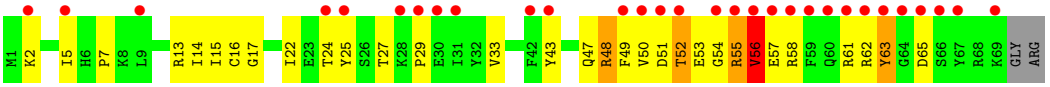
• Molecule 26: 50S ribosomal protein L31

Chain 14:



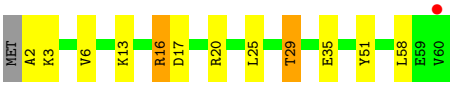
• Molecule 26: 50S ribosomal protein L31

Chain 24:



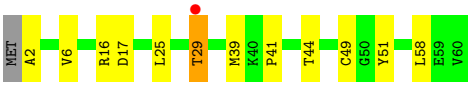
• Molecule 27: 50S ribosomal protein L32

Chain 15:



• Molecule 27: 50S ribosomal protein L32

Chain 25:



• Molecule 28: 50S ribosomal protein L33

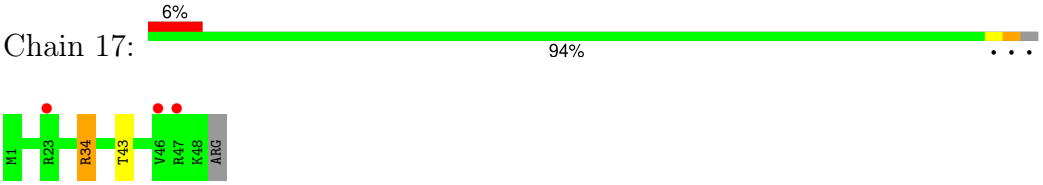
Chain 16:

• Molecule 28: 50S ribosomal protein L33

Chain 26:

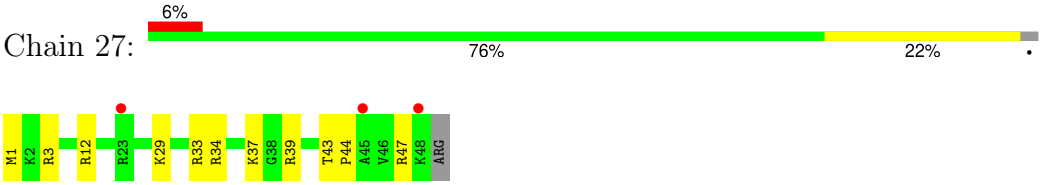
• Molecule 29: 50S ribosomal protein L34

Chain 17:



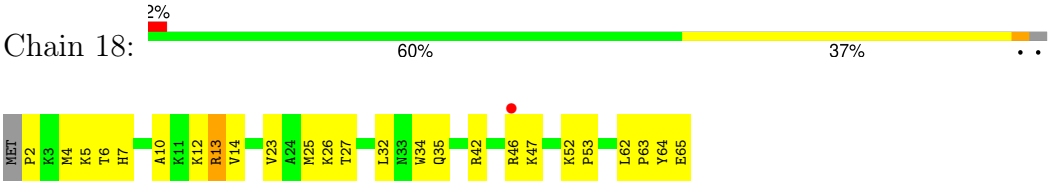
• Molecule 29: 50S ribosomal protein L34

Chain 27:



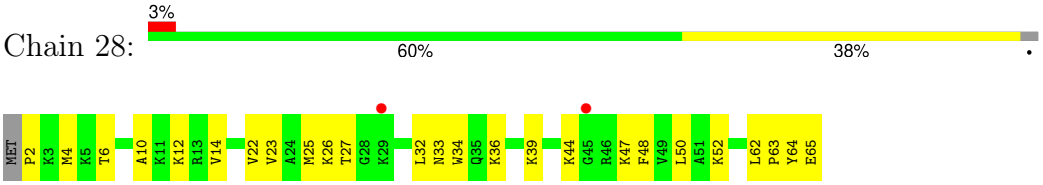
• Molecule 30: 50S ribosomal protein L35

Chain 18:



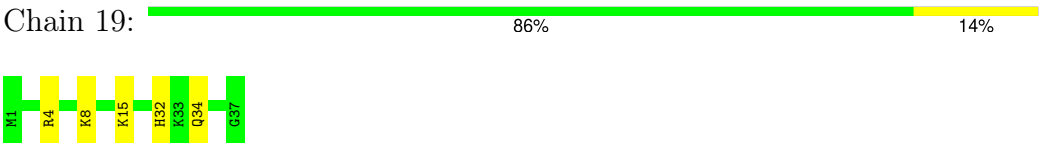
• Molecule 30: 50S ribosomal protein L35

Chain 28:



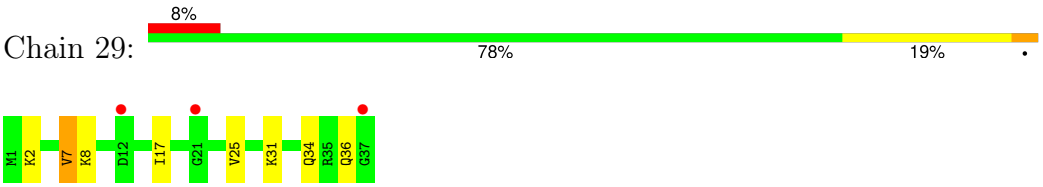
• Molecule 31: 50S ribosomal protein L36

Chain 19:



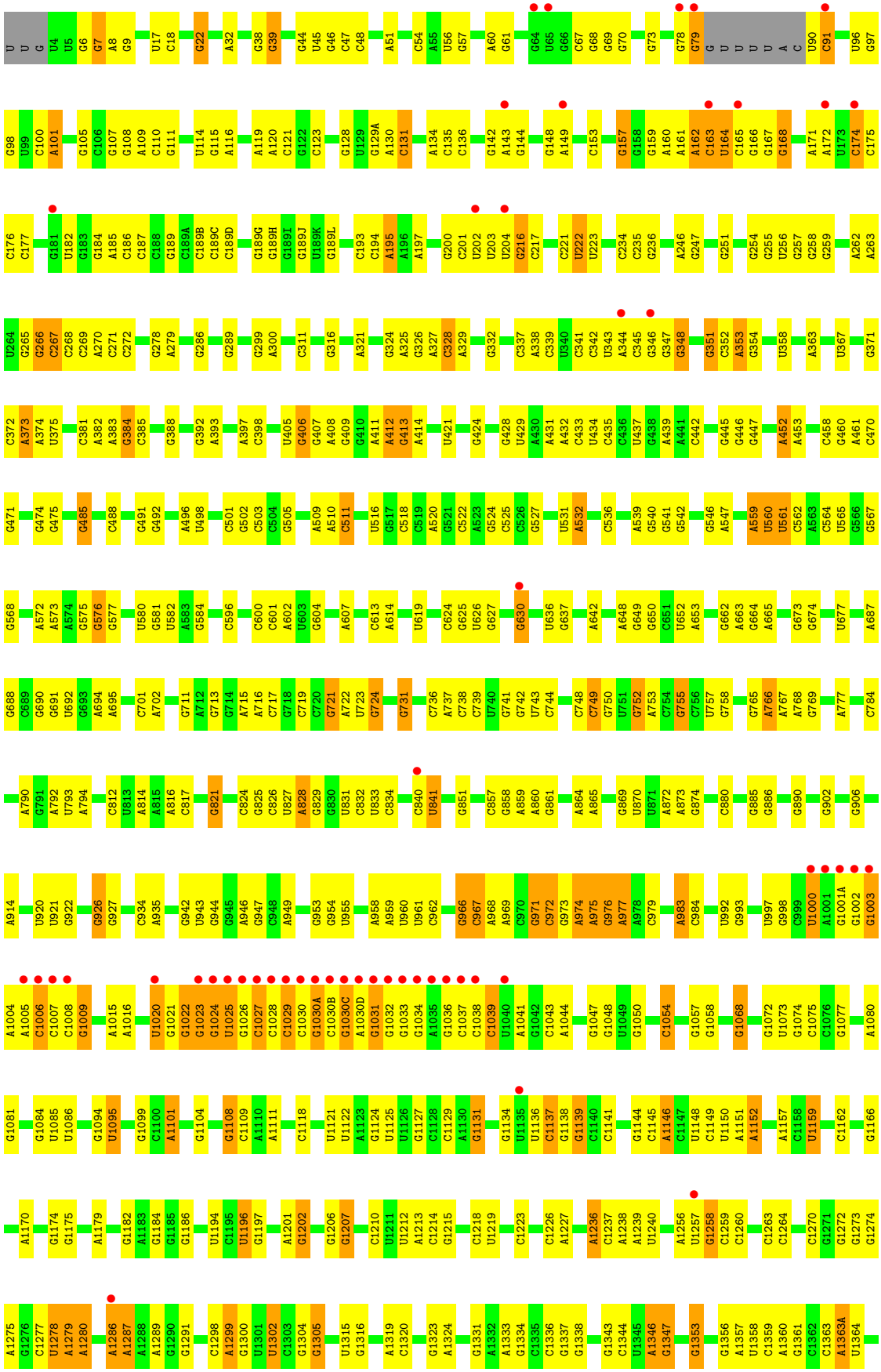
• Molecule 31: 50S ribosomal protein L36

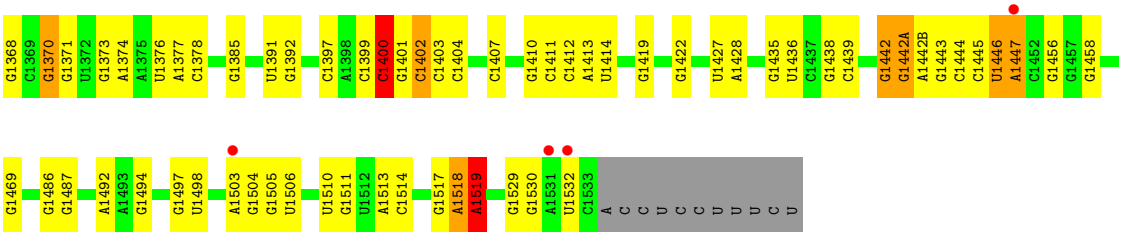
Chain 29:



• Molecule 32: 16S Ribosomal RNA

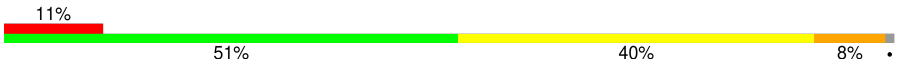
Chain 1a:

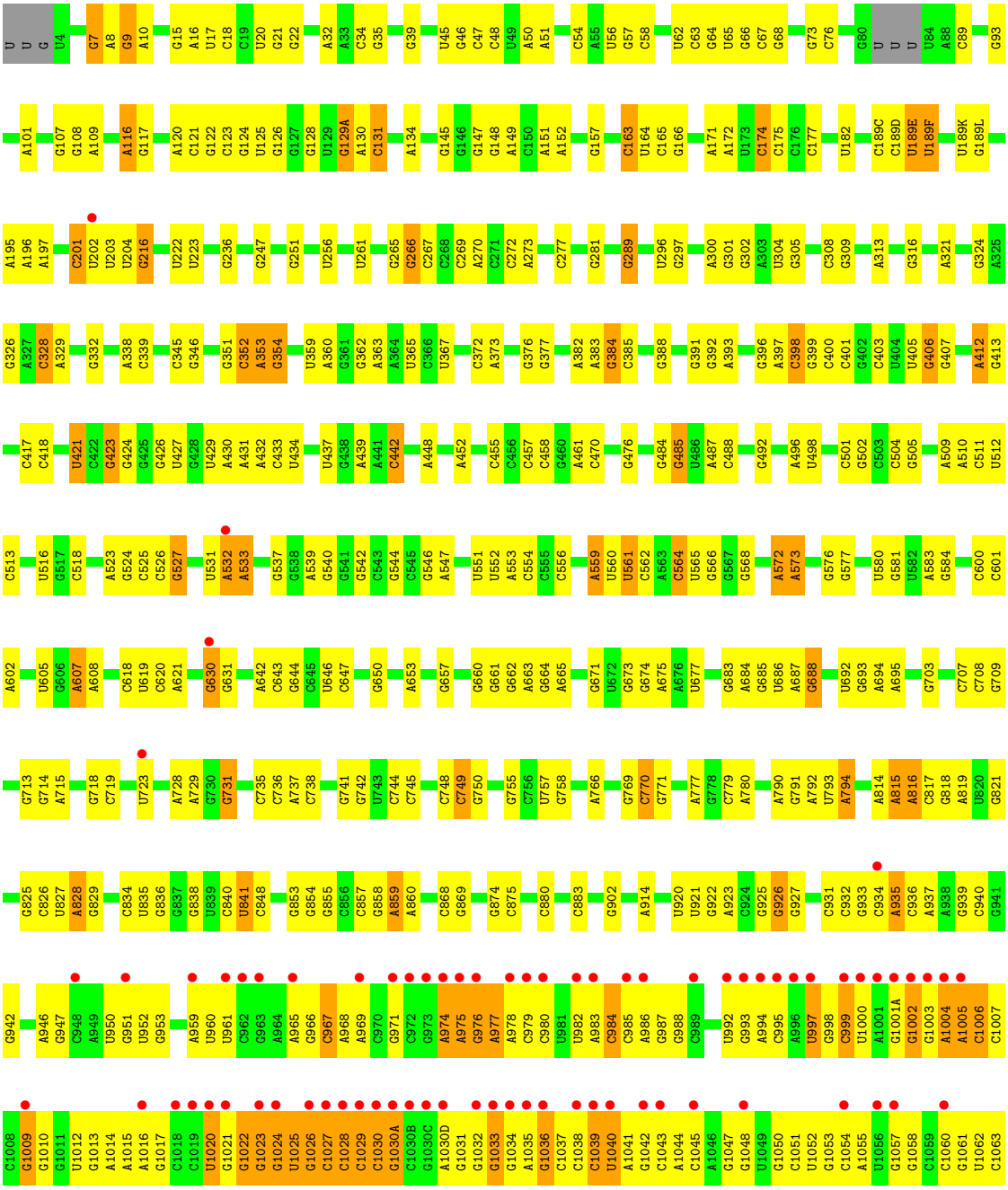


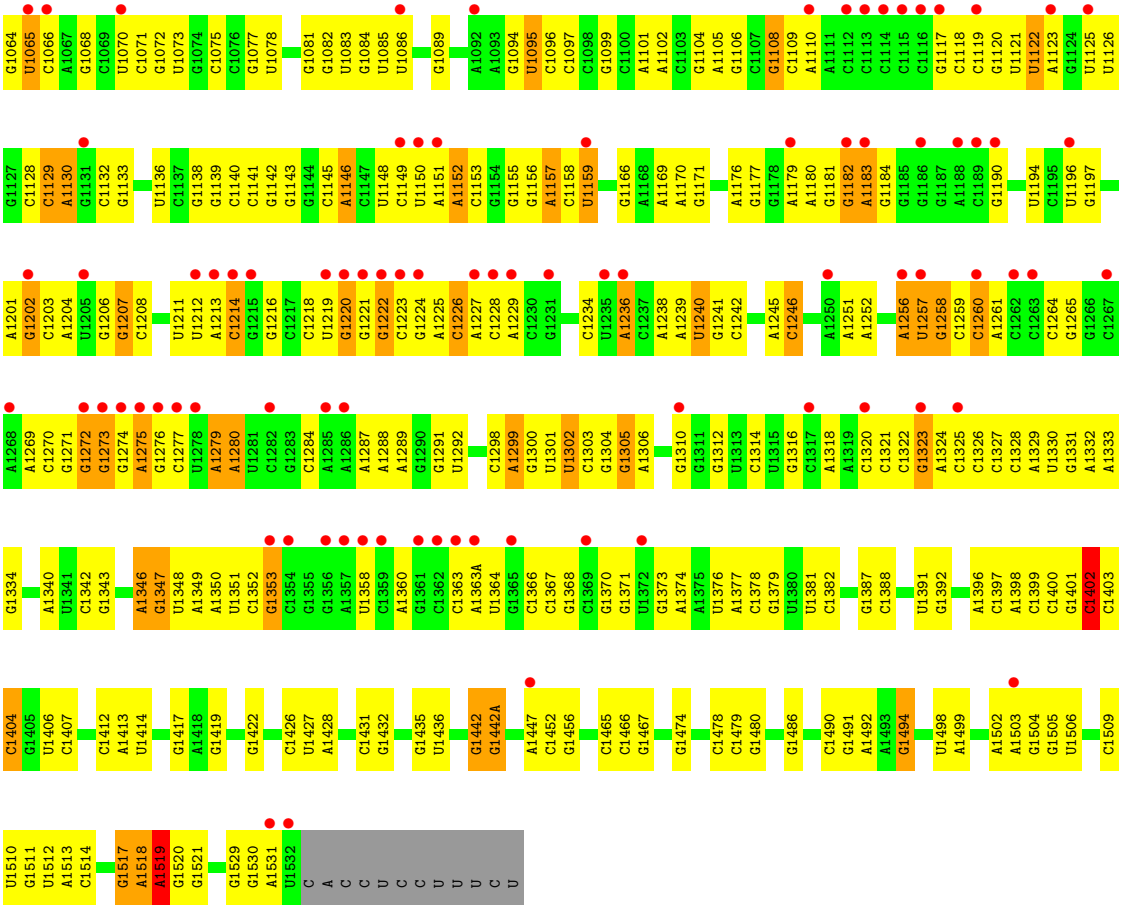


• Molecule 32: 16S Ribosomal RNA

Chain 2a:

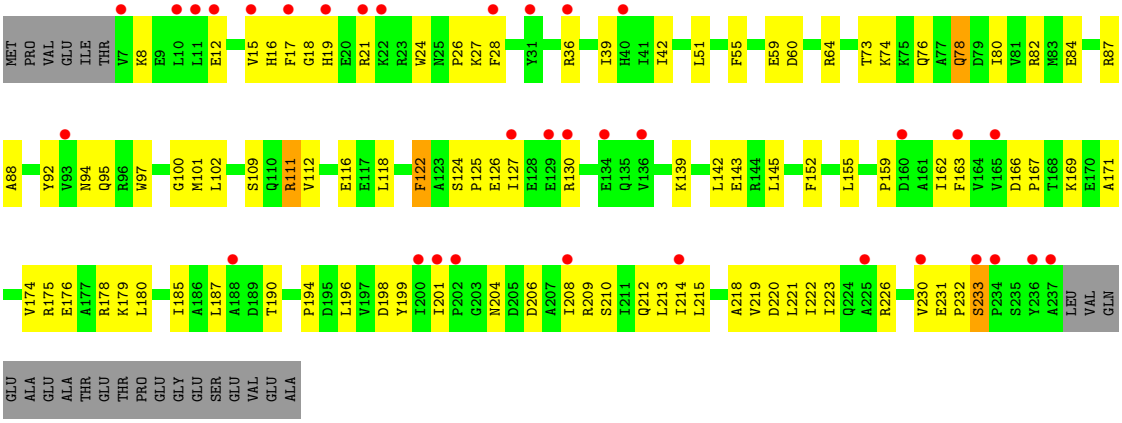






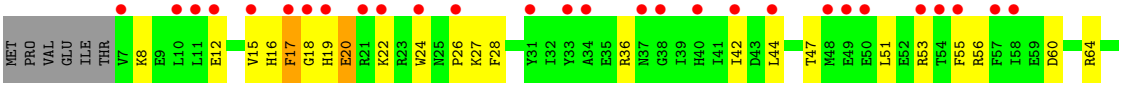
• Molecule 33: 30S ribosomal protein S2

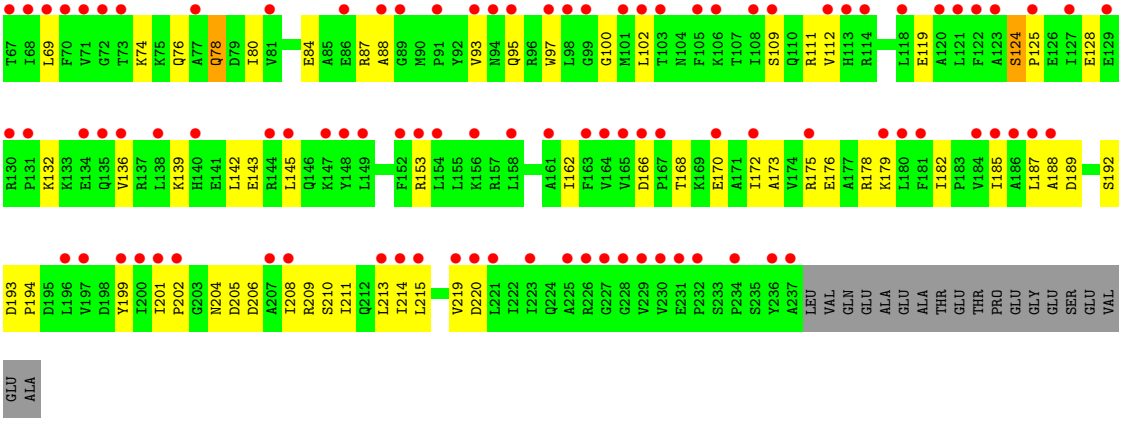
Chain 1b:



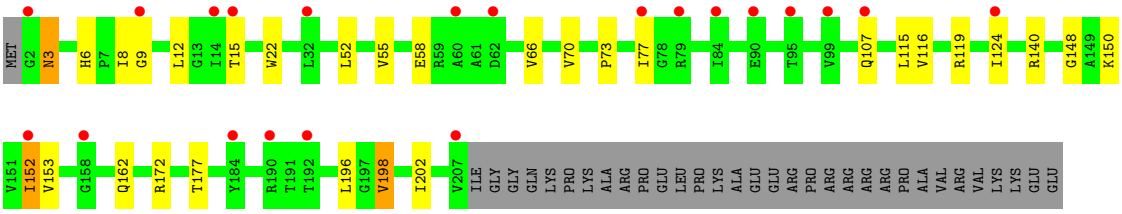
• Molecule 33: 30S ribosomal protein S2

Chain 2b:

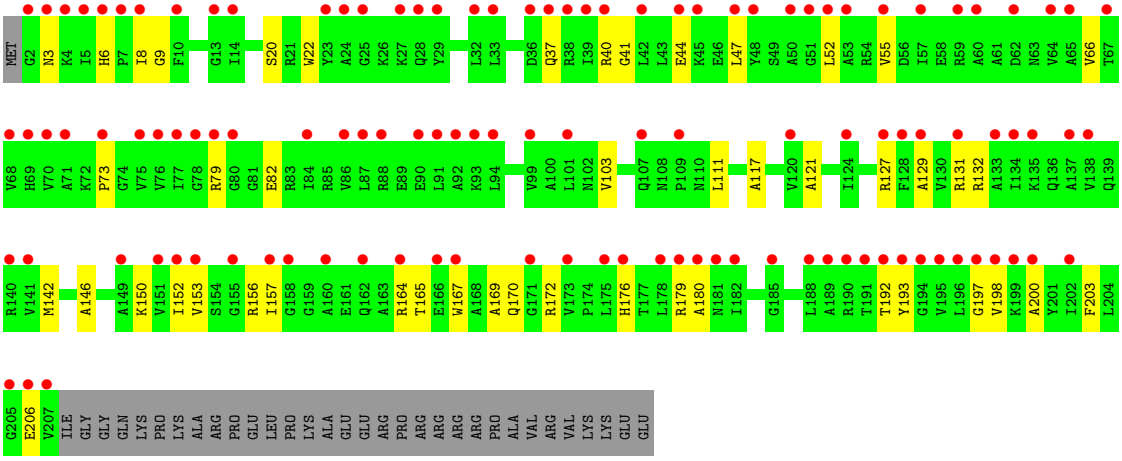




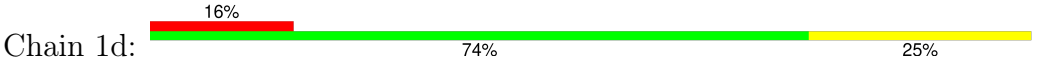
• Molecule 34: 30S ribosomal protein S3

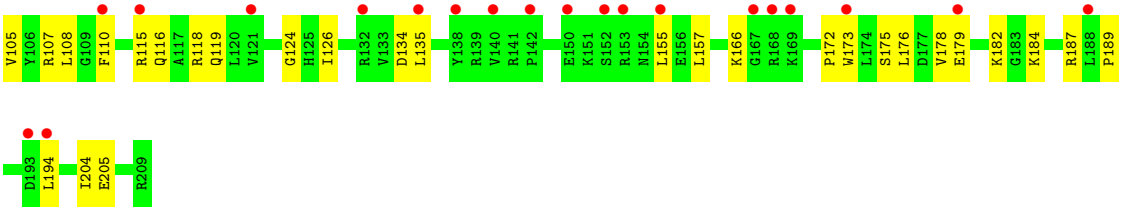


• Molecule 34: 30S ribosomal protein S3



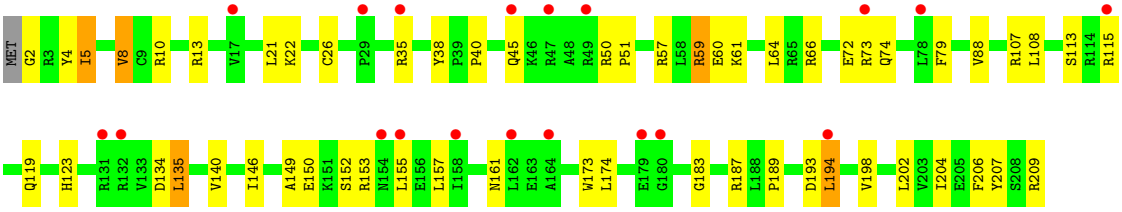
• Molecule 35: 30S ribosomal protein S4





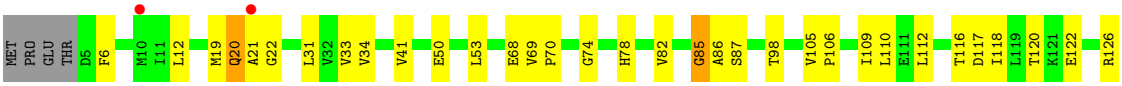
• Molecule 35: 30S ribosomal protein S4

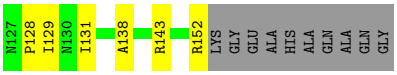
Chain 2d:



• Molecule 36: 30S ribosomal protein S5

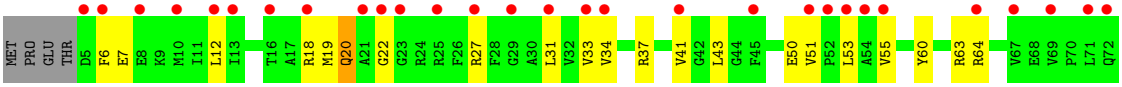
Chain 1e:

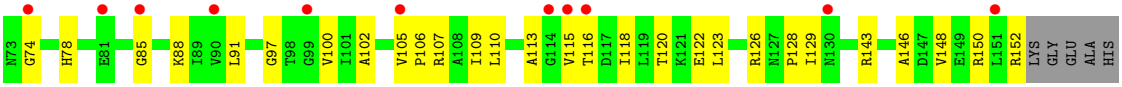




• Molecule 36: 30S ribosomal protein S5

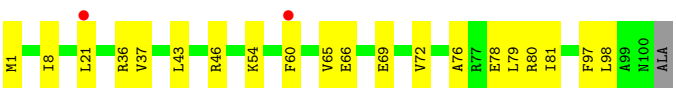
Chain 2e:





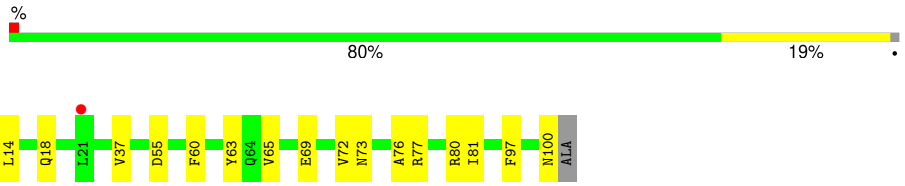
• Molecule 37: 30S ribosomal protein S6

Chain 1f:



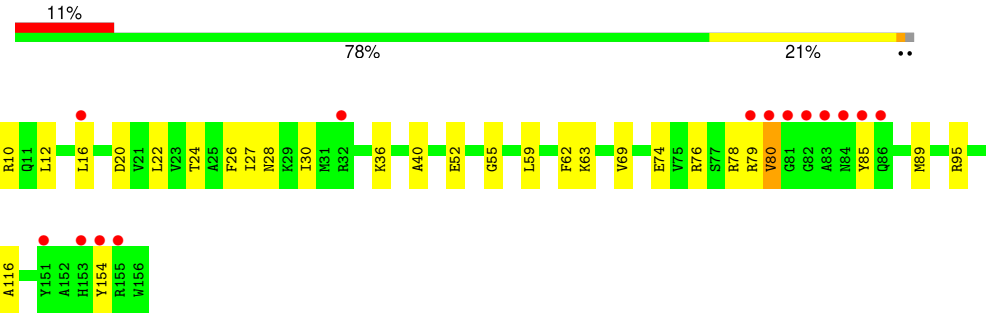
• Molecule 37: 30S ribosomal protein S6

Chain 2f:



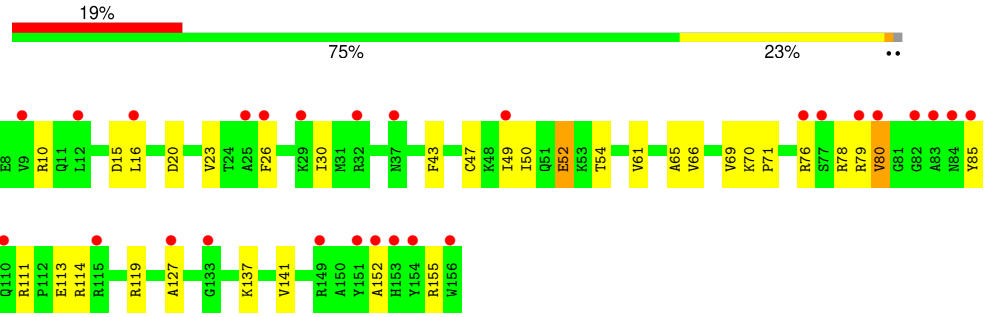
• Molecule 38: 30S ribosomal protein S7

Chain 1g:



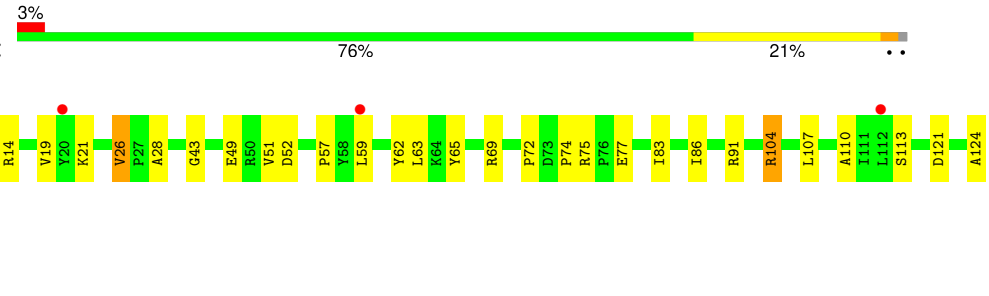
• Molecule 38: 30S ribosomal protein S7

Chain 2g:



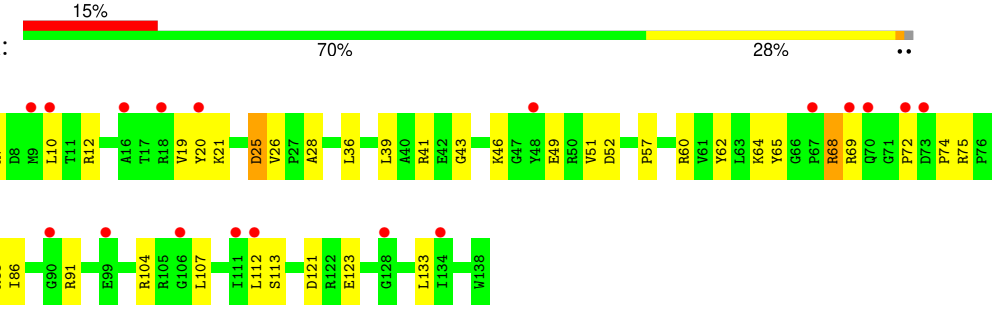
• Molecule 39: 30S ribosomal protein S8

Chain 1h:



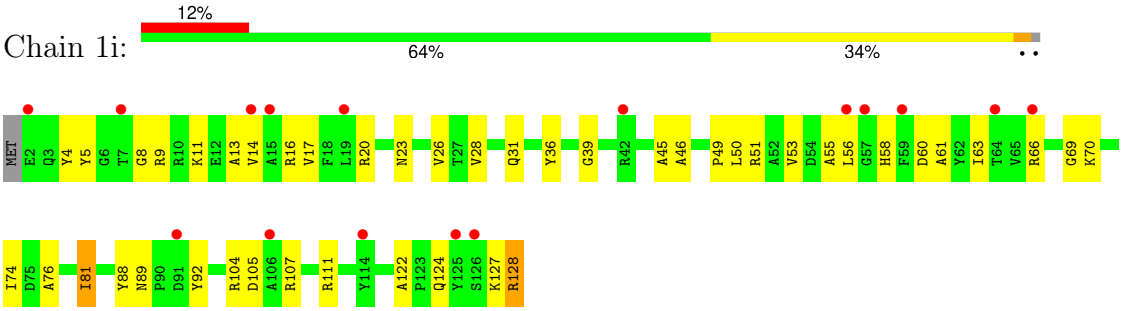
• Molecule 39: 30S ribosomal protein S8

Chain 2h:



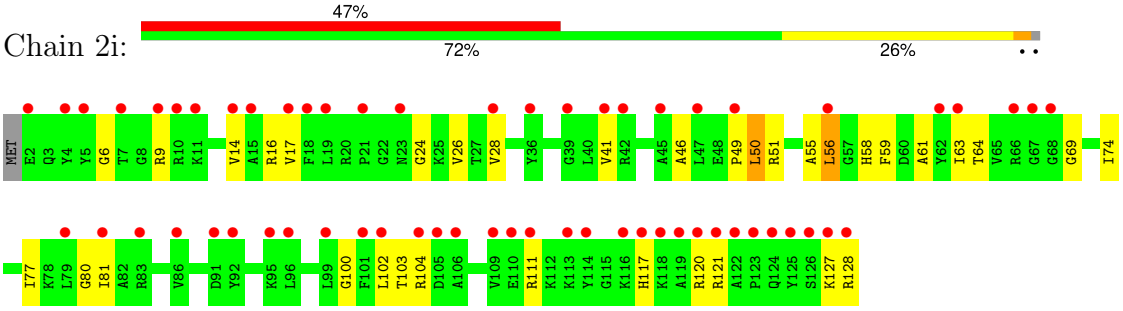
• Molecule 40: 30S ribosomal protein S9

Chain 1i:



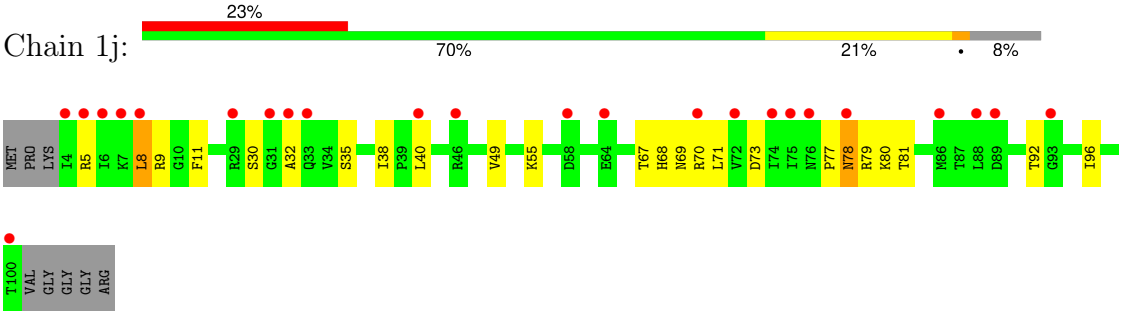
• Molecule 40: 30S ribosomal protein S9

Chain 2i:



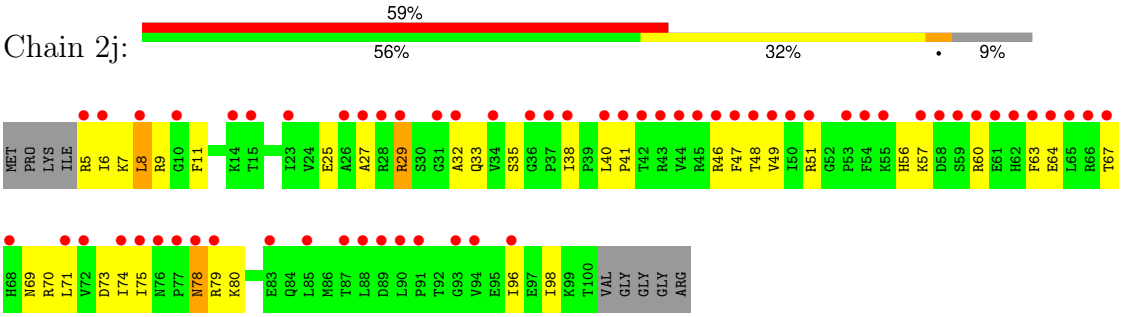
• Molecule 41: 30S ribosomal protein S10

Chain 1j:



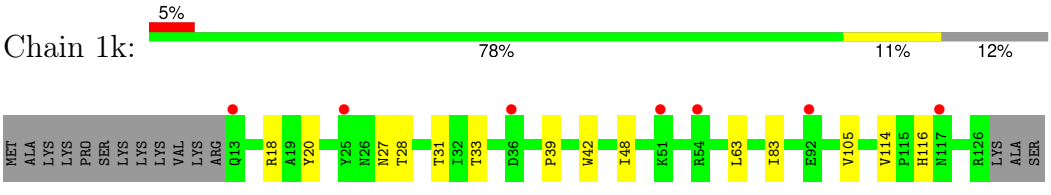
• Molecule 41: 30S ribosomal protein S10

Chain 2j:



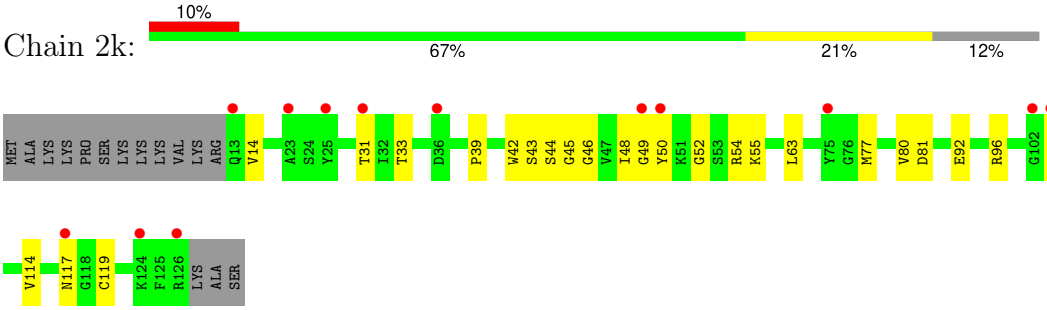
• Molecule 42: 30S ribosomal protein S11

Chain 1k:



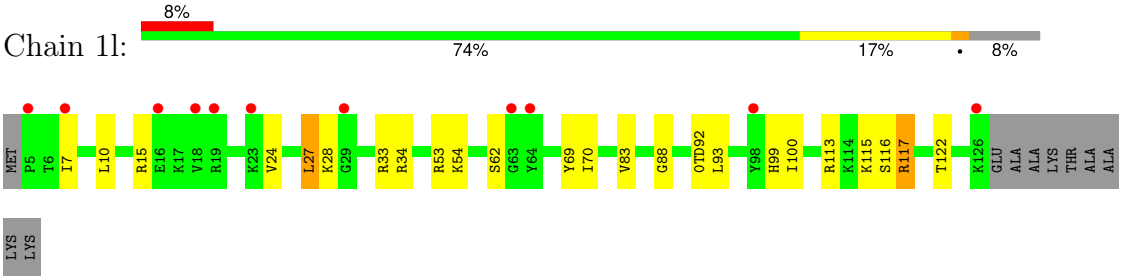
• Molecule 42: 30S ribosomal protein S11

Chain 2k:



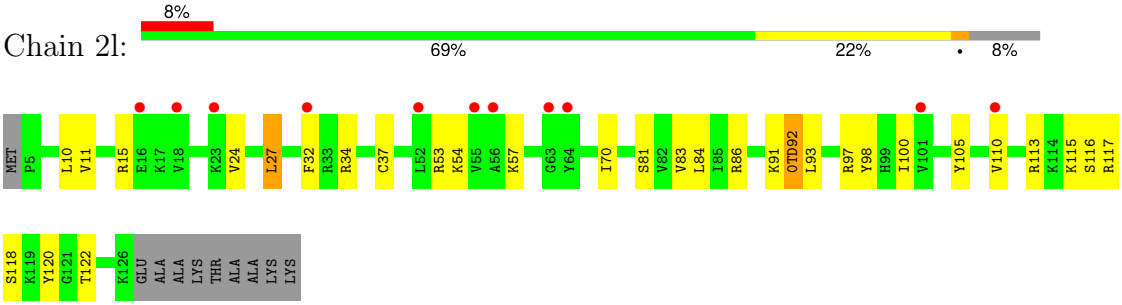
• Molecule 43: 30S ribosomal protein S12

Chain 1l:



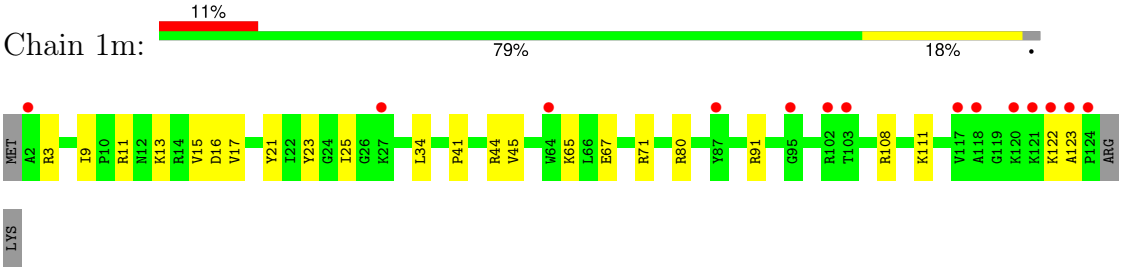
• Molecule 43: 30S ribosomal protein S12

Chain 2l:



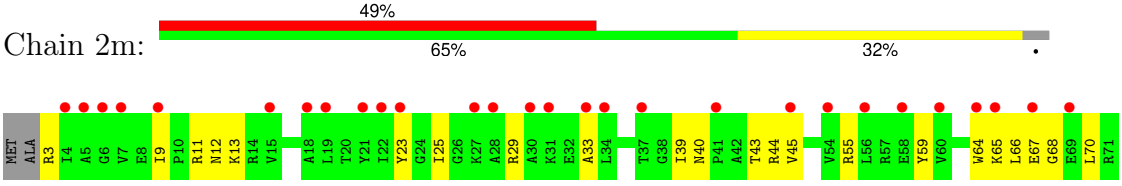
• Molecule 44: 30S ribosomal protein S13

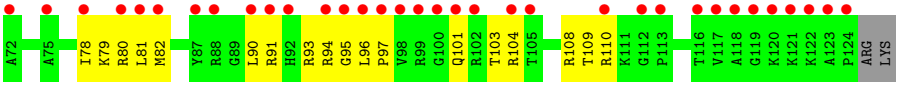
Chain 1m:



• Molecule 44: 30S ribosomal protein S13

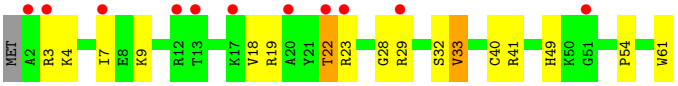
Chain 2m:





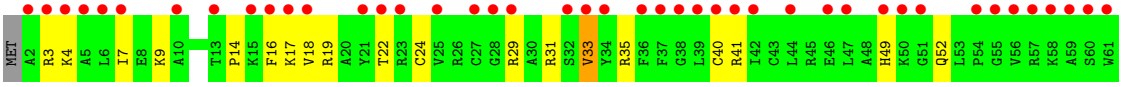
• Molecule 45: 30S ribosomal protein S14 type Z

Chain 1n:



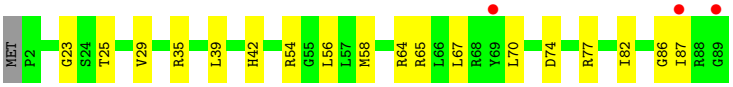
• Molecule 45: 30S ribosomal protein S14 type Z

Chain 2n:



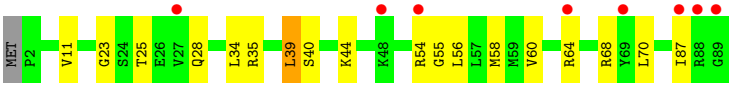
• Molecule 46: 30S ribosomal protein S15

Chain 1o:



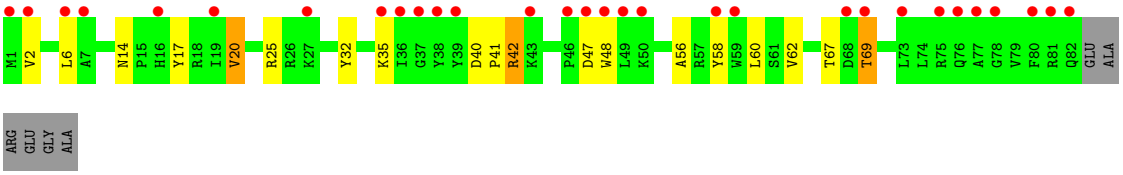
• Molecule 46: 30S ribosomal protein S15

Chain 2o:



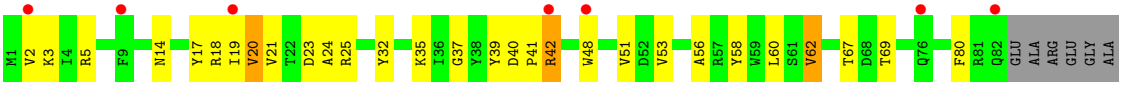
• Molecule 47: 30S ribosomal protein S16

Chain 1p:



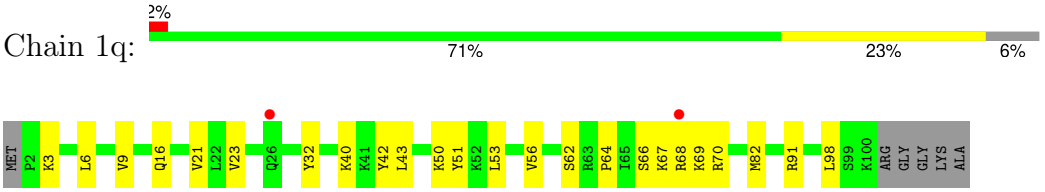
• Molecule 47: 30S ribosomal protein S16

Chain 2p:



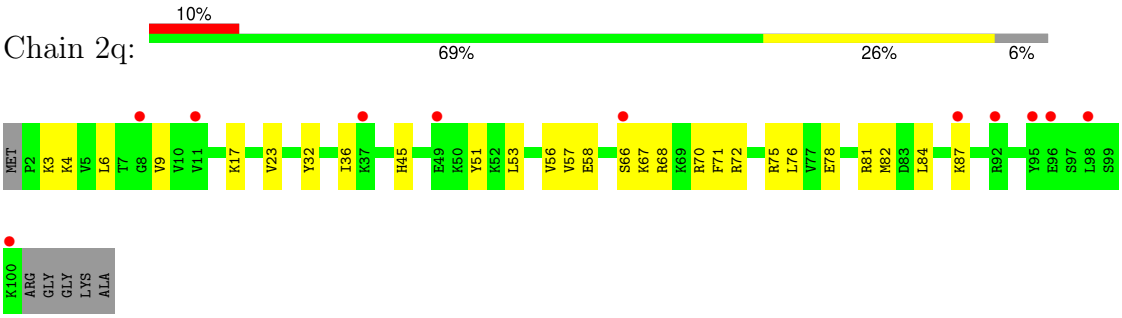
• Molecule 48: 30S ribosomal protein S17

Chain 1q:



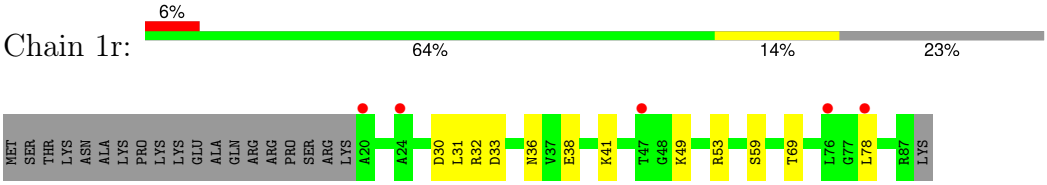
• Molecule 48: 30S ribosomal protein S17

Chain 2q:



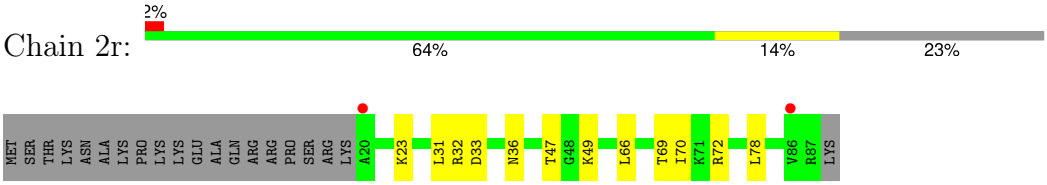
• Molecule 49: 30S ribosomal protein S18

Chain 1r:



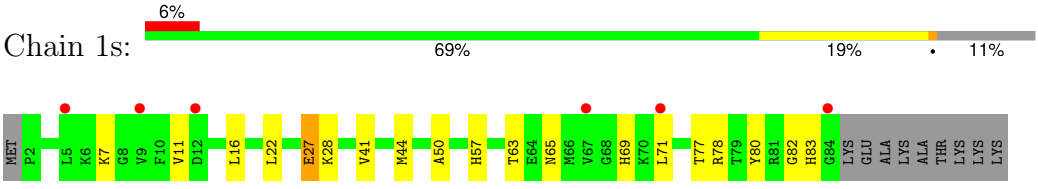
• Molecule 49: 30S ribosomal protein S18

Chain 2r:



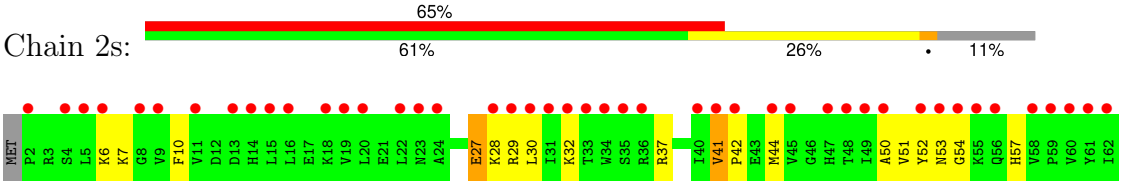
• Molecule 50: 30S ribosomal protein S19

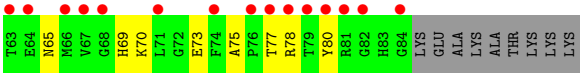
Chain 1s:



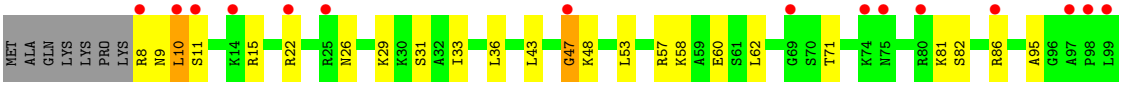
• Molecule 50: 30S ribosomal protein S19

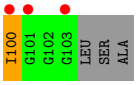
Chain 2s:



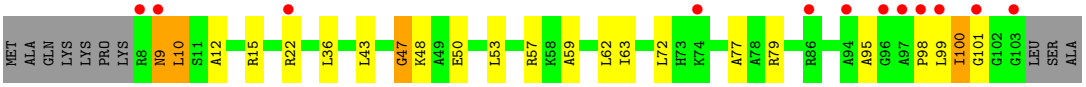


• Molecule 51: 30S ribosomal protein S20





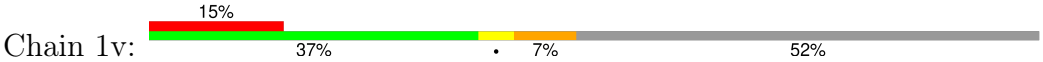
• Molecule 51: 30S ribosomal protein S20

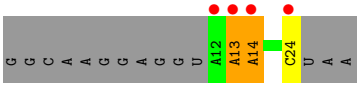


• Molecule 52: 30S ribosomal protein Thx

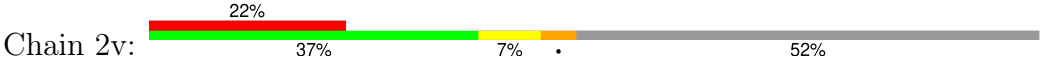
• Molecule 52: 30S ribosomal protein Thx

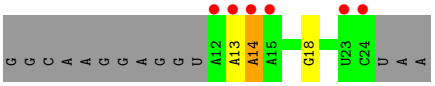
• Molecule 53: mRNA





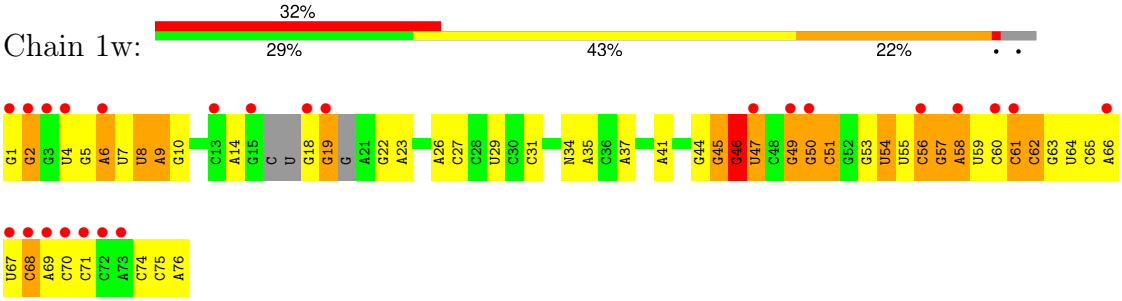
• Molecule 53: mRNA





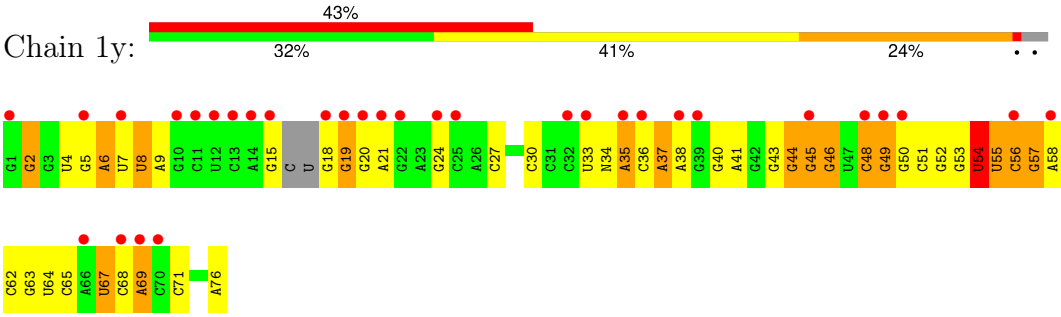
• Molecule 54: A-site and E-site tRNAs

Chain 1w:



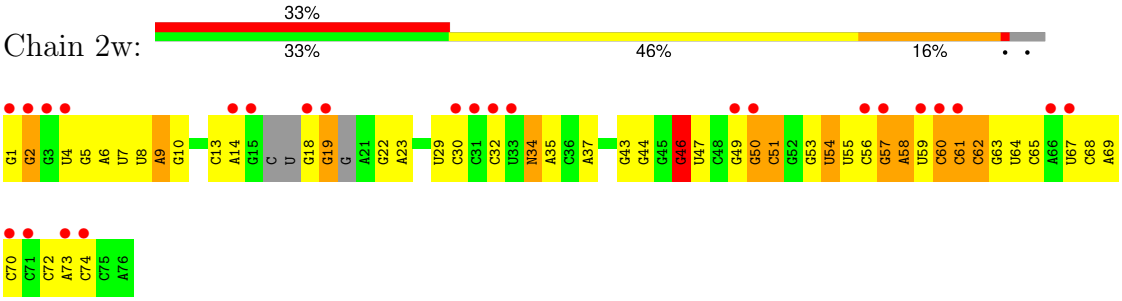
• Molecule 54: A-site and E-site tRNAs

Chain 1y:



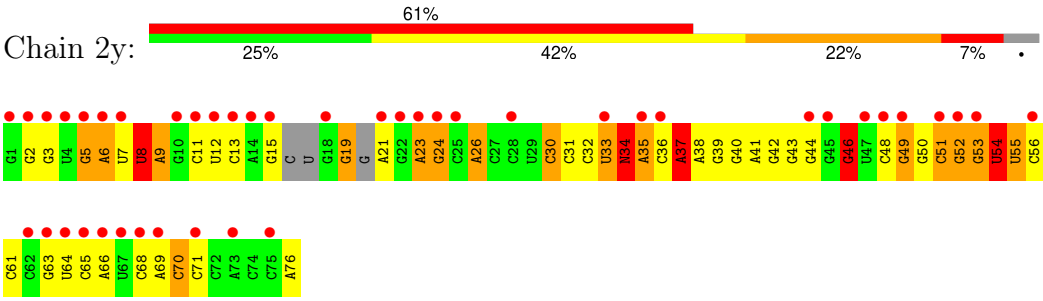
• Molecule 54: A-site and E-site tRNAs

Chain 2w:



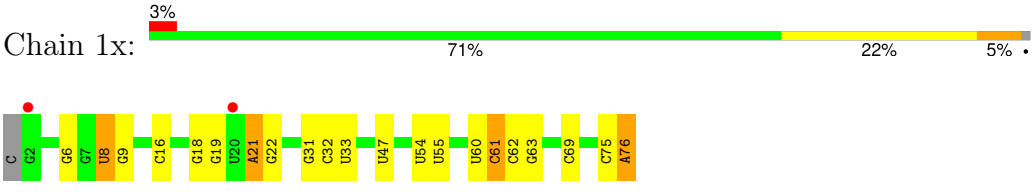
• Molecule 54: A-site and E-site tRNAs

Chain 2y:



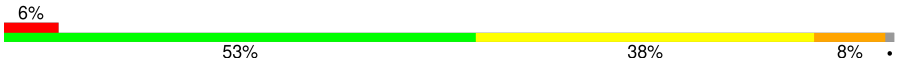
• Molecule 55: P-site tRNA

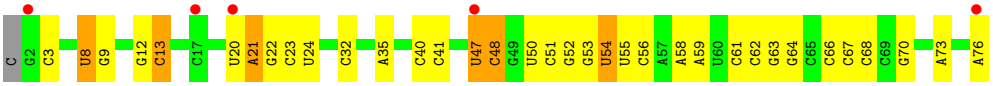
Chain 1x:



• Molecule 55: P-site tRNA

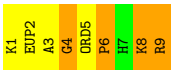
Chain 2x:





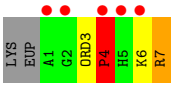
• Molecule 56: NOSO-95179 antibiotic

Chain A:



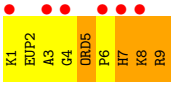
• Molecule 56: NOSO-95179 antibiotic

Chain B:



• Molecule 56: NOSO-95179 antibiotic

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	209.17Å 448.69Å 618.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	154.63 – 2.60 154.63 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.9 (154.63-2.60) 98.9 (154.63-2.60)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.24 (at 2.62Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.212 , 0.249 0.211 , 0.248	Depositor DCC
R_{free} test set	87360 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	56.9	Xtriage
Anisotropy	0.181	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 64.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	301143	wwPDB-VP
Average B, all atoms (Å^2)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.54% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 2MU, K, MA6, 4OC, CM0, 2MA, 5MC, IAR, OMG, 4SU, PSU, 2MG, EUP, ORD, ZN, M2G, 5MU, 0TD, 6MZ, SF4, MG, 7MG, UR3

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	1A	0.29	0/69009	0.46	2/107712 (0.0%)
1	2A	0.22	0/67293	0.39	1/105034 (0.0%)
2	1B	0.22	0/2882	0.40	0/4494
2	2B	0.19	0/2879	0.36	0/4487
3	1D	0.30	0/2186	0.54	0/2944
3	2D	0.24	0/2186	0.50	0/2944
4	1E	0.30	0/1592	0.54	0/2149
4	2E	0.22	0/1592	0.47	0/2149
5	1F	0.27	0/1619	0.48	0/2193
5	2F	0.20	0/1615	0.42	0/2188
6	1G	0.21	0/1448	0.44	0/1957
6	2G	0.19	0/1453	0.42	0/1963
7	1H	0.22	0/1356	0.40	0/1834
7	2H	0.18	0/1356	0.35	0/1834
8	1I	0.18	0/1112	0.39	0/1514
8	2I	0.18	0/1079	0.37	0/1475
9	1N	0.27	0/1144	0.46	0/1543
9	2N	0.18	0/1144	0.39	0/1543
10	1O	0.26	0/943	0.47	0/1269
10	2O	0.21	0/943	0.46	0/1269
11	1P	0.28	0/1152	0.49	0/1533
11	2P	0.20	0/1152	0.43	0/1533
12	1Q	0.27	0/1143	0.47	0/1527
12	2Q	0.20	0/1143	0.41	0/1527
13	1R	0.28	0/982	0.49	0/1312
13	2R	0.20	0/982	0.44	0/1312
14	1S	0.21	0/883	0.44	0/1176
14	2S	0.19	0/880	0.40	0/1172
15	1T	0.25	0/1105	0.49	0/1477
15	2T	0.21	0/1097	0.42	0/1468
16	1U	0.30	0/977	0.48	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
16	2U	0.21	0/977	0.42	0/1301
17	1V	0.37	1/782 (0.1%)	0.50	0/1049
17	2V	0.20	0/782	0.41	0/1049
18	1W	0.30	0/897	0.48	0/1205
18	2W	0.21	0/897	0.41	0/1205
19	1X	0.28	0/764	0.54	2/1025 (0.2%)
19	2X	0.19	0/764	0.40	0/1025
20	1Y	0.24	0/819	0.50	0/1095
20	2Y	0.19	0/819	0.45	0/1095
21	1Z	0.25	0/1267	0.45	0/1717
21	2Z	0.19	0/1299	0.44	0/1763
22	10	0.28	0/662	0.55	0/881
22	20	0.20	0/662	0.45	0/881
23	11	0.29	0/762	0.45	0/1014
23	21	0.21	0/762	0.40	0/1014
24	12	0.25	0/590	0.44	0/781
24	22	0.19	0/590	0.36	0/781
25	13	0.25	0/474	0.48	0/635
25	23	0.21	0/469	0.42	0/630
26	14	0.30	0/565	0.53	0/761
26	24	0.28	0/545	0.73	2/737 (0.3%)
27	15	0.29	0/469	0.56	0/635
27	25	0.24	0/469	0.48	0/635
28	16	0.28	0/460	0.47	0/613
28	26	0.21	0/456	0.40	0/608
29	17	0.29	0/426	0.54	0/561
29	27	0.23	0/426	0.51	0/561
30	18	0.28	0/525	0.50	0/691
30	28	0.22	0/525	0.40	0/691
31	19	0.25	0/310	0.45	0/407
31	29	0.20	0/310	0.44	0/407
32	1a	0.20	1/35795 (0.0%)	0.38	0/55864
32	2a	0.19	0/35886	0.36	0/56005
33	1b	0.26	1/1881 (0.1%)	0.43	0/2542
33	2b	0.21	0/1860	0.47	0/2518
34	1c	0.18	0/1572	0.40	0/2126
34	2c	0.20	0/1566	0.39	0/2119
35	1d	0.19	0/1685	0.43	0/2262
35	2d	0.19	0/1704	0.43	0/2284
36	1e	0.20	0/1145	0.45	0/1543
36	2e	0.20	0/1149	0.46	0/1548
37	1f	0.18	0/823	0.37	0/1115
37	2f	0.19	0/829	0.37	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
38	1g	0.17	0/1250	0.37	0/1679
38	2g	0.18	0/1254	0.38	0/1683
39	1h	0.18	0/1108	0.40	0/1494
39	2h	0.18	0/1108	0.40	0/1494
40	1i	0.20	0/1002	0.46	0/1346
40	2i	0.21	0/997	0.45	0/1343
41	1j	0.20	0/722	0.47	0/982
41	2j	0.20	0/727	0.42	0/988
42	1k	0.19	0/844	0.38	0/1145
42	2k	0.18	0/848	0.37	0/1149
43	1l	0.20	0/937	0.43	0/1260
43	2l	0.19	0/937	0.41	0/1260
44	1m	0.18	0/969	0.43	0/1302
44	2m	0.23	0/961	0.39	0/1291
45	1n	0.20	0/501	0.46	0/664
45	2n	0.19	0/501	0.43	0/664
46	1o	0.18	0/739	0.36	0/985
46	2o	0.16	0/739	0.37	0/985
47	1p	0.20	0/697	0.48	0/939
47	2p	0.19	0/693	0.44	0/935
48	1q	0.19	0/836	0.37	0/1117
48	2q	0.18	0/836	0.39	0/1117
49	1r	0.19	0/560	0.39	0/746
49	2r	0.17	0/560	0.37	0/746
50	1s	0.21	0/667	0.46	0/900
50	2s	0.27	0/661	0.55	0/893
51	1t	0.18	0/730	0.44	0/965
51	2t	0.20	0/729	0.46	0/965
52	1u	0.20	0/203	0.43	0/266
52	2u	0.20	0/203	0.44	0/266
53	1v	0.24	0/308	0.43	0/477
53	2v	0.21	0/308	0.34	0/477
54	1w	0.26	1/1600 (0.1%)	0.36	0/2482
54	1y	0.26	1/1627 (0.1%)	0.37	0/2527
54	2w	0.26	1/1600 (0.1%)	0.35	0/2482
54	2y	0.29	1/1600 (0.1%)	0.38	0/2482
55	1x	0.26	0/1725	0.39	0/2689
55	2x	0.24	0/1725	0.39	0/2689
56	A	1.60	1/43 (2.3%)	1.93	0/51
56	B	2.20	2/35 (5.7%)	1.85	1/43 (2.3%)
56	C	1.71	1/43 (2.3%)	2.56	3/51 (5.9%)
All	All	0.24	11/316879 (0.0%)	0.42	11/474354 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
26	14	0	1
26	24	0	1
33	1b	0	1
33	2b	0	1
All	All	0	4

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	1b	233	SER	C-N	7.51	1.51	1.33
56	A	6	PRO	CA-C	-6.58	1.39	1.52
56	B	4	PRO	N-CA	6.11	1.56	1.47
54	2y	8	4SU	O3'-P	6.03	1.62	1.56
17	1V	34	GLU	C-N	-5.89	1.21	1.33

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
56	C	6	PRO	CA-C-N	9.01	137.92	121.70
56	C	6	PRO	C-N-CA	9.01	137.92	121.70
56	B	4	PRO	CA-N-CD	-7.00	102.19	112.00
26	24	63	TYR	N-CA-C	-6.84	101.81	111.24
1	1A	2014	G	C2'-C3'-O3'	6.62	119.42	109.50

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
26	14	63	TYR	Peptide
33	1b	124	SER	Peptide
26	24	63	TYR	Peptide
33	2b	124	SER	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	31191	568	0
1	2A	60322	0	30425	641	0
2	1B	2577	0	1305	18	0
2	2B	2575	0	1303	36	0
3	1D	2136	0	2218	32	0
3	2D	2136	0	2218	32	0
4	1E	1559	0	1618	40	0
4	2E	1559	0	1618	29	0
5	1F	1584	0	1625	32	0
5	2F	1580	0	1619	44	0
6	1G	1423	0	1436	24	0
6	2G	1428	0	1438	43	0
7	1H	1330	0	1407	25	0
7	2H	1330	0	1407	29	0
8	1I	1097	0	1140	24	0
8	2I	1064	0	1082	21	1
9	1N	1117	0	1184	14	0
9	2N	1117	0	1184	19	0
10	1O	933	0	996	17	0
10	2O	933	0	996	24	0
11	1P	1135	0	1212	25	0
11	2P	1135	0	1212	23	0
12	1Q	1122	0	1179	21	0
12	2Q	1122	0	1179	23	0
13	1R	968	0	1033	20	0
13	2R	968	0	1033	24	0
14	1S	873	0	927	15	0
14	2S	870	0	923	15	0
15	1T	1091	0	1151	21	0
15	2T	1083	0	1136	30	0
16	1U	959	0	1019	16	0
16	2U	959	0	1019	16	0
17	1V	771	0	830	10	0
17	2V	771	0	830	13	0
18	1W	886	0	940	13	0
18	2W	886	0	940	11	0
19	1X	750	0	814	17	0
19	2X	750	0	814	18	0
20	1Y	806	0	881	15	0
20	2Y	806	0	881	18	0
21	1Z	1240	0	1240	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	2Z	1271	0	1273	26	0
22	10	653	0	674	16	0
22	20	653	0	674	12	0
23	11	755	0	826	11	0
23	21	755	0	826	14	0
24	12	588	0	643	4	0
24	22	588	0	643	6	0
25	13	469	0	518	6	0
25	23	464	0	514	8	0
26	14	552	0	533	17	0
26	24	532	0	503	18	0
27	15	455	0	465	9	0
27	25	455	0	465	9	0
28	16	453	0	473	6	0
28	26	449	0	469	7	0
29	17	418	0	467	1	0
29	27	418	0	467	12	0
30	18	517	0	582	24	0
30	28	517	0	582	22	0
31	19	307	0	335	3	0
31	29	307	0	335	7	0
32	1a	32246	0	16294	452	1
32	2a	32327	0	16339	528	0
33	1b	1846	0	1867	69	0
33	2b	1825	0	1828	65	0
34	1c	1548	0	1535	19	0
34	2c	1542	0	1517	35	0
35	1d	1655	0	1672	41	0
35	2d	1674	0	1714	47	0
36	1e	1129	0	1185	33	0
36	2e	1133	0	1191	41	0
37	1f	810	0	804	15	0
37	2f	816	0	808	15	0
38	1g	1231	0	1238	23	0
38	2g	1235	0	1249	27	0
39	1h	1088	0	1126	26	0
39	2h	1088	0	1126	32	0
40	1i	983	0	986	35	0
40	2i	978	0	966	24	0
41	1j	709	0	650	17	0
41	2j	714	0	672	28	0
42	1k	829	0	825	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	2k	833	0	836	17	0
43	1l	932	0	981	15	0
43	2l	932	0	981	24	0
44	1m	958	0	1002	18	0
44	2m	950	0	988	28	0
45	1n	492	0	529	16	0
45	2n	492	0	529	22	0
46	1o	728	0	760	12	0
46	2o	728	0	760	11	0
47	1p	681	0	697	13	0
47	2p	677	0	686	18	0
48	1q	823	0	891	20	0
48	2q	823	0	891	27	0
49	1r	555	0	618	9	0
49	2r	555	0	618	11	0
50	1s	652	0	662	15	0
50	2s	646	0	644	29	0
51	1t	728	0	798	16	0
51	2t	727	0	796	18	0
52	1u	199	0	208	5	0
52	2u	199	0	208	11	0
53	1v	276	0	139	3	0
53	2v	276	0	139	2	0
54	1w	1568	0	802	36	0
54	1y	1591	0	812	42	0
54	2w	1568	0	802	29	0
54	2y	1568	0	802	54	0
55	1x	1625	0	829	7	0
55	2x	1625	0	828	17	0
56	A	72	0	67	7	0
56	B	55	0	56	4	0
56	C	72	0	64	6	0
57	10	6	0	0	0	0
57	11	2	0	0	0	0
57	12	2	0	0	0	0
57	13	2	0	0	0	0
57	15	2	0	0	0	0
57	16	1	0	0	0	0
57	17	2	0	0	0	0
57	18	4	0	0	0	0
57	19	1	0	0	0	0
57	1A	1149	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	1B	36	0	0	0	0
57	1D	9	0	0	0	0
57	1E	10	0	0	0	0
57	1F	8	0	0	0	0
57	1G	5	0	0	0	0
57	1I	1	0	0	0	0
57	1N	7	0	0	0	0
57	1O	4	0	0	0	0
57	1P	4	0	0	0	0
57	1Q	5	0	0	0	0
57	1R	3	0	0	0	0
57	1S	3	0	0	0	0
57	1T	2	0	0	0	0
57	1U	6	0	0	0	0
57	1V	2	0	0	0	0
57	1W	5	0	0	0	0
57	1X	6	0	0	0	0
57	1Y	3	0	0	0	0
57	1Z	4	0	0	0	0
57	1a	314	0	0	0	0
57	1b	2	0	0	0	0
57	1d	2	0	0	0	0
57	1e	2	0	0	0	0
57	1f	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	1r	1	0	0	0	0
57	1s	1	0	0	0	0
57	1t	1	0	0	0	0
57	1v	1	0	0	0	0
57	1w	8	0	0	0	0
57	1x	14	0	0	0	0
57	1y	6	0	0	0	0
57	20	2	0	0	0	0
57	21	2	0	0	0	0
57	23	2	0	0	0	0
57	25	3	0	0	0	0
57	26	1	0	0	0	0
57	28	3	0	0	0	0
57	29	1	0	0	0	0
57	2A	861	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	2B	21	0	0	0	0
57	2D	4	0	0	0	0
57	2E	10	0	0	0	0
57	2F	3	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	2Q	3	0	0	0	0
57	2R	2	0	0	0	0
57	2T	4	0	0	0	0
57	2U	4	0	0	0	0
57	2V	2	0	0	0	0
57	2W	2	0	0	0	0
57	2X	3	0	0	0	0
57	2Z	1	0	0	0	0
57	2a	202	0	0	0	0
57	2d	1	0	0	0	0
57	2e	2	0	0	0	0
57	2f	2	0	0	0	0
57	2g	1	0	0	0	0
57	2i	1	0	0	0	0
57	2j	2	0	0	0	0
57	2l	3	0	0	0	0
57	2n	1	0	0	0	0
57	2q	3	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	2x	6	0	0	0	0
57	2y	7	0	0	0	0
57	C	2	0	0	0	0
58	1A	1	0	0	0	0
58	2A	1	0	0	0	0
59	14	1	0	0	0	0
59	15	1	0	0	0	0
59	16	1	0	0	0	0
59	19	1	0	0	0	0
59	1Y	1	0	0	0	0
59	1n	1	0	0	0	0
59	24	1	0	0	0	0
59	25	1	0	0	0	0
59	26	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	29	1	0	0	0	0
59	2Y	1	0	0	0	0
59	2n	1	0	0	0	0
60	1d	8	0	0	0	0
60	2d	8	0	0	0	0
61	10	11	0	0	2	0
61	11	9	0	0	0	0
61	12	5	0	0	0	0
61	13	6	0	0	0	0
61	15	5	0	0	0	0
61	16	4	0	0	1	0
61	17	7	0	0	0	0
61	18	12	0	0	1	0
61	19	1	0	0	0	0
61	1A	2172	0	0	54	0
61	1B	71	0	0	2	0
61	1D	28	0	0	3	0
61	1E	29	0	0	2	0
61	1F	18	0	0	1	0
61	1G	7	0	0	0	0
61	1H	2	0	0	0	0
61	1I	2	0	0	0	0
61	1N	5	0	0	0	0
61	1O	8	0	0	0	0
61	1P	23	0	0	2	0
61	1Q	11	0	0	0	0
61	1R	18	0	0	2	0
61	1S	3	0	0	0	0
61	1T	10	0	0	1	0
61	1U	11	0	0	0	0
61	1V	8	0	0	0	0
61	1W	7	0	0	1	0
61	1X	7	0	0	1	0
61	1Y	4	0	0	1	0
61	1Z	1	0	0	0	0
61	1a	686	0	0	39	0
61	1b	1	0	0	0	0
61	1d	3	0	0	0	0
61	1f	1	0	0	0	0
61	1g	1	0	0	0	0
61	1i	1	0	0	0	0
61	1l	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	1m	1	0	0	0	0
61	1o	2	0	0	0	0
61	1p	3	0	0	0	0
61	1q	5	0	0	0	0
61	1u	1	0	0	1	0
61	1v	6	0	0	0	0
61	1w	7	0	0	2	0
61	1x	17	0	0	0	0
61	1y	4	0	0	0	0
61	20	5	0	0	0	0
61	21	12	0	0	1	0
61	22	1	0	0	0	0
61	23	1	0	0	0	0
61	25	4	0	0	1	0
61	26	1	0	0	0	0
61	27	3	0	0	0	0
61	28	5	0	0	0	0
61	29	1	0	0	0	0
61	2A	1348	0	0	58	0
61	2B	27	0	0	0	0
61	2D	26	0	0	0	0
61	2E	12	0	0	2	0
61	2F	17	0	0	0	0
61	2I	4	0	0	0	0
61	2N	2	0	0	0	0
61	2O	2	0	0	0	0
61	2P	14	0	0	0	0
61	2Q	2	0	0	0	0
61	2R	3	0	0	0	0
61	2T	6	0	0	0	0
61	2U	4	0	0	1	0
61	2V	1	0	0	0	0
61	2W	5	0	0	0	0
61	2X	6	0	0	1	0
61	2Y	1	0	0	0	0
61	2Z	2	0	0	0	0
61	2a	270	0	0	13	0
61	2d	1	0	0	0	0
61	2g	1	0	0	0	0
61	2j	4	0	0	2	0
61	2l	5	0	0	2	0
61	2m	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	2o	1	0	0	1	0
61	2p	2	0	0	0	0
61	2q	1	0	0	0	0
61	2r	1	0	0	0	0
61	2t	2	0	0	0	0
61	2v	4	0	0	0	0
61	2w	4	0	0	0	0
61	2x	7	0	0	0	0
61	2y	19	0	0	0	0
61	C	4	0	0	0	0
All	All	301143	0	196885	3857	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

The worst 5 of 3857 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1128:U:H3	1:1A:1132:A:N6	1.28	1.28
1:1A:1100:A:N6	1:1A:1151:U:H3	1.47	1.10
1:2A:2137:C:N4	1:2A:2154:G:H1	1.50	1.10
54:2y:30:C:N4	54:2y:40:G:H1	1.51	1.08
54:1w:51:C:N4	54:1w:63:G:H1	1.53	1.05

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:358:U:OP1	8:2I:121:LYS:NZ[2_655]	2.19	0.01

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%)	260 (95%)	12 (4%)	1 (0%)	30	51
3	2D	273/276 (99%)	258 (94%)	14 (5%)	1 (0%)	30	51
4	1E	202/206 (98%)	193 (96%)	8 (4%)	1 (0%)	24	46
4	2E	202/206 (98%)	194 (96%)	7 (4%)	1 (0%)	24	46
5	1F	201/210 (96%)	197 (98%)	3 (2%)	1 (0%)	24	46
5	2F	201/210 (96%)	193 (96%)	6 (3%)	2 (1%)	12	28
6	1G	179/182 (98%)	167 (93%)	10 (6%)	2 (1%)	11	25
6	2G	179/182 (98%)	162 (90%)	15 (8%)	2 (1%)	11	25
7	1H	172/180 (96%)	163 (95%)	9 (5%)	0	100	100
7	2H	172/180 (96%)	162 (94%)	9 (5%)	1 (1%)	21	42
8	1I	144/148 (97%)	126 (88%)	15 (10%)	3 (2%)	5	11
8	2I	144/148 (97%)	131 (91%)	13 (9%)	0	100	100
9	1N	138/140 (99%)	135 (98%)	3 (2%)	0	100	100
9	2N	138/140 (99%)	131 (95%)	7 (5%)	0	100	100
10	1O	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
10	2O	120/122 (98%)	113 (94%)	5 (4%)	2 (2%)	7	15
11	1P	147/150 (98%)	138 (94%)	9 (6%)	0	100	100
11	2P	147/150 (98%)	140 (95%)	5 (3%)	2 (1%)	9	19
12	1Q	139/141 (99%)	132 (95%)	7 (5%)	0	100	100
12	2Q	139/141 (99%)	132 (95%)	7 (5%)	0	100	100
13	1R	116/118 (98%)	111 (96%)	5 (4%)	0	100	100
13	2R	116/118 (98%)	113 (97%)	3 (3%)	0	100	100
14	1S	108/112 (96%)	102 (94%)	6 (6%)	0	100	100
14	2S	108/112 (96%)	103 (95%)	4 (4%)	1 (1%)	14	30
15	1T	129/146 (88%)	122 (95%)	7 (5%)	0	100	100
15	2T	129/146 (88%)	121 (94%)	7 (5%)	1 (1%)	16	34
16	1U	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
16	2U	114/118 (97%)	109 (96%)	5 (4%)	0	100	100
17	1V	99/101 (98%)	94 (95%)	4 (4%)	1 (1%)	12	28
17	2V	99/101 (98%)	94 (95%)	4 (4%)	1 (1%)	12	28
18	1W	110/113 (97%)	109 (99%)	1 (1%)	0	100	100
18	2W	110/113 (97%)	109 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
19	1X	93/96 (97%)	91 (98%)	1 (1%)	1 (1%)	11 25
19	2X	93/96 (97%)	89 (96%)	4 (4%)	0	100 100
20	1Y	105/110 (96%)	99 (94%)	4 (4%)	2 (2%)	6 13
20	2Y	105/110 (96%)	101 (96%)	3 (3%)	1 (1%)	12 28
21	1Z	148/206 (72%)	127 (86%)	21 (14%)	0	100 100
21	2Z	156/206 (76%)	143 (92%)	10 (6%)	3 (2%)	6 13
22	10	81/85 (95%)	81 (100%)	0	0	100 100
22	20	81/85 (95%)	81 (100%)	0	0	100 100
23	11	95/98 (97%)	92 (97%)	2 (2%)	1 (1%)	11 25
23	21	95/98 (97%)	94 (99%)	0	1 (1%)	11 25
24	12	68/72 (94%)	68 (100%)	0	0	100 100
24	22	68/72 (94%)	67 (98%)	1 (2%)	0	100 100
25	13	57/60 (95%)	55 (96%)	2 (4%)	0	100 100
25	23	57/60 (95%)	55 (96%)	2 (4%)	0	100 100
26	14	67/71 (94%)	54 (81%)	9 (13%)	4 (6%)	1 1
26	24	67/71 (94%)	56 (84%)	6 (9%)	5 (8%)	1 1
27	15	57/60 (95%)	54 (95%)	3 (5%)	0	100 100
27	25	57/60 (95%)	55 (96%)	2 (4%)	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%)	202 (88%)	22 (10%)	5 (2%)	5 10
33	2b	229/256 (90%)	204 (89%)	20 (9%)	5 (2%)	5 10
34	1c	204/239 (85%)	183 (90%)	19 (9%)	2 (1%)	12 28
34	2c	204/239 (85%)	187 (92%)	16 (8%)	1 (0%)	24 46
35	1d	206/209 (99%)	197 (96%)	8 (4%)	1 (0%)	24 46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
35	2d	206/209 (99%)	196 (95%)	9 (4%)	1 (0%)	24 46
36	1e	146/162 (90%)	138 (94%)	4 (3%)	4 (3%)	4 7
36	2e	146/162 (90%)	135 (92%)	10 (7%)	1 (1%)	18 38
37	1f	98/101 (97%)	94 (96%)	4 (4%)	0	100 100
37	2f	98/101 (97%)	95 (97%)	3 (3%)	0	100 100
38	1g	153/156 (98%)	144 (94%)	5 (3%)	4 (3%)	4 7
38	2g	153/156 (98%)	141 (92%)	8 (5%)	4 (3%)	4 7
39	1h	135/138 (98%)	131 (97%)	4 (3%)	0	100 100
39	2h	135/138 (98%)	127 (94%)	7 (5%)	1 (1%)	18 38
40	1i	125/128 (98%)	111 (89%)	14 (11%)	0	100 100
40	2i	125/128 (98%)	116 (93%)	8 (6%)	1 (1%)	16 34
41	1j	95/105 (90%)	85 (90%)	6 (6%)	4 (4%)	2 3
41	2j	94/105 (90%)	82 (87%)	7 (7%)	5 (5%)	1 1
42	1k	112/129 (87%)	108 (96%)	3 (3%)	1 (1%)	14 30
42	2k	112/129 (87%)	103 (92%)	7 (6%)	2 (2%)	6 14
43	1l	119/132 (90%)	117 (98%)	2 (2%)	0	100 100
43	2l	119/132 (90%)	112 (94%)	7 (6%)	0	100 100
44	1m	121/126 (96%)	112 (93%)	9 (7%)	0	100 100
44	2m	120/126 (95%)	113 (94%)	7 (6%)	0	100 100
45	1n	58/61 (95%)	55 (95%)	3 (5%)	0	100 100
45	2n	58/61 (95%)	55 (95%)	3 (5%)	0	100 100
46	1o	86/89 (97%)	83 (96%)	3 (4%)	0	100 100
46	2o	86/89 (97%)	84 (98%)	2 (2%)	0	100 100
47	1p	80/88 (91%)	76 (95%)	4 (5%)	0	100 100
47	2p	80/88 (91%)	76 (95%)	4 (5%)	0	100 100
48	1q	97/105 (92%)	92 (95%)	5 (5%)	0	100 100
48	2q	97/105 (92%)	90 (93%)	7 (7%)	0	100 100
49	1r	66/88 (75%)	64 (97%)	2 (3%)	0	100 100
49	2r	66/88 (75%)	65 (98%)	1 (2%)	0	100 100
50	1s	81/93 (87%)	71 (88%)	9 (11%)	1 (1%)	10 23
50	2s	81/93 (87%)	70 (86%)	10 (12%)	1 (1%)	10 23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
51	1t	94/106 (89%)	86 (92%)	5 (5%)	3 (3%)	3 5
51	2t	94/106 (89%)	86 (92%)	3 (3%)	5 (5%)	1 1
52	1u	21/27 (78%)	18 (86%)	3 (14%)	0	100 100
52	2u	21/27 (78%)	20 (95%)	1 (5%)	0	100 100
56	A	5/9 (56%)	3 (60%)	1 (20%)	1 (20%)	0 0
56	B	4/9 (44%)	2 (50%)	2 (50%)	0	100 100
56	C	5/9 (56%)	1 (20%)	2 (40%)	2 (40%)	0 0
All	All	11384/12155 (94%)	10713 (94%)	575 (5%)	96 (1%)	16 34

5 of 96 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	1F	130	ALA
26	14	65	ASP
5	2F	130	ALA
6	2G	52	ILE
17	2V	79	VAL

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%)	205 (95%)	10 (5%)	23 48
3	2D	215/218 (99%)	206 (96%)	9 (4%)	26 52
4	1E	164/166 (99%)	149 (91%)	15 (9%)	9 19
4	2E	164/166 (99%)	152 (93%)	12 (7%)	13 29
5	1F	160/166 (96%)	148 (92%)	12 (8%)	12 28
5	2F	159/166 (96%)	155 (98%)	4 (2%)	42 69
6	1G	143/156 (92%)	136 (95%)	7 (5%)	22 47
6	2G	143/156 (92%)	139 (97%)	4 (3%)	38 66
7	1H	144/148 (97%)	141 (98%)	3 (2%)	47 73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
7	2H	144/148 (97%)	142 (99%)	2 (1%)	59 81
8	1I	113/124 (91%)	110 (97%)	3 (3%)	39 67
8	2I	105/124 (85%)	102 (97%)	3 (3%)	37 65
9	1N	118/119 (99%)	108 (92%)	10 (8%)	10 22
9	2N	118/119 (99%)	112 (95%)	6 (5%)	21 45
10	1O	100/100 (100%)	96 (96%)	4 (4%)	28 55
10	2O	100/100 (100%)	99 (99%)	1 (1%)	68 86
11	1P	115/116 (99%)	110 (96%)	5 (4%)	26 51
11	2P	115/116 (99%)	114 (99%)	1 (1%)	70 87
12	1Q	111/111 (100%)	109 (98%)	2 (2%)	51 76
12	2Q	111/111 (100%)	109 (98%)	2 (2%)	51 76
13	1R	101/101 (100%)	89 (88%)	12 (12%)	5 10
13	2R	101/101 (100%)	94 (93%)	7 (7%)	14 32
14	1S	86/88 (98%)	79 (92%)	7 (8%)	11 24
14	2S	85/88 (97%)	83 (98%)	2 (2%)	43 70
15	1T	115/127 (91%)	111 (96%)	4 (4%)	32 59
15	2T	113/127 (89%)	111 (98%)	2 (2%)	51 76
16	1U	93/94 (99%)	87 (94%)	6 (6%)	15 35
16	2U	93/94 (99%)	90 (97%)	3 (3%)	34 62
17	1V	80/82 (98%)	73 (91%)	7 (9%)	9 21
17	2V	80/82 (98%)	75 (94%)	5 (6%)	16 36
18	1W	90/92 (98%)	83 (92%)	7 (8%)	11 26
18	2W	90/92 (98%)	86 (96%)	4 (4%)	25 50
19	1X	77/78 (99%)	76 (99%)	1 (1%)	61 82
19	2X	77/78 (99%)	77 (100%)	0	100 100
20	1Y	85/91 (93%)	80 (94%)	5 (6%)	18 38
20	2Y	85/91 (93%)	82 (96%)	3 (4%)	32 59
21	1Z	135/179 (75%)	132 (98%)	3 (2%)	45 72
21	2Z	137/179 (76%)	134 (98%)	3 (2%)	45 72
22	10	65/67 (97%)	63 (97%)	2 (3%)	35 63
22	20	65/67 (97%)	64 (98%)	1 (2%)	57 80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
23	11	80/83 (96%)	78 (98%)	2 (2%)	42 69
23	21	80/83 (96%)	78 (98%)	2 (2%)	42 69
24	12	65/67 (97%)	65 (100%)	0	100 100
24	22	65/67 (97%)	65 (100%)	0	100 100
25	13	51/52 (98%)	48 (94%)	3 (6%)	18 38
25	23	50/52 (96%)	50 (100%)	0	100 100
26	14	59/63 (94%)	56 (95%)	3 (5%)	21 45
26	24	53/63 (84%)	49 (92%)	4 (8%)	12 28
27	15	50/52 (96%)	46 (92%)	4 (8%)	11 25
27	25	50/52 (96%)	47 (94%)	3 (6%)	17 37
28	16	51/52 (98%)	46 (90%)	5 (10%)	7 17
28	26	50/52 (96%)	48 (96%)	2 (4%)	28 55
29	17	41/42 (98%)	39 (95%)	2 (5%)	22 47
29	27	41/42 (98%)	40 (98%)	1 (2%)	43 70
30	18	54/55 (98%)	51 (94%)	3 (6%)	19 40
30	28	54/55 (98%)	53 (98%)	1 (2%)	50 75
31	19	34/34 (100%)	33 (97%)	1 (3%)	37 65
31	29	34/34 (100%)	32 (94%)	2 (6%)	18 38
33	1b	192/220 (87%)	189 (98%)	3 (2%)	55 79
33	2b	187/220 (85%)	184 (98%)	3 (2%)	55 79
34	1c	142/188 (76%)	136 (96%)	6 (4%)	26 52
34	2c	140/188 (74%)	140 (100%)	0	100 100
35	1d	169/181 (93%)	163 (96%)	6 (4%)	31 58
35	2d	173/181 (96%)	169 (98%)	4 (2%)	44 71
36	1e	113/123 (92%)	111 (98%)	2 (2%)	51 76
36	2e	114/123 (93%)	112 (98%)	2 (2%)	51 76
37	1f	84/90 (93%)	83 (99%)	1 (1%)	63 83
37	2f	85/90 (94%)	85 (100%)	0	100 100
38	1g	119/127 (94%)	119 (100%)	0	100 100
38	2g	120/127 (94%)	120 (100%)	0	100 100
39	1h	114/119 (96%)	110 (96%)	4 (4%)	32 59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
39	2h	114/119 (96%)	111 (97%)	3 (3%)	40 68
40	1i	90/99 (91%)	88 (98%)	2 (2%)	45 72
40	2i	89/99 (90%)	87 (98%)	2 (2%)	45 72
41	1j	66/92 (72%)	65 (98%)	1 (2%)	57 80
41	2j	69/92 (75%)	68 (99%)	1 (1%)	59 81
42	1k	82/99 (83%)	81 (99%)	1 (1%)	63 83
42	2k	83/99 (84%)	81 (98%)	2 (2%)	43 70
43	1l	96/108 (89%)	93 (97%)	3 (3%)	35 63
43	2l	96/108 (89%)	94 (98%)	2 (2%)	47 73
44	1m	93/101 (92%)	92 (99%)	1 (1%)	65 84
44	2m	92/101 (91%)	92 (100%)	0	100 100
45	1n	49/50 (98%)	46 (94%)	3 (6%)	17 37
45	2n	49/50 (98%)	47 (96%)	2 (4%)	27 54
46	1o	78/80 (98%)	77 (99%)	1 (1%)	61 82
46	2o	78/80 (98%)	76 (97%)	2 (3%)	40 68
47	1p	69/74 (93%)	64 (93%)	5 (7%)	13 30
47	2p	68/74 (92%)	61 (90%)	7 (10%)	7 15
48	1q	94/97 (97%)	93 (99%)	1 (1%)	65 84
48	2q	94/97 (97%)	94 (100%)	0	100 100
49	1r	59/77 (77%)	59 (100%)	0	100 100
49	2r	59/77 (77%)	59 (100%)	0	100 100
50	1s	69/80 (86%)	68 (99%)	1 (1%)	59 81
50	2s	67/80 (84%)	66 (98%)	1 (2%)	57 80
51	1t	70/82 (85%)	68 (97%)	2 (3%)	37 65
51	2t	70/82 (85%)	70 (100%)	0	100 100
52	1u	18/22 (82%)	18 (100%)	0	100 100
52	2u	18/22 (82%)	18 (100%)	0	100 100
56	A	4/4 (100%)	2 (50%)	2 (50%)	0 0
56	B	3/4 (75%)	2 (67%)	1 (33%)	0 0
56	C	4/4 (100%)	3 (75%)	1 (25%)	0 1
All	All	9314/10076 (92%)	8999 (97%)	315 (3%)	32 60

5 of 315 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	2O	98	VAL
35	2d	194	LEU
13	2R	65	LEU
20	2Y	85	VAL
45	2n	33	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 118 such sidechains are listed below:

Mol	Chain	Res	Type
50	1s	69	HIS
42	2k	93	GLN
8	2I	105	HIS
41	2j	56	HIS
35	2d	161	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2864/2915 (98%)	411 (14%)	29 (1%)
1	2A	2791/2915 (95%)	468 (16%)	22 (0%)
2	1B	120/121 (99%)	7 (5%)	1 (0%)
2	2B	118/121 (97%)	24 (20%)	0
32	1a	1497/1521 (98%)	237 (15%)	0
32	2a	1501/1521 (98%)	249 (16%)	0
53	1v	12/27 (44%)	2 (16%)	0
53	2v	12/27 (44%)	2 (16%)	0
54	1w	70/76 (92%)	23 (32%)	0
54	1y	72/76 (94%)	25 (34%)	0
54	2w	70/76 (92%)	23 (32%)	0
54	2y	71/76 (93%)	32 (45%)	0
55	1x	75/77 (97%)	12 (16%)	0
55	2x	75/77 (97%)	12 (16%)	0
All	All	9348/9626 (97%)	1527 (16%)	52 (0%)

5 of 1527 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	12	U
1	1A	13	A
1	1A	34	C

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Mol	Chain	Res	Type
1	1A	45	C
1	1A	54	G

5 of 52 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	2451	A
1	2A	271(M)	G
1	2A	1992	G
2	1B	1	U
1	2A	228	A

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	MA6	1a	1518	32	23,26,27	1.56	5 (21%)	33,38,41	2.18	11 (33%)
54	6MZ	2w	37	54	22,25,26	1.55	4 (18%)	29,36,39	2.19	9 (31%)
55	PSU	1x	55	55	18,21,22	1.33	2 (11%)	21,30,33	2.11	4 (19%)
1	4OC	1A	1942	1	19,22,24	0.80	0	25,31,35	0.97	1 (4%)
56	ORD	A	5	56	6,7,8	0.50	0	2,7,9	0.61	0
54	7MG	2w	46	54	23,26,27	1.38	4 (17%)	27,39,42	2.54	7 (25%)
32	5MC	2a	1407	32,57	19,22,23	1.65	3 (15%)	26,32,35	1.15	3 (11%)
32	M2G	2a	966	32	24,27,28	1.33	4 (16%)	33,40,43	1.94	6 (18%)
55	5MC	2x	32	55	19,22,23	1.66	3 (15%)	26,32,35	1.21	3 (11%)
32	5MC	1a	967	32	19,22,23	1.51	3 (15%)	26,32,35	1.09	3 (11%)
1	OMG	1A	2263	55,1,57	23,26,27	1.24	3 (13%)	32,38,41	2.03	6 (18%)
56	IAR	B	7	56	10,11,11	1.88	2 (20%)	7,13,13	2.18	2 (28%)
32	4OC	1a	1402	32	20,23,24	0.74	0	25,32,35	0.99	2 (8%)
54	5MU	1w	54	54	19,22,23	1.37	5 (26%)	27,32,35	2.21	6 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
56	EUP	C	2	56	4,7,8	0.52	0	4,8,10	1.44	1 (25%)
1	5MU	2A	1939	1	19,22,23	1.39	5 (26%)	27,32,35	2.42	6 (22%)
54	4SU	2w	8	54	18,21,22	1.74	4 (22%)	25,30,33	2.43	5 (20%)
32	5MC	1a	1407	32	19,22,23	1.68	3 (15%)	26,32,35	1.18	3 (11%)
54	PSU	2y	55	54	18,21,22	1.39	2 (11%)	21,30,33	2.01	3 (14%)
54	7MG	2y	46	54	23,26,27	1.39	3 (13%)	27,39,42	2.71	6 (22%)
54	7MG	1w	46	54	23,26,27	1.37	3 (13%)	27,39,42	2.59	7 (25%)
54	6MZ	1y	37	54	22,25,26	1.58	3 (13%)	29,36,39	2.19	10 (34%)
54	7MG	1y	46	54	23,26,27	1.42	3 (13%)	27,39,42	2.69	6 (22%)
32	5MC	1a	1400	32	19,22,23	1.70	3 (15%)	26,32,35	1.16	2 (7%)
55	4SU	1x	8	55	18,21,22	2.17	4 (22%)	25,30,33	1.61	6 (24%)
1	4OC	2A	1920	1	19,22,24	0.78	0	25,31,35	1.03	1 (4%)
32	PSU	2a	516	32,57	18,21,22	1.35	2 (11%)	21,30,33	2.02	5 (23%)
54	CM0	2y	34	54	21,26,27	1.21	3 (14%)	26,37,40	1.84	4 (15%)
32	MA6	1a	1519	32	23,26,27	1.60	4 (17%)	33,38,41	2.29	11 (33%)
1	5MC	1A	1984	1,57	19,22,23	1.67	3 (15%)	26,32,35	1.12	1 (3%)
54	CM0	1y	34	54	21,26,27	1.25	3 (14%)	26,37,40	2.19	5 (19%)
55	4SU	2x	8	55	18,21,22	2.00	5 (27%)	25,30,33	1.35	5 (20%)
1	PSU	2A	1917	1	18,21,22	1.40	2 (11%)	21,30,33	2.12	4 (19%)
54	4SU	1w	8	54	18,21,22	1.78	4 (22%)	25,30,33	2.07	5 (20%)
56	ORD	B	3	56	6,7,8	0.52	0	2,7,9	0.49	0
1	2MA	1A	2515	1,57	22,25,26	1.41	4 (18%)	32,37,40	2.33	8 (25%)
56	EUP	A	2	56	4,7,8	0.55	0	4,8,10	1.00	0
1	2MU	2A	2552	1,57	19,22,24	1.29	3 (15%)	25,31,36	1.84	6 (24%)
32	UR3	1a	1498	32	19,22,23	1.05	2 (10%)	26,32,35	1.80	4 (15%)
54	6MZ	1w	37	54	22,25,26	1.54	5 (22%)	29,36,39	2.14	9 (31%)
54	5MU	2y	54	54	19,22,23	1.44	5 (26%)	27,32,35	2.15	6 (22%)
55	5MU	1x	54	55,57	19,22,23	1.45	5 (26%)	27,32,35	1.86	6 (22%)
1	5MU	1A	1961	1	19,22,23	1.38	4 (21%)	27,32,35	2.25	6 (22%)
55	5MU	2x	54	55	19,22,23	1.43	4 (21%)	27,32,35	2.10	6 (22%)
1	2MA	2A	2503	1	22,25,26	1.48	4 (18%)	32,37,40	2.29	8 (25%)
32	2MG	2a	1207	32	23,26,27	1.26	3 (13%)	33,38,41	2.19	7 (21%)
1	2MU	1A	2564	1	19,22,24	1.19	3 (15%)	25,31,36	1.98	6 (24%)
54	CM0	2w	34	54	21,26,27	1.16	2 (9%)	26,37,40	1.77	5 (19%)
54	4SU	2y	8	54	18,21,22	1.70	4 (22%)	25,30,33	2.21	5 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
56	ORD	C	5	56,32	6,7,8	1.23	1 (16%)	2,7,9	0.78	0
1	OMG	2A	2251	55,1,57	23,26,27	1.20	3 (13%)	32,38,41	1.93	6 (18%)
1	5MU	1A	1937	1	19,22,23	1.42	5 (26%)	27,32,35	2.11	7 (25%)
32	7MG	2a	527	32,57	23,26,27	1.34	4 (17%)	27,39,42	2.54	6 (22%)
56	IAR	A	9	56	10,11,11	1.86	3 (30%)	7,13,13	2.78	1 (14%)
32	5MC	2a	1404	32	19,22,23	1.77	3 (15%)	26,32,35	1.21	3 (11%)
1	PSU	2A	1911	1	18,21,22	1.36	2 (11%)	21,30,33	1.99	3 (14%)
32	4OC	2a	1402	32,57	20,23,24	0.79	0	25,32,35	1.08	3 (12%)
54	5MU	1y	54	54	19,22,23	1.45	5 (26%)	27,32,35	2.12	6 (22%)
32	5MC	1a	1404	32	19,22,23	1.48	3 (15%)	26,32,35	1.03	2 (7%)
1	PSU	1A	1939	1	18,21,22	1.40	2 (11%)	21,30,33	1.88	4 (19%)
54	PSU	1y	55	54	18,21,22	1.33	2 (11%)	21,30,33	2.09	4 (19%)
32	5MC	2a	1400	32	19,22,23	1.71	3 (15%)	26,32,35	1.18	3 (11%)
1	PSU	1A	1933	1	18,21,22	1.38	3 (16%)	21,30,33	2.01	4 (19%)
54	4SU	1y	8	54	18,21,22	1.85	4 (22%)	25,30,33	1.98	5 (20%)
43	0TD	1l	92	43	8,9,10	4.59	1 (12%)	6,11,13	5.05	2 (33%)
54	5MU	2w	54	54	19,22,23	1.41	4 (21%)	27,32,35	1.94	6 (22%)
55	PSU	2x	55	55	18,21,22	1.36	2 (11%)	21,30,33	2.12	5 (23%)
32	MA6	2a	1519	32	23,26,27	1.59	4 (17%)	33,38,41	2.27	12 (36%)
54	PSU	2w	55	54	18,21,22	1.41	2 (11%)	21,30,33	1.95	4 (19%)
32	PSU	1a	516	32	18,21,22	1.40	2 (11%)	21,30,33	2.04	5 (23%)
54	PSU	1w	55	54	18,21,22	1.39	1 (5%)	21,30,33	1.95	4 (19%)
32	MA6	2a	1518	32	23,26,27	1.61	4 (17%)	33,38,41	2.30	13 (39%)
1	5MC	2A	1942	1	19,22,23	1.62	3 (15%)	26,32,35	1.15	2 (7%)
1	5MC	2A	1962	1,57	19,22,23	1.63	3 (15%)	26,32,35	1.23	2 (7%)
1	PSU	1A	2617	1	18,21,22	1.39	3 (16%)	21,30,33	2.16	5 (23%)
32	7MG	1a	527	32,57	23,26,27	1.40	3 (13%)	27,39,42	2.54	6 (22%)
1	5MU	2A	1915	1	19,22,23	1.44	4 (21%)	27,32,35	2.05	6 (22%)
32	M2G	1a	966	32	24,27,28	1.32	4 (16%)	33,40,43	1.92	5 (15%)
56	IAR	C	9	54,56	10,11,11	1.81	2 (20%)	7,13,13	1.64	2 (28%)
54	CM0	1w	34	54	21,26,27	1.11	2 (9%)	26,37,40	1.88	5 (19%)
54	6MZ	2y	37	54,32	22,25,26	1.59	4 (18%)	29,36,39	2.16	9 (31%)
55	5MC	1x	32	55,57	19,22,23	1.69	3 (15%)	26,32,35	1.31	3 (11%)
43	0TD	2l	92	43	8,9,10	4.65	1 (12%)	6,11,13	7.24	3 (50%)
1	PSU	2A	2605	1	18,21,22	1.35	2 (11%)	21,30,33	1.94	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
32	5MC	2a	967	32	19,22,23	1.79	3 (15%)	26,32,35	1.15	2 (7%)
1	5MC	1A	1964	1	19,22,23	1.54	3 (15%)	26,32,35	1.09	2 (7%)
32	UR3	2a	1498	32	19,22,23	1.07	2 (10%)	26,32,35	1.61	4 (15%)
32	2MG	1a	1207	32	23,26,27	1.23	2 (8%)	33,38,41	2.27	9 (27%)

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	MA6	1a	1518	32	-	2/11/29/30	0/3/3/3
54	6MZ	2w	37	54	-	0/9/27/28	0/3/3/3
55	PSU	1x	55	55	-	0/7/25/26	0/2/2/2
1	4OC	1A	1942	1	-	1/9/27/30	0/2/2/2
56	ORD	A	5	56	-	2/5/6/8	-
54	7MG	2w	46	54	-	2/7/37/38	0/3/3/3
32	5MC	2a	1407	32,57	-	0/7/25/26	0/2/2/2
32	M2G	2a	966	32	-	0/11/29/30	0/3/3/3
55	5MC	2x	32	55	-	0/7/25/26	0/2/2/2
32	5MC	1a	967	32	-	2/7/25/26	0/2/2/2
1	OMG	1A	2263	55,1,57	-	1/9/27/28	0/3/3/3
56	IAR	B	7	56	-	2/8/11/11	-
32	4OC	1a	1402	32	-	1/9/29/30	0/2/2/2
54	5MU	1w	54	54	-	0/7/25/26	0/2/2/2
56	EUP	C	2	56	-	3/7/8/10	-
1	5MU	2A	1939	1	-	0/7/25/26	0/2/2/2
54	4SU	2w	8	54	-	0/7/25/26	0/2/2/2
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
54	PSU	2y	55	54	-	1/7/25/26	0/2/2/2
54	7MG	2y	46	54	-	2/7/37/38	0/3/3/3
54	7MG	1w	46	54	-	2/7/37/38	0/3/3/3
54	6MZ	1y	37	54	-	0/9/27/28	0/3/3/3
54	7MG	1y	46	54	-	5/7/37/38	0/3/3/3
32	5MC	1a	1400	32	-	2/7/25/26	0/2/2/2
55	4SU	1x	8	55	-	0/7/25/26	0/2/2/2
1	4OC	2A	1920	1	-	1/9/27/30	0/2/2/2
32	PSU	2a	516	32,57	-	0/7/25/26	0/2/2/2
54	CM0	2y	34	54	-	3/12/30/31	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	MA6	1a	1519	32	-	4/11/29/30	0/3/3/3
1	5MC	1A	1984	1,57	-	0/7/25/26	0/2/2/2
54	CM0	1y	34	54	-	2/12/30/31	0/2/2/2
55	4SU	2x	8	55	-	0/7/25/26	0/2/2/2
1	PSU	2A	1917	1	-	1/7/25/26	0/2/2/2
54	4SU	1w	8	54	-	0/7/25/26	0/2/2/2
56	ORD	B	3	56	-	4/5/6/8	-
1	2MA	1A	2515	1,57	-	1/7/25/26	0/3/3/3
56	EUP	A	2	56	-	1/7/8/10	-
1	2MU	2A	2552	1,57	-	0/9/27/28	0/2/2/2
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
54	6MZ	1w	37	54	-	0/9/27/28	0/3/3/3
54	5MU	2y	54	54	-	2/7/25/26	0/2/2/2
55	5MU	1x	54	55,57	-	0/7/25/26	0/2/2/2
1	5MU	1A	1961	1	-	0/7/25/26	0/2/2/2
55	5MU	2x	54	55	-	0/7/25/26	0/2/2/2
1	2MA	2A	2503	1	-	1/7/25/26	0/3/3/3
32	2MG	2a	1207	32	-	2/9/27/28	0/3/3/3
1	2MU	1A	2564	1	-	0/9/27/28	0/2/2/2
54	CM0	2w	34	54	-	7/12/30/31	0/2/2/2
54	4SU	2y	8	54	-	1/7/25/26	0/2/2/2
56	ORD	C	5	56,32	-	3/5/6/8	-
1	OMG	2A	2251	55,1,57	-	0/9/27/28	0/3/3/3
1	5MU	1A	1937	1	-	0/7/25/26	0/2/2/2
32	7MG	2a	527	32,57	-	3/7/37/38	0/3/3/3
56	IAR	A	9	56	-	2/8/11/11	-
32	5MC	2a	1404	32	-	0/7/25/26	0/2/2/2
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
32	4OC	2a	1402	32,57	-	3/9/29/30	0/2/2/2
54	5MU	1y	54	54	-	2/7/25/26	0/2/2/2
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
1	PSU	1A	1939	1	-	0/7/25/26	0/2/2/2
54	PSU	1y	55	54	-	0/7/25/26	0/2/2/2
32	5MC	2a	1400	32	-	0/7/25/26	0/2/2/2
1	PSU	1A	1933	1	-	0/7/25/26	0/2/2/2
54	4SU	1y	8	54	-	1/7/25/26	0/2/2/2
43	0TD	1l	92	43	-	1/7/12/14	-
54	5MU	2w	54	54	-	0/7/25/26	0/2/2/2
55	PSU	2x	55	55	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	MA6	2a	1519	32	-	4/11/29/30	0/3/3/3
54	PSU	2w	55	54	-	0/7/25/26	0/2/2/2
32	PSU	1a	516	32	-	0/7/25/26	0/2/2/2
54	PSU	1w	55	54	-	0/7/25/26	0/2/2/2
32	MA6	2a	1518	32	-	2/11/29/30	0/3/3/3
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
1	5MC	2A	1962	1,57	-	0/7/25/26	0/2/2/2
1	PSU	1A	2617	1	-	0/7/25/26	0/2/2/2
32	7MG	1a	527	32,57	-	3/7/37/38	0/3/3/3
1	5MU	2A	1915	1	-	0/7/25/26	0/2/2/2
32	M2G	1a	966	32	-	0/11/29/30	0/3/3/3
56	IAR	C	9	54,56	-	2/8/11/11	-
54	CM0	1w	34	54	-	7/12/30/31	0/2/2/2
54	6MZ	2y	37	54,32	-	1/9/27/28	0/3/3/3
55	5MC	1x	32	55,57	-	0/7/25/26	0/2/2/2
43	0TD	2l	92	43	-	2/7/12/14	-
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
32	5MC	2a	967	32	-	0/7/25/26	0/2/2/2
1	5MC	1A	1964	1	-	0/7/25/26	0/2/2/2
32	UR3	2a	1498	32	-	0/7/25/26	0/2/2/2
32	2MG	1a	1207	32	-	0/9/27/28	0/3/3/3

The worst 5 of 252 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	2l	92	0TD	CB-SB	-12.82	1.69	1.82
43	1l	92	0TD	CB-SB	-12.57	1.69	1.82
32	2a	967	5MC	C5-C4	6.71	1.49	1.44
32	2a	1404	5MC	C5-C4	6.63	1.49	1.44
32	2a	1400	5MC	C5-C4	6.33	1.48	1.44

The worst 5 of 418 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	2l	92	0TD	CSB-SB-CB	-17.23	71.40	102.36
43	1l	92	0TD	CSB-SB-CB	-11.72	81.30	102.36
54	1y	46	7MG	N9-C4-N3	9.67	139.64	125.46
54	2y	46	7MG	N9-C4-N3	9.61	139.54	125.46
54	1w	46	7MG	N9-C4-N3	8.64	138.11	125.46

There are no chirality outliers.

5 of 94 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1A	2263	OMG	C1'-C2'-O2'-CM2
32	1a	967	5MC	O4'-C4'-C5'-O5'
32	1a	1400	5MC	O4'-C4'-C5'-O5'
32	1a	1519	MA6	O4'-C4'-C5'-O5'
32	2a	1402	4OC	O4'-C4'-C5'-O5'

There are no ring outliers.

41 monomers are involved in 64 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	1a	1518	MA6	2	0
56	A	5	ORD	1	0
54	2w	46	7MG	1	0
56	B	7	IAR	1	0
32	1a	1402	4OC	2	0
54	1w	54	5MU	3	0
1	2A	1939	5MU	2	0
54	2y	55	PSU	1	0
54	2y	46	7MG	1	0
54	1w	46	7MG	2	0
54	1y	37	6MZ	2	0
32	1a	1400	5MC	1	0
55	1x	8	4SU	3	0
54	2y	34	CM0	1	0
32	1a	1519	MA6	2	0
55	2x	8	4SU	1	0
56	B	3	ORD	2	0
56	A	2	EUP	1	0
1	2A	2552	2MU	2	0
54	2y	54	5MU	1	0
1	1A	1961	5MU	1	0
55	2x	54	5MU	1	0
1	2A	2503	2MA	1	0
32	2a	1207	2MG	1	0
1	1A	2564	2MU	1	0
54	2y	8	4SU	1	0
56	C	5	ORD	2	0
56	A	9	IAR	3	0
32	2a	1402	4OC	2	0
54	1y	54	5MU	2	0
54	1y	55	PSU	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
54	1y	8	4SU	1	0
54	2w	54	5MU	2	0
32	2a	1519	MA6	2	0
32	2a	1518	MA6	3	0
32	1a	966	M2G	2	0
56	C	9	IAR	3	0
54	2y	37	6MZ	3	0
43	2l	92	0TD	1	0
32	2a	967	5MC	1	0
32	1a	1207	2MG	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2842 ligands modelled in this entry, 2840 are monoatomic - leaving 2 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	$\#\|Z\| > 2$
60	SF4	2d	501	35	0,12,12	-	-	-		
60	SF4	1d	501	35	0,12,12	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
60	SF4	2d	501	35	-	-	0/6/5/5
60	SF4	1d	501	35	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	1A	2860/2915 (98%)	-0.54	129 (4%) 38 32	21, 37, 96, 109	0
1	2A	2789/2915 (95%)	0.05	117 (4%) 40 35	35, 60, 95, 109	0
2	1B	120/121 (99%)	-0.48	0 100 100	31, 51, 63, 88	0
2	2B	120/121 (99%)	1.08	7 (5%) 29 23	66, 83, 90, 101	0
3	1D	275/276 (99%)	-0.05	5 (1%) 67 63	23, 38, 54, 83	0
3	2D	275/276 (99%)	0.37	4 (1%) 72 68	32, 52, 66, 85	0
4	1E	204/206 (99%)	-0.06	2 (0%) 79 76	20, 41, 62, 80	0
4	2E	204/206 (99%)	0.33	3 (1%) 72 68	36, 61, 75, 89	0
5	1F	203/210 (96%)	-0.07	1 (0%) 87 85	21, 43, 70, 85	0
5	2F	203/210 (96%)	0.64	6 (2%) 52 47	37, 72, 84, 89	0
6	1G	181/182 (99%)	0.52	10 (5%) 30 25	42, 64, 78, 88	0
6	2G	181/182 (99%)	1.80	63 (34%) 1 1	77, 86, 92, 98	0
7	1H	174/180 (96%)	0.25	4 (2%) 61 55	39, 56, 69, 79	0
7	2H	174/180 (96%)	1.27	24 (13%) 6 5	72, 85, 93, 97	0
8	1I	146/148 (98%)	0.75	4 (2%) 56 50	43, 75, 85, 88	0
8	2I	146/148 (98%)	1.20	17 (11%) 9 7	56, 77, 87, 94	0
9	1N	140/140 (100%)	-0.21	0 100 100	28, 38, 65, 79	0
9	2N	140/140 (100%)	0.83	11 (7%) 18 14	50, 67, 81, 87	0
10	1O	122/122 (100%)	0.07	1 (0%) 82 80	30, 42, 58, 66	0
10	2O	122/122 (100%)	0.62	3 (2%) 58 52	45, 60, 72, 78	0
11	1P	149/150 (99%)	0.06	0 100 100	21, 48, 69, 80	0
11	2P	149/150 (99%)	0.62	7 (4%) 36 30	40, 71, 86, 91	0
12	1Q	141/141 (100%)	-0.04	1 (0%) 84 82	27, 43, 59, 79	0
12	2Q	141/141 (100%)	1.05	16 (11%) 10 8	48, 71, 81, 87	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	1R	118/118 (100%)	-0.26	0 100 100	26, 35, 52, 62	0
13	2R	118/118 (100%)	0.30	1 (0%) 82 80	42, 56, 67, 75	0
14	1S	110/112 (98%)	0.10	1 (0%) 81 78	39, 51, 65, 68	0
14	2S	110/112 (98%)	1.34	16 (14%) 6 4	67, 78, 85, 91	0
15	1T	131/146 (89%)	0.28	10 (7%) 20 16	34, 45, 73, 83	0
15	2T	131/146 (89%)	0.58	2 (1%) 72 68	52, 63, 80, 85	0
16	1U	116/118 (98%)	-0.42	1 (0%) 81 78	22, 31, 46, 69	0
16	2U	116/118 (98%)	0.76	2 (1%) 69 64	48, 65, 80, 88	0
17	1V	101/101 (100%)	-0.29	1 (0%) 79 76	22, 41, 57, 71	0
17	2V	101/101 (100%)	0.94	8 (7%) 18 14	47, 76, 84, 88	0
18	1W	112/113 (99%)	-0.29	3 (2%) 56 50	24, 33, 55, 82	0
18	2W	112/113 (99%)	0.50	3 (2%) 56 50	43, 53, 71, 88	0
19	1X	95/96 (98%)	0.03	2 (2%) 63 58	28, 40, 58, 77	0
19	2X	95/96 (98%)	0.64	5 (5%) 32 26	45, 63, 79, 87	0
20	1Y	107/110 (97%)	0.29	1 (0%) 81 78	37, 52, 72, 81	0
20	2Y	107/110 (97%)	1.35	22 (20%) 2 2	64, 75, 84, 90	0
21	1Z	154/206 (74%)	0.84	20 (12%) 7 5	41, 67, 93, 100	0
21	2Z	160/206 (77%)	1.74	50 (31%) 1 1	70, 87, 98, 101	0
22	10	83/85 (97%)	0.17	5 (6%) 27 22	30, 40, 63, 78	0
22	20	83/85 (97%)	1.32	15 (18%) 3 3	45, 69, 82, 85	0
23	11	97/98 (98%)	0.22	2 (2%) 63 58	28, 47, 73, 77	0
23	21	97/98 (98%)	0.58	4 (4%) 41 36	40, 57, 78, 84	0
24	12	70/72 (97%)	0.36	4 (5%) 29 24	36, 51, 62, 78	0
24	22	70/72 (97%)	0.84	4 (5%) 29 24	62, 74, 81, 84	0
25	13	59/60 (98%)	-0.16	2 (3%) 48 42	28, 37, 65, 85	0
25	23	59/60 (98%)	0.76	3 (5%) 33 28	55, 69, 83, 92	0
26	14	69/71 (97%)	0.89	10 (14%) 6 4	59, 78, 94, 98	0
26	24	69/71 (97%)	2.07	30 (43%) 0 0	80, 91, 97, 98	0
27	15	59/60 (98%)	-0.32	1 (1%) 69 64	21, 32, 53, 63	0
27	25	59/60 (98%)	0.26	1 (1%) 69 64	38, 52, 72, 79	0
28	16	53/54 (98%)	0.01	1 (1%) 66 61	35, 44, 60, 63	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
28	26	53/54 (98%)	0.88	0 100 100	55, 63, 74, 77	0
29	17	48/49 (97%)	-0.23	3 (6%) 26 20	23, 29, 55, 67	0
29	27	48/49 (97%)	0.17	3 (6%) 26 20	34, 42, 67, 76	0
30	18	64/65 (98%)	-0.12	1 (1%) 70 66	29, 35, 43, 58	0
30	28	64/65 (98%)	0.47	2 (3%) 51 45	51, 59, 66, 71	0
31	19	37/37 (100%)	-0.11	0 100 100	31, 42, 60, 62	0
31	29	37/37 (100%)	1.21	3 (8%) 18 14	62, 70, 82, 86	0
32	1a	1488/1521 (97%)	0.32	56 (3%) 44 38	36, 69, 95, 107	0
32	2a	1491/1521 (98%)	0.78	160 (10%) 11 9	50, 80, 99, 109	0
33	1b	231/256 (90%)	1.18	34 (14%) 6 4	66, 82, 93, 98	0
33	2b	231/256 (90%)	2.15	125 (54%) 0 0	76, 90, 96, 101	0
34	1c	206/239 (86%)	1.03	21 (10%) 12 9	64, 76, 85, 91	0
34	2c	206/239 (86%)	2.26	116 (56%) 0 0	79, 89, 94, 98	0
35	1d	208/209 (99%)	1.27	33 (15%) 5 4	59, 74, 85, 90	0
35	2d	208/209 (99%)	1.03	19 (9%) 15 11	63, 74, 83, 91	0
36	1e	148/162 (91%)	0.66	2 (1%) 73 69	51, 66, 77, 84	0
36	2e	148/162 (91%)	1.50	40 (27%) 1 1	72, 80, 88, 95	0
37	1f	100/101 (99%)	0.69	2 (2%) 65 60	57, 70, 79, 82	0
37	2f	100/101 (99%)	0.65	1 (1%) 79 76	64, 74, 84, 87	0
38	1g	155/156 (99%)	0.92	17 (10%) 10 8	64, 74, 87, 95	0
38	2g	155/156 (99%)	1.35	30 (19%) 3 2	75, 83, 91, 95	0
39	1h	137/138 (99%)	0.74	4 (2%) 53 48	58, 69, 76, 80	0
39	2h	137/138 (99%)	1.26	21 (15%) 5 4	70, 80, 86, 88	0
40	1i	127/128 (99%)	1.19	16 (12%) 8 6	58, 80, 89, 93	0
40	2i	127/128 (99%)	2.03	60 (47%) 0 0	78, 88, 94, 97	0
41	1j	97/105 (92%)	1.57	24 (24%) 2 1	60, 79, 91, 94	0
41	2j	96/105 (91%)	2.44	62 (64%) 0 0	81, 90, 97, 98	0
42	1k	114/129 (88%)	0.88	7 (6%) 27 22	43, 69, 79, 84	0
42	2k	114/129 (88%)	1.20	13 (11%) 10 7	58, 77, 85, 87	0
43	1l	121/132 (91%)	0.53	11 (9%) 15 11	50, 58, 71, 80	0
43	2l	121/132 (91%)	0.96	11 (9%) 15 11	62, 72, 79, 84	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
44	1m	123/126 (97%)	0.90	14 (11%) 10 7	62, 75, 86, 94	0
44	2m	122/126 (96%)	2.30	62 (50%) 0 0	78, 88, 96, 102	0
45	1n	60/61 (98%)	1.34	11 (18%) 3 3	62, 72, 79, 81	0
45	2n	60/61 (98%)	2.63	43 (71%) 0 0	81, 89, 94, 97	0
46	1o	88/89 (98%)	0.69	3 (3%) 48 42	50, 67, 78, 83	0
46	2o	88/89 (98%)	1.02	8 (9%) 15 11	66, 76, 86, 91	0
47	1p	82/88 (93%)	1.80	30 (36%) 1 0	59, 74, 84, 86	0
47	2p	82/88 (93%)	1.05	7 (8%) 16 13	61, 71, 80, 83	0
48	1q	99/105 (94%)	0.82	2 (2%) 65 60	57, 70, 79, 84	0
48	2q	99/105 (94%)	1.09	11 (11%) 10 8	66, 76, 85, 86	0
49	1r	68/88 (77%)	0.76	5 (7%) 20 16	61, 70, 80, 86	0
49	2r	68/88 (77%)	0.68	2 (2%) 53 48	69, 76, 85, 89	0
50	1s	83/93 (89%)	0.99	6 (7%) 21 17	66, 76, 86, 90	0
50	2s	83/93 (89%)	2.65	60 (72%) 0 0	83, 91, 97, 99	0
51	1t	96/106 (90%)	1.35	18 (18%) 3 2	62, 73, 84, 89	0
51	2t	96/106 (90%)	0.97	12 (12%) 8 6	60, 73, 86, 89	0
52	1u	23/27 (85%)	1.15	2 (8%) 16 12	65, 69, 77, 80	0
52	2u	23/27 (85%)	2.67	16 (69%) 0 0	78, 86, 90, 91	0
53	1v	13/27 (48%)	1.03	4 (30%) 1 1	48, 67, 93, 102	0
53	2v	13/27 (48%)	2.09	6 (46%) 0 0	70, 91, 102, 110	0
54	1w	67/76 (88%)	1.66	24 (35%) 1 1	55, 96, 102, 106	0
54	1y	68/76 (89%)	1.92	33 (48%) 0 0	40, 98, 103, 108	0
54	2w	67/76 (88%)	1.94	25 (37%) 1 0	73, 100, 104, 108	0
54	2y	67/76 (88%)	2.26	46 (68%) 0 0	58, 101, 105, 106	0
55	1x	72/77 (93%)	0.40	2 (2%) 55 49	36, 71, 85, 93	0
55	2x	72/77 (93%)	0.92	5 (6%) 23 18	56, 85, 94, 98	0
56	A	6/9 (66%)	1.18	0 100 100	70, 73, 78, 79	0
56	B	5/9 (55%)	2.86	5 (100%) 0 0	70, 75, 79, 79	0
56	C	6/9 (66%)	4.06	6 (100%) 0 0	90, 91, 95, 97	0
All	All	20896/21781 (95%)	0.50	2030 (9%) 13 10	20, 67, 94, 110	0

The worst 5 of 2030 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
44	2m	124	PRO	11.6
44	2m	123	ALA	8.3
44	2m	102	ARG	7.4
44	1m	124	PRO	7.1
38	1g	80	VAL	6.9

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
54	PSU	2w	55	20/21	0.33	0.20	95,102,111,112	0
56	IAR	B	7	12/12	0.38	0.30	76,91,98,99	0
54	7MG	1y	46	24/25	0.43	0.19	90,101,105,118	0
54	7MG	1w	46	24/25	0.48	0.18	88,96,107,117	0
54	7MG	2w	46	24/25	0.48	0.17	92,102,108,119	0
54	PSU	2y	55	20/21	0.50	0.17	94,101,106,117	0
54	4SU	2y	8	20/21	0.50	0.17	99,104,116,125	0
54	PSU	1w	55	20/21	0.52	0.20	71,97,102,104	0
54	CM0	2y	34	25/26	0.55	0.20	85,102,110,128	0
54	7MG	2y	46	24/25	0.55	0.16	94,104,109,114	0
54	4SU	1y	8	20/21	0.57	0.16	95,99,109,118	0
54	PSU	1y	55	20/21	0.58	0.16	93,98,104,117	0
54	5MU	2y	54	21/22	0.61	0.17	93,102,109,126	0
54	4SU	2w	8	20/21	0.61	0.15	97,102,109,122	0
54	6MZ	2y	37	23/24	0.65	0.16	89,99,106,125	0
56	IAR	C	9	12/12	0.65	0.19	81,88,101,103	0
56	ORD	C	5	8/9	0.69	0.20	90,95,96,98	0
54	5MU	2w	54	21/22	0.69	0.14	87,92,100,102	0
54	CM0	1y	34	25/26	0.69	0.17	84,94,101,121	0
54	CM0	2w	34	25/26	0.70	0.18	83,92,98,110	0
54	4SU	1w	8	20/21	0.71	0.13	93,97,110,113	0
54	5MU	1w	54	21/22	0.73	0.14	69,85,91,95	0
54	6MZ	1y	37	23/24	0.73	0.17	85,94,103,117	0
32	2MG	2a	1207	24/25	0.77	0.16	84,94,98,101	0
54	5MU	1y	54	21/22	0.78	0.12	90,95,100,110	0
56	ORD	B	3	8/9	0.79	0.24	72,75,81,82	0
55	PSU	2x	55	20/21	0.79	0.12	78,86,93,99	0
55	4SU	2x	8	20/21	0.80	0.13	83,89,97,98	0
56	IAR	A	9	12/12	0.81	0.26	67,79,91,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	EUP	C	2	8/9	0.83	0.21	87,92,94,94	0
54	CM0	1w	34	25/26	0.83	0.17	74,78,85,93	0
55	5MU	2x	54	21/22	0.84	0.13	82,88,92,102	0
32	M2G	2a	966	25/26	0.84	0.17	63,73,89,97	0
43	0TD	2l	92	10/11	0.85	0.14	70,70,74,88	0
1	5MU	2A	1915	21/22	0.85	0.12	74,77,85,90	0
32	PSU	2a	516	20/21	0.86	0.12	78,81,88,90	0
32	5MC	2a	967	21/22	0.87	0.14	67,75,84,91	0
32	7MG	2a	527	24/25	0.88	0.14	64,72,81,89	0
56	EUP	A	2	8/9	0.88	0.14	59,75,76,78	0
56	ORD	A	5	8/9	0.89	0.15	72,74,77,77	0
43	0TD	1l	92	10/11	0.89	0.12	50,54,58,79	0
32	5MC	2a	1404	21/22	0.89	0.12	52,61,70,76	0
54	6MZ	2w	37	23/24	0.90	0.11	82,87,91,96	0
55	5MC	2x	32	21/22	0.90	0.15	74,79,84,85	0
55	5MU	1x	54	21/22	0.91	0.10	63,72,76,83	0
1	5MU	1A	1937	21/22	0.91	0.12	56,62,67,74	0
55	PSU	1x	55	20/21	0.91	0.09	64,70,77,78	0
55	4SU	1x	8	20/21	0.91	0.12	61,68,82,83	0
1	PSU	2A	1911	20/21	0.91	0.10	64,68,75,79	0
32	4OC	2a	1402	22/23	0.91	0.13	57,67,73,79	0
1	PSU	2A	1917	20/21	0.92	0.08	64,69,82,86	0
32	5MC	2a	1400	21/22	0.93	0.13	67,72,76,82	0
1	4OC	2A	1920	21/23	0.93	0.10	57,66,69,70	0
32	UR3	2a	1498	21/22	0.94	0.11	52,60,69,72	0
54	6MZ	1w	37	23/24	0.94	0.09	59,65,70,71	0
32	2MG	1a	1207	24/25	0.94	0.10	70,74,80,80	0
32	PSU	1a	516	20/21	0.94	0.08	61,68,71,72	0
32	MA6	2a	1518	24/25	0.95	0.11	58,67,72,75	0
55	5MC	1x	32	21/22	0.95	0.11	47,57,61,67	0
32	MA6	2a	1519	24/25	0.95	0.12	56,68,70,73	0
1	2MA	2A	2503	23/24	0.95	0.10	31,39,43,53	0
1	5MC	2A	1942	21/22	0.95	0.10	56,63,67,79	0
32	5MC	2a	1407	21/22	0.96	0.09	49,60,64,76	0
1	PSU	1A	1933	20/21	0.96	0.08	45,49,53,59	0
32	7MG	1a	527	24/25	0.96	0.08	46,52,57,59	0
32	M2G	1a	966	25/26	0.96	0.10	51,57,63,72	0
32	5MC	1a	967	21/22	0.96	0.09	52,59,67,70	0
1	PSU	1A	1939	20/21	0.96	0.08	52,56,63,70	0
32	5MC	1a	1400	21/22	0.96	0.10	46,54,59,62	0
1	5MC	2A	1962	21/22	0.96	0.09	43,53,59,75	0
32	MA6	1a	1519	24/25	0.96	0.10	40,43,47,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
32	4OC	1a	1402	22/23	0.97	0.08	42,47,55,57	0
1	OMG	2A	2251	24/25	0.97	0.08	38,43,47,57	0
32	5MC	1a	1404	21/22	0.97	0.07	35,40,47,51	0
32	5MC	1a	1407	21/22	0.97	0.09	35,41,44,46	0
1	4OC	1A	1942	21/23	0.97	0.07	38,47,50,55	0
1	5MU	2A	1939	21/22	0.97	0.07	37,40,46,48	0
1	5MC	1A	1964	21/22	0.97	0.07	40,43,47,53	0
32	UR3	1a	1498	21/22	0.98	0.07	34,41,47,50	0
32	MA6	1a	1518	24/25	0.98	0.08	35,42,46,47	0
1	2MA	1A	2515	23/24	0.98	0.06	21,24,28,31	0
1	2MU	1A	2564	21/23	0.98	0.07	24,30,35,36	0
1	PSU	1A	2617	20/21	0.98	0.06	23,29,33,33	0
1	2MU	2A	2552	21/23	0.98	0.08	38,42,49,54	0
1	PSU	2A	2605	20/21	0.98	0.06	38,43,46,49	0
1	5MU	1A	1961	21/22	0.98	0.06	24,28,33,35	0
1	5MC	1A	1984	21/22	0.98	0.06	22,36,41,45	0
1	OMG	1A	2263	24/25	0.98	0.06	23,27,31,35	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	2y	3007	1/1	0.13	0.31	92,92,92,92	0
57	MG	1x	3014	1/1	0.36	0.19	82,82,82,82	0
57	MG	2B	3012	1/1	0.39	0.24	102,102,102,102	0
57	MG	1v	3001	1/1	0.42	0.31	85,85,85,85	0
57	MG	2A	3302	1/1	0.44	0.28	90,90,90,90	0
57	MG	1w	103	1/1	0.47	0.19	85,85,85,85	0
57	MG	2O	8002	1/1	0.49	0.28	82,82,82,82	0
57	MG	1a	1898	1/1	0.49	0.16	89,89,89,89	0
57	MG	2a	1802	1/1	0.51	0.30	100,100,100,100	0
57	MG	1A	3948	1/1	0.52	0.22	76,76,76,76	0
57	MG	1a	1834	1/1	0.53	0.31	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2y	3005	1/1	0.54	0.25	101,101,101,101	0
57	MG	2A	3528	1/1	0.54	0.29	58,58,58,58	0
57	MG	2A	3332	1/1	0.57	0.28	77,77,77,77	0
57	MG	18	101	1/1	0.57	0.23	80,80,80,80	0
57	MG	1a	1669	1/1	0.57	0.16	93,93,93,93	0
57	MG	2G	3001	1/1	0.57	0.28	81,81,81,81	0
57	MG	2A	3300	1/1	0.58	0.12	84,84,84,84	0
57	MG	1y	102	1/1	0.58	0.32	80,80,80,80	0
57	MG	2A	3576	1/1	0.59	0.19	84,84,84,84	0
57	MG	2A	3724	1/1	0.59	0.16	88,88,88,88	0
57	MG	1a	1866	1/1	0.59	0.27	76,76,76,76	0
57	MG	1A	4042	1/1	0.59	0.16	69,69,69,69	0
57	MG	C	8002	1/1	0.59	0.33	98,98,98,98	0
57	MG	2a	1773	1/1	0.61	0.20	88,88,88,88	0
57	MG	2A	3484	1/1	0.62	0.32	84,84,84,84	0
57	MG	1A	3421	1/1	0.62	0.27	74,74,74,74	0
57	MG	2A	3615	1/1	0.63	0.13	92,92,92,92	0
57	MG	1B	227	1/1	0.63	0.15	73,73,73,73	0
57	MG	1y	106	1/1	0.63	0.17	84,84,84,84	0
57	MG	1w	106	1/1	0.63	0.22	89,89,89,89	0
57	MG	1a	1737	1/1	0.63	0.24	81,81,81,81	0
57	MG	2A	3843	1/1	0.64	0.16	86,86,86,86	0
57	MG	1a	1802	1/1	0.64	0.23	92,92,92,92	0
57	MG	2B	3013	1/1	0.64	0.23	70,70,70,70	0
57	MG	1a	1665	1/1	0.64	0.18	67,67,67,67	0
57	MG	2A	3178	1/1	0.64	0.20	74,74,74,74	0
57	MG	2A	3253	1/1	0.64	0.15	79,79,79,79	0
57	MG	1S	3003	1/1	0.64	0.17	73,73,73,73	0
57	MG	2A	3669	1/1	0.64	0.20	62,62,62,62	0
57	MG	1A	3782	1/1	0.64	0.17	60,60,60,60	0
57	MG	2A	3797	1/1	0.64	0.20	72,72,72,72	0
57	MG	1A	3957	1/1	0.65	0.28	70,70,70,70	0
57	MG	2A	3101	1/1	0.65	0.31	73,73,73,73	0
57	MG	1y	103	1/1	0.65	0.26	86,86,86,86	0
57	MG	1A	3433	1/1	0.66	0.19	60,60,60,60	0
57	MG	2y	3006	1/1	0.66	0.14	106,106,106,106	0
57	MG	2D	304	1/1	0.66	0.24	73,73,73,73	0
57	MG	C	8001	1/1	0.66	0.41	95,95,95,95	0
57	MG	1A	3515	1/1	0.66	0.22	69,69,69,69	0
57	MG	2a	1757	1/1	0.67	0.27	77,77,77,77	0
57	MG	1a	1875	1/1	0.67	0.39	90,90,90,90	0
57	MG	1A	3873	1/1	0.68	0.22	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1a	1868	1/1	0.68	0.18	71,71,71,71	0
57	MG	2A	3236	1/1	0.68	0.17	84,84,84,84	0
57	MG	1a	1870	1/1	0.68	0.33	80,80,80,80	0
57	MG	2A	3818	1/1	0.68	0.16	76,76,76,76	0
57	MG	2R	8001	1/1	0.68	0.20	83,83,83,83	0
57	MG	1A	3453	1/1	0.68	0.23	70,70,70,70	0
57	MG	1A	3754	1/1	0.69	0.47	75,75,75,75	0
57	MG	1B	223	1/1	0.69	0.13	80,80,80,80	0
57	MG	1A	3995	1/1	0.69	0.17	52,52,52,52	0
57	MG	2A	3268	1/1	0.69	0.23	68,68,68,68	0
57	MG	1a	1815	1/1	0.69	0.28	87,87,87,87	0
57	MG	1a	1872	1/1	0.69	0.17	93,93,93,93	0
57	MG	2A	3320	1/1	0.69	0.26	81,81,81,81	0
57	MG	2A	3327	1/1	0.69	0.31	73,73,73,73	0
57	MG	1Y	203	1/1	0.70	0.23	80,80,80,80	0
57	MG	2a	1793	1/1	0.70	0.21	75,75,75,75	0
57	MG	1A	3357	1/1	0.70	0.26	71,71,71,71	0
57	MG	2v	101	1/1	0.70	0.16	85,85,85,85	0
57	MG	2x	103	1/1	0.70	0.23	92,92,92,92	0
57	MG	2A	3647	1/1	0.70	0.18	81,81,81,81	0
57	MG	2A	3249	1/1	0.70	0.25	81,81,81,81	0
57	MG	2Z	8001	1/1	0.70	0.18	89,89,89,89	0
57	MG	2a	1689	1/1	0.70	0.25	83,83,83,83	0
57	MG	2A	3553	1/1	0.70	0.20	52,52,52,52	0
57	MG	2a	1683	1/1	0.71	0.25	76,76,76,76	0
57	MG	2A	3018	1/1	0.71	0.24	78,78,78,78	0
57	MG	1a	1871	1/1	0.71	0.21	96,96,96,96	0
57	MG	2a	1769	1/1	0.71	0.22	72,72,72,72	0
57	MG	1A	4035	1/1	0.71	0.27	76,76,76,76	0
57	MG	2A	3231	1/1	0.71	0.25	67,67,67,67	0
57	MG	1x	3010	1/1	0.71	0.29	80,80,80,80	0
57	MG	1A	3975	1/1	0.71	0.26	74,74,74,74	0
57	MG	1a	1814	1/1	0.71	0.22	89,89,89,89	0
57	MG	1l	8002	1/1	0.71	0.20	79,79,79,79	0
57	MG	2A	3579	1/1	0.71	0.14	62,62,62,62	0
57	MG	2A	3598	1/1	0.71	0.17	71,71,71,71	0
57	MG	2A	3296	1/1	0.71	0.23	73,73,73,73	0
57	MG	1A	3571	1/1	0.71	0.24	62,62,62,62	0
57	MG	1a	1839	1/1	0.72	0.22	77,77,77,77	0
57	MG	2A	3541	1/1	0.72	0.17	62,62,62,62	0
57	MG	1A	3459	1/1	0.72	0.28	71,71,71,71	0
57	MG	2A	3559	1/1	0.72	0.19	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2j	8001	1/1	0.72	0.16	86,86,86,86	0
57	MG	2A	3045	1/1	0.72	0.40	78,78,78,78	0
57	MG	2a	1667	1/1	0.72	0.29	83,83,83,83	0
57	MG	2a	1673	1/1	0.72	0.17	83,83,83,83	0
57	MG	1A	3428	1/1	0.72	0.16	72,72,72,72	0
57	MG	1A	3924	1/1	0.72	0.19	63,63,63,63	0
57	MG	2a	1749	1/1	0.72	0.26	75,75,75,75	0
57	MG	2A	3185	1/1	0.72	0.15	69,69,69,69	0
57	MG	1a	1796	1/1	0.73	0.16	69,69,69,69	0
57	MG	2A	3243	1/1	0.73	0.34	69,69,69,69	0
57	MG	2A	3594	1/1	0.73	0.22	75,75,75,75	0
57	MG	1a	1801	1/1	0.73	0.15	77,77,77,77	0
57	MG	1a	1842	1/1	0.73	0.25	74,74,74,74	0
57	MG	1a	1655	1/1	0.73	0.22	74,74,74,74	0
57	MG	1a	1714	1/1	0.73	0.17	76,76,76,76	0
57	MG	1A	4021	1/1	0.73	0.14	60,60,60,60	0
57	MG	1y	105	1/1	0.73	0.22	93,93,93,93	0
57	MG	1a	1704	1/1	0.74	0.17	83,83,83,83	0
57	MG	2a	1786	1/1	0.74	0.20	85,85,85,85	0
57	MG	2A	3773	1/1	0.74	0.17	83,83,83,83	0
57	MG	1A	3721	1/1	0.74	0.18	59,59,59,59	0
57	MG	2a	1636	1/1	0.74	0.15	86,86,86,86	0
57	MG	2A	3098	1/1	0.74	0.19	76,76,76,76	0
57	MG	2x	101	1/1	0.74	0.33	89,89,89,89	0
57	MG	1A	3724	1/1	0.74	0.16	67,67,67,67	0
57	MG	2y	3003	1/1	0.74	0.20	102,102,102,102	0
57	MG	2A	3521	1/1	0.74	0.19	66,66,66,66	0
57	MG	2A	3301	1/1	0.74	0.10	88,88,88,88	0
57	MG	1A	3415	1/1	0.74	0.32	56,56,56,56	0
57	MG	2E	302	1/1	0.74	0.40	80,80,80,80	0
57	MG	2A	3305	1/1	0.74	0.11	76,76,76,76	0
57	MG	2A	3630	1/1	0.75	0.12	50,50,50,50	0
57	MG	2a	1665	1/1	0.75	0.22	70,70,70,70	0
57	MG	1a	1897	1/1	0.75	0.15	83,83,83,83	0
57	MG	1a	1843	1/1	0.75	0.24	84,84,84,84	0
57	MG	1A	3983	1/1	0.75	0.19	63,63,63,63	0
57	MG	2a	1684	1/1	0.75	0.22	76,76,76,76	0
57	MG	2a	1687	1/1	0.75	0.42	78,78,78,78	0
57	MG	2A	3519	1/1	0.75	0.16	77,77,77,77	0
57	MG	2A	3011	1/1	0.75	0.28	64,64,64,64	0
57	MG	2A	3803	1/1	0.75	0.15	71,71,71,71	0
57	MG	1V	202	1/1	0.75	0.16	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2a	1771	1/1	0.75	0.31	78,78,78,78	0
57	MG	2A	3824	1/1	0.75	0.12	93,93,93,93	0
57	MG	2A	3825	1/1	0.75	0.15	73,73,73,73	0
57	MG	2A	3829	1/1	0.75	0.17	75,75,75,75	0
57	MG	1A	3988	1/1	0.75	0.19	67,67,67,67	0
57	MG	2i	8001	1/1	0.75	0.12	72,72,72,72	0
57	MG	2A	3273	1/1	0.75	0.26	82,82,82,82	0
57	MG	2A	3051	1/1	0.75	0.16	80,80,80,80	0
57	MG	2B	3015	1/1	0.75	0.19	81,81,81,81	0
57	MG	2A	3091	1/1	0.75	0.18	75,75,75,75	0
57	MG	1A	3833	1/1	0.75	0.12	64,64,64,64	0
57	MG	1A	3372	1/1	0.75	0.15	65,65,65,65	0
57	MG	1B	229	1/1	0.75	0.18	77,77,77,77	0
57	MG	2A	3601	1/1	0.75	0.29	75,75,75,75	0
57	MG	1a	1876	1/1	0.75	0.21	83,83,83,83	0
57	MG	2a	1628	1/1	0.75	0.29	68,68,68,68	0
57	MG	1A	4071	1/1	0.76	0.21	82,82,82,82	0
57	MG	2A	3712	1/1	0.76	0.09	94,94,94,94	0
57	MG	2A	3163	1/1	0.76	0.23	78,78,78,78	0
57	MG	1A	3998	1/1	0.76	0.23	71,71,71,71	0
57	MG	2a	1777	1/1	0.76	0.21	82,82,82,82	0
57	MG	2A	3778	1/1	0.76	0.24	75,75,75,75	0
57	MG	2a	1791	1/1	0.76	0.37	72,72,72,72	0
57	MG	1a	1621	1/1	0.76	0.22	52,52,52,52	0
57	MG	1A	3984	1/1	0.76	0.16	55,55,55,55	0
57	MG	2a	1629	1/1	0.76	0.25	80,80,80,80	0
57	MG	2A	3807	1/1	0.76	0.16	84,84,84,84	0
57	MG	1A	3597	1/1	0.76	0.21	56,56,56,56	0
57	MG	1A	3359	1/1	0.76	0.21	67,67,67,67	0
57	MG	2A	3245	1/1	0.76	0.19	79,79,79,79	0
57	MG	2y	3002	1/1	0.76	0.21	86,86,86,86	0
57	MG	1a	1685	1/1	0.76	0.37	74,74,74,74	0
57	MG	2A	3353	1/1	0.76	0.26	78,78,78,78	0
57	MG	2A	3397	1/1	0.76	0.19	72,72,72,72	0
57	MG	1a	1692	1/1	0.76	0.31	73,73,73,73	0
57	MG	2a	1693	1/1	0.76	0.35	87,87,87,87	0
57	MG	1A	4062	1/1	0.76	0.14	80,80,80,80	0
57	MG	1a	1893	1/1	0.77	0.14	73,73,73,73	0
57	MG	2A	3719	1/1	0.77	0.12	78,78,78,78	0
57	MG	1a	1860	1/1	0.77	0.14	83,83,83,83	0
57	MG	1A	4037	1/1	0.77	0.18	43,43,43,43	0
57	MG	1d	503	1/1	0.77	0.12	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2R	8002	1/1	0.77	0.17	60,60,60,60	0
57	MG	2A	3794	1/1	0.77	0.16	71,71,71,71	0
57	MG	1a	1716	1/1	0.77	0.17	74,74,74,74	0
57	MG	1A	3999	1/1	0.77	0.19	66,66,66,66	0
57	MG	1B	228	1/1	0.77	0.16	69,69,69,69	0
57	MG	2A	3812	1/1	0.77	0.17	80,80,80,80	0
57	MG	2A	3344	1/1	0.77	0.09	85,85,85,85	0
57	MG	1A	3529	1/1	0.77	0.21	62,62,62,62	0
57	MG	2A	3370	1/1	0.77	0.24	63,63,63,63	0
57	MG	1A	3349	1/1	0.77	0.22	59,59,59,59	0
57	MG	2A	3451	1/1	0.77	0.14	78,78,78,78	0
57	MG	2B	3002	1/1	0.77	0.16	81,81,81,81	0
57	MG	1a	1857	1/1	0.77	0.17	74,74,74,74	0
57	MG	1a	1880	1/1	0.77	0.20	72,72,72,72	0
57	MG	2A	3693	1/1	0.77	0.18	75,75,75,75	0
57	MG	2A	3259	1/1	0.78	0.28	83,83,83,83	0
57	MG	1a	1799	1/1	0.78	0.16	70,70,70,70	0
57	MG	1A	4054	1/1	0.78	0.27	79,79,79,79	0
57	MG	2A	3823	1/1	0.78	0.14	51,51,51,51	0
57	MG	1A	3568	1/1	0.78	0.21	57,57,57,57	0
57	MG	1A	3413	1/1	0.78	0.20	84,84,84,84	0
57	MG	1A	3256	1/1	0.78	0.37	65,65,65,65	0
57	MG	2A	3832	1/1	0.78	0.27	67,67,67,67	0
57	MG	2A	3836	1/1	0.78	0.18	72,72,72,72	0
57	MG	1a	1824	1/1	0.78	0.21	74,74,74,74	0
57	MG	1A	3845	1/1	0.78	0.12	23,23,23,23	0
57	MG	1a	1838	1/1	0.78	0.20	71,71,71,71	0
57	MG	2A	3616	1/1	0.78	0.20	82,82,82,82	0
57	MG	1A	3616	1/1	0.78	0.22	72,72,72,72	0
57	MG	2A	3104	1/1	0.78	0.31	73,73,73,73	0
57	MG	1A	3917	1/1	0.78	0.20	67,67,67,67	0
57	MG	2A	3671	1/1	0.78	0.13	65,65,65,65	0
57	MG	2A	3347	1/1	0.78	0.12	72,72,72,72	0
57	MG	1A	3719	1/1	0.78	0.14	66,66,66,66	0
57	MG	2A	3713	1/1	0.78	0.13	68,68,68,68	0
57	MG	1A	3275	1/1	0.78	0.23	61,61,61,61	0
57	MG	1A	3538	1/1	0.78	0.15	68,68,68,68	0
57	MG	1x	3009	1/1	0.78	0.25	76,76,76,76	0
57	MG	1a	1865	1/1	0.78	0.15	85,85,85,85	0
57	MG	1a	1741	1/1	0.78	0.20	83,83,83,83	0
57	MG	1a	1795	1/1	0.78	0.19	71,71,71,71	0
57	MG	1A	3749	1/1	0.78	0.21	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1a	1684	1/1	0.79	0.18	79,79,79,79	0
57	MG	2a	1624	1/1	0.79	0.20	81,81,81,81	0
57	MG	2A	3704	1/1	0.79	0.19	89,89,89,89	0
57	MG	2A	3198	1/1	0.79	0.26	76,76,76,76	0
57	MG	2A	3207	1/1	0.79	0.24	73,73,73,73	0
57	MG	2A	3213	1/1	0.79	0.16	65,65,65,65	0
57	MG	2A	3720	1/1	0.79	0.12	81,81,81,81	0
57	MG	1a	1859	1/1	0.79	0.26	72,72,72,72	0
57	MG	2a	1681	1/1	0.79	0.17	85,85,85,85	0
57	MG	2A	3421	1/1	0.79	0.17	44,44,44,44	0
57	MG	2A	3776	1/1	0.79	0.15	70,70,70,70	0
57	MG	1A	3675	1/1	0.79	0.22	60,60,60,60	0
57	MG	1b	3002	1/1	0.79	0.18	87,87,87,87	0
57	MG	1A	3723	1/1	0.79	0.15	67,67,67,67	0
57	MG	2a	1742	1/1	0.79	0.28	83,83,83,83	0
57	MG	1A	3967	1/1	0.79	0.16	65,65,65,65	0
57	MG	2a	1755	1/1	0.79	0.14	75,75,75,75	0
57	MG	1A	4076	1/1	0.79	0.27	64,64,64,64	0
57	MG	2a	1762	1/1	0.79	0.21	75,75,75,75	0
57	MG	2A	3539	1/1	0.79	0.17	83,83,83,83	0
57	MG	2A	3079	1/1	0.79	0.23	82,82,82,82	0
57	MG	2A	3082	1/1	0.79	0.29	56,56,56,56	0
57	MG	1A	3689	1/1	0.79	0.23	75,75,75,75	0
57	MG	2A	3568	1/1	0.79	0.14	88,88,88,88	0
57	MG	2A	3575	1/1	0.79	0.13	82,82,82,82	0
57	MG	2A	3274	1/1	0.79	0.20	79,79,79,79	0
57	MG	1A	3713	1/1	0.79	0.25	72,72,72,72	0
57	MG	1A	3281	1/1	0.79	0.28	79,79,79,79	0
57	MG	2A	3597	1/1	0.79	0.13	64,64,64,64	0
57	MG	2n	502	1/1	0.79	0.18	84,84,84,84	0
57	MG	1a	1756	1/1	0.79	0.15	72,72,72,72	0
57	MG	2A	3140	1/1	0.79	0.20	72,72,72,72	0
57	MG	2A	3160	1/1	0.79	0.18	85,85,85,85	0
57	MG	2A	3317	1/1	0.79	0.23	71,71,71,71	0
57	MG	1A	3774	1/1	0.79	0.10	49,49,49,49	0
57	MG	1a	1676	1/1	0.79	0.28	76,76,76,76	0
57	MG	2A	3664	1/1	0.79	0.15	69,69,69,69	0
57	MG	2A	3328	1/1	0.79	0.21	82,82,82,82	0
57	MG	2A	3184	1/1	0.79	0.17	68,68,68,68	0
57	MG	2X	3002	1/1	0.79	0.56	78,78,78,78	0
57	MG	2a	1637	1/1	0.80	0.39	67,67,67,67	0
57	MG	2A	3779	1/1	0.80	0.25	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	10	105	1/1	0.80	0.16	66,66,66,66	0
57	MG	15	103	1/1	0.80	0.17	68,68,68,68	0
57	MG	2a	1677	1/1	0.80	0.24	69,69,69,69	0
57	MG	2a	1680	1/1	0.80	0.25	88,88,88,88	0
57	MG	1a	1727	1/1	0.80	0.21	79,79,79,79	0
57	MG	1A	3401	1/1	0.80	0.19	55,55,55,55	0
57	MG	1a	1840	1/1	0.80	0.22	74,74,74,74	0
57	MG	2A	3816	1/1	0.80	0.17	80,80,80,80	0
57	MG	1a	1841	1/1	0.80	0.14	58,58,58,58	0
57	MG	1B	220	1/1	0.80	0.17	63,63,63,63	0
57	MG	1A	3289	1/1	0.80	0.16	60,60,60,60	0
57	MG	2A	3226	1/1	0.80	0.25	73,73,73,73	0
57	MG	2a	1751	1/1	0.80	0.19	77,77,77,77	0
57	MG	2A	3046	1/1	0.80	0.16	57,57,57,57	0
57	MG	2A	3629	1/1	0.80	0.17	64,64,64,64	0
57	MG	2a	1761	1/1	0.80	0.23	86,86,86,86	0
57	MG	2A	3235	1/1	0.80	0.23	79,79,79,79	0
57	MG	2A	3632	1/1	0.80	0.18	70,70,70,70	0
57	MG	2A	3860	1/1	0.80	0.33	64,64,64,64	0
57	MG	1A	3935	1/1	0.80	0.17	57,57,57,57	0
57	MG	2B	3006	1/1	0.80	0.17	84,84,84,84	0
57	MG	2a	1778	1/1	0.80	0.18	91,91,91,91	0
57	MG	2B	3008	1/1	0.80	0.26	70,70,70,70	0
57	MG	1A	3473	1/1	0.80	0.26	62,62,62,62	0
57	MG	2A	3667	1/1	0.80	0.19	63,63,63,63	0
57	MG	2a	1795	1/1	0.80	0.23	83,83,83,83	0
57	MG	1A	4060	1/1	0.80	0.17	69,69,69,69	0
57	MG	2A	3086	1/1	0.80	0.12	73,73,73,73	0
57	MG	2A	3684	1/1	0.80	0.30	82,82,82,82	0
57	MG	2A	3090	1/1	0.80	0.22	89,89,89,89	0
57	MG	1E	306	1/1	0.80	0.22	74,74,74,74	0
57	MG	2A	3493	1/1	0.80	0.15	65,65,65,65	0
57	MG	2x	102	1/1	0.80	0.24	77,77,77,77	0
57	MG	2A	3266	1/1	0.80	0.36	78,78,78,78	0
57	MG	1A	4002	1/1	0.80	0.33	77,77,77,77	0
57	MG	2A	3270	1/1	0.80	0.19	64,64,64,64	0
57	MG	2a	1623	1/1	0.80	0.37	78,78,78,78	0
57	MG	1A	4064	1/1	0.80	0.13	78,78,78,78	0
57	MG	1a	1869	1/1	0.80	0.17	70,70,70,70	0
57	MG	2A	3291	1/1	0.80	0.15	69,69,69,69	0
57	MG	1A	3949	1/1	0.80	0.16	68,68,68,68	0
57	MG	1A	3321	1/1	0.81	0.15	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	3815	1/1	0.81	0.25	72,72,72,72	0
57	MG	1A	3154	1/1	0.81	0.16	59,59,59,59	0
57	MG	2A	3587	1/1	0.81	0.16	64,64,64,64	0
57	MG	1a	1867	1/1	0.81	0.17	80,80,80,80	0
57	MG	1a	1678	1/1	0.81	0.18	62,62,62,62	0
57	MG	2A	3197	1/1	0.81	0.28	71,71,71,71	0
57	MG	1a	1808	1/1	0.81	0.09	86,86,86,86	0
57	MG	2a	1733	1/1	0.81	0.12	82,82,82,82	0
57	MG	2A	3204	1/1	0.81	0.33	75,75,75,75	0
57	MG	2A	3834	1/1	0.81	0.23	68,68,68,68	0
57	MG	1A	3458	1/1	0.81	0.13	47,47,47,47	0
57	MG	2A	3340	1/1	0.81	0.18	77,77,77,77	0
57	MG	1A	3887	1/1	0.81	0.14	58,58,58,58	0
57	MG	1a	1818	1/1	0.81	0.22	74,74,74,74	0
57	MG	1a	1823	1/1	0.81	0.15	72,72,72,72	0
57	MG	2A	3663	1/1	0.81	0.15	53,53,53,53	0
57	MG	2A	3358	1/1	0.81	0.30	50,50,50,50	0
57	MG	2A	3019	1/1	0.81	0.39	75,75,75,75	0
57	MG	1a	1688	1/1	0.81	0.16	76,76,76,76	0
57	MG	1A	4065	1/1	0.81	0.11	66,66,66,66	0
57	MG	2A	3444	1/1	0.81	0.17	71,71,71,71	0
57	MG	1A	3381	1/1	0.81	0.13	68,68,68,68	0
57	MG	2a	1792	1/1	0.81	0.14	75,75,75,75	0
57	MG	1A	3166	1/1	0.81	0.24	70,70,70,70	0
57	MG	1A	4090	1/1	0.81	0.23	52,52,52,52	0
57	MG	2A	3513	1/1	0.81	0.22	68,68,68,68	0
57	MG	2e	3001	1/1	0.81	0.17	81,81,81,81	0
57	MG	1a	1905	1/1	0.81	0.23	75,75,75,75	0
57	MG	1B	202	1/1	0.81	0.17	62,62,62,62	0
57	MG	2a	1607	1/1	0.81	0.28	81,81,81,81	0
57	MG	2a	1617	1/1	0.81	0.14	68,68,68,68	0
57	MG	1B	207	1/1	0.81	0.28	71,71,71,71	0
57	MG	2A	3094	1/1	0.81	0.28	83,83,83,83	0
57	MG	1B	212	1/1	0.81	0.11	69,69,69,69	0
57	MG	1A	3929	1/1	0.81	0.25	85,85,85,85	0
57	MG	2A	3556	1/1	0.81	0.12	56,56,56,56	0
57	MG	1a	1656	1/1	0.81	0.17	69,69,69,69	0
57	MG	2a	1658	1/1	0.81	0.18	82,82,82,82	0
57	MG	1w	104	1/1	0.81	0.12	87,87,87,87	0
57	MG	2A	3574	1/1	0.81	0.22	69,69,69,69	0
57	MG	1A	3500	1/1	0.81	0.15	55,55,55,55	0
57	MG	1A	3267	1/1	0.82	0.16	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	1630	1/1	0.82	0.20	64,64,64,64	0
57	MG	2A	3256	1/1	0.82	0.16	74,74,74,74	0
57	MG	2A	3728	1/1	0.82	0.17	71,71,71,71	0
57	MG	2a	1638	1/1	0.82	0.27	64,64,64,64	0
57	MG	2a	1646	1/1	0.82	0.35	67,67,67,67	0
57	MG	2A	3504	1/1	0.82	0.11	67,67,67,67	0
57	MG	1A	4008	1/1	0.82	0.16	54,54,54,54	0
57	MG	2A	3260	1/1	0.82	0.22	77,77,77,77	0
57	MG	1x	3003	1/1	0.82	0.23	77,77,77,77	0
57	MG	1a	1626	1/1	0.82	0.24	71,71,71,71	0
57	MG	1a	1825	1/1	0.82	0.14	76,76,76,76	0
57	MG	2A	3271	1/1	0.82	0.33	69,69,69,69	0
57	MG	2A	3805	1/1	0.82	0.20	73,73,73,73	0
57	MG	2A	3806	1/1	0.82	0.16	76,76,76,76	0
57	MG	1x	3012	1/1	0.82	0.26	69,69,69,69	0
57	MG	2A	3151	1/1	0.82	0.34	69,69,69,69	0
57	MG	2A	3282	1/1	0.82	0.13	74,74,74,74	0
57	MG	2A	3287	1/1	0.82	0.24	70,70,70,70	0
57	MG	2a	1741	1/1	0.82	0.15	70,70,70,70	0
57	MG	1a	1830	1/1	0.82	0.11	62,62,62,62	0
57	MG	1a	1833	1/1	0.82	0.26	69,69,69,69	0
57	MG	1a	1873	1/1	0.82	0.17	79,79,79,79	0
57	MG	2A	3182	1/1	0.82	0.30	67,67,67,67	0
57	MG	1A	3457	1/1	0.82	0.12	52,52,52,52	0
57	MG	1A	3852	1/1	0.82	0.13	43,43,43,43	0
57	MG	1B	231	1/1	0.82	0.18	70,70,70,70	0
57	MG	1A	3335	1/1	0.82	0.17	55,55,55,55	0
57	MG	2A	3322	1/1	0.82	0.18	71,71,71,71	0
57	MG	1a	1673	1/1	0.82	0.23	78,78,78,78	0
57	MG	2A	3026	1/1	0.82	0.19	63,63,63,63	0
57	MG	2A	3209	1/1	0.82	0.18	70,70,70,70	0
57	MG	2a	1780	1/1	0.82	0.22	65,65,65,65	0
57	MG	1G	3003	1/1	0.82	0.09	71,71,71,71	0
57	MG	1A	4108	1/1	0.82	0.24	76,76,76,76	0
57	MG	2A	3638	1/1	0.82	0.17	77,77,77,77	0
57	MG	2A	3227	1/1	0.82	0.21	69,69,69,69	0
57	MG	2A	3661	1/1	0.82	0.19	84,84,84,84	0
57	MG	2a	1800	1/1	0.82	0.23	68,68,68,68	0
57	MG	2A	3350	1/1	0.82	0.20	76,76,76,76	0
57	MG	2E	303	1/1	0.82	0.31	71,71,71,71	0
57	MG	1A	3417	1/1	0.82	0.13	69,69,69,69	0
57	MG	2A	3234	1/1	0.82	0.41	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	3054	1/1	0.82	0.19	59,59,59,59	0
57	MG	1A	3888	1/1	0.82	0.11	50,50,50,50	0
57	MG	2U	201	1/1	0.82	0.29	59,59,59,59	0
57	MG	2A	3400	1/1	0.82	0.31	57,57,57,57	0
57	MG	2A	3685	1/1	0.82	0.23	75,75,75,75	0
57	MG	29	101	1/1	0.82	0.38	79,79,79,79	0
57	MG	1A	3906	1/1	0.82	0.22	47,47,47,47	0
57	MG	2a	1610	1/1	0.82	0.56	78,78,78,78	0
57	MG	2A	3435	1/1	0.82	0.16	59,59,59,59	0
57	MG	1a	1691	1/1	0.82	0.17	68,68,68,68	0
57	MG	1A	3961	1/1	0.82	0.16	49,49,49,49	0
57	MG	2A	3471	1/1	0.82	0.20	45,45,45,45	0
57	MG	1a	1888	1/1	0.83	0.34	66,66,66,66	0
57	MG	1a	1759	1/1	0.83	0.13	60,60,60,60	0
57	MG	2A	3602	1/1	0.83	0.17	69,69,69,69	0
57	MG	1a	1761	1/1	0.83	0.17	59,59,59,59	0
57	MG	1E	308	1/1	0.83	0.14	73,73,73,73	0
57	MG	1A	3205	1/1	0.83	0.24	76,76,76,76	0
57	MG	1O	3004	1/1	0.83	0.15	73,73,73,73	0
57	MG	1a	1855	1/1	0.83	0.18	80,80,80,80	0
57	MG	2A	3635	1/1	0.83	0.16	82,82,82,82	0
57	MG	2A	3393	1/1	0.83	0.16	69,69,69,69	0
57	MG	2A	3845	1/1	0.83	0.24	69,69,69,69	0
57	MG	1a	1683	1/1	0.83	0.28	86,86,86,86	0
57	MG	1r	3001	1/1	0.83	0.26	66,66,66,66	0
57	MG	2A	3662	1/1	0.83	0.16	63,63,63,63	0
57	MG	2a	1748	1/1	0.83	0.15	69,69,69,69	0
57	MG	1A	3822	1/1	0.83	0.10	40,40,40,40	0
57	MG	1A	3912	1/1	0.83	0.12	56,56,56,56	0
57	MG	1a	1861	1/1	0.83	0.20	57,57,57,57	0
57	MG	2A	3447	1/1	0.83	0.29	62,62,62,62	0
57	MG	2A	3111	1/1	0.83	0.18	86,86,86,86	0
57	MG	1B	203	1/1	0.83	0.09	51,51,51,51	0
57	MG	2a	1765	1/1	0.83	0.25	75,75,75,75	0
57	MG	2a	1766	1/1	0.83	0.24	69,69,69,69	0
57	MG	1A	3973	1/1	0.83	0.11	72,72,72,72	0
57	MG	2A	3159	1/1	0.83	0.17	86,86,86,86	0
57	MG	1x	3007	1/1	0.83	0.24	72,72,72,72	0
57	MG	2A	3708	1/1	0.83	0.13	81,81,81,81	0
57	MG	1A	3829	1/1	0.83	0.15	56,56,56,56	0
57	MG	1A	3217	1/1	0.83	0.17	46,46,46,46	0
57	MG	2a	1781	1/1	0.83	0.24	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3729	1/1	0.83	0.23	62,62,62,62	0
57	MG	1A	3269	1/1	0.83	0.18	62,62,62,62	0
57	MG	1a	1827	1/1	0.83	0.24	58,58,58,58	0
57	MG	2A	3194	1/1	0.83	0.19	73,73,73,73	0
57	MG	1A	3250	1/1	0.83	0.21	62,62,62,62	0
57	MG	2a	1615	1/1	0.83	0.34	73,73,73,73	0
57	MG	1a	1832	1/1	0.83	0.14	81,81,81,81	0
57	MG	2a	1620	1/1	0.83	0.38	73,73,73,73	0
57	MG	2g	8001	1/1	0.83	0.12	76,76,76,76	0
57	MG	2A	3309	1/1	0.83	0.41	85,85,85,85	0
57	MG	2A	3316	1/1	0.83	0.13	62,62,62,62	0
57	MG	2A	3572	1/1	0.83	0.16	79,79,79,79	0
57	MG	1A	3532	1/1	0.83	0.17	69,69,69,69	0
57	MG	1A	3952	1/1	0.83	0.13	52,52,52,52	0
57	MG	1a	1877	1/1	0.83	0.11	81,81,81,81	0
57	MG	1a	1878	1/1	0.83	0.14	95,95,95,95	0
57	MG	1A	3953	1/1	0.83	0.14	62,62,62,62	0
57	MG	2a	1640	1/1	0.83	0.42	77,77,77,77	0
57	MG	2a	1642	1/1	0.83	0.14	74,74,74,74	0
57	MG	1a	1882	1/1	0.83	0.15	67,67,67,67	0
57	MG	2a	1649	1/1	0.83	0.38	85,85,85,85	0
57	MG	2a	1652	1/1	0.83	0.28	72,72,72,72	0
57	MG	2A	3337	1/1	0.83	0.19	74,74,74,74	0
57	MG	1A	3955	1/1	0.84	0.15	54,54,54,54	0
57	MG	1A	3469	1/1	0.84	0.33	70,70,70,70	0
57	MG	1A	3599	1/1	0.84	0.19	61,61,61,61	0
57	MG	28	102	1/1	0.84	0.23	73,73,73,73	0
57	MG	1a	1689	1/1	0.84	0.31	70,70,70,70	0
57	MG	2A	3299	1/1	0.84	0.17	79,79,79,79	0
57	MG	1A	3962	1/1	0.84	0.14	56,56,56,56	0
57	MG	2A	3622	1/1	0.84	0.15	73,73,73,73	0
57	MG	1A	3601	1/1	0.84	0.21	68,68,68,68	0
57	MG	2a	1618	1/1	0.84	0.37	70,70,70,70	0
57	MG	1A	3787	1/1	0.84	0.10	75,75,75,75	0
57	MG	1a	1710	1/1	0.84	0.34	73,73,73,73	0
57	MG	1A	3608	1/1	0.84	0.18	70,70,70,70	0
57	MG	2A	3314	1/1	0.84	0.20	68,68,68,68	0
57	MG	2A	3315	1/1	0.84	0.26	62,62,62,62	0
57	MG	1A	3292	1/1	0.84	0.15	49,49,49,49	0
57	MG	1A	3654	1/1	0.84	0.12	23,23,23,23	0
57	MG	1a	1731	1/1	0.84	0.23	90,90,90,90	0
57	MG	1A	3987	1/1	0.84	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	3674	1/1	0.84	0.20	61,61,61,61	0
57	MG	1A	3393	1/1	0.84	0.12	55,55,55,55	0
57	MG	1A	3857	1/1	0.84	0.23	43,43,43,43	0
57	MG	1F	306	1/1	0.84	0.17	55,55,55,55	0
57	MG	1A	3865	1/1	0.84	0.12	34,34,34,34	0
57	MG	1a	1892	1/1	0.84	0.19	69,69,69,69	0
57	MG	1A	4000	1/1	0.84	0.25	77,77,77,77	0
57	MG	2a	1666	1/1	0.84	0.20	87,87,87,87	0
57	MG	2A	3348	1/1	0.84	0.10	78,78,78,78	0
57	MG	1P	203	1/1	0.84	0.21	47,47,47,47	0
57	MG	1R	203	1/1	0.84	0.17	46,46,46,46	0
57	MG	1a	1899	1/1	0.84	0.15	73,73,73,73	0
57	MG	2A	3364	1/1	0.84	0.29	58,58,58,58	0
57	MG	2A	3189	1/1	0.84	0.17	70,70,70,70	0
57	MG	2A	3725	1/1	0.84	0.15	58,58,58,58	0
57	MG	2a	1686	1/1	0.84	0.18	65,65,65,65	0
57	MG	2A	3377	1/1	0.84	0.18	79,79,79,79	0
57	MG	2A	3769	1/1	0.84	0.17	83,83,83,83	0
57	MG	2A	3379	1/1	0.84	0.24	58,58,58,58	0
57	MG	2a	1702	1/1	0.84	0.09	73,73,73,73	0
57	MG	2a	1703	1/1	0.84	0.12	67,67,67,67	0
57	MG	2a	1730	1/1	0.84	0.24	72,72,72,72	0
57	MG	2A	3385	1/1	0.84	0.25	69,69,69,69	0
57	MG	2A	3388	1/1	0.84	0.28	67,67,67,67	0
57	MG	1a	1903	1/1	0.84	0.44	77,77,77,77	0
57	MG	2A	3789	1/1	0.84	0.09	68,68,68,68	0
57	MG	2A	3790	1/1	0.84	0.12	58,58,58,58	0
57	MG	1S	3001	1/1	0.84	0.28	57,57,57,57	0
57	MG	2A	3796	1/1	0.84	0.13	72,72,72,72	0
57	MG	1A	3318	1/1	0.84	0.18	45,45,45,45	0
57	MG	1A	3691	1/1	0.84	0.10	44,44,44,44	0
57	MG	1A	3709	1/1	0.84	0.24	56,56,56,56	0
57	MG	1a	1816	1/1	0.84	0.15	84,84,84,84	0
57	MG	1s	3001	1/1	0.84	0.20	71,71,71,71	0
57	MG	2a	1767	1/1	0.84	0.16	76,76,76,76	0
57	MG	2A	3449	1/1	0.84	0.20	54,54,54,54	0
57	MG	2A	3219	1/1	0.84	0.18	67,67,67,67	0
57	MG	1Z	303	1/1	0.84	0.08	74,74,74,74	0
57	MG	1A	3712	1/1	0.84	0.12	48,48,48,48	0
57	MG	11	102	1/1	0.84	0.14	76,76,76,76	0
57	MG	1A	3521	1/1	0.84	0.12	34,34,34,34	0
57	MG	1A	3526	1/1	0.84	0.13	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	4043	1/1	0.84	0.19	63,63,63,63	0
57	MG	1A	4053	1/1	0.84	0.19	64,64,64,64	0
57	MG	1a	1642	1/1	0.84	0.33	70,70,70,70	0
57	MG	2A	3533	1/1	0.84	0.13	48,48,48,48	0
57	MG	2A	3839	1/1	0.84	0.55	66,66,66,66	0
57	MG	2a	1798	1/1	0.84	0.20	69,69,69,69	0
57	MG	1a	1651	1/1	0.84	0.13	76,76,76,76	0
57	MG	2A	3252	1/1	0.84	0.24	70,70,70,70	0
57	MG	1A	3447	1/1	0.84	0.18	82,82,82,82	0
57	MG	2A	3254	1/1	0.84	0.14	69,69,69,69	0
57	MG	2A	3557	1/1	0.84	0.23	57,57,57,57	0
57	MG	1A	3403	1/1	0.84	0.19	63,63,63,63	0
57	MG	2B	3011	1/1	0.84	0.22	80,80,80,80	0
57	MG	2q	203	1/1	0.84	0.14	87,87,87,87	0
57	MG	2r	3001	1/1	0.84	0.26	84,84,84,84	0
57	MG	2A	3561	1/1	0.84	0.11	80,80,80,80	0
57	MG	1A	3931	1/1	0.84	0.20	69,69,69,69	0
57	MG	1a	1668	1/1	0.84	0.39	67,67,67,67	0
57	MG	1A	3202	1/1	0.84	0.49	50,50,50,50	0
57	MG	2A	3001	1/1	0.84	0.34	78,78,78,78	0
57	MG	1A	3044	1/1	0.84	0.23	65,65,65,65	0
57	MG	2E	308	1/1	0.84	0.19	73,73,73,73	0
57	MG	1A	3730	1/1	0.84	0.09	66,66,66,66	0
57	MG	1A	3736	1/1	0.84	0.10	69,69,69,69	0
57	MG	2A	3592	1/1	0.84	0.17	77,77,77,77	0
57	MG	1A	3375	1/1	0.84	0.24	66,66,66,66	0
57	MG	2a	1634	1/1	0.85	0.19	92,92,92,92	0
57	MG	2A	3138	1/1	0.85	0.17	70,70,70,70	0
57	MG	2A	3737	1/1	0.85	0.13	67,67,67,67	0
57	MG	2A	3524	1/1	0.85	0.14	59,59,59,59	0
57	MG	1a	1724	1/1	0.85	0.13	71,71,71,71	0
57	MG	1A	3121	1/1	0.85	0.14	52,52,52,52	0
57	MG	2A	3535	1/1	0.85	0.11	57,57,57,57	0
57	MG	2a	1648	1/1	0.85	0.36	74,74,74,74	0
57	MG	2A	3157	1/1	0.85	0.15	70,70,70,70	0
57	MG	1a	1602	1/1	0.85	0.12	65,65,65,65	0
57	MG	2A	3545	1/1	0.85	0.12	53,53,53,53	0
57	MG	2a	1660	1/1	0.85	0.26	72,72,72,72	0
57	MG	1a	1851	1/1	0.85	0.10	73,73,73,73	0
57	MG	1a	1607	1/1	0.85	0.11	69,69,69,69	0
57	MG	1B	219	1/1	0.85	0.12	60,60,60,60	0
57	MG	2A	3799	1/1	0.85	0.11	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3179	1/1	0.85	0.24	79,79,79,79	0
57	MG	1w	105	1/1	0.85	0.19	69,69,69,69	0
57	MG	2A	3313	1/1	0.85	0.22	75,75,75,75	0
57	MG	1A	4032	1/1	0.85	0.13	71,71,71,71	0
57	MG	2A	3573	1/1	0.85	0.14	67,67,67,67	0
57	MG	1x	3001	1/1	0.85	0.35	74,74,74,74	0
57	MG	1a	1758	1/1	0.85	0.13	85,85,85,85	0
57	MG	1A	3194	1/1	0.85	0.19	61,61,61,61	0
57	MG	1a	1650	1/1	0.85	0.25	69,69,69,69	0
57	MG	1a	1774	1/1	0.85	0.12	78,78,78,78	0
57	MG	2A	3588	1/1	0.85	0.16	67,67,67,67	0
57	MG	2a	1719	1/1	0.85	0.15	82,82,82,82	0
57	MG	2a	1728	1/1	0.85	0.14	65,65,65,65	0
57	MG	2A	3591	1/1	0.85	0.13	76,76,76,76	0
57	MG	1A	4036	1/1	0.85	0.12	51,51,51,51	0
57	MG	2A	3206	1/1	0.85	0.22	72,72,72,72	0
57	MG	1A	3635	1/1	0.85	0.13	56,56,56,56	0
57	MG	1A	3344	1/1	0.85	0.21	64,64,64,64	0
57	MG	2A	3599	1/1	0.85	0.11	57,57,57,57	0
57	MG	1a	1659	1/1	0.85	0.26	85,85,85,85	0
57	MG	2a	1752	1/1	0.85	0.26	74,74,74,74	0
57	MG	1A	3734	1/1	0.85	0.16	64,64,64,64	0
57	MG	2a	1756	1/1	0.85	0.23	72,72,72,72	0
57	MG	2A	3606	1/1	0.85	0.21	53,53,53,53	0
57	MG	1A	3451	1/1	0.85	0.24	66,66,66,66	0
57	MG	1A	3395	1/1	0.85	0.17	66,66,66,66	0
57	MG	1A	4056	1/1	0.85	0.16	53,53,53,53	0
57	MG	2A	3233	1/1	0.85	0.33	75,75,75,75	0
57	MG	1A	3262	1/1	0.85	0.19	54,54,54,54	0
57	MG	2B	3014	1/1	0.85	0.23	74,74,74,74	0
57	MG	1a	1817	1/1	0.85	0.17	65,65,65,65	0
57	MG	2B	3018	1/1	0.85	0.11	80,80,80,80	0
57	MG	1A	3206	1/1	0.85	0.18	32,32,32,32	0
57	MG	2A	3240	1/1	0.85	0.22	69,69,69,69	0
57	MG	2A	3037	1/1	0.85	0.22	75,75,75,75	0
57	MG	1a	1879	1/1	0.85	0.10	89,89,89,89	0
57	MG	2a	1782	1/1	0.85	0.23	84,84,84,84	0
57	MG	2a	1785	1/1	0.85	0.21	73,73,73,73	0
57	MG	2F	303	1/1	0.85	0.21	78,78,78,78	0
57	MG	2a	1788	1/1	0.85	0.20	76,76,76,76	0
57	MG	2a	1790	1/1	0.85	0.21	74,74,74,74	0
57	MG	1a	1822	1/1	0.85	0.22	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3251	1/1	0.85	0.15	75,75,75,75	0
57	MG	1A	3918	1/1	0.85	0.13	65,65,65,65	0
57	MG	1A	3703	1/1	0.85	0.10	43,43,43,43	0
57	MG	2A	3668	1/1	0.85	0.27	50,50,50,50	0
57	MG	2U	202	1/1	0.85	0.20	65,65,65,65	0
57	MG	2U	203	1/1	0.85	0.33	67,67,67,67	0
57	MG	2d	502	1/1	0.85	0.08	75,75,75,75	0
57	MG	1A	3195	1/1	0.85	0.30	67,67,67,67	0
57	MG	1A	4073	1/1	0.85	0.16	63,63,63,63	0
57	MG	1T	202	1/1	0.85	0.24	70,70,70,70	0
57	MG	1A	3793	1/1	0.85	0.18	55,55,55,55	0
57	MG	2j	8002	1/1	0.85	0.08	79,79,79,79	0
57	MG	2A	3689	1/1	0.85	0.17	72,72,72,72	0
57	MG	2a	1609	1/1	0.85	0.22	68,68,68,68	0
57	MG	1A	3596	1/1	0.85	0.14	44,44,44,44	0
57	MG	2a	1614	1/1	0.85	0.11	70,70,70,70	0
57	MG	1A	3944	1/1	0.85	0.11	62,62,62,62	0
57	MG	1A	3368	1/1	0.85	0.11	51,51,51,51	0
57	MG	1a	1908	1/1	0.85	0.16	75,75,75,75	0
57	MG	2A	3486	1/1	0.85	0.19	81,81,81,81	0
57	MG	2a	1621	1/1	0.85	0.24	64,64,64,64	0
57	MG	1A	3319	1/1	0.85	0.17	53,53,53,53	0
57	MG	1A	3374	1/1	0.85	0.13	68,68,68,68	0
57	MG	2A	3721	1/1	0.85	0.11	62,62,62,62	0
57	MG	2A	3277	1/1	0.85	0.34	67,67,67,67	0
57	MG	2A	3279	1/1	0.85	0.18	67,67,67,67	0
57	MG	1A	4057	1/1	0.86	0.12	73,73,73,73	0
57	MG	2A	3686	1/1	0.86	0.10	62,62,62,62	0
57	MG	2a	1626	1/1	0.86	0.32	74,74,74,74	0
57	MG	1A	3263	1/1	0.86	0.20	61,61,61,61	0
57	MG	2A	3085	1/1	0.86	0.23	70,70,70,70	0
57	MG	2A	3701	1/1	0.86	0.10	61,61,61,61	0
57	MG	1A	3979	1/1	0.86	0.10	53,53,53,53	0
57	MG	1A	3652	1/1	0.86	0.12	37,37,37,37	0
57	MG	1A	3747	1/1	0.86	0.17	43,43,43,43	0
57	MG	2A	3093	1/1	0.86	0.17	71,71,71,71	0
57	MG	1A	4070	1/1	0.86	0.15	66,66,66,66	0
57	MG	1A	3020	1/1	0.86	0.13	45,45,45,45	0
57	MG	2A	3497	1/1	0.86	0.25	63,63,63,63	0
57	MG	1A	3246	1/1	0.86	0.29	63,63,63,63	0
57	MG	2A	3512	1/1	0.86	0.18	71,71,71,71	0
57	MG	1A	4075	1/1	0.86	0.43	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	3732	1/1	0.86	0.09	59,59,59,59	0
57	MG	2A	3515	1/1	0.86	0.10	37,37,37,37	0
57	MG	2a	1662	1/1	0.86	0.19	66,66,66,66	0
57	MG	2A	3516	1/1	0.86	0.14	70,70,70,70	0
57	MG	2A	3110	1/1	0.86	0.12	54,54,54,54	0
57	MG	2A	3275	1/1	0.86	0.18	75,75,75,75	0
57	MG	2a	1670	1/1	0.86	0.35	62,62,62,62	0
57	MG	2a	1672	1/1	0.86	0.33	74,74,74,74	0
57	MG	1A	3764	1/1	0.86	0.09	23,23,23,23	0
57	MG	2A	3135	1/1	0.86	0.27	63,63,63,63	0
57	MG	1A	3765	1/1	0.86	0.11	65,65,65,65	0
57	MG	2A	3534	1/1	0.86	0.19	72,72,72,72	0
57	MG	1A	3025	1/1	0.86	0.09	46,46,46,46	0
57	MG	1A	3553	1/1	0.86	0.11	44,44,44,44	0
57	MG	1w	102	1/1	0.86	0.31	73,73,73,73	0
57	MG	2A	3543	1/1	0.86	0.22	68,68,68,68	0
57	MG	1A	3280	1/1	0.86	0.18	57,57,57,57	0
57	MG	1B	206	1/1	0.86	0.20	74,74,74,74	0
57	MG	1A	3029	1/1	0.86	0.15	61,61,61,61	0
57	MG	1a	1635	1/1	0.86	0.14	64,64,64,64	0
57	MG	2a	1709	1/1	0.86	0.11	69,69,69,69	0
57	MG	2A	3303	1/1	0.86	0.27	77,77,77,77	0
57	MG	1A	3594	1/1	0.86	0.13	35,35,35,35	0
57	MG	1a	1863	1/1	0.86	0.24	73,73,73,73	0
57	MG	1A	4024	1/1	0.86	0.09	60,60,60,60	0
57	MG	1a	1782	1/1	0.86	0.16	77,77,77,77	0
57	MG	2A	3188	1/1	0.86	0.22	73,73,73,73	0
57	MG	1a	1786	1/1	0.86	0.14	62,62,62,62	0
57	MG	1a	1791	1/1	0.86	0.12	82,82,82,82	0
57	MG	1A	4031	1/1	0.86	0.19	67,67,67,67	0
57	MG	1A	3355	1/1	0.86	0.10	60,60,60,60	0
57	MG	1B	224	1/1	0.86	0.19	71,71,71,71	0
57	MG	2A	3590	1/1	0.86	0.12	70,70,70,70	0
57	MG	1A	3260	1/1	0.86	0.11	55,55,55,55	0
57	MG	2A	3329	1/1	0.86	0.10	67,67,67,67	0
57	MG	1A	3290	1/1	0.86	0.13	63,63,63,63	0
57	MG	1a	1666	1/1	0.86	0.32	73,73,73,73	0
57	MG	2B	3003	1/1	0.86	0.32	73,73,73,73	0
57	MG	2A	3339	1/1	0.86	0.14	73,73,73,73	0
57	MG	1A	3365	1/1	0.86	0.11	59,59,59,59	0
57	MG	2A	3214	1/1	0.86	0.14	56,56,56,56	0
57	MG	2a	1772	1/1	0.86	0.24	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3291	1/1	0.86	0.25	61,61,61,61	0
57	MG	2A	3224	1/1	0.86	0.34	72,72,72,72	0
57	MG	1A	3215	1/1	0.86	0.25	66,66,66,66	0
57	MG	2A	3025	1/1	0.86	0.13	53,53,53,53	0
57	MG	2A	3621	1/1	0.86	0.19	86,86,86,86	0
57	MG	1A	3965	1/1	0.86	0.20	59,59,59,59	0
57	MG	2A	3036	1/1	0.86	0.28	72,72,72,72	0
57	MG	1A	3623	1/1	0.86	0.12	63,63,63,63	0
57	MG	2E	304	1/1	0.86	0.16	69,69,69,69	0
57	MG	2A	3371	1/1	0.86	0.27	70,70,70,70	0
57	MG	2E	310	1/1	0.86	0.12	43,43,43,43	0
57	MG	1a	1681	1/1	0.86	0.25	64,64,64,64	0
57	MG	1a	1885	1/1	0.86	0.17	71,71,71,71	0
57	MG	2A	3641	1/1	0.86	0.13	69,69,69,69	0
57	MG	2A	3644	1/1	0.86	0.15	82,82,82,82	0
57	MG	2A	3646	1/1	0.86	0.23	78,78,78,78	0
57	MG	2A	3047	1/1	0.86	0.23	64,64,64,64	0
57	MG	2A	3651	1/1	0.86	0.12	75,75,75,75	0
57	MG	2A	3657	1/1	0.86	0.17	70,70,70,70	0
57	MG	2W	3001	1/1	0.86	0.13	62,62,62,62	0
57	MG	2X	3001	1/1	0.86	0.17	86,86,86,86	0
57	MG	2A	3659	1/1	0.86	0.15	74,74,74,74	0
57	MG	2A	3660	1/1	0.86	0.14	69,69,69,69	0
57	MG	2l	202	1/1	0.86	0.21	62,62,62,62	0
57	MG	21	101	1/1	0.86	0.18	73,73,73,73	0
57	MG	1A	4055	1/1	0.86	0.15	72,72,72,72	0
57	MG	28	103	1/1	0.86	0.26	65,65,65,65	0
57	MG	2A	3389	1/1	0.86	0.22	54,54,54,54	0
57	MG	2a	1603	1/1	0.86	0.17	64,64,64,64	0
57	MG	2A	3053	1/1	0.86	0.19	75,75,75,75	0
57	MG	2A	3247	1/1	0.86	0.24	62,62,62,62	0
57	MG	2A	3666	1/1	0.86	0.12	46,46,46,46	0
57	MG	2A	3398	1/1	0.86	0.16	58,58,58,58	0
57	MG	1A	3632	1/1	0.86	0.16	66,66,66,66	0
57	MG	2A	3407	1/1	0.86	0.23	75,75,75,75	0
57	MG	2A	3416	1/1	0.86	0.17	70,70,70,70	0
57	MG	2A	3677	1/1	0.86	0.15	64,64,64,64	0
57	MG	2A	3077	1/1	0.86	0.25	71,71,71,71	0
57	MG	2a	1633	1/1	0.87	0.17	78,78,78,78	0
57	MG	2A	3747	1/1	0.87	0.15	45,45,45,45	0
57	MG	2A	3766	1/1	0.87	0.14	67,67,67,67	0
57	MG	2A	3311	1/1	0.87	0.17	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3827	1/1	0.87	0.15	45,45,45,45	0
57	MG	2A	3013	1/1	0.87	0.22	62,62,62,62	0
57	MG	2A	3777	1/1	0.87	0.14	69,69,69,69	0
57	MG	19	101	1/1	0.87	0.12	52,52,52,52	0
57	MG	1a	1826	1/1	0.87	0.22	60,60,60,60	0
57	MG	1A	3345	1/1	0.87	0.15	72,72,72,72	0
57	MG	2a	1650	1/1	0.87	0.20	76,76,76,76	0
57	MG	2A	3319	1/1	0.87	0.27	70,70,70,70	0
57	MG	2a	1653	1/1	0.87	0.30	75,75,75,75	0
57	MG	2A	3201	1/1	0.87	0.19	54,54,54,54	0
57	MG	1a	1605	1/1	0.87	0.17	66,66,66,66	0
57	MG	2A	3325	1/1	0.87	0.12	74,74,74,74	0
57	MG	2A	3031	1/1	0.87	0.18	62,62,62,62	0
57	MG	2A	3800	1/1	0.87	0.22	68,68,68,68	0
57	MG	2A	3034	1/1	0.87	0.21	69,69,69,69	0
57	MG	1A	3990	1/1	0.87	0.21	63,63,63,63	0
57	MG	2A	3583	1/1	0.87	0.10	68,68,68,68	0
57	MG	2A	3585	1/1	0.87	0.19	71,71,71,71	0
57	MG	2A	3809	1/1	0.87	0.13	73,73,73,73	0
57	MG	2A	3811	1/1	0.87	0.23	76,76,76,76	0
57	MG	2A	3211	1/1	0.87	0.24	71,71,71,71	0
57	MG	2A	3212	1/1	0.87	0.24	49,49,49,49	0
57	MG	1A	3735	1/1	0.87	0.22	36,36,36,36	0
57	MG	2a	1685	1/1	0.87	0.13	67,67,67,67	0
57	MG	1a	1623	1/1	0.87	0.27	64,64,64,64	0
57	MG	1a	1725	1/1	0.87	0.16	62,62,62,62	0
57	MG	1A	3997	1/1	0.87	0.22	61,61,61,61	0
57	MG	2A	3596	1/1	0.87	0.14	68,68,68,68	0
57	MG	2A	3049	1/1	0.87	0.22	75,75,75,75	0
57	MG	1a	1631	1/1	0.87	0.23	63,63,63,63	0
57	MG	2a	1705	1/1	0.87	0.11	75,75,75,75	0
57	MG	1A	3232	1/1	0.87	0.16	64,64,64,64	0
57	MG	2a	1713	1/1	0.87	0.12	74,74,74,74	0
57	MG	2a	1717	1/1	0.87	0.15	85,85,85,85	0
57	MG	1a	1911	1/1	0.87	0.10	79,79,79,79	0
57	MG	2a	1722	1/1	0.87	0.15	87,87,87,87	0
57	MG	2A	3062	1/1	0.87	0.36	64,64,64,64	0
57	MG	2a	1729	1/1	0.87	0.12	71,71,71,71	0
57	MG	2A	3605	1/1	0.87	0.12	66,66,66,66	0
57	MG	2A	3366	1/1	0.87	0.18	49,49,49,49	0
57	MG	1A	3295	1/1	0.87	0.19	54,54,54,54	0
57	MG	1B	234	1/1	0.87	0.20	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2a	1746	1/1	0.87	0.17	70,70,70,70	0
57	MG	1e	202	1/1	0.87	0.22	77,77,77,77	0
57	MG	2B	3005	1/1	0.87	0.11	76,76,76,76	0
57	MG	1A	3245	1/1	0.87	0.17	60,60,60,60	0
57	MG	1A	3751	1/1	0.87	0.17	64,64,64,64	0
57	MG	2B	3009	1/1	0.87	0.22	75,75,75,75	0
57	MG	2A	3246	1/1	0.87	0.18	63,63,63,63	0
57	MG	1A	4003	1/1	0.87	0.14	58,58,58,58	0
57	MG	1t	3001	1/1	0.87	0.28	67,67,67,67	0
57	MG	2A	3394	1/1	0.87	0.15	46,46,46,46	0
57	MG	2a	1764	1/1	0.87	0.22	65,65,65,65	0
57	MG	1A	3539	1/1	0.87	0.14	61,61,61,61	0
57	MG	1a	1660	1/1	0.87	0.18	73,73,73,73	0
57	MG	1I	3001	1/1	0.87	0.18	80,80,80,80	0
57	MG	1A	3199	1/1	0.87	0.18	70,70,70,70	0
57	MG	2A	3255	1/1	0.87	0.21	58,58,58,58	0
57	MG	2A	3103	1/1	0.87	0.19	70,70,70,70	0
57	MG	2A	3425	1/1	0.87	0.14	61,61,61,61	0
57	MG	2A	3433	1/1	0.87	0.13	67,67,67,67	0
57	MG	1a	1794	1/1	0.87	0.12	79,79,79,79	0
57	MG	2A	3436	1/1	0.87	0.11	49,49,49,49	0
57	MG	2A	3107	1/1	0.87	0.18	59,59,59,59	0
57	MG	1A	3498	1/1	0.87	0.09	48,48,48,48	0
57	MG	2A	3665	1/1	0.87	0.14	66,66,66,66	0
57	MG	1A	4029	1/1	0.87	0.15	58,58,58,58	0
57	MG	2A	3121	1/1	0.87	0.36	80,80,80,80	0
57	MG	1A	3499	1/1	0.87	0.11	24,24,24,24	0
57	MG	1A	3781	1/1	0.87	0.10	26,26,26,26	0
57	MG	1x	3008	1/1	0.87	0.16	81,81,81,81	0
57	MG	1A	4131	1/1	0.87	0.23	36,36,36,36	0
57	MG	2A	3679	1/1	0.87	0.10	66,66,66,66	0
57	MG	20	8002	1/1	0.87	0.12	75,75,75,75	0
57	MG	2a	1799	1/1	0.87	0.48	78,78,78,78	0
57	MG	1A	3165	1/1	0.87	0.15	62,62,62,62	0
57	MG	26	502	1/1	0.87	0.22	73,73,73,73	0
57	MG	1a	1682	1/1	0.87	0.25	65,65,65,65	0
57	MG	2A	3506	1/1	0.87	0.18	63,63,63,63	0
57	MG	2e	3002	1/1	0.87	0.21	76,76,76,76	0
57	MG	2A	3281	1/1	0.87	0.18	69,69,69,69	0
57	MG	1A	3038	1/1	0.87	0.14	52,52,52,52	0
57	MG	2a	1604	1/1	0.87	0.11	75,75,75,75	0
57	MG	2A	3698	1/1	0.87	0.09	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3162	1/1	0.87	0.15	58,58,58,58	0
57	MG	1A	3274	1/1	0.87	0.16	60,60,60,60	0
57	MG	2A	3705	1/1	0.87	0.10	83,83,83,83	0
57	MG	2A	3167	1/1	0.87	0.24	66,66,66,66	0
57	MG	2A	3172	1/1	0.87	0.13	72,72,72,72	0
57	MG	1A	3800	1/1	0.87	0.13	60,60,60,60	0
57	MG	1y	104	1/1	0.87	0.43	79,79,79,79	0
57	MG	1a	1687	1/1	0.87	0.20	68,68,68,68	0
57	MG	2x	105	1/1	0.87	0.26	78,78,78,78	0
57	MG	2y	3001	1/1	0.87	0.21	65,65,65,65	0
57	MG	1A	3680	1/1	0.87	0.11	19,19,19,19	0
57	MG	2A	3304	1/1	0.87	0.28	87,87,87,87	0
57	MG	2A	3536	1/1	0.87	0.22	66,66,66,66	0
57	MG	1A	4044	1/1	0.87	0.15	57,57,57,57	0
57	MG	2A	3306	1/1	0.87	0.14	71,71,71,71	0
57	MG	2A	3187	1/1	0.87	0.22	68,68,68,68	0
57	MG	2a	1632	1/1	0.87	0.17	78,78,78,78	0
57	MG	1A	3745	1/1	0.88	0.17	44,44,44,44	0
57	MG	1a	1805	1/1	0.88	0.10	73,73,73,73	0
57	MG	1A	3978	1/1	0.88	0.17	69,69,69,69	0
57	MG	1a	1810	1/1	0.88	0.12	72,72,72,72	0
57	MG	1a	1890	1/1	0.88	0.11	63,63,63,63	0
57	MG	2A	3782	1/1	0.88	0.12	66,66,66,66	0
57	MG	2A	3785	1/1	0.88	0.14	69,69,69,69	0
57	MG	2a	1644	1/1	0.88	0.18	58,58,58,58	0
57	MG	1a	1811	1/1	0.88	0.10	73,73,73,73	0
57	MG	2a	1647	1/1	0.88	0.22	64,64,64,64	0
57	MG	1a	1667	1/1	0.88	0.27	66,66,66,66	0
57	MG	1A	3185	1/1	0.88	0.23	64,64,64,64	0
57	MG	2A	3056	1/1	0.88	0.10	61,61,61,61	0
57	MG	2A	3058	1/1	0.88	0.27	57,57,57,57	0
57	MG	2A	3232	1/1	0.88	0.18	66,66,66,66	0
57	MG	1A	3411	1/1	0.88	0.24	65,65,65,65	0
57	MG	1N	201	1/1	0.88	0.23	52,52,52,52	0
57	MG	1a	1901	1/1	0.88	0.27	64,64,64,64	0
57	MG	1O	3001	1/1	0.88	0.11	70,70,70,70	0
57	MG	2A	3237	1/1	0.88	0.13	70,70,70,70	0
57	MG	2A	3359	1/1	0.88	0.29	55,55,55,55	0
57	MG	2a	1668	1/1	0.88	0.23	63,63,63,63	0
57	MG	2A	3239	1/1	0.88	0.20	67,67,67,67	0
57	MG	2a	1671	1/1	0.88	0.14	66,66,66,66	0
57	MG	1a	1904	1/1	0.88	0.15	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3242	1/1	0.88	0.15	63,63,63,63	0
57	MG	2a	1676	1/1	0.88	0.21	73,73,73,73	0
57	MG	1A	3879	1/1	0.88	0.12	75,75,75,75	0
57	MG	2a	1679	1/1	0.88	0.18	75,75,75,75	0
57	MG	2A	3817	1/1	0.88	0.09	64,64,64,64	0
57	MG	1A	3091	1/1	0.88	0.12	43,43,43,43	0
57	MG	1A	3257	1/1	0.88	0.19	61,61,61,61	0
57	MG	2A	3380	1/1	0.88	0.33	71,71,71,71	0
57	MG	2A	3604	1/1	0.88	0.11	55,55,55,55	0
57	MG	2A	3826	1/1	0.88	0.12	70,70,70,70	0
57	MG	1A	3700	1/1	0.88	0.14	43,43,43,43	0
57	MG	2A	3387	1/1	0.88	0.15	52,52,52,52	0
57	MG	2A	3248	1/1	0.88	0.17	56,56,56,56	0
57	MG	1A	3097	1/1	0.88	0.17	65,65,65,65	0
57	MG	2A	3838	1/1	0.88	0.18	79,79,79,79	0
57	MG	1A	3261	1/1	0.88	0.10	58,58,58,58	0
57	MG	2A	3099	1/1	0.88	0.32	62,62,62,62	0
57	MG	2A	3844	1/1	0.88	0.22	65,65,65,65	0
57	MG	2A	3395	1/1	0.88	0.24	61,61,61,61	0
57	MG	2A	3850	1/1	0.88	0.35	56,56,56,56	0
57	MG	2a	1721	1/1	0.88	0.13	63,63,63,63	0
57	MG	1a	1686	1/1	0.88	0.29	69,69,69,69	0
57	MG	2A	3862	1/1	0.88	0.18	68,68,68,68	0
57	MG	1A	3598	1/1	0.88	0.11	50,50,50,50	0
57	MG	1A	3276	1/1	0.88	0.36	55,55,55,55	0
57	MG	2B	3004	1/1	0.88	0.28	79,79,79,79	0
57	MG	2A	3401	1/1	0.88	0.22	62,62,62,62	0
57	MG	1A	3928	1/1	0.88	0.22	41,41,41,41	0
57	MG	2B	3007	1/1	0.88	0.12	70,70,70,70	0
57	MG	2a	1747	1/1	0.88	0.14	76,76,76,76	0
57	MG	2A	3409	1/1	0.88	0.09	75,75,75,75	0
57	MG	1a	1837	1/1	0.88	0.31	70,70,70,70	0
57	MG	1A	3783	1/1	0.88	0.16	62,62,62,62	0
57	MG	1A	3501	1/1	0.88	0.12	40,40,40,40	0
57	MG	2A	3656	1/1	0.88	0.09	67,67,67,67	0
57	MG	2A	3432	1/1	0.88	0.12	62,62,62,62	0
57	MG	1A	3788	1/1	0.88	0.19	76,76,76,76	0
57	MG	2B	3016	1/1	0.88	0.14	74,74,74,74	0
57	MG	2B	3017	1/1	0.88	0.12	75,75,75,75	0
57	MG	2A	3269	1/1	0.88	0.36	77,77,77,77	0
57	MG	2B	3020	1/1	0.88	0.28	72,72,72,72	0
57	MG	2B	3021	1/1	0.88	0.16	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	4013	1/1	0.88	0.20	63,63,63,63	0
57	MG	1a	1713	1/1	0.88	0.10	77,77,77,77	0
57	MG	2A	3446	1/1	0.88	0.15	69,69,69,69	0
57	MG	1A	4014	1/1	0.88	0.17	57,57,57,57	0
57	MG	1a	1847	1/1	0.88	0.14	63,63,63,63	0
57	MG	1A	4016	1/1	0.88	0.17	51,51,51,51	0
57	MG	2F	301	1/1	0.88	0.15	57,57,57,57	0
57	MG	2A	3460	1/1	0.88	0.10	55,55,55,55	0
57	MG	1A	3279	1/1	0.88	0.23	65,65,65,65	0
57	MG	2A	3480	1/1	0.88	0.12	44,44,44,44	0
57	MG	1B	208	1/1	0.88	0.17	53,53,53,53	0
57	MG	2A	3675	1/1	0.88	0.26	74,74,74,74	0
57	MG	1a	1616	1/1	0.88	0.10	68,68,68,68	0
57	MG	1A	3797	1/1	0.88	0.10	51,51,51,51	0
57	MG	1A	3519	1/1	0.88	0.09	47,47,47,47	0
57	MG	2A	3290	1/1	0.88	0.19	57,57,57,57	0
57	MG	1A	3806	1/1	0.88	0.09	41,41,41,41	0
57	MG	2A	3509	1/1	0.88	0.14	64,64,64,64	0
57	MG	2A	3690	1/1	0.88	0.09	87,87,87,87	0
57	MG	1A	3248	1/1	0.88	0.12	51,51,51,51	0
57	MG	1a	1632	1/1	0.88	0.17	72,72,72,72	0
57	MG	2A	3514	1/1	0.88	0.17	67,67,67,67	0
57	MG	1A	3449	1/1	0.88	0.30	66,66,66,66	0
57	MG	1a	1641	1/1	0.88	0.23	76,76,76,76	0
57	MG	1A	3450	1/1	0.88	0.21	59,59,59,59	0
57	MG	2a	1601	1/1	0.88	0.23	67,67,67,67	0
57	MG	1A	3398	1/1	0.88	0.11	64,64,64,64	0
57	MG	1A	3839	1/1	0.88	0.12	76,76,76,76	0
57	MG	2A	3717	1/1	0.88	0.14	60,60,60,60	0
57	MG	2A	3718	1/1	0.88	0.21	70,70,70,70	0
57	MG	2l	203	1/1	0.88	0.16	69,69,69,69	0
57	MG	2A	3191	1/1	0.88	0.13	74,74,74,74	0
57	MG	1a	1654	1/1	0.88	0.29	72,72,72,72	0
57	MG	2A	3196	1/1	0.88	0.25	60,60,60,60	0
57	MG	2A	3722	1/1	0.88	0.17	75,75,75,75	0
57	MG	1a	1792	1/1	0.88	0.16	69,69,69,69	0
57	MG	2a	1619	1/1	0.88	0.10	89,89,89,89	0
57	MG	2A	3312	1/1	0.88	0.15	71,71,71,71	0
57	MG	2x	104	1/1	0.88	0.22	77,77,77,77	0
57	MG	1A	3399	1/1	0.88	0.24	44,44,44,44	0
57	MG	1B	233	1/1	0.88	0.12	73,73,73,73	0
57	MG	2A	3203	1/1	0.88	0.28	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1a	1657	1/1	0.88	0.19	61,61,61,61	0
57	MG	2A	3758	1/1	0.88	0.12	77,77,77,77	0
57	MG	1A	3364	1/1	0.88	0.17	66,66,66,66	0
57	MG	2A	3767	1/1	0.88	0.09	95,95,95,95	0
57	MG	2a	1631	1/1	0.88	0.13	75,75,75,75	0
57	MG	1A	3855	1/1	0.88	0.10	27,27,27,27	0
57	MG	1A	3325	1/1	0.89	0.23	47,47,47,47	0
57	MG	1A	3383	1/1	0.89	0.10	53,53,53,53	0
57	MG	1A	4074	1/1	0.89	0.21	67,67,67,67	0
57	MG	2a	1613	1/1	0.89	0.17	63,63,63,63	0
57	MG	2A	3205	1/1	0.89	0.21	66,66,66,66	0
57	MG	1A	3789	1/1	0.89	0.12	49,49,49,49	0
57	MG	2a	1616	1/1	0.89	0.21	71,71,71,71	0
57	MG	1a	1813	1/1	0.89	0.11	72,72,72,72	0
57	MG	1A	3387	1/1	0.89	0.10	63,63,63,63	0
57	MG	1a	1637	1/1	0.89	0.20	64,64,64,64	0
57	MG	2A	3403	1/1	0.89	0.26	63,63,63,63	0
57	MG	1A	4077	1/1	0.89	0.11	51,51,51,51	0
57	MG	2a	1622	1/1	0.89	0.37	63,63,63,63	0
57	MG	1A	3692	1/1	0.89	0.14	46,46,46,46	0
57	MG	1a	1646	1/1	0.89	0.10	70,70,70,70	0
57	MG	2a	1625	1/1	0.89	0.30	67,67,67,67	0
57	MG	2A	3702	1/1	0.89	0.08	57,57,57,57	0
57	MG	1a	1649	1/1	0.89	0.14	75,75,75,75	0
57	MG	2A	3423	1/1	0.89	0.19	77,77,77,77	0
57	MG	1A	4091	1/1	0.89	0.49	50,50,50,50	0
57	MG	2A	3710	1/1	0.89	0.09	82,82,82,82	0
57	MG	1A	4105	1/1	0.89	0.18	61,61,61,61	0
57	MG	1A	3699	1/1	0.89	0.09	31,31,31,31	0
57	MG	2A	3716	1/1	0.89	0.18	79,79,79,79	0
57	MG	2A	3229	1/1	0.89	0.38	63,63,63,63	0
57	MG	2A	3230	1/1	0.89	0.29	67,67,67,67	0
57	MG	2A	3439	1/1	0.89	0.12	55,55,55,55	0
57	MG	1A	4109	1/1	0.89	0.11	62,62,62,62	0
57	MG	1A	3805	1/1	0.89	0.10	61,61,61,61	0
57	MG	1A	3555	1/1	0.89	0.14	26,26,26,26	0
57	MG	1A	3976	1/1	0.89	0.13	65,65,65,65	0
57	MG	1A	3809	1/1	0.89	0.09	23,23,23,23	0
57	MG	2A	3459	1/1	0.89	0.17	58,58,58,58	0
57	MG	1A	3818	1/1	0.89	0.13	72,72,72,72	0
57	MG	2A	3469	1/1	0.89	0.10	49,49,49,49	0
57	MG	1A	3452	1/1	0.89	0.16	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	1B	211	1/1	0.89	0.15	51,51,51,51	0
57	MG	1A	3826	1/1	0.89	0.10	56,56,56,56	0
57	MG	1B	216	1/1	0.89	0.14	51,51,51,51	0
57	MG	2a	1661	1/1	0.89	0.18	71,71,71,71	0
57	MG	1A	3986	1/1	0.89	0.16	68,68,68,68	0
57	MG	1a	1674	1/1	0.89	0.17	69,69,69,69	0
57	MG	1A	3330	1/1	0.89	0.11	50,50,50,50	0
57	MG	1a	1677	1/1	0.89	0.09	69,69,69,69	0
57	MG	1A	3588	1/1	0.89	0.19	62,62,62,62	0
57	MG	2a	1669	1/1	0.89	0.17	69,69,69,69	0
57	MG	1a	1854	1/1	0.89	0.15	68,68,68,68	0
57	MG	1a	1680	1/1	0.89	0.26	61,61,61,61	0
57	MG	2A	3783	1/1	0.89	0.12	73,73,73,73	0
57	MG	1a	1856	1/1	0.89	0.22	68,68,68,68	0
57	MG	2a	1675	1/1	0.89	0.20	76,76,76,76	0
57	MG	1A	3831	1/1	0.89	0.12	48,48,48,48	0
57	MG	1a	1858	1/1	0.89	0.13	57,57,57,57	0
57	MG	2A	3793	1/1	0.89	0.24	79,79,79,79	0
57	MG	1A	3144	1/1	0.89	0.17	72,72,72,72	0
57	MG	2A	3520	1/1	0.89	0.19	62,62,62,62	0
57	MG	1A	3086	1/1	0.89	0.23	49,49,49,49	0
57	MG	2A	3523	1/1	0.89	0.14	49,49,49,49	0
57	MG	1A	3841	1/1	0.89	0.11	57,57,57,57	0
57	MG	2A	3801	1/1	0.89	0.16	69,69,69,69	0
57	MG	2A	3802	1/1	0.89	0.09	68,68,68,68	0
57	MG	2a	1688	1/1	0.89	0.24	62,62,62,62	0
57	MG	2A	3526	1/1	0.89	0.17	69,69,69,69	0
57	MG	2A	3057	1/1	0.89	0.24	66,66,66,66	0
57	MG	2a	1701	1/1	0.89	0.26	76,76,76,76	0
57	MG	1B	230	1/1	0.89	0.11	72,72,72,72	0
57	MG	2A	3060	1/1	0.89	0.16	53,53,53,53	0
57	MG	1A	3843	1/1	0.89	0.11	29,29,29,29	0
57	MG	2A	3065	1/1	0.89	0.13	53,53,53,53	0
57	MG	1A	3039	1/1	0.89	0.24	59,59,59,59	0
57	MG	1A	3848	1/1	0.89	0.08	66,66,66,66	0
57	MG	1A	3050	1/1	0.89	0.14	59,59,59,59	0
57	MG	1A	3111	1/1	0.89	0.11	48,48,48,48	0
57	MG	1A	3409	1/1	0.89	0.15	57,57,57,57	0
57	MG	2a	1727	1/1	0.89	0.09	82,82,82,82	0
57	MG	2A	3555	1/1	0.89	0.17	48,48,48,48	0
57	MG	2A	3087	1/1	0.89	0.12	59,59,59,59	0
57	MG	2A	3089	1/1	0.89	0.15	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1a	1694	1/1	0.89	0.17	63,63,63,63	0
57	MG	1A	3604	1/1	0.89	0.13	58,58,58,58	0
57	MG	2A	3288	1/1	0.89	0.21	70,70,70,70	0
57	MG	1A	3605	1/1	0.89	0.15	55,55,55,55	0
57	MG	1A	3235	1/1	0.89	0.17	55,55,55,55	0
57	MG	1A	3266	1/1	0.89	0.20	60,60,60,60	0
57	MG	1A	3741	1/1	0.89	0.12	70,70,70,70	0
57	MG	1A	3744	1/1	0.89	0.14	56,56,56,56	0
57	MG	1A	3617	1/1	0.89	0.08	55,55,55,55	0
57	MG	2a	1753	1/1	0.89	0.28	64,64,64,64	0
57	MG	1A	3114	1/1	0.89	0.13	41,41,41,41	0
57	MG	1A	3626	1/1	0.89	0.10	20,20,20,20	0
57	MG	2A	3851	1/1	0.89	0.11	36,36,36,36	0
57	MG	2A	3856	1/1	0.89	0.17	49,49,49,49	0
57	MG	1a	1883	1/1	0.89	0.14	69,69,69,69	0
57	MG	1A	3920	1/1	0.89	0.19	50,50,50,50	0
57	MG	2B	3001	1/1	0.89	0.17	80,80,80,80	0
57	MG	2A	3114	1/1	0.89	0.11	63,63,63,63	0
57	MG	2A	3115	1/1	0.89	0.07	63,63,63,63	0
57	MG	2A	3116	1/1	0.89	0.10	75,75,75,75	0
57	MG	2A	3593	1/1	0.89	0.12	65,65,65,65	0
57	MG	2A	3117	1/1	0.89	0.26	54,54,54,54	0
57	MG	1a	1887	1/1	0.89	0.10	76,76,76,76	0
57	MG	2a	1774	1/1	0.89	0.27	68,68,68,68	0
57	MG	1U	202	1/1	0.89	0.11	58,58,58,58	0
57	MG	2A	3136	1/1	0.89	0.24	48,48,48,48	0
57	MG	1a	1751	1/1	0.89	0.16	65,65,65,65	0
57	MG	1A	3629	1/1	0.89	0.07	17,17,17,17	0
57	MG	2A	3143	1/1	0.89	0.29	64,64,64,64	0
57	MG	2a	1783	1/1	0.89	0.19	85,85,85,85	0
57	MG	2A	3144	1/1	0.89	0.28	67,67,67,67	0
57	MG	1A	3115	1/1	0.89	0.17	56,56,56,56	0
57	MG	1A	3273	1/1	0.89	0.27	62,62,62,62	0
57	MG	2a	1789	1/1	0.89	0.25	77,77,77,77	0
57	MG	2A	3614	1/1	0.89	0.17	80,80,80,80	0
57	MG	1a	1760	1/1	0.89	0.17	66,66,66,66	0
57	MG	1A	3084	1/1	0.89	0.26	47,47,47,47	0
57	MG	1a	1900	1/1	0.89	0.12	70,70,70,70	0
57	MG	1a	1765	1/1	0.89	0.12	87,87,87,87	0
57	MG	2A	3623	1/1	0.89	0.15	71,71,71,71	0
57	MG	2A	3165	1/1	0.89	0.15	59,59,59,59	0
57	MG	1A	3766	1/1	0.89	0.11	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3171	1/1	0.89	0.33	63,63,63,63	0
57	MG	2E	309	1/1	0.89	0.13	62,62,62,62	0
57	MG	2A	3634	1/1	0.89	0.10	52,52,52,52	0
57	MG	15	102	1/1	0.89	0.10	66,66,66,66	0
57	MG	1A	3940	1/1	0.89	0.10	56,56,56,56	0
57	MG	1a	1789	1/1	0.89	0.22	67,67,67,67	0
57	MG	2A	3349	1/1	0.89	0.11	74,74,74,74	0
57	MG	2Q	3003	1/1	0.89	0.12	55,55,55,55	0
57	MG	1a	1790	1/1	0.89	0.20	69,69,69,69	0
57	MG	1A	3429	1/1	0.89	0.20	67,67,67,67	0
57	MG	2A	3648	1/1	0.89	0.12	69,69,69,69	0
57	MG	2q	201	1/1	0.89	0.18	64,64,64,64	0
57	MG	1d	502	1/1	0.89	0.23	81,81,81,81	0
57	MG	2A	3655	1/1	0.89	0.11	36,36,36,36	0
57	MG	2t	3001	1/1	0.89	0.17	58,58,58,58	0
57	MG	2A	3186	1/1	0.89	0.13	55,55,55,55	0
57	MG	2v	102	1/1	0.89	0.20	87,87,87,87	0
57	MG	2A	3362	1/1	0.89	0.22	55,55,55,55	0
57	MG	2A	3363	1/1	0.89	0.34	64,64,64,64	0
57	MG	1A	3945	1/1	0.89	0.19	69,69,69,69	0
57	MG	1A	3669	1/1	0.89	0.08	38,38,38,38	0
57	MG	1A	3135	1/1	0.89	0.09	43,43,43,43	0
57	MG	1n	502	1/1	0.89	0.38	66,66,66,66	0
57	MG	28	101	1/1	0.89	0.16	78,78,78,78	0
57	MG	2A	3192	1/1	0.89	0.07	62,62,62,62	0
57	MG	2A	3193	1/1	0.89	0.17	58,58,58,58	0
57	MG	1A	3950	1/1	0.89	0.10	62,62,62,62	0
57	MG	1A	3323	1/1	0.89	0.10	56,56,56,56	0
57	MG	1a	1617	1/1	0.89	0.14	59,59,59,59	0
57	MG	1A	3786	1/1	0.89	0.16	74,74,74,74	0
57	MG	1a	1612	1/1	0.90	0.08	71,71,71,71	0
57	MG	1A	4059	1/1	0.90	0.09	60,60,60,60	0
57	MG	1A	3479	1/1	0.90	0.24	49,49,49,49	0
57	MG	2A	3413	1/1	0.90	0.09	70,70,70,70	0
57	MG	1a	1619	1/1	0.90	0.28	70,70,70,70	0
57	MG	1A	3497	1/1	0.90	0.11	21,21,21,21	0
57	MG	1A	4063	1/1	0.90	0.11	54,54,54,54	0
57	MG	1a	1625	1/1	0.90	0.18	68,68,68,68	0
57	MG	1A	3396	1/1	0.90	0.12	55,55,55,55	0
57	MG	1a	1627	1/1	0.90	0.37	62,62,62,62	0
57	MG	1A	3397	1/1	0.90	0.23	62,62,62,62	0
57	MG	1A	3131	1/1	0.90	0.18	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1a	1634	1/1	0.90	0.12	62,62,62,62	0
57	MG	1A	3336	1/1	0.90	0.35	54,54,54,54	0
57	MG	1a	1636	1/1	0.90	0.29	70,70,70,70	0
57	MG	1A	3506	1/1	0.90	0.09	12,12,12,12	0
57	MG	1A	3513	1/1	0.90	0.17	49,49,49,49	0
57	MG	1A	3400	1/1	0.90	0.32	61,61,61,61	0
57	MG	1a	1829	1/1	0.90	0.16	50,50,50,50	0
57	MG	1A	3337	1/1	0.90	0.17	64,64,64,64	0
57	MG	2A	3464	1/1	0.90	0.17	67,67,67,67	0
57	MG	2A	3729	1/1	0.90	0.16	76,76,76,76	0
57	MG	1a	1831	1/1	0.90	0.16	82,82,82,82	0
57	MG	1a	1647	1/1	0.90	0.18	72,72,72,72	0
57	MG	2A	3742	1/1	0.90	0.10	50,50,50,50	0
57	MG	1A	3402	1/1	0.90	0.13	44,44,44,44	0
57	MG	2A	3481	1/1	0.90	0.09	52,52,52,52	0
57	MG	1A	3693	1/1	0.90	0.10	64,64,64,64	0
57	MG	1A	3963	1/1	0.90	0.08	44,44,44,44	0
57	MG	2A	3487	1/1	0.90	0.10	44,44,44,44	0
57	MG	1a	1653	1/1	0.90	0.11	65,65,65,65	0
57	MG	2a	1655	1/1	0.90	0.18	67,67,67,67	0
57	MG	1A	3105	1/1	0.90	0.20	30,30,30,30	0
57	MG	2a	1659	1/1	0.90	0.20	65,65,65,65	0
57	MG	1A	3045	1/1	0.90	0.14	54,54,54,54	0
57	MG	2A	3505	1/1	0.90	0.10	67,67,67,67	0
57	MG	1A	3970	1/1	0.90	0.14	55,55,55,55	0
57	MG	2a	1664	1/1	0.90	0.28	71,71,71,71	0
57	MG	1A	4110	1/1	0.90	0.12	69,69,69,69	0
57	MG	1A	4116	1/1	0.90	0.32	37,37,37,37	0
57	MG	1a	1845	1/1	0.90	0.15	79,79,79,79	0
57	MG	1a	1846	1/1	0.90	0.14	73,73,73,73	0
57	MG	2A	3257	1/1	0.90	0.14	59,59,59,59	0
57	MG	2A	3791	1/1	0.90	0.18	62,62,62,62	0
57	MG	2A	3792	1/1	0.90	0.17	72,72,72,72	0
57	MG	1A	3702	1/1	0.90	0.18	71,71,71,71	0
57	MG	2A	3064	1/1	0.90	0.10	54,54,54,54	0
57	MG	2A	3262	1/1	0.90	0.16	68,68,68,68	0
57	MG	2A	3265	1/1	0.90	0.17	67,67,67,67	0
57	MG	1A	3824	1/1	0.90	0.07	23,23,23,23	0
57	MG	2A	3070	1/1	0.90	0.15	57,57,57,57	0
57	MG	2A	3071	1/1	0.90	0.14	62,62,62,62	0
57	MG	1A	3258	1/1	0.90	0.32	60,60,60,60	0
57	MG	1A	3704	1/1	0.90	0.15	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3352	1/1	0.90	0.25	39,39,39,39	0
57	MG	2A	3083	1/1	0.90	0.29	63,63,63,63	0
57	MG	1A	3981	1/1	0.90	0.20	60,60,60,60	0
57	MG	1B	209	1/1	0.90	0.13	65,65,65,65	0
57	MG	1A	3287	1/1	0.90	0.11	64,64,64,64	0
57	MG	1A	3148	1/1	0.90	0.28	38,38,38,38	0
57	MG	2a	1691	1/1	0.90	0.28	68,68,68,68	0
57	MG	1A	3834	1/1	0.90	0.11	41,41,41,41	0
57	MG	2a	1696	1/1	0.90	0.22	69,69,69,69	0
57	MG	2A	3283	1/1	0.90	0.14	61,61,61,61	0
57	MG	2A	3284	1/1	0.90	0.14	63,63,63,63	0
57	MG	1A	3838	1/1	0.90	0.11	70,70,70,70	0
57	MG	2A	3822	1/1	0.90	0.14	78,78,78,78	0
57	MG	2a	1708	1/1	0.90	0.07	95,95,95,95	0
57	MG	1A	3042	1/1	0.90	0.20	57,57,57,57	0
57	MG	2a	1711	1/1	0.90	0.15	80,80,80,80	0
57	MG	2a	1712	1/1	0.90	0.12	71,71,71,71	0
57	MG	1A	3989	1/1	0.90	0.23	58,58,58,58	0
57	MG	1A	3426	1/1	0.90	0.12	63,63,63,63	0
57	MG	2A	3292	1/1	0.90	0.24	62,62,62,62	0
57	MG	2A	3828	1/1	0.90	0.22	74,74,74,74	0
57	MG	1A	3991	1/1	0.90	0.11	54,54,54,54	0
57	MG	2a	1725	1/1	0.90	0.19	77,77,77,77	0
57	MG	2A	3297	1/1	0.90	0.22	61,61,61,61	0
57	MG	2A	3298	1/1	0.90	0.22	55,55,55,55	0
57	MG	1A	3994	1/1	0.90	0.10	54,54,54,54	0
57	MG	1A	3099	1/1	0.90	0.11	68,68,68,68	0
57	MG	2a	1731	1/1	0.90	0.12	77,77,77,77	0
57	MG	1A	3578	1/1	0.90	0.14	27,27,27,27	0
57	MG	2A	3582	1/1	0.90	0.16	72,72,72,72	0
57	MG	1A	3725	1/1	0.90	0.15	61,61,61,61	0
57	MG	1A	3850	1/1	0.90	0.12	58,58,58,58	0
57	MG	1A	3728	1/1	0.90	0.12	56,56,56,56	0
57	MG	1E	304	1/1	0.90	0.16	57,57,57,57	0
57	MG	1A	3581	1/1	0.90	0.10	73,73,73,73	0
57	MG	2A	3307	1/1	0.90	0.14	54,54,54,54	0
57	MG	1A	3118	1/1	0.90	0.21	47,47,47,47	0
57	MG	1a	1695	1/1	0.90	0.10	69,69,69,69	0
57	MG	1a	1701	1/1	0.90	0.24	73,73,73,73	0
57	MG	2A	3122	1/1	0.90	0.14	86,86,86,86	0
57	MG	2A	3126	1/1	0.90	0.22	49,49,49,49	0
57	MG	1a	1881	1/1	0.90	0.14	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1a	1702	1/1	0.90	0.12	66,66,66,66	0
57	MG	2A	3600	1/1	0.90	0.18	74,74,74,74	0
57	MG	1F	304	1/1	0.90	0.14	54,54,54,54	0
57	MG	1A	3178	1/1	0.90	0.17	54,54,54,54	0
57	MG	1F	308	1/1	0.90	0.12	57,57,57,57	0
57	MG	1A	3869	1/1	0.90	0.08	44,44,44,44	0
57	MG	1A	3446	1/1	0.90	0.14	67,67,67,67	0
57	MG	2A	3613	1/1	0.90	0.12	76,76,76,76	0
57	MG	1A	3309	1/1	0.90	0.36	39,39,39,39	0
57	MG	1N	202	1/1	0.90	0.10	53,53,53,53	0
57	MG	1A	4017	1/1	0.90	0.09	56,56,56,56	0
57	MG	2A	3617	1/1	0.90	0.14	64,64,64,64	0
57	MG	2a	1779	1/1	0.90	0.16	75,75,75,75	0
57	MG	1A	3179	1/1	0.90	0.15	47,47,47,47	0
57	MG	1a	1732	1/1	0.90	0.15	64,64,64,64	0
57	MG	2A	3338	1/1	0.90	0.21	73,73,73,73	0
57	MG	1a	1734	1/1	0.90	0.11	63,63,63,63	0
57	MG	1A	3237	1/1	0.90	0.15	64,64,64,64	0
57	MG	2A	3342	1/1	0.90	0.15	65,65,65,65	0
57	MG	2A	3343	1/1	0.90	0.11	57,57,57,57	0
57	MG	1A	3900	1/1	0.90	0.13	75,75,75,75	0
57	MG	1A	3270	1/1	0.90	0.14	66,66,66,66	0
57	MG	2A	3173	1/1	0.90	0.18	58,58,58,58	0
57	MG	2A	3177	1/1	0.90	0.28	65,65,65,65	0
57	MG	1S	3002	1/1	0.90	0.15	47,47,47,47	0
57	MG	2O	8001	1/1	0.90	0.14	62,62,62,62	0
57	MG	2A	3352	1/1	0.90	0.15	70,70,70,70	0
57	MG	1A	3907	1/1	0.90	0.07	25,25,25,25	0
57	MG	1a	1909	1/1	0.90	0.27	68,68,68,68	0
57	MG	2a	1801	1/1	0.90	0.16	63,63,63,63	0
57	MG	1A	3382	1/1	0.90	0.16	56,56,56,56	0
57	MG	2T	3002	1/1	0.90	0.11	61,61,61,61	0
57	MG	2A	3361	1/1	0.90	0.24	44,44,44,44	0
57	MG	1A	3180	1/1	0.90	0.24	49,49,49,49	0
57	MG	2f	3002	1/1	0.90	0.10	76,76,76,76	0
57	MG	1U	204	1/1	0.90	0.11	58,58,58,58	0
57	MG	1A	3101	1/1	0.90	0.12	44,44,44,44	0
57	MG	1e	201	1/1	0.90	0.08	75,75,75,75	0
57	MG	1a	1767	1/1	0.90	0.13	78,78,78,78	0
57	MG	1A	4038	1/1	0.90	0.10	59,59,59,59	0
57	MG	1a	1775	1/1	0.90	0.07	72,72,72,72	0
57	MG	1A	3388	1/1	0.90	0.20	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	21	102	1/1	0.90	0.17	63,63,63,63	0
57	MG	23	101	1/1	0.90	0.15	64,64,64,64	0
57	MG	25	103	1/1	0.90	0.12	68,68,68,68	0
57	MG	1A	3760	1/1	0.90	0.14	25,25,25,25	0
57	MG	1A	3927	1/1	0.90	0.33	44,44,44,44	0
57	MG	13	101	1/1	0.90	0.12	76,76,76,76	0
57	MG	1A	4045	1/1	0.90	0.13	72,72,72,72	0
57	MG	2A	3199	1/1	0.90	0.19	62,62,62,62	0
57	MG	2A	3672	1/1	0.90	0.14	66,66,66,66	0
57	MG	1A	4047	1/1	0.90	0.16	62,62,62,62	0
57	MG	1a	1793	1/1	0.90	0.18	61,61,61,61	0
57	MG	1A	3390	1/1	0.90	0.18	56,56,56,56	0
57	MG	2a	1608	1/1	0.90	0.47	77,77,77,77	0
57	MG	1A	3326	1/1	0.90	0.16	64,64,64,64	0
57	MG	1A	3472	1/1	0.90	0.10	50,50,50,50	0
57	MG	2a	1612	1/1	0.90	0.23	65,65,65,65	0
57	MG	1A	3129	1/1	0.90	0.13	46,46,46,46	0
57	MG	2A	3688	1/1	0.90	0.08	61,61,61,61	0
57	MG	1A	3936	1/1	0.90	0.12	60,60,60,60	0
57	MG	1E	309	1/1	0.91	0.34	45,45,45,45	0
57	MG	1A	3531	1/1	0.91	0.11	15,15,15,15	0
57	MG	1A	3332	1/1	0.91	0.13	54,54,54,54	0
57	MG	2A	3166	1/1	0.91	0.18	72,72,72,72	0
57	MG	1A	3040	1/1	0.91	0.11	55,55,55,55	0
57	MG	2A	3795	1/1	0.91	0.17	78,78,78,78	0
57	MG	2A	3168	1/1	0.91	0.25	61,61,61,61	0
57	MG	1A	3676	1/1	0.91	0.14	60,60,60,60	0
57	MG	1A	3679	1/1	0.91	0.16	29,29,29,29	0
57	MG	1A	3448	1/1	0.91	0.33	62,62,62,62	0
57	MG	2A	3562	1/1	0.91	0.28	52,52,52,52	0
57	MG	1x	3002	1/1	0.91	0.14	74,74,74,74	0
57	MG	1A	3681	1/1	0.91	0.08	37,37,37,37	0
57	MG	1A	3939	1/1	0.91	0.09	65,65,65,65	0
57	MG	2A	3321	1/1	0.91	0.17	64,64,64,64	0
57	MG	2A	3181	1/1	0.91	0.18	62,62,62,62	0
57	MG	1A	3544	1/1	0.91	0.10	56,56,56,56	0
57	MG	2A	3326	1/1	0.91	0.23	72,72,72,72	0
57	MG	2A	3580	1/1	0.91	0.10	57,57,57,57	0
57	MG	1A	3174	1/1	0.91	0.19	45,45,45,45	0
57	MG	1P	204	1/1	0.91	0.15	62,62,62,62	0
57	MG	1A	3795	1/1	0.91	0.11	60,60,60,60	0
57	MG	2A	3331	1/1	0.91	0.29	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	3819	1/1	0.91	0.18	57,57,57,57	0
57	MG	2a	1674	1/1	0.91	0.11	69,69,69,69	0
57	MG	1x	3013	1/1	0.91	0.19	77,77,77,77	0
57	MG	1A	3198	1/1	0.91	0.27	41,41,41,41	0
57	MG	1A	3564	1/1	0.91	0.12	29,29,29,29	0
57	MG	2a	1678	1/1	0.91	0.12	76,76,76,76	0
57	MG	1A	3265	1/1	0.91	0.28	56,56,56,56	0
57	MG	1A	3951	1/1	0.91	0.08	31,31,31,31	0
57	MG	1A	3074	1/1	0.91	0.18	47,47,47,47	0
57	MG	1A	3244	1/1	0.91	0.20	52,52,52,52	0
57	MG	1a	1848	1/1	0.91	0.12	82,82,82,82	0
57	MG	1A	3816	1/1	0.91	0.13	60,60,60,60	0
57	MG	1a	1700	1/1	0.91	0.18	67,67,67,67	0
57	MG	1X	3005	1/1	0.91	0.16	52,52,52,52	0
57	MG	1A	3268	1/1	0.91	0.19	51,51,51,51	0
57	MG	2A	3351	1/1	0.91	0.08	73,73,73,73	0
57	MG	2A	3024	1/1	0.91	0.14	63,63,63,63	0
57	MG	2a	1692	1/1	0.91	0.21	51,51,51,51	0
57	MG	1A	3354	1/1	0.91	0.14	71,71,71,71	0
57	MG	2A	3848	1/1	0.91	0.18	70,70,70,70	0
57	MG	2a	1698	1/1	0.91	0.12	68,68,68,68	0
57	MG	1A	3303	1/1	0.91	0.23	47,47,47,47	0
57	MG	1A	3595	1/1	0.91	0.14	52,52,52,52	0
57	MG	1A	4066	1/1	0.91	0.15	54,54,54,54	0
57	MG	1A	3468	1/1	0.91	0.13	36,36,36,36	0
57	MG	1A	3717	1/1	0.91	0.24	58,58,58,58	0
57	MG	2A	3038	1/1	0.91	0.10	63,63,63,63	0
57	MG	2A	3039	1/1	0.91	0.27	68,68,68,68	0
57	MG	2A	3369	1/1	0.91	0.19	65,65,65,65	0
57	MG	1A	3077	1/1	0.91	0.22	39,39,39,39	0
57	MG	2A	3627	1/1	0.91	0.14	45,45,45,45	0
57	MG	2A	3218	1/1	0.91	0.12	62,62,62,62	0
57	MG	18	104	1/1	0.91	0.15	58,58,58,58	0
57	MG	1A	3313	1/1	0.91	0.15	52,52,52,52	0
57	MG	1A	3974	1/1	0.91	0.09	76,76,76,76	0
57	MG	1A	3722	1/1	0.91	0.11	52,52,52,52	0
57	MG	2A	3636	1/1	0.91	0.11	60,60,60,60	0
57	MG	1A	3156	1/1	0.91	0.14	47,47,47,47	0
57	MG	1a	1608	1/1	0.91	0.25	68,68,68,68	0
57	MG	1a	1748	1/1	0.91	0.09	68,68,68,68	0
57	MG	2a	1732	1/1	0.91	0.12	90,90,90,90	0
57	MG	1a	1611	1/1	0.91	0.10	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3977	1/1	0.91	0.13	75,75,75,75	0
57	MG	1a	1614	1/1	0.91	0.15	60,60,60,60	0
57	MG	2a	1744	1/1	0.91	0.17	51,51,51,51	0
57	MG	2A	3649	1/1	0.91	0.07	61,61,61,61	0
57	MG	1A	3143	1/1	0.91	0.13	56,56,56,56	0
57	MG	2A	3063	1/1	0.91	0.17	60,60,60,60	0
57	MG	1A	3603	1/1	0.91	0.11	45,45,45,45	0
57	MG	1A	3207	1/1	0.91	0.10	48,48,48,48	0
57	MG	2A	3402	1/1	0.91	0.13	68,68,68,68	0
57	MG	2E	307	1/1	0.91	0.20	64,64,64,64	0
57	MG	2A	3067	1/1	0.91	0.31	52,52,52,52	0
57	MG	2A	3241	1/1	0.91	0.14	60,60,60,60	0
57	MG	2A	3069	1/1	0.91	0.16	27,27,27,27	0
57	MG	2a	1760	1/1	0.91	0.19	77,77,77,77	0
57	MG	1A	3982	1/1	0.91	0.12	59,59,59,59	0
57	MG	1A	3369	1/1	0.91	0.19	62,62,62,62	0
57	MG	2A	3420	1/1	0.91	0.11	60,60,60,60	0
57	MG	2A	3075	1/1	0.91	0.08	56,56,56,56	0
57	MG	1A	3606	1/1	0.91	0.11	46,46,46,46	0
57	MG	1A	3849	1/1	0.91	0.12	46,46,46,46	0
57	MG	2A	3080	1/1	0.91	0.32	72,72,72,72	0
57	MG	1a	1884	1/1	0.91	0.10	72,72,72,72	0
57	MG	2T	3001	1/1	0.91	0.11	68,68,68,68	0
57	MG	1A	3322	1/1	0.91	0.10	65,65,65,65	0
57	MG	1a	1886	1/1	0.91	0.17	83,83,83,83	0
57	MG	2A	3676	1/1	0.91	0.13	74,74,74,74	0
57	MG	1a	1630	1/1	0.91	0.31	62,62,62,62	0
57	MG	1A	3613	1/1	0.91	0.08	47,47,47,47	0
57	MG	1A	3854	1/1	0.91	0.12	52,52,52,52	0
57	MG	1A	3416	1/1	0.91	0.15	36,36,36,36	0
57	MG	1A	3739	1/1	0.91	0.15	66,66,66,66	0
57	MG	1a	1894	1/1	0.91	0.09	64,64,64,64	0
57	MG	2A	3455	1/1	0.91	0.10	66,66,66,66	0
57	MG	2A	3456	1/1	0.91	0.11	50,50,50,50	0
57	MG	2A	3458	1/1	0.91	0.10	38,38,38,38	0
57	MG	1a	1895	1/1	0.91	0.14	88,88,88,88	0
57	MG	1a	1896	1/1	0.91	0.13	63,63,63,63	0
57	MG	1A	3860	1/1	0.91	0.07	80,80,80,80	0
57	MG	2A	3468	1/1	0.91	0.14	73,73,73,73	0
57	MG	2A	3267	1/1	0.91	0.20	71,71,71,71	0
57	MG	2a	1794	1/1	0.91	0.19	76,76,76,76	0
57	MG	1A	3373	1/1	0.91	0.16	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2a	1796	1/1	0.91	0.12	79,79,79,79	0
57	MG	1A	3742	1/1	0.91	0.06	25,25,25,25	0
57	MG	1A	3871	1/1	0.91	0.11	50,50,50,50	0
57	MG	1A	3208	1/1	0.91	0.14	48,48,48,48	0
57	MG	2A	3715	1/1	0.91	0.11	55,55,55,55	0
57	MG	2A	3272	1/1	0.91	0.22	67,67,67,67	0
57	MG	1A	3209	1/1	0.91	0.14	61,61,61,61	0
57	MG	1A	3211	1/1	0.91	0.09	55,55,55,55	0
57	MG	2A	3494	1/1	0.91	0.20	73,73,73,73	0
57	MG	2A	3496	1/1	0.91	0.11	72,72,72,72	0
57	MG	1A	3186	1/1	0.91	0.10	53,53,53,53	0
57	MG	2A	3500	1/1	0.91	0.25	70,70,70,70	0
57	MG	1B	226	1/1	0.91	0.08	46,46,46,46	0
57	MG	1A	3331	1/1	0.91	0.10	57,57,57,57	0
57	MG	1A	4012	1/1	0.91	0.11	52,52,52,52	0
57	MG	1a	1913	1/1	0.91	0.18	63,63,63,63	0
57	MG	2A	3731	1/1	0.91	0.10	63,63,63,63	0
57	MG	1b	3001	1/1	0.91	0.13	87,87,87,87	0
57	MG	2A	3734	1/1	0.91	0.08	60,60,60,60	0
57	MG	1A	3901	1/1	0.91	0.12	19,19,19,19	0
57	MG	1A	3649	1/1	0.91	0.08	31,31,31,31	0
57	MG	1A	3434	1/1	0.91	0.29	51,51,51,51	0
57	MG	1A	3763	1/1	0.91	0.08	35,35,35,35	0
57	MG	2A	3139	1/1	0.91	0.12	46,46,46,46	0
57	MG	1A	3653	1/1	0.91	0.08	33,33,33,33	0
57	MG	2A	3141	1/1	0.91	0.12	59,59,59,59	0
57	MG	1f	3001	1/1	0.91	0.23	61,61,61,61	0
57	MG	1D	3004	1/1	0.91	0.15	42,42,42,42	0
57	MG	2A	3147	1/1	0.91	0.18	68,68,68,68	0
57	MG	1a	1821	1/1	0.91	0.18	69,69,69,69	0
57	MG	2A	3154	1/1	0.91	0.27	71,71,71,71	0
57	MG	2A	3155	1/1	0.91	0.20	62,62,62,62	0
57	MG	1A	3445	1/1	0.91	0.13	61,61,61,61	0
57	MG	2a	1639	1/1	0.91	0.09	55,55,55,55	0
57	MG	1A	4028	1/1	0.91	0.09	60,60,60,60	0
57	MG	1A	3667	1/1	0.91	0.07	78,78,78,78	0
57	MG	1A	4040	1/1	0.92	0.12	82,82,82,82	0
57	MG	1A	3714	1/1	0.92	0.13	61,61,61,61	0
57	MG	1A	3559	1/1	0.92	0.10	39,39,39,39	0
57	MG	1A	3875	1/1	0.92	0.10	60,60,60,60	0
57	MG	2A	3078	1/1	0.92	0.10	51,51,51,51	0
57	MG	1A	3718	1/1	0.92	0.15	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	4046	1/1	0.92	0.11	70,70,70,70	0
57	MG	2V	202	1/1	0.92	0.14	58,58,58,58	0
57	MG	1A	3563	1/1	0.92	0.07	21,21,21,21	0
57	MG	2A	3603	1/1	0.92	0.14	69,69,69,69	0
57	MG	1a	1629	1/1	0.92	0.24	69,69,69,69	0
57	MG	1A	4051	1/1	0.92	0.11	48,48,48,48	0
57	MG	1A	4052	1/1	0.92	0.11	59,59,59,59	0
57	MG	2A	3609	1/1	0.92	0.15	72,72,72,72	0
57	MG	1A	3430	1/1	0.92	0.17	51,51,51,51	0
57	MG	2A	3308	1/1	0.92	0.12	62,62,62,62	0
57	MG	25	102	1/1	0.92	0.23	58,58,58,58	0
57	MG	1a	1633	1/1	0.92	0.10	66,66,66,66	0
57	MG	1A	3297	1/1	0.92	0.23	44,44,44,44	0
57	MG	1A	3570	1/1	0.92	0.08	31,31,31,31	0
57	MG	1A	3903	1/1	0.92	0.08	49,49,49,49	0
57	MG	1A	3904	1/1	0.92	0.13	66,66,66,66	0
57	MG	1A	3259	1/1	0.92	0.25	59,59,59,59	0
57	MG	1A	3441	1/1	0.92	0.20	59,59,59,59	0
57	MG	1a	1644	1/1	0.92	0.13	74,74,74,74	0
57	MG	2A	3102	1/1	0.92	0.22	69,69,69,69	0
57	MG	1A	3726	1/1	0.92	0.20	47,47,47,47	0
57	MG	1A	3914	1/1	0.92	0.11	33,33,33,33	0
57	MG	2A	3106	1/1	0.92	0.15	58,58,58,58	0
57	MG	1A	3210	1/1	0.92	0.20	74,74,74,74	0
57	MG	1A	3310	1/1	0.92	0.15	64,64,64,64	0
57	MG	1A	3590	1/1	0.92	0.08	22,22,22,22	0
57	MG	1A	3593	1/1	0.92	0.08	25,25,25,25	0
57	MG	1A	3063	1/1	0.92	0.43	50,50,50,50	0
57	MG	1A	3316	1/1	0.92	0.12	52,52,52,52	0
57	MG	1A	3212	1/1	0.92	0.08	50,50,50,50	0
57	MG	2A	3334	1/1	0.92	0.28	63,63,63,63	0
57	MG	2A	3336	1/1	0.92	0.24	52,52,52,52	0
57	MG	2A	3652	1/1	0.92	0.32	72,72,72,72	0
57	MG	1A	3092	1/1	0.92	0.18	48,48,48,48	0
57	MG	1A	3117	1/1	0.92	0.11	40,40,40,40	0
57	MG	1A	3743	1/1	0.92	0.11	58,58,58,58	0
57	MG	2A	3130	1/1	0.92	0.25	63,63,63,63	0
57	MG	2A	3341	1/1	0.92	0.21	71,71,71,71	0
57	MG	1a	1874	1/1	0.92	0.19	72,72,72,72	0
57	MG	2a	1627	1/1	0.92	0.28	71,71,71,71	0
57	MG	1a	1664	1/1	0.92	0.28	54,54,54,54	0
57	MG	1A	4080	1/1	0.92	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	1A	4087	1/1	0.92	0.10	59,59,59,59	0
57	MG	1A	3218	1/1	0.92	0.18	49,49,49,49	0
57	MG	1A	3384	1/1	0.92	0.23	44,44,44,44	0
57	MG	1A	3941	1/1	0.92	0.10	50,50,50,50	0
57	MG	1A	4106	1/1	0.92	0.26	67,67,67,67	0
57	MG	2a	1635	1/1	0.92	0.29	60,60,60,60	0
57	MG	1A	3454	1/1	0.92	0.15	67,67,67,67	0
57	MG	2A	3148	1/1	0.92	0.13	62,62,62,62	0
57	MG	2A	3354	1/1	0.92	0.25	71,71,71,71	0
57	MG	2A	3673	1/1	0.92	0.12	62,62,62,62	0
57	MG	2A	3674	1/1	0.92	0.13	63,63,63,63	0
57	MG	1A	3455	1/1	0.92	0.09	50,50,50,50	0
57	MG	2A	3152	1/1	0.92	0.15	59,59,59,59	0
57	MG	1A	3946	1/1	0.92	0.18	64,64,64,64	0
57	MG	2A	3678	1/1	0.92	0.11	54,54,54,54	0
57	MG	1A	3456	1/1	0.92	0.10	37,37,37,37	0
57	MG	1A	4124	1/1	0.92	0.12	37,37,37,37	0
57	MG	2A	3158	1/1	0.92	0.11	63,63,63,63	0
57	MG	1A	3385	1/1	0.92	0.12	53,53,53,53	0
57	MG	2A	3368	1/1	0.92	0.38	66,66,66,66	0
57	MG	1A	3757	1/1	0.92	0.12	46,46,46,46	0
57	MG	1a	1889	1/1	0.92	0.10	75,75,75,75	0
57	MG	2A	3691	1/1	0.92	0.10	64,64,64,64	0
57	MG	1A	3386	1/1	0.92	0.12	55,55,55,55	0
57	MG	2A	3374	1/1	0.92	0.29	64,64,64,64	0
57	MG	1A	3610	1/1	0.92	0.11	59,59,59,59	0
57	MG	1A	3611	1/1	0.92	0.06	44,44,44,44	0
57	MG	1A	3230	1/1	0.92	0.18	48,48,48,48	0
57	MG	2A	3381	1/1	0.92	0.09	53,53,53,53	0
57	MG	1A	3463	1/1	0.92	0.26	58,58,58,58	0
57	MG	2A	3386	1/1	0.92	0.28	56,56,56,56	0
57	MG	1A	3959	1/1	0.92	0.14	61,61,61,61	0
57	MG	1A	3772	1/1	0.92	0.15	45,45,45,45	0
57	MG	1A	3773	1/1	0.92	0.17	61,61,61,61	0
57	MG	1B	218	1/1	0.92	0.12	62,62,62,62	0
57	MG	1A	3465	1/1	0.92	0.34	72,72,72,72	0
57	MG	1A	3964	1/1	0.92	0.15	33,33,33,33	0
57	MG	1a	1902	1/1	0.92	0.13	56,56,56,56	0
57	MG	1a	1699	1/1	0.92	0.18	56,56,56,56	0
57	MG	1B	221	1/1	0.92	0.14	54,54,54,54	0
57	MG	1B	222	1/1	0.92	0.07	57,57,57,57	0
57	MG	1A	3620	1/1	0.92	0.12	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3095	1/1	0.92	0.25	39,39,39,39	0
57	MG	1a	1910	1/1	0.92	0.28	59,59,59,59	0
57	MG	2a	1682	1/1	0.92	0.20	63,63,63,63	0
57	MG	1A	3968	1/1	0.92	0.12	72,72,72,72	0
57	MG	1A	3625	1/1	0.92	0.12	42,42,42,42	0
57	MG	1A	3234	1/1	0.92	0.09	38,38,38,38	0
57	MG	2A	3417	1/1	0.92	0.09	58,58,58,58	0
57	MG	2A	3735	1/1	0.92	0.09	62,62,62,62	0
57	MG	1A	3328	1/1	0.92	0.09	53,53,53,53	0
57	MG	2A	3740	1/1	0.92	0.10	48,48,48,48	0
57	MG	2a	1690	1/1	0.92	0.26	65,65,65,65	0
57	MG	1A	3197	1/1	0.92	0.15	61,61,61,61	0
57	MG	1A	3634	1/1	0.92	0.13	45,45,45,45	0
57	MG	2A	3748	1/1	0.92	0.09	38,38,38,38	0
57	MG	1a	1726	1/1	0.92	0.11	60,60,60,60	0
57	MG	2A	3759	1/1	0.92	0.13	42,42,42,42	0
57	MG	2a	1700	1/1	0.92	0.19	71,71,71,71	0
57	MG	1B	232	1/1	0.92	0.10	57,57,57,57	0
57	MG	1A	3474	1/1	0.92	0.11	42,42,42,42	0
57	MG	2A	3200	1/1	0.92	0.13	66,66,66,66	0
57	MG	2A	3770	1/1	0.92	0.07	78,78,78,78	0
57	MG	1l	8001	1/1	0.92	0.10	84,84,84,84	0
57	MG	2A	3202	1/1	0.92	0.15	61,61,61,61	0
57	MG	2A	3443	1/1	0.92	0.14	62,62,62,62	0
57	MG	1A	3640	1/1	0.92	0.12	64,64,64,64	0
57	MG	1m	201	1/1	0.92	0.18	72,72,72,72	0
57	MG	1D	3002	1/1	0.92	0.12	45,45,45,45	0
57	MG	1A	3796	1/1	0.92	0.11	55,55,55,55	0
57	MG	1a	1740	1/1	0.92	0.22	55,55,55,55	0
57	MG	1A	3980	1/1	0.92	0.09	57,57,57,57	0
57	MG	1a	1746	1/1	0.92	0.13	61,61,61,61	0
57	MG	1w	101	1/1	0.92	0.30	65,65,65,65	0
57	MG	1A	3643	1/1	0.92	0.11	23,23,23,23	0
57	MG	1a	1749	1/1	0.92	0.09	85,85,85,85	0
57	MG	2A	3216	1/1	0.92	0.31	44,44,44,44	0
57	MG	1a	1750	1/1	0.92	0.16	63,63,63,63	0
57	MG	1A	3646	1/1	0.92	0.12	21,21,21,21	0
57	MG	2A	3222	1/1	0.92	0.14	61,61,61,61	0
57	MG	2a	1735	1/1	0.92	0.14	66,66,66,66	0
57	MG	2a	1739	1/1	0.92	0.10	59,59,59,59	0
57	MG	1A	3271	1/1	0.92	0.14	35,35,35,35	0
57	MG	2A	3225	1/1	0.92	0.21	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	1F	301	1/1	0.92	0.12	44,44,44,44	0
57	MG	1A	3163	1/1	0.92	0.09	55,55,55,55	0
57	MG	1A	3334	1/1	0.92	0.12	42,42,42,42	0
57	MG	2A	3492	1/1	0.92	0.11	51,51,51,51	0
57	MG	1x	3004	1/1	0.92	0.19	70,70,70,70	0
57	MG	1x	3005	1/1	0.92	0.28	68,68,68,68	0
57	MG	1A	3241	1/1	0.92	0.09	52,52,52,52	0
57	MG	1A	3817	1/1	0.92	0.08	55,55,55,55	0
57	MG	1A	3657	1/1	0.92	0.08	26,26,26,26	0
57	MG	2A	3502	1/1	0.92	0.23	74,74,74,74	0
57	MG	1a	1773	1/1	0.92	0.11	89,89,89,89	0
57	MG	1A	3664	1/1	0.92	0.09	52,52,52,52	0
57	MG	1A	3242	1/1	0.92	0.15	51,51,51,51	0
57	MG	1A	3243	1/1	0.92	0.07	29,29,29,29	0
57	MG	1O	3002	1/1	0.92	0.16	56,56,56,56	0
57	MG	1A	3338	1/1	0.92	0.10	44,44,44,44	0
57	MG	1A	3034	1/1	0.92	0.09	38,38,38,38	0
57	MG	1A	3200	1/1	0.92	0.16	53,53,53,53	0
57	MG	1Q	203	1/1	0.92	0.21	73,73,73,73	0
57	MG	2A	3827	1/1	0.92	0.09	58,58,58,58	0
57	MG	2A	3518	1/1	0.92	0.26	63,63,63,63	0
57	MG	1Q	204	1/1	0.92	0.12	61,61,61,61	0
57	MG	2A	3830	1/1	0.92	0.11	41,41,41,41	0
57	MG	1A	3832	1/1	0.92	0.08	59,59,59,59	0
57	MG	1A	3127	1/1	0.92	0.28	65,65,65,65	0
57	MG	1A	4001	1/1	0.92	0.11	49,49,49,49	0
57	MG	1A	3412	1/1	0.92	0.26	54,54,54,54	0
57	MG	1A	3076	1/1	0.92	0.09	32,32,32,32	0
57	MG	2A	3842	1/1	0.92	0.23	67,67,67,67	0
57	MG	1A	4005	1/1	0.92	0.09	63,63,63,63	0
57	MG	2a	1784	1/1	0.92	0.14	77,77,77,77	0
57	MG	2A	3530	1/1	0.92	0.19	57,57,57,57	0
57	MG	1A	4006	1/1	0.92	0.10	58,58,58,58	0
57	MG	2A	3030	1/1	0.92	0.17	44,44,44,44	0
57	MG	1a	1807	1/1	0.92	0.07	71,71,71,71	0
57	MG	1A	3528	1/1	0.92	0.11	42,42,42,42	0
57	MG	2A	3853	1/1	0.92	0.10	57,57,57,57	0
57	MG	2A	3854	1/1	0.92	0.16	53,53,53,53	0
57	MG	2A	3035	1/1	0.92	0.17	56,56,56,56	0
57	MG	2A	3540	1/1	0.92	0.13	59,59,59,59	0
57	MG	2A	3861	1/1	0.92	0.12	50,50,50,50	0
57	MG	1A	4009	1/1	0.92	0.10	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3261	1/1	0.92	0.22	59,59,59,59	0
57	MG	2A	3544	1/1	0.92	0.13	42,42,42,42	0
57	MG	1A	4011	1/1	0.92	0.12	58,58,58,58	0
57	MG	2A	3549	1/1	0.92	0.13	52,52,52,52	0
57	MG	1A	3690	1/1	0.92	0.14	62,62,62,62	0
57	MG	1Z	304	1/1	0.92	0.10	58,58,58,58	0
57	MG	2A	3041	1/1	0.92	0.22	67,67,67,67	0
57	MG	2A	3044	1/1	0.92	0.28	49,49,49,49	0
57	MG	1A	3175	1/1	0.92	0.26	49,49,49,49	0
57	MG	1A	3255	1/1	0.92	0.09	40,40,40,40	0
57	MG	1A	3847	1/1	0.92	0.07	36,36,36,36	0
57	MG	2A	3565	1/1	0.92	0.30	69,69,69,69	0
57	MG	2A	3566	1/1	0.92	0.20	51,51,51,51	0
57	MG	1A	3017	1/1	0.92	0.09	56,56,56,56	0
57	MG	2A	3569	1/1	0.92	0.19	68,68,68,68	0
57	MG	2A	3570	1/1	0.92	0.13	55,55,55,55	0
57	MG	2A	3571	1/1	0.92	0.13	77,77,77,77	0
57	MG	2B	3019	1/1	0.92	0.11	85,85,85,85	0
57	MG	2A	3050	1/1	0.92	0.13	59,59,59,59	0
57	MG	1A	3052	1/1	0.92	0.17	34,34,34,34	0
57	MG	1A	3423	1/1	0.92	0.28	54,54,54,54	0
57	MG	1A	4027	1/1	0.92	0.14	55,55,55,55	0
57	MG	1A	3851	1/1	0.92	0.11	46,46,46,46	0
57	MG	1A	3542	1/1	0.92	0.11	44,44,44,44	0
57	MG	1A	3360	1/1	0.92	0.10	58,58,58,58	0
57	MG	1A	3549	1/1	0.92	0.07	24,24,24,24	0
57	MG	1a	1828	1/1	0.92	0.11	69,69,69,69	0
57	MG	2A	3285	1/1	0.92	0.24	66,66,66,66	0
57	MG	1A	4034	1/1	0.92	0.09	34,34,34,34	0
57	MG	1A	3705	1/1	0.92	0.10	48,48,48,48	0
57	MG	2A	3289	1/1	0.92	0.26	81,81,81,81	0
57	MG	1A	3552	1/1	0.92	0.09	59,59,59,59	0
57	MG	1A	3362	1/1	0.92	0.12	54,54,54,54	0
57	MG	2Q	3002	1/1	0.92	0.26	61,61,61,61	0
57	MG	1A	3062	1/1	0.92	0.23	36,36,36,36	0
57	MG	2A	3431	1/1	0.93	0.13	57,57,57,57	0
57	MG	2a	1611	1/1	0.93	0.32	67,67,67,67	0
57	MG	1a	1671	1/1	0.93	0.10	57,57,57,57	0
57	MG	1D	3009	1/1	0.93	0.23	28,28,28,28	0
57	MG	2A	3048	1/1	0.93	0.21	77,77,77,77	0
57	MG	1A	3812	1/1	0.93	0.12	60,60,60,60	0
57	MG	2A	3697	1/1	0.93	0.06	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	1849	1/1	0.93	0.08	95,95,95,95	0
57	MG	1a	1850	1/1	0.93	0.12	76,76,76,76	0
57	MG	1A	3376	1/1	0.93	0.15	62,62,62,62	0
57	MG	1a	1853	1/1	0.93	0.12	63,63,63,63	0
57	MG	1A	3379	1/1	0.93	0.17	49,49,49,49	0
57	MG	1A	3277	1/1	0.93	0.36	43,43,43,43	0
57	MG	1A	3819	1/1	0.93	0.09	48,48,48,48	0
57	MG	2A	3711	1/1	0.93	0.07	59,59,59,59	0
57	MG	2A	3059	1/1	0.93	0.33	68,68,68,68	0
57	MG	1A	3820	1/1	0.93	0.15	63,63,63,63	0
57	MG	1A	3254	1/1	0.93	0.17	41,41,41,41	0
57	MG	1F	307	1/1	0.93	0.15	52,52,52,52	0
57	MG	1A	3164	1/1	0.93	0.21	44,44,44,44	0
57	MG	2A	3461	1/1	0.93	0.09	44,44,44,44	0
57	MG	1G	3002	1/1	0.93	0.22	62,62,62,62	0
57	MG	1A	3621	1/1	0.93	0.07	48,48,48,48	0
57	MG	1A	3070	1/1	0.93	0.18	60,60,60,60	0
57	MG	1A	3533	1/1	0.93	0.10	68,68,68,68	0
57	MG	1A	3228	1/1	0.93	0.09	48,48,48,48	0
57	MG	2A	3074	1/1	0.93	0.15	67,67,67,67	0
57	MG	1A	4049	1/1	0.93	0.07	42,42,42,42	0
57	MG	1A	3108	1/1	0.93	0.12	46,46,46,46	0
57	MG	1a	1693	1/1	0.93	0.13	58,58,58,58	0
57	MG	2A	3490	1/1	0.93	0.10	49,49,49,49	0
57	MG	2a	1641	1/1	0.93	0.23	62,62,62,62	0
57	MG	2A	3733	1/1	0.93	0.10	65,65,65,65	0
57	MG	2A	3491	1/1	0.93	0.14	58,58,58,58	0
57	MG	2A	3263	1/1	0.93	0.11	50,50,50,50	0
57	MG	2A	3264	1/1	0.93	0.10	60,60,60,60	0
57	MG	2A	3738	1/1	0.93	0.08	45,45,45,45	0
57	MG	1O	3003	1/1	0.93	0.08	71,71,71,71	0
57	MG	1A	3960	1/1	0.93	0.15	47,47,47,47	0
57	MG	2A	3746	1/1	0.93	0.06	79,79,79,79	0
57	MG	1a	1698	1/1	0.93	0.19	66,66,66,66	0
57	MG	2a	1654	1/1	0.93	0.10	71,71,71,71	0
57	MG	2A	3499	1/1	0.93	0.17	61,61,61,61	0
57	MG	2a	1657	1/1	0.93	0.33	64,64,64,64	0
57	MG	2A	3750	1/1	0.93	0.07	48,48,48,48	0
57	MG	1P	201	1/1	0.93	0.15	34,34,34,34	0
57	MG	1A	3231	1/1	0.93	0.13	70,70,70,70	0
57	MG	2A	3761	1/1	0.93	0.09	41,41,41,41	0
57	MG	2A	3765	1/1	0.93	0.07	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3170	1/1	0.93	0.13	59,59,59,59	0
57	MG	1A	3546	1/1	0.93	0.21	59,59,59,59	0
57	MG	2A	3088	1/1	0.93	0.15	51,51,51,51	0
57	MG	1A	3132	1/1	0.93	0.12	50,50,50,50	0
57	MG	1a	1709	1/1	0.93	0.07	61,61,61,61	0
57	MG	1R	201	1/1	0.93	0.09	42,42,42,42	0
57	MG	1A	3550	1/1	0.93	0.08	21,21,21,21	0
57	MG	1A	3340	1/1	0.93	0.10	53,53,53,53	0
57	MG	1A	3043	1/1	0.93	0.10	37,37,37,37	0
57	MG	1A	4061	1/1	0.93	0.09	47,47,47,47	0
57	MG	1A	3969	1/1	0.93	0.17	70,70,70,70	0
57	MG	1A	3650	1/1	0.93	0.10	25,25,25,25	0
57	MG	1A	3972	1/1	0.93	0.17	62,62,62,62	0
57	MG	1a	1728	1/1	0.93	0.12	52,52,52,52	0
57	MG	2A	3105	1/1	0.93	0.12	54,54,54,54	0
57	MG	1A	3296	1/1	0.93	0.20	52,52,52,52	0
57	MG	1W	201	1/1	0.93	0.17	44,44,44,44	0
57	MG	2A	3108	1/1	0.93	0.08	71,71,71,71	0
57	MG	1X	3001	1/1	0.93	0.05	54,54,54,54	0
57	MG	1A	3236	1/1	0.93	0.20	58,58,58,58	0
57	MG	1A	4069	1/1	0.93	0.09	53,53,53,53	0
57	MG	2A	3798	1/1	0.93	0.12	59,59,59,59	0
57	MG	1Z	301	1/1	0.93	0.22	43,43,43,43	0
57	MG	1a	1745	1/1	0.93	0.14	66,66,66,66	0
57	MG	1A	3350	1/1	0.93	0.14	57,57,57,57	0
57	MG	2A	3119	1/1	0.93	0.08	53,53,53,53	0
57	MG	1A	3351	1/1	0.93	0.15	45,45,45,45	0
57	MG	10	102	1/1	0.93	0.10	50,50,50,50	0
57	MG	2A	3124	1/1	0.93	0.11	45,45,45,45	0
57	MG	2A	3548	1/1	0.93	0.20	44,44,44,44	0
57	MG	1A	3264	1/1	0.93	0.13	49,49,49,49	0
57	MG	11	101	1/1	0.93	0.12	45,45,45,45	0
57	MG	2A	3133	1/1	0.93	0.19	49,49,49,49	0
57	MG	1a	1753	1/1	0.93	0.09	71,71,71,71	0
57	MG	1A	3305	1/1	0.93	0.08	52,52,52,52	0
57	MG	2A	3310	1/1	0.93	0.12	65,65,65,65	0
57	MG	12	3001	1/1	0.93	0.11	52,52,52,52	0
57	MG	2a	1707	1/1	0.93	0.09	82,82,82,82	0
57	MG	1A	3307	1/1	0.93	0.13	48,48,48,48	0
57	MG	1A	3574	1/1	0.93	0.11	29,29,29,29	0
57	MG	2a	1710	1/1	0.93	0.08	83,83,83,83	0
57	MG	1A	3075	1/1	0.93	0.08	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1a	1762	1/1	0.93	0.09	77,77,77,77	0
57	MG	1A	3862	1/1	0.93	0.09	37,37,37,37	0
57	MG	2a	1714	1/1	0.93	0.10	58,58,58,58	0
57	MG	2A	3146	1/1	0.93	0.20	59,59,59,59	0
57	MG	2A	3318	1/1	0.93	0.25	70,70,70,70	0
57	MG	1a	1912	1/1	0.93	0.06	66,66,66,66	0
57	MG	1A	3864	1/1	0.93	0.06	31,31,31,31	0
57	MG	2A	3150	1/1	0.93	0.13	42,42,42,42	0
57	MG	1a	1772	1/1	0.93	0.08	85,85,85,85	0
57	MG	2A	3324	1/1	0.93	0.11	57,57,57,57	0
57	MG	2A	3577	1/1	0.93	0.12	60,60,60,60	0
57	MG	1A	4088	1/1	0.93	0.10	62,62,62,62	0
57	MG	1A	4089	1/1	0.93	0.30	38,38,38,38	0
57	MG	1a	1604	1/1	0.93	0.12	67,67,67,67	0
57	MG	1A	3054	1/1	0.93	0.28	65,65,65,65	0
57	MG	1a	1783	1/1	0.93	0.16	58,58,58,58	0
57	MG	2A	3586	1/1	0.93	0.11	54,54,54,54	0
57	MG	2A	3847	1/1	0.93	0.22	59,59,59,59	0
57	MG	1a	1784	1/1	0.93	0.09	67,67,67,67	0
57	MG	1a	1785	1/1	0.93	0.12	71,71,71,71	0
57	MG	1A	3585	1/1	0.93	0.08	26,26,26,26	0
57	MG	2A	3335	1/1	0.93	0.21	56,56,56,56	0
57	MG	1A	4093	1/1	0.93	0.13	73,73,73,73	0
57	MG	2A	3855	1/1	0.93	0.08	72,72,72,72	0
57	MG	2a	1750	1/1	0.93	0.11	83,83,83,83	0
57	MG	1A	3311	1/1	0.93	0.09	38,38,38,38	0
57	MG	2A	3857	1/1	0.93	0.22	48,48,48,48	0
57	MG	2A	3858	1/1	0.93	0.09	55,55,55,55	0
57	MG	2A	3859	1/1	0.93	0.10	56,56,56,56	0
57	MG	1A	3066	1/1	0.93	0.29	39,39,39,39	0
57	MG	1A	3768	1/1	0.93	0.08	60,60,60,60	0
57	MG	2a	1758	1/1	0.93	0.18	55,55,55,55	0
57	MG	1A	3770	1/1	0.93	0.10	52,52,52,52	0
57	MG	1A	3363	1/1	0.93	0.38	50,50,50,50	0
57	MG	1A	3992	1/1	0.93	0.13	45,45,45,45	0
57	MG	1A	3477	1/1	0.93	0.09	26,26,26,26	0
57	MG	1a	1622	1/1	0.93	0.17	57,57,57,57	0
57	MG	2A	3346	1/1	0.93	0.09	65,65,65,65	0
57	MG	1a	1800	1/1	0.93	0.13	67,67,67,67	0
57	MG	2a	1768	1/1	0.93	0.24	63,63,63,63	0
57	MG	1A	4127	1/1	0.93	0.14	33,33,33,33	0
57	MG	1A	3890	1/1	0.93	0.06	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	4148	1/1	0.93	0.15	37,37,37,37	0
57	MG	2A	3183	1/1	0.93	0.16	63,63,63,63	0
57	MG	1a	1806	1/1	0.93	0.10	80,80,80,80	0
57	MG	1B	201	1/1	0.93	0.19	56,56,56,56	0
57	MG	1A	3893	1/1	0.93	0.12	31,31,31,31	0
57	MG	2A	3357	1/1	0.93	0.27	49,49,49,49	0
57	MG	1A	3894	1/1	0.93	0.07	71,71,71,71	0
57	MG	2A	3620	1/1	0.93	0.11	34,34,34,34	0
57	MG	1A	3897	1/1	0.93	0.09	47,47,47,47	0
57	MG	1A	3182	1/1	0.93	0.23	34,34,34,34	0
57	MG	1A	3776	1/1	0.93	0.10	55,55,55,55	0
57	MG	1A	3778	1/1	0.93	0.15	43,43,43,43	0
57	MG	1A	3482	1/1	0.93	0.13	52,52,52,52	0
57	MG	1A	3078	1/1	0.93	0.17	40,40,40,40	0
57	MG	2A	3195	1/1	0.93	0.10	67,67,67,67	0
57	MG	1B	215	1/1	0.93	0.12	42,42,42,42	0
57	MG	1a	1819	1/1	0.93	0.22	62,62,62,62	0
57	MG	1A	3694	1/1	0.93	0.16	73,73,73,73	0
57	MG	2A	3372	1/1	0.93	0.30	71,71,71,71	0
57	MG	2A	3640	1/1	0.93	0.09	45,45,45,45	0
57	MG	1A	3068	1/1	0.93	0.11	46,46,46,46	0
57	MG	1A	3913	1/1	0.93	0.16	57,57,57,57	0
57	MG	2a	1797	1/1	0.93	0.21	67,67,67,67	0
57	MG	1a	1645	1/1	0.93	0.17	65,65,65,65	0
57	MG	1A	3160	1/1	0.93	0.09	42,42,42,42	0
57	MG	2A	3002	1/1	0.93	0.14	57,57,57,57	0
57	MG	2A	3383	1/1	0.93	0.21	56,56,56,56	0
57	MG	2A	3384	1/1	0.93	0.37	64,64,64,64	0
57	MG	2A	3005	1/1	0.93	0.17	64,64,64,64	0
57	MG	2A	3654	1/1	0.93	0.08	83,83,83,83	0
57	MG	1A	3600	1/1	0.93	0.08	67,67,67,67	0
57	MG	1A	3371	1/1	0.93	0.10	58,58,58,58	0
57	MG	1A	3103	1/1	0.93	0.14	41,41,41,41	0
57	MG	1A	3502	1/1	0.93	0.17	54,54,54,54	0
57	MG	2A	3022	1/1	0.93	0.09	44,44,44,44	0
57	MG	2A	3023	1/1	0.93	0.32	56,56,56,56	0
57	MG	1A	3249	1/1	0.93	0.12	56,56,56,56	0
57	MG	2A	3396	1/1	0.93	0.09	61,61,61,61	0
57	MG	1A	4019	1/1	0.93	0.23	73,73,73,73	0
57	MG	1A	3711	1/1	0.93	0.06	37,37,37,37	0
57	MG	1A	4023	1/1	0.93	0.12	53,53,53,53	0
57	MG	1A	3216	1/1	0.93	0.23	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3220	1/1	0.93	0.34	65,65,65,65	0
57	MG	1A	3252	1/1	0.93	0.35	36,36,36,36	0
57	MG	2A	3406	1/1	0.93	0.26	72,72,72,72	0
57	MG	1A	3431	1/1	0.93	0.28	37,37,37,37	0
57	MG	25	104	1/1	0.93	0.10	62,62,62,62	0
57	MG	1A	3807	1/1	0.93	0.10	63,63,63,63	0
57	MG	1A	3716	1/1	0.93	0.09	39,39,39,39	0
57	MG	2A	3415	1/1	0.93	0.16	69,69,69,69	0
57	MG	1D	3001	1/1	0.93	0.11	43,43,43,43	0
57	MG	1A	3810	1/1	0.93	0.09	40,40,40,40	0
57	MG	2A	3040	1/1	0.93	0.09	62,62,62,62	0
57	MG	1A	4033	1/1	0.93	0.08	48,48,48,48	0
57	MG	2A	3682	1/1	0.93	0.08	41,41,41,41	0
57	MG	2A	3422	1/1	0.93	0.19	56,56,56,56	0
57	MG	1a	1844	1/1	0.93	0.08	92,92,92,92	0
57	MG	1D	3008	1/1	0.93	0.18	47,47,47,47	0
57	MG	1A	3304	1/1	0.94	0.07	57,57,57,57	0
57	MG	1A	4068	1/1	0.94	0.16	36,36,36,36	0
57	MG	1A	3085	1/1	0.94	0.05	38,38,38,38	0
57	MG	2A	3375	1/1	0.94	0.16	62,62,62,62	0
57	MG	1A	3172	1/1	0.94	0.27	45,45,45,45	0
57	MG	1A	3799	1/1	0.94	0.05	14,14,14,14	0
57	MG	1A	3308	1/1	0.94	0.31	31,31,31,31	0
57	MG	2A	3653	1/1	0.94	0.22	58,58,58,58	0
57	MG	16	102	1/1	0.94	0.07	57,57,57,57	0
57	MG	23	102	1/1	0.94	0.11	68,68,68,68	0
57	MG	1x	3006	1/1	0.94	0.11	62,62,62,62	0
57	MG	1A	3685	1/1	0.94	0.09	23,23,23,23	0
57	MG	1A	3100	1/1	0.94	0.25	42,42,42,42	0
57	MG	1A	3460	1/1	0.94	0.21	34,34,34,34	0
57	MG	1A	3461	1/1	0.94	0.22	34,34,34,34	0
57	MG	1a	1603	1/1	0.94	0.20	58,58,58,58	0
57	MG	1A	4079	1/1	0.94	0.08	73,73,73,73	0
57	MG	2A	3390	1/1	0.94	0.07	64,64,64,64	0
57	MG	2A	3392	1/1	0.94	0.34	73,73,73,73	0
57	MG	2a	1602	1/1	0.94	0.08	72,72,72,72	0
57	MG	1A	3142	1/1	0.94	0.19	55,55,55,55	0
57	MG	1a	1606	1/1	0.94	0.15	62,62,62,62	0
57	MG	1A	4084	1/1	0.94	0.11	35,35,35,35	0
57	MG	1A	4085	1/1	0.94	0.11	48,48,48,48	0
57	MG	1a	1804	1/1	0.94	0.07	53,53,53,53	0
57	MG	1A	3811	1/1	0.94	0.11	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3399	1/1	0.94	0.28	69,69,69,69	0
57	MG	1A	3577	1/1	0.94	0.12	41,41,41,41	0
57	MG	1A	3813	1/1	0.94	0.07	58,58,58,58	0
57	MG	2A	3003	1/1	0.94	0.18	67,67,67,67	0
57	MG	1A	3464	1/1	0.94	0.11	70,70,70,70	0
57	MG	2A	3006	1/1	0.94	0.14	54,54,54,54	0
57	MG	2A	3215	1/1	0.94	0.15	46,46,46,46	0
57	MG	2A	3007	1/1	0.94	0.06	41,41,41,41	0
57	MG	2A	3681	1/1	0.94	0.17	59,59,59,59	0
57	MG	2A	3410	1/1	0.94	0.25	46,46,46,46	0
57	MG	2A	3411	1/1	0.94	0.29	55,55,55,55	0
57	MG	2A	3010	1/1	0.94	0.09	41,41,41,41	0
57	MG	1a	1809	1/1	0.94	0.11	69,69,69,69	0
57	MG	1A	3697	1/1	0.94	0.07	29,29,29,29	0
57	MG	2A	3015	1/1	0.94	0.10	58,58,58,58	0
57	MG	2A	3419	1/1	0.94	0.07	70,70,70,70	0
57	MG	1A	4092	1/1	0.94	0.30	42,42,42,42	0
57	MG	1a	1812	1/1	0.94	0.21	66,66,66,66	0
57	MG	2A	3696	1/1	0.94	0.15	80,80,80,80	0
57	MG	1A	3579	1/1	0.94	0.10	17,17,17,17	0
57	MG	1A	4095	1/1	0.94	0.27	44,44,44,44	0
57	MG	2A	3228	1/1	0.94	0.16	57,57,57,57	0
57	MG	1A	4098	1/1	0.94	0.19	52,52,52,52	0
57	MG	1a	1624	1/1	0.94	0.15	51,51,51,51	0
57	MG	1A	3580	1/1	0.94	0.09	28,28,28,28	0
57	MG	2A	3706	1/1	0.94	0.07	57,57,57,57	0
57	MG	1A	3037	1/1	0.94	0.18	52,52,52,52	0
57	MG	1A	4107	1/1	0.94	0.11	48,48,48,48	0
57	MG	2A	3033	1/1	0.94	0.10	32,32,32,32	0
57	MG	2A	3440	1/1	0.94	0.12	46,46,46,46	0
57	MG	1a	1820	1/1	0.94	0.16	70,70,70,70	0
57	MG	1A	3312	1/1	0.94	0.26	35,35,35,35	0
57	MG	1A	3586	1/1	0.94	0.14	41,41,41,41	0
57	MG	2A	3238	1/1	0.94	0.20	69,69,69,69	0
57	MG	1A	3825	1/1	0.94	0.09	68,68,68,68	0
57	MG	1A	4113	1/1	0.94	0.09	29,29,29,29	0
57	MG	1A	3404	1/1	0.94	0.16	51,51,51,51	0
57	MG	1A	3707	1/1	0.94	0.19	61,61,61,61	0
57	MG	2a	1651	1/1	0.94	0.11	61,61,61,61	0
57	MG	1A	3708	1/1	0.94	0.13	59,59,59,59	0
57	MG	2A	3723	1/1	0.94	0.11	60,60,60,60	0
57	MG	2A	3244	1/1	0.94	0.07	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3408	1/1	0.94	0.28	39,39,39,39	0
57	MG	2A	3726	1/1	0.94	0.08	71,71,71,71	0
57	MG	1A	4132	1/1	0.94	0.41	37,37,37,37	0
57	MG	2A	3462	1/1	0.94	0.09	47,47,47,47	0
57	MG	2A	3463	1/1	0.94	0.10	44,44,44,44	0
57	MG	1A	4135	1/1	0.94	0.23	44,44,44,44	0
57	MG	1A	4145	1/1	0.94	0.14	47,47,47,47	0
57	MG	1A	3710	1/1	0.94	0.12	63,63,63,63	0
57	MG	2A	3470	1/1	0.94	0.11	41,41,41,41	0
57	MG	1A	4149	1/1	0.94	0.20	48,48,48,48	0
57	MG	2A	3473	1/1	0.94	0.08	37,37,37,37	0
57	MG	2A	3475	1/1	0.94	0.08	62,62,62,62	0
57	MG	2A	3476	1/1	0.94	0.09	35,35,35,35	0
57	MG	1A	3592	1/1	0.94	0.08	48,48,48,48	0
57	MG	1a	1835	1/1	0.94	0.07	66,66,66,66	0
57	MG	1A	3067	1/1	0.94	0.11	63,63,63,63	0
57	MG	1a	1648	1/1	0.94	0.13	58,58,58,58	0
57	MG	2A	3751	1/1	0.94	0.07	47,47,47,47	0
57	MG	1A	3145	1/1	0.94	0.05	37,37,37,37	0
57	MG	1A	3146	1/1	0.94	0.09	60,60,60,60	0
57	MG	1A	3715	1/1	0.94	0.08	53,53,53,53	0
57	MG	2A	3763	1/1	0.94	0.09	42,42,42,42	0
57	MG	1A	3842	1/1	0.94	0.11	30,30,30,30	0
57	MG	1A	3184	1/1	0.94	0.10	47,47,47,47	0
57	MG	1B	210	1/1	0.94	0.19	47,47,47,47	0
57	MG	1A	3481	1/1	0.94	0.19	34,34,34,34	0
57	MG	1A	3320	1/1	0.94	0.28	54,54,54,54	0
57	MG	1B	213	1/1	0.94	0.06	46,46,46,46	0
57	MG	1A	3486	1/1	0.94	0.07	53,53,53,53	0
57	MG	1a	1663	1/1	0.94	0.24	50,50,50,50	0
57	MG	1A	3490	1/1	0.94	0.10	61,61,61,61	0
57	MG	1A	3993	1/1	0.94	0.08	42,42,42,42	0
57	MG	2A	3781	1/1	0.94	0.18	59,59,59,59	0
57	MG	2A	3072	1/1	0.94	0.12	53,53,53,53	0
57	MG	1A	3492	1/1	0.94	0.10	26,26,26,26	0
57	MG	2A	3784	1/1	0.94	0.10	56,56,56,56	0
57	MG	1A	3602	1/1	0.94	0.06	15,15,15,15	0
57	MG	2a	1694	1/1	0.94	0.10	90,90,90,90	0
57	MG	2a	1695	1/1	0.94	0.11	69,69,69,69	0
57	MG	1A	3120	1/1	0.94	0.18	42,42,42,42	0
57	MG	1A	3016	1/1	0.94	0.09	38,38,38,38	0
57	MG	1A	3420	1/1	0.94	0.22	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3727	1/1	0.94	0.07	16,16,16,16	0
57	MG	1A	3370	1/1	0.94	0.14	51,51,51,51	0
57	MG	1A	3193	1/1	0.94	0.09	50,50,50,50	0
57	MG	2A	3084	1/1	0.94	0.06	41,41,41,41	0
57	MG	1A	3424	1/1	0.94	0.09	59,59,59,59	0
57	MG	1A	3731	1/1	0.94	0.07	20,20,20,20	0
57	MG	1a	1864	1/1	0.94	0.09	48,48,48,48	0
57	MG	2A	3525	1/1	0.94	0.12	65,65,65,65	0
57	MG	2A	3286	1/1	0.94	0.16	63,63,63,63	0
57	MG	1A	3732	1/1	0.94	0.08	27,27,27,27	0
57	MG	1A	3503	1/1	0.94	0.08	54,54,54,54	0
57	MG	1A	3224	1/1	0.94	0.28	29,29,29,29	0
57	MG	2a	1715	1/1	0.94	0.20	60,60,60,60	0
57	MG	2A	3804	1/1	0.94	0.13	75,75,75,75	0
57	MG	1A	3427	1/1	0.94	0.18	61,61,61,61	0
57	MG	1A	3514	1/1	0.94	0.12	57,57,57,57	0
57	MG	1A	3282	1/1	0.94	0.11	67,67,67,67	0
57	MG	2a	1723	1/1	0.94	0.12	52,52,52,52	0
57	MG	2a	1724	1/1	0.94	0.07	84,84,84,84	0
57	MG	2A	3095	1/1	0.94	0.11	55,55,55,55	0
57	MG	1A	3286	1/1	0.94	0.18	66,66,66,66	0
57	MG	1A	4015	1/1	0.94	0.10	56,56,56,56	0
57	MG	2A	3813	1/1	0.94	0.12	72,72,72,72	0
57	MG	1A	3123	1/1	0.94	0.10	41,41,41,41	0
57	MG	1A	3892	1/1	0.94	0.10	28,28,28,28	0
57	MG	1a	1690	1/1	0.94	0.27	60,60,60,60	0
57	MG	2A	3546	1/1	0.94	0.20	60,60,60,60	0
57	MG	2A	3547	1/1	0.94	0.07	40,40,40,40	0
57	MG	2a	1738	1/1	0.94	0.11	60,60,60,60	0
57	MG	1E	301	1/1	0.94	0.23	42,42,42,42	0
57	MG	1E	302	1/1	0.94	0.21	36,36,36,36	0
57	MG	2A	3552	1/1	0.94	0.10	43,43,43,43	0
57	MG	2a	1743	1/1	0.94	0.10	72,72,72,72	0
57	MG	1A	3523	1/1	0.94	0.13	60,60,60,60	0
57	MG	1A	3288	1/1	0.94	0.11	65,65,65,65	0
57	MG	1A	4022	1/1	0.94	0.16	63,63,63,63	0
57	MG	1A	3896	1/1	0.94	0.13	50,50,50,50	0
57	MG	2A	3558	1/1	0.94	0.14	39,39,39,39	0
57	MG	1A	3048	1/1	0.94	0.17	54,54,54,54	0
57	MG	2A	3560	1/1	0.94	0.07	63,63,63,63	0
57	MG	2A	3833	1/1	0.94	0.10	70,70,70,70	0
57	MG	2A	3112	1/1	0.94	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	3113	1/1	0.94	0.21	69,69,69,69	0
57	MG	2A	3837	1/1	0.94	0.07	58,58,58,58	0
57	MG	2A	3563	1/1	0.94	0.14	46,46,46,46	0
57	MG	1A	3898	1/1	0.94	0.08	47,47,47,47	0
57	MG	1A	3380	1/1	0.94	0.21	37,37,37,37	0
57	MG	2A	3567	1/1	0.94	0.11	68,68,68,68	0
57	MG	1A	3530	1/1	0.94	0.06	17,17,17,17	0
57	MG	1A	4030	1/1	0.94	0.19	59,59,59,59	0
57	MG	1a	1706	1/1	0.94	0.22	69,69,69,69	0
57	MG	1a	1707	1/1	0.94	0.22	67,67,67,67	0
57	MG	1A	3752	1/1	0.94	0.09	32,32,32,32	0
57	MG	1A	3437	1/1	0.94	0.24	49,49,49,49	0
57	MG	2A	3852	1/1	0.94	0.23	50,50,50,50	0
57	MG	2a	1770	1/1	0.94	0.17	74,74,74,74	0
57	MG	1a	1891	1/1	0.94	0.09	69,69,69,69	0
57	MG	1a	1712	1/1	0.94	0.12	48,48,48,48	0
57	MG	1A	3755	1/1	0.94	0.06	28,28,28,28	0
57	MG	1A	3196	1/1	0.94	0.16	56,56,56,56	0
57	MG	2a	1776	1/1	0.94	0.22	67,67,67,67	0
57	MG	1A	3641	1/1	0.94	0.13	48,48,48,48	0
57	MG	1a	1717	1/1	0.94	0.13	65,65,65,65	0
57	MG	1a	1719	1/1	0.94	0.12	55,55,55,55	0
57	MG	1N	204	1/1	0.94	0.36	53,53,53,53	0
57	MG	2A	3584	1/1	0.94	0.09	43,43,43,43	0
57	MG	1A	3128	1/1	0.94	0.09	45,45,45,45	0
57	MG	1A	3534	1/1	0.94	0.07	39,39,39,39	0
57	MG	1A	3647	1/1	0.94	0.08	35,35,35,35	0
57	MG	1A	4039	1/1	0.94	0.17	40,40,40,40	0
57	MG	1A	3535	1/1	0.94	0.07	32,32,32,32	0
57	MG	2a	1787	1/1	0.94	0.19	67,67,67,67	0
57	MG	1A	3018	1/1	0.94	0.18	76,76,76,76	0
57	MG	1a	1733	1/1	0.94	0.13	70,70,70,70	0
57	MG	1A	3922	1/1	0.94	0.10	62,62,62,62	0
57	MG	1A	3769	1/1	0.94	0.07	58,58,58,58	0
57	MG	1A	3925	1/1	0.94	0.08	68,68,68,68	0
57	MG	2B	3010	1/1	0.94	0.07	70,70,70,70	0
57	MG	1A	3294	1/1	0.94	0.23	46,46,46,46	0
57	MG	2A	3156	1/1	0.94	0.14	45,45,45,45	0
57	MG	1R	202	1/1	0.94	0.55	45,45,45,45	0
57	MG	1A	3130	1/1	0.94	0.11	43,43,43,43	0
57	MG	1a	1914	1/1	0.94	0.10	74,74,74,74	0
57	MG	2A	3345	1/1	0.94	0.22	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	4048	1/1	0.94	0.08	51,51,51,51	0
57	MG	1A	3339	1/1	0.94	0.08	52,52,52,52	0
57	MG	1A	3655	1/1	0.94	0.06	50,50,50,50	0
57	MG	2A	3164	1/1	0.94	0.13	41,41,41,41	0
57	MG	1T	201	1/1	0.94	0.20	51,51,51,51	0
57	MG	2D	303	1/1	0.94	0.51	51,51,51,51	0
57	MG	2A	3612	1/1	0.94	0.10	56,56,56,56	0
57	MG	1A	3934	1/1	0.94	0.10	57,57,57,57	0
57	MG	1A	3656	1/1	0.94	0.09	33,33,33,33	0
57	MG	1A	3112	1/1	0.94	0.23	34,34,34,34	0
57	MG	1A	3938	1/1	0.94	0.11	52,52,52,52	0
57	MG	2A	3355	1/1	0.94	0.18	43,43,43,43	0
57	MG	2A	3356	1/1	0.94	0.20	58,58,58,58	0
57	MG	1A	3659	1/1	0.94	0.09	61,61,61,61	0
57	MG	1A	3547	1/1	0.94	0.10	38,38,38,38	0
57	MG	2F	302	1/1	0.94	0.12	59,59,59,59	0
57	MG	1A	3342	1/1	0.94	0.27	49,49,49,49	0
57	MG	2A	3360	1/1	0.94	0.23	47,47,47,47	0
57	MG	2N	8001	1/1	0.94	0.12	63,63,63,63	0
57	MG	2A	3628	1/1	0.94	0.10	55,55,55,55	0
57	MG	1A	3942	1/1	0.94	0.08	64,64,64,64	0
57	MG	2Q	3001	1/1	0.94	0.08	66,66,66,66	0
57	MG	1a	1766	1/1	0.94	0.08	54,54,54,54	0
57	MG	1A	3167	1/1	0.94	0.09	46,46,46,46	0
57	MG	1A	3671	1/1	0.94	0.06	41,41,41,41	0
57	MG	1A	3672	1/1	0.94	0.09	39,39,39,39	0
57	MG	2A	3367	1/1	0.94	0.13	53,53,53,53	0
57	MG	2A	3637	1/1	0.94	0.08	47,47,47,47	0
57	MG	2T	3004	1/1	0.94	0.13	67,67,67,67	0
57	MG	1A	3204	1/1	0.94	0.07	61,61,61,61	0
57	MG	1A	3347	1/1	0.94	0.36	40,40,40,40	0
57	MG	1a	1778	1/1	0.94	0.07	60,60,60,60	0
57	MG	2V	201	1/1	0.94	0.19	52,52,52,52	0
58	K	2A	3849	1/1	0.94	0.11	72,72,72,72	0
59	ZN	24	501	1/1	0.94	0.11	125,125,125,125	0
57	MG	1A	3485	1/1	0.95	0.33	36,36,36,36	0
57	MG	2T	3003	1/1	0.95	0.20	57,57,57,57	0
57	MG	2A	3174	1/1	0.95	0.09	57,57,57,57	0
57	MG	2A	3175	1/1	0.95	0.06	64,64,64,64	0
57	MG	2A	3176	1/1	0.95	0.15	66,66,66,66	0
57	MG	2A	3373	1/1	0.95	0.30	63,63,63,63	0
57	MG	2U	204	1/1	0.95	0.10	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	4067	1/1	0.95	0.07	60,60,60,60	0
57	MG	1A	3188	1/1	0.95	0.28	33,33,33,33	0
57	MG	2A	3643	1/1	0.95	0.13	64,64,64,64	0
57	MG	1a	1747	1/1	0.95	0.10	67,67,67,67	0
57	MG	2A	3180	1/1	0.95	0.27	59,59,59,59	0
57	MG	2X	3003	1/1	0.95	0.09	60,60,60,60	0
57	MG	1A	3487	1/1	0.95	0.14	47,47,47,47	0
57	MG	20	8001	1/1	0.95	0.10	59,59,59,59	0
57	MG	1A	3488	1/1	0.95	0.13	38,38,38,38	0
57	MG	2A	3382	1/1	0.95	0.27	49,49,49,49	0
57	MG	1A	3489	1/1	0.95	0.12	44,44,44,44	0
57	MG	1A	4072	1/1	0.95	0.09	47,47,47,47	0
57	MG	1a	1752	1/1	0.95	0.06	55,55,55,55	0
57	MG	1A	3706	1/1	0.95	0.16	47,47,47,47	0
57	MG	1W	202	1/1	0.95	0.13	51,51,51,51	0
57	MG	1A	3422	1/1	0.95	0.09	50,50,50,50	0
57	MG	1X	3004	1/1	0.95	0.15	41,41,41,41	0
57	MG	1A	3491	1/1	0.95	0.11	45,45,45,45	0
57	MG	1w	108	1/1	0.95	0.15	68,68,68,68	0
57	MG	1A	3821	1/1	0.95	0.07	36,36,36,36	0
57	MG	1A	3079	1/1	0.95	0.06	28,28,28,28	0
57	MG	1Z	302	1/1	0.95	0.12	60,60,60,60	0
57	MG	1A	3298	1/1	0.95	0.09	57,57,57,57	0
57	MG	1A	3377	1/1	0.95	0.18	59,59,59,59	0
57	MG	1A	4081	1/1	0.95	0.07	46,46,46,46	0
57	MG	10	103	1/1	0.95	0.17	63,63,63,63	0
57	MG	1A	4082	1/1	0.95	0.12	14,14,14,14	0
57	MG	1A	3065	1/1	0.95	0.12	39,39,39,39	0
57	MG	1a	1776	1/1	0.95	0.07	74,74,74,74	0
57	MG	1a	1777	1/1	0.95	0.07	77,77,77,77	0
57	MG	1A	3213	1/1	0.95	0.14	45,45,45,45	0
57	MG	1A	3214	1/1	0.95	0.11	46,46,46,46	0
57	MG	2A	3408	1/1	0.95	0.25	56,56,56,56	0
57	MG	1A	3306	1/1	0.95	0.08	49,49,49,49	0
57	MG	1A	3272	1/1	0.95	0.23	53,53,53,53	0
57	MG	1A	3432	1/1	0.95	0.23	43,43,43,43	0
57	MG	2A	3210	1/1	0.95	0.11	56,56,56,56	0
57	MG	2A	3680	1/1	0.95	0.08	69,69,69,69	0
57	MG	1A	3509	1/1	0.95	0.08	57,57,57,57	0
57	MG	1A	3836	1/1	0.95	0.06	71,71,71,71	0
57	MG	18	102	1/1	0.95	0.08	63,63,63,63	0
57	MG	18	103	1/1	0.95	0.16	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3510	1/1	0.95	0.07	30,30,30,30	0
57	MG	1A	3720	1/1	0.95	0.06	51,51,51,51	0
57	MG	1a	1601	1/1	0.95	0.07	53,53,53,53	0
57	MG	1A	4097	1/1	0.95	0.13	68,68,68,68	0
57	MG	1A	3840	1/1	0.95	0.09	62,62,62,62	0
57	MG	2A	3221	1/1	0.95	0.13	76,76,76,76	0
57	MG	2A	3694	1/1	0.95	0.07	58,58,58,58	0
57	MG	2A	3695	1/1	0.95	0.17	60,60,60,60	0
57	MG	1a	1798	1/1	0.95	0.08	63,63,63,63	0
57	MG	1A	4102	1/1	0.95	0.33	39,39,39,39	0
57	MG	2A	3434	1/1	0.95	0.07	49,49,49,49	0
57	MG	2A	3699	1/1	0.95	0.20	73,73,73,73	0
57	MG	1A	3609	1/1	0.95	0.11	49,49,49,49	0
57	MG	1A	3343	1/1	0.95	0.31	57,57,57,57	0
57	MG	2A	3703	1/1	0.95	0.06	79,79,79,79	0
57	MG	2A	3438	1/1	0.95	0.10	36,36,36,36	0
57	MG	1A	3124	1/1	0.95	0.14	37,37,37,37	0
57	MG	1A	3436	1/1	0.95	0.15	55,55,55,55	0
57	MG	2A	3707	1/1	0.95	0.12	69,69,69,69	0
57	MG	1A	3036	1/1	0.95	0.07	34,34,34,34	0
57	MG	2a	1645	1/1	0.95	0.09	61,61,61,61	0
57	MG	1A	3520	1/1	0.95	0.06	19,19,19,19	0
57	MG	1A	4111	1/1	0.95	0.19	38,38,38,38	0
57	MG	1a	1615	1/1	0.95	0.06	50,50,50,50	0
57	MG	2A	3448	1/1	0.95	0.14	55,55,55,55	0
57	MG	1A	3985	1/1	0.95	0.10	59,59,59,59	0
57	MG	1A	4114	1/1	0.95	0.23	46,46,46,46	0
57	MG	2A	3452	1/1	0.95	0.10	62,62,62,62	0
57	MG	1A	3440	1/1	0.95	0.09	48,48,48,48	0
57	MG	1A	4117	1/1	0.95	0.13	39,39,39,39	0
57	MG	1A	4119	1/1	0.95	0.22	39,39,39,39	0
57	MG	1A	3060	1/1	0.95	0.13	54,54,54,54	0
57	MG	1A	3622	1/1	0.95	0.10	54,54,54,54	0
57	MG	1A	4129	1/1	0.95	0.18	35,35,35,35	0
57	MG	1A	3444	1/1	0.95	0.12	53,53,53,53	0
57	MG	1A	3527	1/1	0.95	0.10	56,56,56,56	0
57	MG	1a	1628	1/1	0.95	0.12	54,54,54,54	0
57	MG	2A	3466	1/1	0.95	0.11	39,39,39,39	0
57	MG	2A	3042	1/1	0.95	0.12	58,58,58,58	0
57	MG	2A	3730	1/1	0.95	0.07	50,50,50,50	0
57	MG	2A	3043	1/1	0.95	0.15	34,34,34,34	0
57	MG	1A	4133	1/1	0.95	0.09	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	3348	1/1	0.95	0.12	50,50,50,50	0
57	MG	1A	4137	1/1	0.95	0.29	40,40,40,40	0
57	MG	2A	3474	1/1	0.95	0.17	64,64,64,64	0
57	MG	1A	4140	1/1	0.95	0.26	38,38,38,38	0
57	MG	1A	4141	1/1	0.95	0.48	30,30,30,30	0
57	MG	2A	3739	1/1	0.95	0.13	73,73,73,73	0
57	MG	2A	3477	1/1	0.95	0.11	61,61,61,61	0
57	MG	2A	3479	1/1	0.95	0.09	48,48,48,48	0
57	MG	1A	3856	1/1	0.95	0.07	13,13,13,13	0
57	MG	1A	3733	1/1	0.95	0.11	40,40,40,40	0
57	MG	2A	3482	1/1	0.95	0.07	41,41,41,41	0
57	MG	2A	3749	1/1	0.95	0.06	54,54,54,54	0
57	MG	1A	3251	1/1	0.95	0.08	40,40,40,40	0
57	MG	1A	3391	1/1	0.95	0.14	49,49,49,49	0
57	MG	1a	1640	1/1	0.95	0.14	50,50,50,50	0
57	MG	2A	3489	1/1	0.95	0.07	41,41,41,41	0
57	MG	2A	3055	1/1	0.95	0.08	46,46,46,46	0
57	MG	2A	3762	1/1	0.95	0.08	56,56,56,56	0
57	MG	2A	3258	1/1	0.95	0.12	67,67,67,67	0
57	MG	1A	3392	1/1	0.95	0.19	34,34,34,34	0
57	MG	1A	3738	1/1	0.95	0.08	59,59,59,59	0
57	MG	1a	1643	1/1	0.95	0.10	54,54,54,54	0
57	MG	1B	204	1/1	0.95	0.17	70,70,70,70	0
57	MG	1A	3173	1/1	0.95	0.07	44,44,44,44	0
57	MG	2A	3772	1/1	0.95	0.08	30,30,30,30	0
57	MG	1A	3639	1/1	0.95	0.06	44,44,44,44	0
57	MG	2A	3774	1/1	0.95	0.06	65,65,65,65	0
57	MG	2A	3775	1/1	0.95	0.11	47,47,47,47	0
57	MG	1a	1836	1/1	0.95	0.20	62,62,62,62	0
57	MG	2a	1699	1/1	0.95	0.08	68,68,68,68	0
57	MG	1A	3278	1/1	0.95	0.21	35,35,35,35	0
57	MG	1A	3315	1/1	0.95	0.15	61,61,61,61	0
57	MG	1A	3353	1/1	0.95	0.10	38,38,38,38	0
57	MG	1A	4004	1/1	0.95	0.13	50,50,50,50	0
57	MG	1A	3644	1/1	0.95	0.12	45,45,45,45	0
57	MG	2A	3510	1/1	0.95	0.12	55,55,55,55	0
57	MG	1a	1652	1/1	0.95	0.10	70,70,70,70	0
57	MG	1A	3536	1/1	0.95	0.05	29,29,29,29	0
57	MG	2A	3787	1/1	0.95	0.10	63,63,63,63	0
57	MG	2A	3073	1/1	0.95	0.09	58,58,58,58	0
57	MG	1A	4007	1/1	0.95	0.11	43,43,43,43	0
57	MG	1A	3889	1/1	0.95	0.05	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	2A	3076	1/1	0.95	0.10	52,52,52,52	0
57	MG	1B	217	1/1	0.95	0.07	37,37,37,37	0
57	MG	2a	1716	1/1	0.95	0.08	60,60,60,60	0
57	MG	2A	3280	1/1	0.95	0.14	50,50,50,50	0
57	MG	1A	3147	1/1	0.95	0.09	43,43,43,43	0
57	MG	2a	1720	1/1	0.95	0.09	75,75,75,75	0
57	MG	1a	1658	1/1	0.95	0.11	52,52,52,52	0
57	MG	1A	3891	1/1	0.95	0.06	46,46,46,46	0
57	MG	1A	3226	1/1	0.95	0.37	39,39,39,39	0
57	MG	1A	3541	1/1	0.95	0.09	42,42,42,42	0
57	MG	1A	3651	1/1	0.95	0.11	47,47,47,47	0
57	MG	2A	3529	1/1	0.95	0.08	53,53,53,53	0
57	MG	1A	3090	1/1	0.95	0.10	39,39,39,39	0
57	MG	2A	3532	1/1	0.95	0.11	41,41,41,41	0
57	MG	1A	3358	1/1	0.95	0.19	50,50,50,50	0
57	MG	1A	3759	1/1	0.95	0.08	41,41,41,41	0
57	MG	1A	4018	1/1	0.95	0.10	48,48,48,48	0
57	MG	1A	3229	1/1	0.95	0.07	50,50,50,50	0
57	MG	2A	3537	1/1	0.95	0.08	41,41,41,41	0
57	MG	2a	1737	1/1	0.95	0.19	61,61,61,61	0
57	MG	1a	1670	1/1	0.95	0.40	64,64,64,64	0
57	MG	2A	3294	1/1	0.95	0.07	53,53,53,53	0
57	MG	2a	1740	1/1	0.95	0.13	52,52,52,52	0
57	MG	2A	3295	1/1	0.95	0.06	53,53,53,53	0
57	MG	2A	3542	1/1	0.95	0.11	45,45,45,45	0
57	MG	1A	3201	1/1	0.95	0.12	53,53,53,53	0
57	MG	2A	3092	1/1	0.95	0.11	34,34,34,34	0
57	MG	2a	1745	1/1	0.95	0.17	64,64,64,64	0
57	MG	1a	1672	1/1	0.95	0.27	62,62,62,62	0
57	MG	1A	3150	1/1	0.95	0.27	42,42,42,42	0
57	MG	2A	3821	1/1	0.95	0.07	54,54,54,54	0
57	MG	1A	3405	1/1	0.95	0.15	29,29,29,29	0
57	MG	2A	3096	1/1	0.95	0.16	51,51,51,51	0
57	MG	1A	3406	1/1	0.95	0.27	37,37,37,37	0
57	MG	2A	3551	1/1	0.95	0.17	45,45,45,45	0
57	MG	1A	3767	1/1	0.95	0.05	33,33,33,33	0
57	MG	2a	1754	1/1	0.95	0.13	70,70,70,70	0
57	MG	2A	3100	1/1	0.95	0.12	51,51,51,51	0
57	MG	2A	3554	1/1	0.95	0.09	58,58,58,58	0
57	MG	1A	3910	1/1	0.95	0.13	62,62,62,62	0
57	MG	1a	1679	1/1	0.95	0.25	65,65,65,65	0
57	MG	2A	3831	1/1	0.95	0.06	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3911	1/1	0.95	0.06	48,48,48,48	0
57	MG	1A	3662	1/1	0.95	0.07	22,22,22,22	0
57	MG	2a	1763	1/1	0.95	0.08	67,67,67,67	0
57	MG	1A	3462	1/1	0.95	0.19	39,39,39,39	0
57	MG	1A	3407	1/1	0.95	0.27	41,41,41,41	0
57	MG	1A	3556	1/1	0.95	0.07	27,27,27,27	0
57	MG	1A	3558	1/1	0.95	0.10	26,26,26,26	0
57	MG	1A	3919	1/1	0.95	0.06	27,27,27,27	0
57	MG	2A	3564	1/1	0.95	0.07	62,62,62,62	0
57	MG	1E	303	1/1	0.95	0.15	29,29,29,29	0
57	MG	1A	3151	1/1	0.95	0.09	51,51,51,51	0
57	MG	1A	3921	1/1	0.95	0.13	57,57,57,57	0
57	MG	1A	3116	1/1	0.95	0.22	37,37,37,37	0
57	MG	1A	3923	1/1	0.95	0.08	62,62,62,62	0
57	MG	2a	1775	1/1	0.95	0.10	69,69,69,69	0
57	MG	1A	3467	1/1	0.95	0.07	52,52,52,52	0
57	MG	1A	3021	1/1	0.95	0.21	34,34,34,34	0
57	MG	2A	3118	1/1	0.95	0.22	71,71,71,71	0
57	MG	1F	305	1/1	0.95	0.14	47,47,47,47	0
57	MG	2A	3323	1/1	0.95	0.07	63,63,63,63	0
57	MG	2A	3120	1/1	0.95	0.09	47,47,47,47	0
57	MG	1A	3569	1/1	0.95	0.09	57,57,57,57	0
57	MG	1a	1696	1/1	0.95	0.14	72,72,72,72	0
57	MG	2A	3578	1/1	0.95	0.06	36,36,36,36	0
57	MG	1A	3327	1/1	0.95	0.26	46,46,46,46	0
57	MG	2A	3125	1/1	0.95	0.16	54,54,54,54	0
57	MG	1A	3470	1/1	0.95	0.12	33,33,33,33	0
57	MG	2A	3330	1/1	0.95	0.08	48,48,48,48	0
57	MG	2A	3127	1/1	0.95	0.24	50,50,50,50	0
57	MG	2A	3129	1/1	0.95	0.18	40,40,40,40	0
57	MG	1G	3001	1/1	0.95	0.10	43,43,43,43	0
57	MG	2A	3132	1/1	0.95	0.19	45,45,45,45	0
57	MG	1A	3930	1/1	0.95	0.11	59,59,59,59	0
57	MG	1A	3682	1/1	0.95	0.08	51,51,51,51	0
57	MG	1a	1703	1/1	0.95	0.07	60,60,60,60	0
57	MG	1G	3004	1/1	0.95	0.07	46,46,46,46	0
57	MG	1A	3683	1/1	0.95	0.06	52,52,52,52	0
57	MG	1A	3684	1/1	0.95	0.09	49,49,49,49	0
57	MG	2A	3595	1/1	0.95	0.07	44,44,44,44	0
57	MG	1a	1708	1/1	0.95	0.28	50,50,50,50	0
57	MG	1A	3104	1/1	0.95	0.12	44,44,44,44	0
57	MG	1A	3794	1/1	0.95	0.10	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	1N	206	1/1	0.95	0.11	50,50,50,50	0
57	MG	1N	207	1/1	0.95	0.17	33,33,33,33	0
57	MG	1A	3414	1/1	0.95	0.08	53,53,53,53	0
57	MG	1A	3329	1/1	0.95	0.09	59,59,59,59	0
57	MG	1A	3475	1/1	0.95	0.21	39,39,39,39	0
57	MG	1A	3014	1/1	0.95	0.04	34,34,34,34	0
57	MG	1a	1720	1/1	0.95	0.10	61,61,61,61	0
57	MG	2D	301	1/1	0.95	0.28	53,53,53,53	0
57	MG	2l	201	1/1	0.95	0.09	72,72,72,72	0
57	MG	1a	1721	1/1	0.95	0.06	31,31,31,31	0
57	MG	2A	3607	1/1	0.95	0.06	68,68,68,68	0
57	MG	1A	3943	1/1	0.95	0.14	68,68,68,68	0
57	MG	1A	4058	1/1	0.95	0.12	31,31,31,31	0
57	MG	1A	3240	1/1	0.95	0.13	35,35,35,35	0
57	MG	2E	305	1/1	0.95	0.09	65,65,65,65	0
57	MG	2E	306	1/1	0.95	0.10	40,40,40,40	0
57	MG	1Q	201	1/1	0.95	0.12	34,34,34,34	0
57	MG	1Q	202	1/1	0.95	0.11	49,49,49,49	0
57	MG	2A	3161	1/1	0.95	0.09	48,48,48,48	0
57	MG	1A	3419	1/1	0.95	0.23	49,49,49,49	0
57	MG	1A	3695	1/1	0.95	0.07	35,35,35,35	0
57	MG	1A	3947	1/1	0.95	0.09	59,59,59,59	0
57	MG	1A	3141	1/1	0.95	0.22	37,37,37,37	0
57	MG	1a	1736	1/1	0.95	0.07	62,62,62,62	0
57	MG	2A	3624	1/1	0.95	0.09	51,51,51,51	0
57	MG	2A	3626	1/1	0.95	0.09	45,45,45,45	0
57	MG	1A	3698	1/1	0.95	0.07	29,29,29,29	0
57	MG	2A	3365	1/1	0.95	0.13	37,37,37,37	0
57	MG	1a	1738	1/1	0.95	0.19	44,44,44,44	0
57	MG	1a	1739	1/1	0.95	0.09	53,53,53,53	0
57	MG	2A	3631	1/1	0.95	0.08	61,61,61,61	0
58	K	1A	3435	1/1	0.95	0.13	57,57,57,57	0
57	MG	1A	3587	1/1	0.95	0.14	35,35,35,35	0
57	MG	2A	3633	1/1	0.95	0.07	55,55,55,55	0
57	MG	2A	3208	1/1	0.96	0.34	41,41,41,41	0
57	MG	1A	4112	1/1	0.96	0.23	37,37,37,37	0
57	MG	1a	1852	1/1	0.96	0.09	67,67,67,67	0
57	MG	1A	3511	1/1	0.96	0.07	26,26,26,26	0
57	MG	1A	3161	1/1	0.96	0.11	24,24,24,24	0
57	MG	1W	205	1/1	0.96	0.11	32,32,32,32	0
57	MG	1A	4115	1/1	0.96	0.17	31,31,31,31	0
57	MG	1A	3784	1/1	0.96	0.08	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1a	1705	1/1	0.96	0.08	62,62,62,62	0
57	MG	2A	3217	1/1	0.96	0.23	37,37,37,37	0
57	MG	1A	3696	1/1	0.96	0.07	39,39,39,39	0
57	MG	1A	3905	1/1	0.96	0.16	41,41,41,41	0
57	MG	2a	1643	1/1	0.96	0.16	54,54,54,54	0
57	MG	2A	3376	1/1	0.96	0.28	55,55,55,55	0
57	MG	1A	4122	1/1	0.96	0.10	54,54,54,54	0
57	MG	2A	3780	1/1	0.96	0.15	57,57,57,57	0
57	MG	2A	3378	1/1	0.96	0.08	52,52,52,52	0
57	MG	1A	3162	1/1	0.96	0.06	30,30,30,30	0
57	MG	1A	4125	1/1	0.96	0.15	33,33,33,33	0
57	MG	1a	1711	1/1	0.96	0.16	49,49,49,49	0
57	MG	1A	3069	1/1	0.96	0.14	59,59,59,59	0
57	MG	2A	3786	1/1	0.96	0.05	59,59,59,59	0
57	MG	10	101	1/1	0.96	0.09	42,42,42,42	0
57	MG	1A	3518	1/1	0.96	0.06	33,33,33,33	0
57	MG	1A	4130	1/1	0.96	0.28	31,31,31,31	0
57	MG	2a	1656	1/1	0.96	0.11	66,66,66,66	0
57	MG	10	104	1/1	0.96	0.08	61,61,61,61	0
57	MG	2A	3581	1/1	0.96	0.06	55,55,55,55	0
57	MG	1a	1718	1/1	0.96	0.08	55,55,55,55	0
57	MG	1A	4010	1/1	0.96	0.07	60,60,60,60	0
57	MG	10	106	1/1	0.96	0.05	54,54,54,54	0
57	MG	1A	3790	1/1	0.96	0.09	38,38,38,38	0
57	MG	2a	1663	1/1	0.96	0.18	47,47,47,47	0
57	MG	2A	3391	1/1	0.96	0.32	46,46,46,46	0
57	MG	1A	3791	1/1	0.96	0.07	64,64,64,64	0
57	MG	1A	3792	1/1	0.96	0.07	66,66,66,66	0
57	MG	1A	3049	1/1	0.96	0.06	31,31,31,31	0
57	MG	1A	4138	1/1	0.96	0.32	42,42,42,42	0
57	MG	1A	3098	1/1	0.96	0.07	35,35,35,35	0
57	MG	1A	3072	1/1	0.96	0.06	36,36,36,36	0
57	MG	17	102	1/1	0.96	0.11	51,51,51,51	0
57	MG	1A	4142	1/1	0.96	0.25	52,52,52,52	0
57	MG	1A	4144	1/1	0.96	0.11	39,39,39,39	0
57	MG	1a	1735	1/1	0.96	0.08	53,53,53,53	0
57	MG	1A	3522	1/1	0.96	0.07	25,25,25,25	0
57	MG	1A	3341	1/1	0.96	0.17	38,38,38,38	0
57	MG	2A	3404	1/1	0.96	0.15	48,48,48,48	0
57	MG	1A	3798	1/1	0.96	0.07	57,57,57,57	0
57	MG	2A	3814	1/1	0.96	0.06	66,66,66,66	0
57	MG	1A	4150	1/1	0.96	0.12	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	4020	1/1	0.96	0.10	57,57,57,57	0
57	MG	1A	3293	1/1	0.96	0.09	44,44,44,44	0
57	MG	1a	1744	1/1	0.96	0.09	54,54,54,54	0
57	MG	1A	3002	1/1	0.96	0.05	19,19,19,19	0
57	MG	2A	3412	1/1	0.96	0.05	75,75,75,75	0
57	MG	2A	3608	1/1	0.96	0.10	37,37,37,37	0
57	MG	1A	3169	1/1	0.96	0.08	53,53,53,53	0
57	MG	2A	3610	1/1	0.96	0.07	58,58,58,58	0
57	MG	2A	3611	1/1	0.96	0.12	49,49,49,49	0
57	MG	1A	3028	1/1	0.96	0.32	36,36,36,36	0
57	MG	1A	3926	1/1	0.96	0.09	43,43,43,43	0
57	MG	2A	3097	1/1	0.96	0.19	51,51,51,51	0
57	MG	1A	3346	1/1	0.96	0.08	56,56,56,56	0
57	MG	1A	3102	1/1	0.96	0.11	44,44,44,44	0
57	MG	1A	3009	1/1	0.96	0.10	38,38,38,38	0
57	MG	2A	3618	1/1	0.96	0.07	70,70,70,70	0
57	MG	2A	3619	1/1	0.96	0.08	58,58,58,58	0
57	MG	1A	3299	1/1	0.96	0.13	39,39,39,39	0
57	MG	2A	3835	1/1	0.96	0.11	56,56,56,56	0
57	MG	1A	3300	1/1	0.96	0.07	48,48,48,48	0
57	MG	2A	3424	1/1	0.96	0.07	31,31,31,31	0
57	MG	1a	1754	1/1	0.96	0.06	67,67,67,67	0
57	MG	2A	3428	1/1	0.96	0.14	52,52,52,52	0
57	MG	2A	3840	1/1	0.96	0.07	64,64,64,64	0
57	MG	2A	3841	1/1	0.96	0.07	61,61,61,61	0
57	MG	2A	3430	1/1	0.96	0.07	56,56,56,56	0
57	MG	1a	1755	1/1	0.96	0.06	71,71,71,71	0
57	MG	1A	3933	1/1	0.96	0.06	75,75,75,75	0
57	MG	1A	3301	1/1	0.96	0.10	51,51,51,51	0
57	MG	1A	3134	1/1	0.96	0.10	51,51,51,51	0
57	MG	1a	1620	1/1	0.96	0.21	60,60,60,60	0
57	MG	1A	3058	1/1	0.96	0.12	34,34,34,34	0
57	MG	1A	3937	1/1	0.96	0.09	42,42,42,42	0
57	MG	1A	3628	1/1	0.96	0.06	41,41,41,41	0
57	MG	2a	1718	1/1	0.96	0.07	74,74,74,74	0
57	MG	1A	3176	1/1	0.96	0.18	53,53,53,53	0
57	MG	2A	3442	1/1	0.96	0.04	38,38,38,38	0
57	MG	1A	3630	1/1	0.96	0.12	67,67,67,67	0
57	MG	1a	1770	1/1	0.96	0.15	74,74,74,74	0
57	MG	1A	4041	1/1	0.96	0.09	56,56,56,56	0
57	MG	1A	3139	1/1	0.96	0.09	22,22,22,22	0
57	MG	2A	3642	1/1	0.96	0.07	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2a	1726	1/1	0.96	0.05	79,79,79,79	0
57	MG	2A	3276	1/1	0.96	0.16	55,55,55,55	0
57	MG	1A	3410	1/1	0.96	0.09	62,62,62,62	0
57	MG	2A	3645	1/1	0.96	0.08	63,63,63,63	0
57	MG	2A	3278	1/1	0.96	0.07	63,63,63,63	0
57	MG	1A	3356	1/1	0.96	0.11	36,36,36,36	0
57	MG	1A	3545	1/1	0.96	0.12	46,46,46,46	0
57	MG	1A	3059	1/1	0.96	0.07	31,31,31,31	0
57	MG	2a	1734	1/1	0.96	0.06	76,76,76,76	0
57	MG	1A	3106	1/1	0.96	0.27	38,38,38,38	0
57	MG	1a	1780	1/1	0.96	0.05	65,65,65,65	0
57	MG	1A	3828	1/1	0.96	0.12	47,47,47,47	0
57	MG	1A	3642	1/1	0.96	0.10	54,54,54,54	0
57	MG	1A	3548	1/1	0.96	0.04	25,25,25,25	0
57	MG	1A	3220	1/1	0.96	0.06	56,56,56,56	0
57	MG	1A	3221	1/1	0.96	0.17	42,42,42,42	0
57	MG	2A	3465	1/1	0.96	0.12	37,37,37,37	0
57	MG	1a	1788	1/1	0.96	0.08	43,43,43,43	0
57	MG	1a	1638	1/1	0.96	0.18	46,46,46,46	0
57	MG	2A	3134	1/1	0.96	0.20	63,63,63,63	0
57	MG	1a	1639	1/1	0.96	0.10	56,56,56,56	0
57	MG	1A	3551	1/1	0.96	0.07	23,23,23,23	0
57	MG	2A	3472	1/1	0.96	0.09	44,44,44,44	0
57	MG	2A	3137	1/1	0.96	0.08	39,39,39,39	0
57	MG	1A	3835	1/1	0.96	0.06	72,72,72,72	0
57	MG	1A	3648	1/1	0.96	0.05	29,29,29,29	0
57	MG	1A	3956	1/1	0.96	0.07	53,53,53,53	0
57	MG	1A	3222	1/1	0.96	0.22	42,42,42,42	0
57	MG	2A	3478	1/1	0.96	0.06	34,34,34,34	0
57	MG	2A	3142	1/1	0.96	0.13	65,65,65,65	0
57	MG	1A	3958	1/1	0.96	0.10	26,26,26,26	0
57	MG	1A	3181	1/1	0.96	0.14	37,37,37,37	0
57	MG	2a	1759	1/1	0.96	0.12	62,62,62,62	0
57	MG	1A	3476	1/1	0.96	0.36	33,33,33,33	0
57	MG	1A	3418	1/1	0.96	0.21	42,42,42,42	0
57	MG	2A	3485	1/1	0.96	0.08	38,38,38,38	0
57	MG	1A	3032	1/1	0.96	0.26	32,32,32,32	0
57	MG	2A	3149	1/1	0.96	0.15	74,74,74,74	0
57	MG	2A	3488	1/1	0.96	0.15	42,42,42,42	0
57	MG	1A	3227	1/1	0.96	0.12	42,42,42,42	0
57	MG	2A	3683	1/1	0.96	0.09	38,38,38,38	0
57	MG	1A	3740	1/1	0.96	0.10	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3183	1/1	0.96	0.34	34,34,34,34	0
57	MG	2A	3153	1/1	0.96	0.13	53,53,53,53	0
57	MG	2A	3687	1/1	0.96	0.12	67,67,67,67	0
57	MG	1F	302	1/1	0.96	0.16	28,28,28,28	0
57	MG	1A	3483	1/1	0.96	0.25	37,37,37,37	0
57	MG	2A	3495	1/1	0.96	0.13	26,26,26,26	0
57	MG	1A	3484	1/1	0.96	0.12	37,37,37,37	0
57	MG	1x	3011	1/1	0.96	0.11	68,68,68,68	0
57	MG	2A	3498	1/1	0.96	0.09	62,62,62,62	0
57	MG	1A	3317	1/1	0.96	0.06	42,42,42,42	0
57	MG	1A	3660	1/1	0.96	0.07	43,43,43,43	0
57	MG	1A	3971	1/1	0.96	0.08	42,42,42,42	0
57	MG	1y	101	1/1	0.96	0.10	48,48,48,48	0
57	MG	1A	3746	1/1	0.96	0.04	36,36,36,36	0
57	MG	2A	3700	1/1	0.96	0.07	76,76,76,76	0
57	MG	1A	3853	1/1	0.96	0.07	52,52,52,52	0
57	MG	1a	1662	1/1	0.96	0.22	54,54,54,54	0
57	MG	1A	3661	1/1	0.96	0.04	29,29,29,29	0
57	MG	2A	3511	1/1	0.96	0.06	63,63,63,63	0
57	MG	1A	3080	1/1	0.96	0.18	35,35,35,35	0
57	MG	1A	3013	1/1	0.96	0.06	28,28,28,28	0
57	MG	1A	3425	1/1	0.96	0.14	48,48,48,48	0
57	MG	2A	3169	1/1	0.96	0.13	54,54,54,54	0
57	MG	1A	3113	1/1	0.96	0.28	31,31,31,31	0
57	MG	2A	3517	1/1	0.96	0.15	63,63,63,63	0
57	MG	1N	203	1/1	0.96	0.11	44,44,44,44	0
57	MG	1A	3035	1/1	0.96	0.16	38,38,38,38	0
57	MG	2A	3714	1/1	0.96	0.10	69,69,69,69	0
57	MG	1N	205	1/1	0.96	0.10	43,43,43,43	0
57	MG	1A	3863	1/1	0.96	0.06	24,24,24,24	0
57	MG	1A	3192	1/1	0.96	0.17	39,39,39,39	0
57	MG	2A	3012	1/1	0.96	0.06	48,48,48,48	0
57	MG	1A	3023	1/1	0.96	0.19	32,32,32,32	0
57	MG	1A	3496	1/1	0.96	0.10	43,43,43,43	0
57	MG	2A	3527	1/1	0.96	0.07	35,35,35,35	0
57	MG	1a	1675	1/1	0.96	0.45	68,68,68,68	0
57	MG	1A	3584	1/1	0.96	0.06	33,33,33,33	0
57	MG	1A	3872	1/1	0.96	0.05	42,42,42,42	0
57	MG	1A	3677	1/1	0.96	0.05	19,19,19,19	0
57	MG	1A	3324	1/1	0.96	0.13	50,50,50,50	0
57	MG	1A	3878	1/1	0.96	0.21	51,51,51,51	0
57	MG	1A	3149	1/1	0.96	0.15	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2a	1605	1/1	0.96	0.24	52,52,52,52	0
57	MG	2a	1606	1/1	0.96	0.34	65,65,65,65	0
57	MG	2A	3027	1/1	0.96	0.08	43,43,43,43	0
57	MG	2A	3028	1/1	0.96	0.10	55,55,55,55	0
57	MG	2A	3029	1/1	0.96	0.08	53,53,53,53	0
57	MG	2q	202	1/1	0.96	0.05	77,77,77,77	0
57	MG	1A	3088	1/1	0.96	0.21	30,30,30,30	0
57	MG	1A	3046	1/1	0.96	0.22	52,52,52,52	0
57	MG	1A	3589	1/1	0.96	0.08	23,23,23,23	0
57	MG	1Q	205	1/1	0.96	0.07	51,51,51,51	0
57	MG	1A	3047	1/1	0.96	0.08	39,39,39,39	0
57	MG	1A	4100	1/1	0.96	0.27	49,49,49,49	0
57	MG	1A	3771	1/1	0.96	0.07	41,41,41,41	0
57	MG	2A	3741	1/1	0.96	0.07	43,43,43,43	0
57	MG	1A	3024	1/1	0.96	0.23	33,33,33,33	0
57	MG	2A	3744	1/1	0.96	0.06	37,37,37,37	0
57	MG	2x	106	1/1	0.96	0.17	69,69,69,69	0
57	MG	2A	3745	1/1	0.96	0.08	57,57,57,57	0
57	MG	1A	3996	1/1	0.96	0.14	56,56,56,56	0
57	MG	1A	3159	1/1	0.96	0.07	31,31,31,31	0
57	MG	2y	3004	1/1	0.96	0.25	64,64,64,64	0
57	MG	2A	3550	1/1	0.96	0.05	40,40,40,40	0
57	MG	1A	3505	1/1	0.96	0.08	41,41,41,41	0
57	MG	1A	3284	1/1	0.96	0.09	63,63,63,63	0
57	MG	1U	201	1/1	0.96	0.19	38,38,38,38	0
57	MG	1A	3285	1/1	0.96	0.09	55,55,55,55	0
57	MG	1A	3094	1/1	0.96	0.28	41,41,41,41	0
57	MG	1a	1697	1/1	0.96	0.06	60,60,60,60	0
57	MG	1V	201	1/1	0.96	0.25	47,47,47,47	0
59	ZN	2n	501	1/1	0.96	0.07	106,106,106,106	0
57	MG	1A	3666	1/1	0.97	0.09	19,19,19,19	0
57	MG	1A	3082	1/1	0.97	0.04	40,40,40,40	0
57	MG	1A	3007	1/1	0.97	0.17	34,34,34,34	0
57	MG	1A	3670	1/1	0.97	0.06	50,50,50,50	0
57	MG	1a	1862	1/1	0.97	0.07	34,34,34,34	0
57	MG	1A	4101	1/1	0.97	0.36	32,32,32,32	0
57	MG	1G	3005	1/1	0.97	0.05	64,64,64,64	0
57	MG	1A	3442	1/1	0.97	0.09	44,44,44,44	0
57	MG	1A	4103	1/1	0.97	0.14	38,38,38,38	0
57	MG	2A	3418	1/1	0.97	0.18	58,58,58,58	0
57	MG	1A	4104	1/1	0.97	0.14	53,53,53,53	0
57	MG	2A	3032	1/1	0.97	0.07	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3537	1/1	0.97	0.05	32,32,32,32	0
57	MG	2a	1697	1/1	0.97	0.08	70,70,70,70	0
57	MG	1A	3673	1/1	0.97	0.07	17,17,17,17	0
57	MG	1A	3022	1/1	0.97	0.22	32,32,32,32	0
57	MG	1A	3171	1/1	0.97	0.24	44,44,44,44	0
57	MG	2D	302	1/1	0.97	0.06	33,33,33,33	0
57	MG	1A	3366	1/1	0.97	0.14	34,34,34,34	0
57	MG	1A	3367	1/1	0.97	0.26	39,39,39,39	0
57	MG	2a	1704	1/1	0.97	0.10	72,72,72,72	0
57	MG	2A	3429	1/1	0.97	0.08	42,42,42,42	0
57	MG	1A	3543	1/1	0.97	0.09	34,34,34,34	0
57	MG	1A	3071	1/1	0.97	0.13	39,39,39,39	0
57	MG	1A	3122	1/1	0.97	0.21	34,34,34,34	0
57	MG	1A	3750	1/1	0.97	0.11	39,39,39,39	0
57	MG	2A	3170	1/1	0.97	0.10	44,44,44,44	0
57	MG	1P	202	1/1	0.97	0.04	35,35,35,35	0
57	MG	1A	3233	1/1	0.97	0.12	34,34,34,34	0
57	MG	1A	3493	1/1	0.97	0.05	34,34,34,34	0
57	MG	1A	3087	1/1	0.97	0.23	39,39,39,39	0
57	MG	2A	3736	1/1	0.97	0.06	60,60,60,60	0
57	MG	1a	1768	1/1	0.97	0.05	75,75,75,75	0
57	MG	1A	3837	1/1	0.97	0.08	62,62,62,62	0
57	MG	1A	3010	1/1	0.97	0.09	57,57,57,57	0
57	MG	1A	3612	1/1	0.97	0.08	47,47,47,47	0
57	MG	2A	3445	1/1	0.97	0.05	29,29,29,29	0
57	MG	1A	3758	1/1	0.97	0.08	44,44,44,44	0
57	MG	2A	3052	1/1	0.97	0.20	62,62,62,62	0
57	MG	1A	4025	1/1	0.97	0.06	73,73,73,73	0
57	MG	1A	3125	1/1	0.97	0.13	29,29,29,29	0
57	MG	2A	3450	1/1	0.97	0.13	49,49,49,49	0
57	MG	1a	1661	1/1	0.97	0.21	61,61,61,61	0
57	MG	1A	3177	1/1	0.97	0.17	45,45,45,45	0
57	MG	2A	3453	1/1	0.97	0.09	52,52,52,52	0
57	MG	2A	3454	1/1	0.97	0.12	64,64,64,64	0
57	MG	2A	3753	1/1	0.97	0.06	65,65,65,65	0
57	MG	1A	3761	1/1	0.97	0.05	23,23,23,23	0
57	MG	1A	3762	1/1	0.97	0.09	25,25,25,25	0
57	MG	2A	3760	1/1	0.97	0.09	51,51,51,51	0
57	MG	2A	3457	1/1	0.97	0.12	52,52,52,52	0
57	MG	2a	1736	1/1	0.97	0.15	67,67,67,67	0
57	MG	1A	3089	1/1	0.97	0.15	39,39,39,39	0
57	MG	1A	3061	1/1	0.97	0.13	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	2W	3002	1/1	0.97	0.09	52,52,52,52	0
57	MG	2A	3061	1/1	0.97	0.05	41,41,41,41	0
57	MG	2A	3190	1/1	0.97	0.20	56,56,56,56	0
57	MG	1A	3554	1/1	0.97	0.08	41,41,41,41	0
57	MG	1A	3153	1/1	0.97	0.21	29,29,29,29	0
57	MG	1a	1787	1/1	0.97	0.04	77,77,77,77	0
57	MG	1A	3030	1/1	0.97	0.04	34,34,34,34	0
57	MG	1A	3504	1/1	0.97	0.09	17,17,17,17	0
57	MG	2A	3467	1/1	0.97	0.16	58,58,58,58	0
57	MG	2A	3068	1/1	0.97	0.08	45,45,45,45	0
57	MG	1A	3155	1/1	0.97	0.05	39,39,39,39	0
57	MG	1A	3627	1/1	0.97	0.18	29,29,29,29	0
57	MG	1A	3561	1/1	0.97	0.09	18,18,18,18	0
57	MG	1A	4147	1/1	0.97	0.11	34,34,34,34	0
57	MG	1A	3701	1/1	0.97	0.06	33,33,33,33	0
57	MG	1A	3954	1/1	0.97	0.05	36,36,36,36	0
57	MG	1a	1906	1/1	0.97	0.07	48,48,48,48	0
57	MG	1X	3002	1/1	0.97	0.14	39,39,39,39	0
57	MG	1a	1797	1/1	0.97	0.07	72,72,72,72	0
57	MG	1X	3003	1/1	0.97	0.08	51,51,51,51	0
57	MG	1A	3110	1/1	0.97	0.10	16,16,16,16	0
57	MG	1A	3858	1/1	0.97	0.12	18,18,18,18	0
57	MG	2A	3788	1/1	0.97	0.07	63,63,63,63	0
57	MG	2A	3081	1/1	0.97	0.07	45,45,45,45	0
57	MG	1Y	201	1/1	0.97	0.19	52,52,52,52	0
57	MG	2A	3483	1/1	0.97	0.14	61,61,61,61	0
57	MG	1A	3031	1/1	0.97	0.29	34,34,34,34	0
57	MG	1a	1803	1/1	0.97	0.05	61,61,61,61	0
57	MG	1A	3631	1/1	0.97	0.06	55,55,55,55	0
57	MG	1A	3566	1/1	0.97	0.06	28,28,28,28	0
57	MG	1A	3567	1/1	0.97	0.05	25,25,25,25	0
57	MG	1A	3093	1/1	0.97	0.18	40,40,40,40	0
57	MG	1A	3868	1/1	0.97	0.05	41,41,41,41	0
57	MG	1A	4050	1/1	0.97	0.06	34,34,34,34	0
57	MG	1A	3636	1/1	0.97	0.04	40,40,40,40	0
57	MG	1A	3012	1/1	0.97	0.15	48,48,48,48	0
57	MG	1A	3785	1/1	0.97	0.06	82,82,82,82	0
57	MG	1A	3966	1/1	0.97	0.05	55,55,55,55	0
57	MG	2A	3223	1/1	0.97	0.16	36,36,36,36	0
57	MG	1B	214	1/1	0.97	0.06	51,51,51,51	0
57	MG	1A	3314	1/1	0.97	0.11	40,40,40,40	0
57	MG	1A	3187	1/1	0.97	0.11	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	3808	1/1	0.97	0.08	64,64,64,64	0
57	MG	1A	3876	1/1	0.97	0.08	66,66,66,66	0
57	MG	2A	3810	1/1	0.97	0.09	61,61,61,61	0
57	MG	13	102	1/1	0.97	0.10	45,45,45,45	0
57	MG	2A	3650	1/1	0.97	0.09	46,46,46,46	0
57	MG	2A	3503	1/1	0.97	0.07	63,63,63,63	0
57	MG	1A	3573	1/1	0.97	0.05	43,43,43,43	0
57	MG	1A	3055	1/1	0.97	0.09	28,28,28,28	0
57	MG	1A	3880	1/1	0.97	0.09	59,59,59,59	0
57	MG	1A	3885	1/1	0.97	0.08	55,55,55,55	0
57	MG	1A	3886	1/1	0.97	0.05	52,52,52,52	0
57	MG	1w	107	1/1	0.97	0.06	49,49,49,49	0
57	MG	2A	3820	1/1	0.97	0.11	54,54,54,54	0
57	MG	1A	3575	1/1	0.97	0.07	27,27,27,27	0
57	MG	1A	3283	1/1	0.97	0.06	39,39,39,39	0
57	MG	1A	3189	1/1	0.97	0.16	34,34,34,34	0
57	MG	2A	3109	1/1	0.97	0.10	39,39,39,39	0
57	MG	1A	3253	1/1	0.97	0.06	48,48,48,48	0
57	MG	1A	3471	1/1	0.97	0.17	28,28,28,28	0
57	MG	1A	3219	1/1	0.97	0.16	40,40,40,40	0
57	MG	1A	3583	1/1	0.97	0.05	42,42,42,42	0
57	MG	1A	3190	1/1	0.97	0.14	35,35,35,35	0
57	MG	1A	3895	1/1	0.97	0.04	32,32,32,32	0
57	MG	2A	3522	1/1	0.97	0.05	73,73,73,73	0
57	MG	2A	3670	1/1	0.97	0.06	54,54,54,54	0
57	MG	2f	3001	1/1	0.97	0.09	58,58,58,58	0
57	MG	1A	3524	1/1	0.97	0.14	32,32,32,32	0
57	MG	1A	3525	1/1	0.97	0.08	25,25,25,25	0
57	MG	1B	236	1/1	0.97	0.05	33,33,33,33	0
57	MG	1a	1715	1/1	0.97	0.11	63,63,63,63	0
57	MG	1A	3137	1/1	0.97	0.30	32,32,32,32	0
57	MG	2A	3250	1/1	0.97	0.09	73,73,73,73	0
57	MG	1A	3899	1/1	0.97	0.07	22,22,22,22	0
57	MG	1A	3801	1/1	0.97	0.07	65,65,65,65	0
57	MG	2A	3531	1/1	0.97	0.08	42,42,42,42	0
57	MG	2A	3123	1/1	0.97	0.07	46,46,46,46	0
57	MG	1A	3803	1/1	0.97	0.05	36,36,36,36	0
57	MG	1A	3902	1/1	0.97	0.08	58,58,58,58	0
57	MG	1A	3804	1/1	0.97	0.04	29,29,29,29	0
57	MG	2A	3846	1/1	0.97	0.10	80,80,80,80	0
57	MG	1a	1723	1/1	0.97	0.16	62,62,62,62	0
57	MG	2A	3128	1/1	0.97	0.14	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1a	1618	1/1	0.97	0.06	46,46,46,46	0
57	MG	1A	3138	1/1	0.97	0.18	36,36,36,36	0
57	MG	1A	3056	1/1	0.97	0.08	41,41,41,41	0
57	MG	1A	4083	1/1	0.97	0.09	57,57,57,57	0
57	MG	1A	3225	1/1	0.97	0.38	35,35,35,35	0
57	MG	1A	3057	1/1	0.97	0.15	45,45,45,45	0
57	MG	1A	3908	1/1	0.97	0.13	56,56,56,56	0
57	MG	1E	310	1/1	0.97	0.12	61,61,61,61	0
57	MG	1A	3480	1/1	0.97	0.15	38,38,38,38	0
57	MG	1A	3361	1/1	0.97	0.13	46,46,46,46	0
57	MG	1A	3663	1/1	0.97	0.08	46,46,46,46	0
57	MG	2A	3014	1/1	0.97	0.08	36,36,36,36	0
57	MG	1A	3438	1/1	0.97	0.20	31,31,31,31	0
57	MG	2A	3016	1/1	0.97	0.04	37,37,37,37	0
57	MG	1A	3665	1/1	0.97	0.07	57,57,57,57	0
57	MG	1A	3915	1/1	0.97	0.19	33,33,33,33	0
57	MG	2A	3405	1/1	0.97	0.14	22,22,22,22	0
59	ZN	2Y	501	1/1	0.97	0.05	94,94,94,94	0
57	MG	2A	3020	1/1	0.97	0.22	56,56,56,56	0
57	MG	2A	3021	1/1	0.97	0.30	50,50,50,50	0
60	SF4	1d	501	8/8	0.97	0.06	63,72,78,81	0
57	MG	1Y	204	1/1	0.98	0.12	46,46,46,46	0
57	MG	2A	3658	1/1	0.98	0.24	47,47,47,47	0
57	MG	1A	3658	1/1	0.98	0.04	40,40,40,40	0
57	MG	1A	4078	1/1	0.98	0.06	44,44,44,44	0
57	MG	2A	3538	1/1	0.98	0.10	39,39,39,39	0
57	MG	1a	1907	1/1	0.98	0.16	46,46,46,46	0
57	MG	2A	3066	1/1	0.98	0.16	51,51,51,51	0
57	MG	1A	3238	1/1	0.98	0.04	37,37,37,37	0
57	MG	1A	3932	1/1	0.98	0.09	56,56,56,56	0
57	MG	1A	3239	1/1	0.98	0.19	36,36,36,36	0
57	MG	1A	3041	1/1	0.98	0.05	24,24,24,24	0
57	MG	1A	3006	1/1	0.98	0.03	24,24,24,24	0
57	MG	1A	3607	1/1	0.98	0.04	25,25,25,25	0
57	MG	1A	3516	1/1	0.98	0.04	17,17,17,17	0
57	MG	1A	3517	1/1	0.98	0.06	51,51,51,51	0
57	MG	1A	3859	1/1	0.98	0.05	34,34,34,34	0
57	MG	2A	3426	1/1	0.98	0.18	26,26,26,26	0
57	MG	1A	3562	1/1	0.98	0.07	27,27,27,27	0
57	MG	1A	3333	1/1	0.98	0.04	33,33,33,33	0
57	MG	12	3002	1/1	0.98	0.15	42,42,42,42	0
57	MG	1A	3668	1/1	0.98	0.06	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3302	1/1	0.98	0.03	26,26,26,26	0
57	MG	1A	3001	1/1	0.98	0.05	50,50,50,50	0
57	MG	1B	235	1/1	0.98	0.04	40,40,40,40	0
57	MG	1A	4094	1/1	0.98	0.09	43,43,43,43	0
57	MG	17	101	1/1	0.98	0.05	45,45,45,45	0
57	MG	2A	3437	1/1	0.98	0.06	60,60,60,60	0
57	MG	1A	3866	1/1	0.98	0.05	28,28,28,28	0
57	MG	1A	4096	1/1	0.98	0.15	36,36,36,36	0
57	MG	1D	3003	1/1	0.98	0.03	18,18,18,18	0
57	MG	1A	3614	1/1	0.98	0.05	21,21,21,21	0
57	MG	1D	3006	1/1	0.98	0.07	34,34,34,34	0
57	MG	1D	3007	1/1	0.98	0.18	47,47,47,47	0
57	MG	1A	3615	1/1	0.98	0.09	24,24,24,24	0
57	MG	1A	4099	1/1	0.98	0.12	34,34,34,34	0
57	MG	2A	3692	1/1	0.98	0.04	69,69,69,69	0
57	MG	1A	3140	1/1	0.98	0.05	35,35,35,35	0
57	MG	1A	3478	1/1	0.98	0.11	32,32,32,32	0
57	MG	1A	3618	1/1	0.98	0.06	56,56,56,56	0
57	MG	1A	3119	1/1	0.98	0.08	38,38,38,38	0
57	MG	1E	305	1/1	0.98	0.11	33,33,33,33	0
57	MG	1A	3008	1/1	0.98	0.06	33,33,33,33	0
57	MG	1a	1609	1/1	0.98	0.06	51,51,51,51	0
57	MG	1a	1610	1/1	0.98	0.09	24,24,24,24	0
57	MG	1E	307	1/1	0.98	0.07	29,29,29,29	0
57	MG	1A	4026	1/1	0.98	0.04	46,46,46,46	0
57	MG	1a	1613	1/1	0.98	0.04	58,58,58,58	0
57	MG	1A	3877	1/1	0.98	0.05	77,77,77,77	0
57	MG	1A	3678	1/1	0.98	0.07	24,24,24,24	0
57	MG	1A	3737	1/1	0.98	0.11	41,41,41,41	0
57	MG	1A	3191	1/1	0.98	0.28	37,37,37,37	0
57	MG	1A	3882	1/1	0.98	0.05	37,37,37,37	0
57	MG	1A	3247	1/1	0.98	0.21	49,49,49,49	0
57	MG	1A	3033	1/1	0.98	0.04	32,32,32,32	0
57	MG	1A	3168	1/1	0.98	0.29	35,35,35,35	0
57	MG	1A	3808	1/1	0.98	0.05	45,45,45,45	0
57	MG	2A	3589	1/1	0.98	0.15	40,40,40,40	0
57	MG	1A	3576	1/1	0.98	0.04	25,25,25,25	0
57	MG	1A	3015	1/1	0.98	0.04	18,18,18,18	0
57	MG	1A	3003	1/1	0.98	0.04	41,41,41,41	0
57	MG	1A	4118	1/1	0.98	0.09	36,36,36,36	0
57	MG	1A	3686	1/1	0.98	0.11	25,25,25,25	0
57	MG	1A	4120	1/1	0.98	0.15	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	4121	1/1	0.98	0.19	31,31,31,31	0
57	MG	2A	3004	1/1	0.98	0.05	46,46,46,46	0
57	MG	1A	3687	1/1	0.98	0.05	39,39,39,39	0
57	MG	1A	4123	1/1	0.98	0.29	33,33,33,33	0
57	MG	1A	3815	1/1	0.98	0.06	58,58,58,58	0
57	MG	2A	3009	1/1	0.98	0.09	50,50,50,50	0
57	MG	2A	3727	1/1	0.98	0.05	67,67,67,67	0
57	MG	1A	3005	1/1	0.98	0.12	42,42,42,42	0
57	MG	1A	4126	1/1	0.98	0.21	38,38,38,38	0
57	MG	1a	1742	1/1	0.98	0.08	57,57,57,57	0
57	MG	1a	1743	1/1	0.98	0.05	41,41,41,41	0
57	MG	1A	3748	1/1	0.98	0.14	37,37,37,37	0
57	MG	1A	3378	1/1	0.98	0.04	37,37,37,37	0
57	MG	1A	3223	1/1	0.98	0.10	44,44,44,44	0
57	MG	1A	3633	1/1	0.98	0.04	34,34,34,34	0
57	MG	1A	3582	1/1	0.98	0.08	20,20,20,20	0
57	MG	1A	3753	1/1	0.98	0.05	40,40,40,40	0
57	MG	1A	3823	1/1	0.98	0.06	65,65,65,65	0
57	MG	1A	4136	1/1	0.98	0.15	45,45,45,45	0
57	MG	1A	3107	1/1	0.98	0.04	38,38,38,38	0
57	MG	1A	3026	1/1	0.98	0.04	37,37,37,37	0
57	MG	1A	4139	1/1	0.98	0.07	37,37,37,37	0
57	MG	2A	3743	1/1	0.98	0.08	44,44,44,44	0
57	MG	1A	3637	1/1	0.98	0.04	46,46,46,46	0
57	MG	1A	3109	1/1	0.98	0.12	34,34,34,34	0
57	MG	1A	3064	1/1	0.98	0.14	32,32,32,32	0
57	MG	1A	4143	1/1	0.98	0.26	37,37,37,37	0
57	MG	2A	3145	1/1	0.98	0.10	38,38,38,38	0
57	MG	1A	3494	1/1	0.98	0.10	35,35,35,35	0
57	MG	1A	3909	1/1	0.98	0.04	38,38,38,38	0
57	MG	1A	3027	1/1	0.98	0.05	20,20,20,20	0
57	MG	1a	1763	1/1	0.98	0.05	65,65,65,65	0
57	MG	2A	3755	1/1	0.98	0.05	55,55,55,55	0
57	MG	2E	301	1/1	0.98	0.17	59,59,59,59	0
57	MG	2A	3757	1/1	0.98	0.05	68,68,68,68	0
57	MG	1A	3152	1/1	0.98	0.21	37,37,37,37	0
57	MG	1A	3203	1/1	0.98	0.17	33,33,33,33	0
57	MG	1A	3645	1/1	0.98	0.09	44,44,44,44	0
57	MG	1A	3591	1/1	0.98	0.04	10,10,10,10	0
57	MG	1A	3011	1/1	0.98	0.10	43,43,43,43	0
57	MG	1a	1771	1/1	0.98	0.04	60,60,60,60	0
57	MG	1A	3916	1/1	0.98	0.05	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1U	203	1/1	0.98	0.24	37,37,37,37	0
57	MG	1A	3096	1/1	0.98	0.21	40,40,40,40	0
57	MG	2A	3768	1/1	0.98	0.06	72,72,72,72	0
57	MG	1U	205	1/1	0.98	0.21	30,30,30,30	0
57	MG	1U	206	1/1	0.98	0.20	40,40,40,40	0
57	MG	2A	3771	1/1	0.98	0.06	52,52,52,52	0
57	MG	1A	3389	1/1	0.98	0.12	42,42,42,42	0
57	MG	2A	3639	1/1	0.98	0.04	33,33,33,33	0
57	MG	1A	3133	1/1	0.98	0.21	42,42,42,42	0
57	MG	1a	1779	1/1	0.98	0.05	68,68,68,68	0
57	MG	1A	3019	1/1	0.98	0.14	31,31,31,31	0
57	MG	1a	1781	1/1	0.98	0.04	55,55,55,55	0
57	MG	1A	3158	1/1	0.98	0.07	30,30,30,30	0
57	MG	1W	203	1/1	0.98	0.12	38,38,38,38	0
57	MG	1W	204	1/1	0.98	0.19	34,34,34,34	0
57	MG	1A	3466	1/1	0.98	0.09	41,41,41,41	0
57	MG	1A	3083	1/1	0.98	0.22	40,40,40,40	0
57	MG	1A	3844	1/1	0.98	0.07	30,30,30,30	0
57	MG	1A	3508	1/1	0.98	0.14	39,39,39,39	0
57	MG	1A	3394	1/1	0.98	0.08	36,36,36,36	0
57	MG	1A	3777	1/1	0.98	0.08	48,48,48,48	0
59	ZN	14	501	1/1	0.98	0.05	99,99,99,99	0
57	MG	1X	3006	1/1	0.98	0.05	35,35,35,35	0
57	MG	1A	3136	1/1	0.98	0.17	40,40,40,40	0
59	ZN	25	101	1/1	0.98	0.06	59,59,59,59	0
57	MG	1A	3779	1/1	0.98	0.05	29,29,29,29	0
57	MG	2A	3293	1/1	0.98	0.05	58,58,58,58	0
60	SF4	2d	501	8/8	0.98	0.05	66,75,87,95	0
57	MG	2A	3414	1/1	0.99	0.03	64,64,64,64	0
57	MG	1A	3780	1/1	0.99	0.05	30,30,30,30	0
57	MG	1A	3881	1/1	0.99	0.03	52,52,52,52	0
57	MG	1A	4086	1/1	0.99	0.10	30,30,30,30	0
57	MG	2A	3709	1/1	0.99	0.05	76,76,76,76	0
57	MG	1A	3572	1/1	0.99	0.08	18,18,18,18	0
57	MG	2A	3764	1/1	0.99	0.03	35,35,35,35	0
57	MG	1A	3884	1/1	0.99	0.06	46,46,46,46	0
57	MG	1A	3557	1/1	0.99	0.05	19,19,19,19	0
57	MG	1A	3051	1/1	0.99	0.08	18,18,18,18	0
57	MG	2A	3333	1/1	0.99	0.08	41,41,41,41	0
57	MG	1A	3830	1/1	0.99	0.06	64,64,64,64	0
57	MG	1B	205	1/1	0.99	0.05	45,45,45,45	0
57	MG	1D	3005	1/1	0.99	0.13	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	3624	1/1	0.99	0.04	54,54,54,54	0
57	MG	2A	3427	1/1	0.99	0.08	71,71,71,71	0
57	MG	1A	3512	1/1	0.99	0.09	26,26,26,26	0
57	MG	1A	3560	1/1	0.99	0.05	34,34,34,34	0
57	MG	1A	3126	1/1	0.99	0.17	32,32,32,32	0
57	MG	1A	3157	1/1	0.99	0.16	24,24,24,24	0
57	MG	2A	3625	1/1	0.99	0.06	30,30,30,30	0
57	MG	2a	1706	1/1	0.99	0.04	73,73,73,73	0
57	MG	1a	1757	1/1	0.99	0.04	49,49,49,49	0
57	MG	1A	3439	1/1	0.99	0.30	31,31,31,31	0
57	MG	1A	4128	1/1	0.99	0.10	31,31,31,31	0
57	MG	1A	3081	1/1	0.99	0.15	28,28,28,28	0
57	MG	1A	3814	1/1	0.99	0.04	51,51,51,51	0
57	MG	2A	3131	1/1	0.99	0.05	55,55,55,55	0
57	MG	1a	1722	1/1	0.99	0.06	36,36,36,36	0
57	MG	1A	3688	1/1	0.99	0.05	30,30,30,30	0
57	MG	1a	1764	1/1	0.99	0.04	49,49,49,49	0
57	MG	2A	3441	1/1	0.99	0.04	48,48,48,48	0
57	MG	2A	3008	1/1	0.99	0.05	45,45,45,45	0
57	MG	1A	3565	1/1	0.99	0.05	21,21,21,21	0
57	MG	1A	3495	1/1	0.99	0.06	42,42,42,42	0
57	MG	1A	4134	1/1	0.99	0.14	32,32,32,32	0
57	MG	1A	3540	1/1	0.99	0.04	29,29,29,29	0
57	MG	1a	1769	1/1	0.99	0.04	54,54,54,54	0
57	MG	1A	3870	1/1	0.99	0.05	35,35,35,35	0
57	MG	1A	3073	1/1	0.99	0.12	21,21,21,21	0
57	MG	1F	303	1/1	0.99	0.14	31,31,31,31	0
57	MG	2A	3017	1/1	0.99	0.04	46,46,46,46	0
57	MG	1A	3004	1/1	0.99	0.04	24,24,24,24	0
57	MG	1A	3775	1/1	0.99	0.07	41,41,41,41	0
57	MG	1A	3874	1/1	0.99	0.02	56,56,56,56	0
57	MG	1A	3846	1/1	0.99	0.07	25,25,25,25	0
57	MG	1A	3443	1/1	0.99	0.11	47,47,47,47	0
59	ZN	1Y	202	1/1	0.99	0.02	63,63,63,63	0
57	MG	1A	3619	1/1	0.99	0.03	53,53,53,53	0
59	ZN	1n	501	1/1	0.99	0.03	67,67,67,67	0
57	MG	1A	3638	1/1	0.99	0.06	24,24,24,24	0
57	MG	2A	3508	1/1	0.99	0.03	46,46,46,46	0
57	MG	2A	3754	1/1	0.99	0.04	43,43,43,43	0
59	ZN	26	501	1/1	0.99	0.04	67,67,67,67	0
59	ZN	29	102	1/1	0.99	0.04	70,70,70,70	0
57	MG	1A	3053	1/1	0.99	0.05	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	3756	1/1	0.99	0.04	46,46,46,46	0
57	MG	1A	4146	1/1	0.99	0.02	29,29,29,29	0
57	MG	1a	1730	1/1	1.00	0.06	35,35,35,35	0
57	MG	1A	3802	1/1	1.00	0.05	24,24,24,24	0
57	MG	1A	3756	1/1	1.00	0.07	27,27,27,27	0
59	ZN	15	101	1/1	1.00	0.04	43,43,43,43	0
59	ZN	16	101	1/1	1.00	0.06	45,45,45,45	0
59	ZN	19	102	1/1	1.00	0.06	47,47,47,47	0
57	MG	1A	3861	1/1	1.00	0.02	58,58,58,58	0
57	MG	2A	3507	1/1	1.00	0.07	37,37,37,37	0
57	MG	1B	225	1/1	1.00	0.02	33,33,33,33	0
57	MG	1A	3507	1/1	1.00	0.07	34,34,34,34	0
57	MG	2A	3752	1/1	1.00	0.07	36,36,36,36	0
57	MG	1A	3867	1/1	1.00	0.02	27,27,27,27	0
57	MG	1A	3883	1/1	1.00	0.03	17,17,17,17	0
57	MG	2A	3501	1/1	1.00	0.03	37,37,37,37	0
57	MG	1a	1729	1/1	1.00	0.06	39,39,39,39	0

6.5 Other polymers (i)

There are no such residues in this entry.