



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 19, 2020 – 12:51 PM BST

PDB ID : 6XQE
Title : Crystal structure of the *Thermus thermophilus* 70S ribosome in complex with sarecycline, UAA-mRNA, and deacylated P-site tRNA at 3.00Å resolution
Authors : Batool, Z.; Lomakin, I.B.; Bunick, C.G.; Polikanov, Y.S.
Deposited on : 2020-07-09
Resolution : 3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.14.6
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.14.6

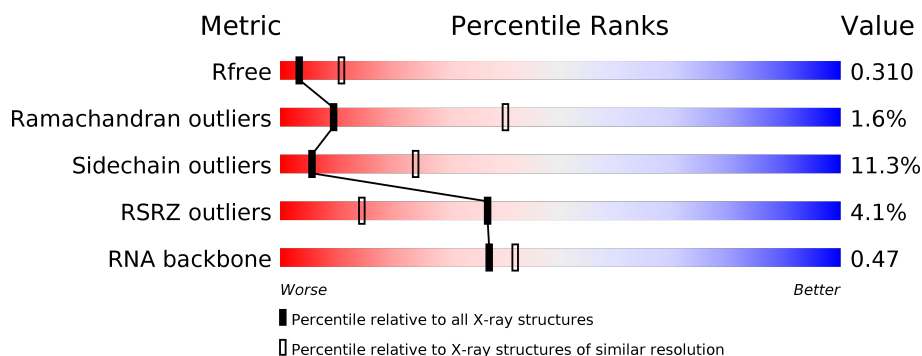
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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.



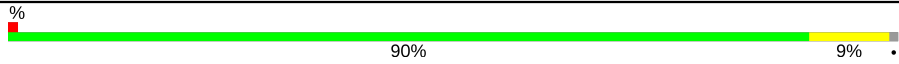

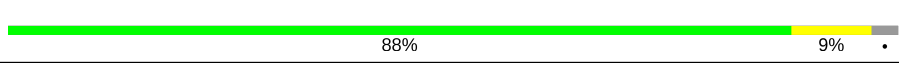

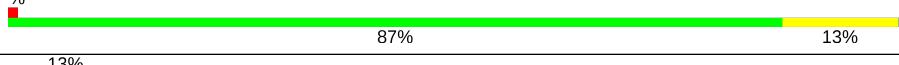
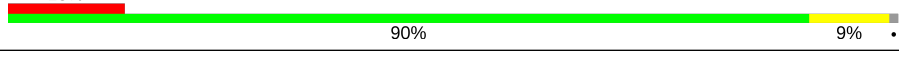
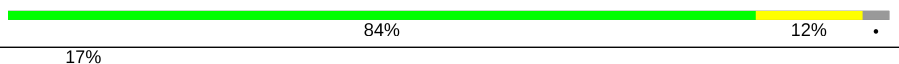

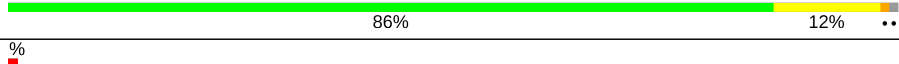

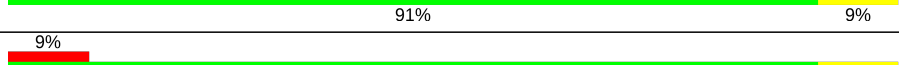
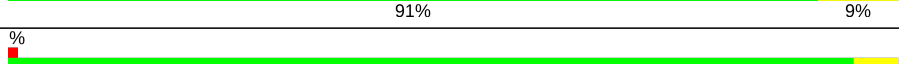
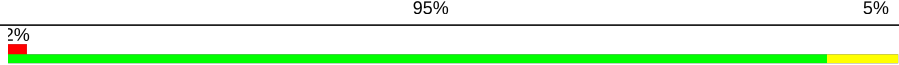
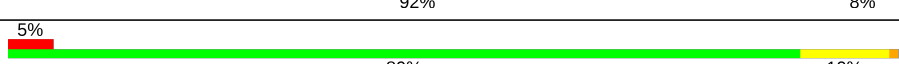
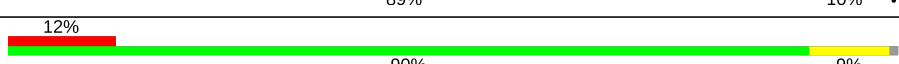
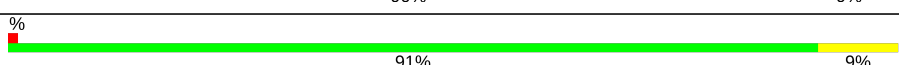
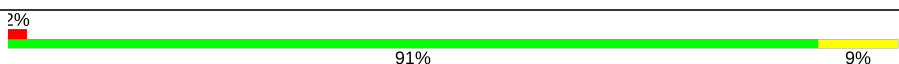
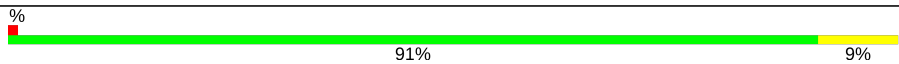
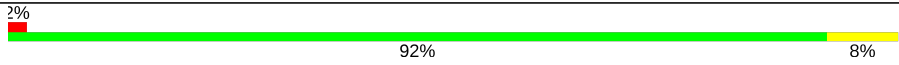

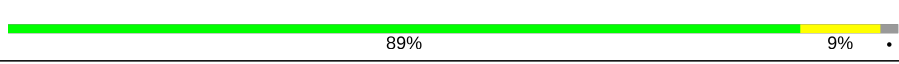
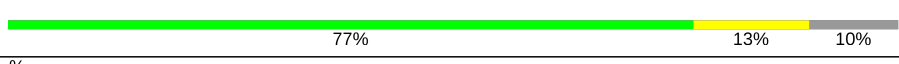
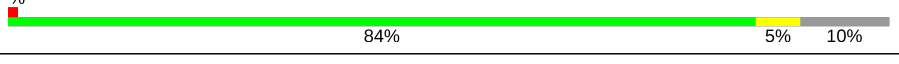
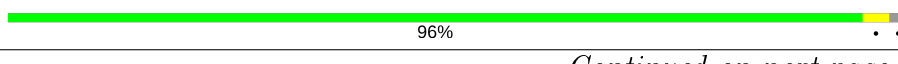

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)
RNA backbone	3102	1173 (3.30-2.70)

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 on 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 $\leq 5\%$. 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	<div> <div>78%</div> <div>20%</div> <div>..</div> </div>
1	2A	2915	<div> <div>75%</div> <div>21%</div> <div>.</div> </div>
2	1B	121	<div> <div>91%</div> <div>7%</div> <div>..</div> </div>
2	2B	121	<div> <div>71%</div> <div>28%</div> <div>.</div> </div>
3	1D	276	<div> <div>91%</div> <div>9%</div> </div>
3	2D	276	<div> <div>%</div> <div>93%</div> <div>7%</div> </div>

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Mol	Chain	Length	Quality of chain
4	1E	206	
4	2E	206	
5	1F	210	
5	2F	210	
6	1G	182	
6	2G	182	
7	1H	180	
7	2H	180	
8	1I	148	
8	2I	148	
9	1N	140	
9	2N	140	
10	1O	122	
10	2O	122	
11	1P	150	
11	2P	150	
12	1Q	141	
12	2Q	141	
13	1R	118	
13	2R	118	
14	1S	112	
14	2S	112	
15	1T	146	
15	2T	146	
16	1U	118	

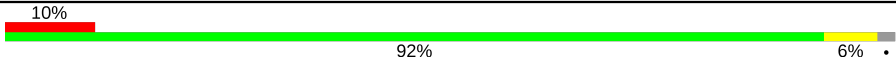
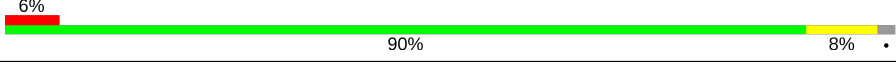
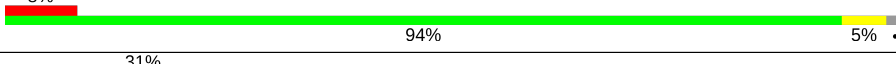
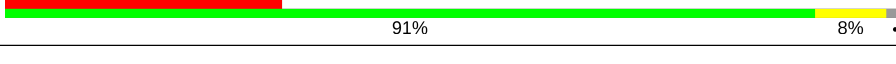
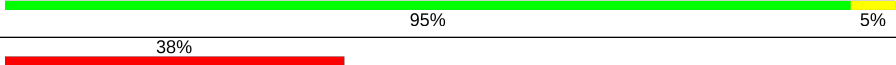
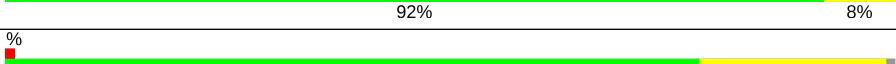
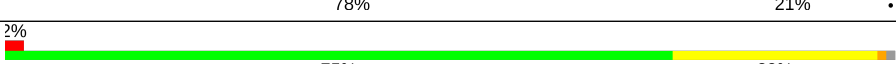
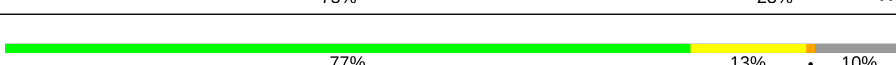
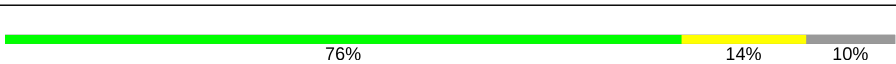


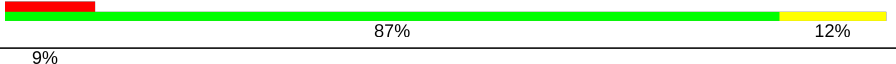
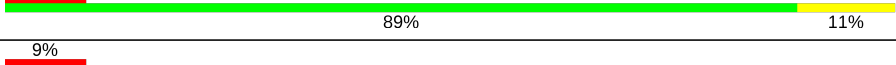
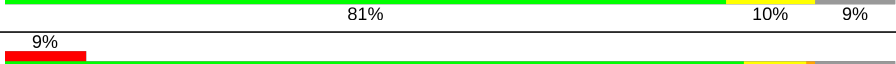
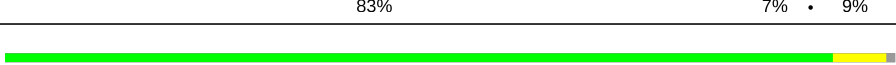
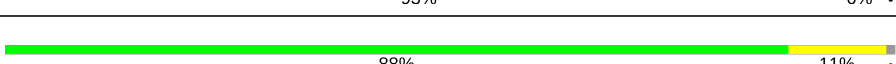


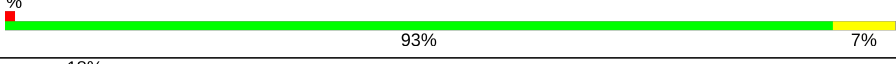
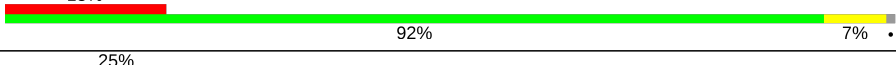





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Mol	Chain	Length	Quality of chain
16	2U	118	
17	1V	101	
17	2V	101	
18	1W	113	
18	2W	113	
19	1X	96	
19	2X	96	
20	1Y	110	
20	2Y	110	
21	1Z	206	
21	2Z	206	
22	10	85	
22	20	85	
23	11	98	
23	21	98	
24	12	72	
24	22	72	
25	13	60	
25	23	60	
26	14	71	
26	24	71	
27	15	60	
27	25	60	
28	16	54	
28	26	54	

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Mol	Chain	Length	Quality of chain
29	17	49	
29	27	49	
30	18	65	
30	28	65	
31	19	37	
31	29	37	
32	1a	1521	
32	2a	1521	
33	1b	256	
33	2b	256	
34	1c	239	
34	2c	239	
35	1d	209	
35	2d	209	
36	1e	162	
36	2e	162	
37	1f	101	
37	2f	101	
38	1g	156	
38	2g	156	
39	1h	138	
39	2h	138	
40	1i	128	
40	2i	128	
41	1j	105	

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Mol	Chain	Length	Quality of chain
41	2j	105	
42	1k	129	
42	2k	129	
43	1l	132	
43	2l	132	
44	1m	126	
44	2m	126	
45	1n	61	
45	2n	61	
46	1o	89	
46	2o	89	
47	1p	88	
47	2p	88	
48	1q	105	
48	2q	105	
49	1r	88	
49	2r	88	
50	1s	93	
50	2s	93	
51	1t	106	
51	2t	106	
52	1u	27	
52	2u	27	
53	1v	24	
53	2v	24	

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Mol	Chain	Length	Quality of chain
54	1x	77	
54	2x	77	

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
55	MG	1A	3304	-	-	-	X
55	MG	1A	3312	-	-	-	X
55	MG	1A	3370	-	-	-	X
55	MG	1A	3842	-	-	-	X
55	MG	1O	203	-	-	-	X
55	MG	1Q	205	-	-	-	X
55	MG	1a	3061	-	-	-	X
55	MG	1a	3172	-	-	-	X
55	MG	1x	102	-	-	-	X
55	MG	2A	3195	-	-	-	X
55	MG	2A	3232	-	-	-	X
55	MG	2A	3278	-	-	-	X
55	MG	2A	3294	-	-	-	X
55	MG	2A	3539	-	-	-	X
55	MG	2a	1790	-	-	-	X
55	MG	2a	1806	-	-	-	X

2 Entry composition [i](#)

There are 60 unique types of molecules in this entry. The entry contains 292071 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	122	Total	C	N	O	S	0	0	0
			951	587	197	165	2			
44	2m	121	Total	C	N	O	S	0	0	0
			943	581	196	164	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	10	Total	C	N	O	P	0	0	0
			217	98	44	65	10			
53	2v	6	Total	C	N	O	P	0	0	0
			113	49	22	36	6			

- Molecule 54 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	1x	76	Total	C	N	O	P	S	0	0
			1625	725	294	529	76	1		
54	2x	76	Total	C	N	O	P	S	0	0
			1625	725	294	529	76	1		

- Molecule 55 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	2E	5	Total	Mg	0	0
			5	5		
55	17	7	Total	Mg	0	0
			7	7		
55	2d	2	Total	Mg	0	0
			2	2		
55	1T	2	Total	Mg	0	0
			2	2		
55	1N	5	Total	Mg	0	0
			5	5		
55	2r	1	Total	Mg	0	0
			1	1		
55	18	6	Total	Mg	0	0
			6	6		
55	2W	1	Total	Mg	0	0
			1	1		
55	1Y	2	Total	Mg	0	0
			2	2		
55	13	5	Total	Mg	0	0
			5	5		
55	1f	2	Total	Mg	0	0
			2	2		
55	1P	6	Total	Mg	0	0
			6	6		
55	2B	20	Total	Mg	0	0
			20	20		
55	2a	216	Total	Mg	0	0
			216	216		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	1E	14	Total 14	Mg 14	0	0
55	1b	1	Total 1	Mg 1	0	0
55	2l	2	Total 2	Mg 2	0	0
55	2F	6	Total 6	Mg 6	0	0
55	16	3	Total 3	Mg 3	0	0
55	28	3	Total 3	Mg 3	0	0
55	2e	2	Total 2	Mg 2	0	0
55	1W	9	Total 9	Mg 9	0	0
55	1A	1040	Total 1040	Mg 1040	0	0
55	1t	1	Total 1	Mg 1	0	0
55	1n	3	Total 3	Mg 3	0	0
55	2P	4	Total 4	Mg 4	0	0
55	1X	4	Total 4	Mg 4	0	0
55	2q	2	Total 2	Mg 2	0	0
55	12	2	Total 2	Mg 2	0	0
55	2i	1	Total 1	Mg 1	0	0
55	1S	3	Total 3	Mg 3	0	0
55	25	4	Total 4	Mg 4	0	0
55	2T	4	Total 4	Mg 4	0	0
55	1D	10	Total 10	Mg 10	0	0
55	23	3	Total 3	Mg 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
55	1e	1	Total Mg 1 1	0	0
55	2G	1	Total Mg 1 1	0	0
55	1I	1	Total Mg 1 1	0	0
55	2f	2	Total Mg 2 2	0	0
55	1V	4	Total Mg 4 4	0	0
55	2X	1	Total Mg 1 1	0	0
55	1a	212	Total Mg 212 212	0	0
55	2Q	4	Total Mg 4 4	0	0
55	15	4	Total Mg 4 4	0	0
55	1x	13	Total Mg 13 13	0	0
55	2j	2	Total Mg 2 2	0	0
55	1R	7	Total Mg 7 7	0	0
55	26	1	Total Mg 1 1	0	0
55	2U	2	Total Mg 2 2	0	0
55	1G	4	Total Mg 4 4	0	0
55	2O	1	Total Mg 1 1	0	0
55	1I	3	Total Mg 3 3	0	0
55	1d	1	Total Mg 1 1	0	0
55	2n	1	Total Mg 1 1	0	0
55	1H	2	Total Mg 2 2	0	0
55	2I	6	Total Mg 6 6	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
55	2g	1	Total Mg 1 1	0	0
55	2Y	2	Total Mg 2 2	0	0
55	1v	5	Total Mg 5 5	0	0
55	2x	7	Total Mg 7 7	0	0
55	2R	1	Total Mg 1 1	0	0
55	1Z	3	Total Mg 3 3	0	0
55	2D	8	Total Mg 8 8	0	0
55	14	1	Total Mg 1 1	0	0
55	2k	1	Total Mg 1 1	0	0
55	1U	8	Total Mg 8 8	0	0
55	1O	5	Total Mg 5 5	0	0
55	27	2	Total Mg 2 2	0	0
55	19	2	Total Mg 2 2	0	0
55	1l	3	Total Mg 3 3	0	0
55	2V	1	Total Mg 1 1	0	0
55	1F	13	Total Mg 13 13	0	0
55	10	7	Total Mg 7 7	0	0
55	2t	1	Total Mg 1 1	0	0
55	1Q	5	Total Mg 5 5	0	0
55	2A	850	Total Mg 850 850	0	0
55	2Z	2	Total Mg 2 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	1B	36	Total	Mg	0	0
			36	36		

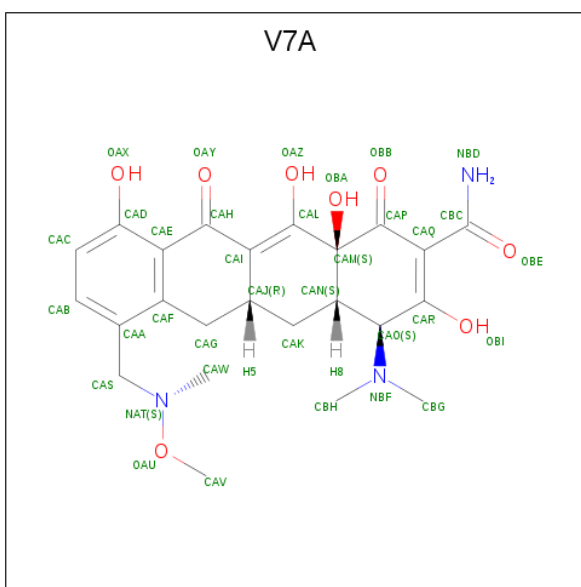
- Molecule 56 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	1A	1	Total	K	0	0
			1	1		
56	2A	1	Total	K	0	0
			1	1		

- Molecule 57 is ZINC ION (three-letter code: ZN) (formula: Zn).

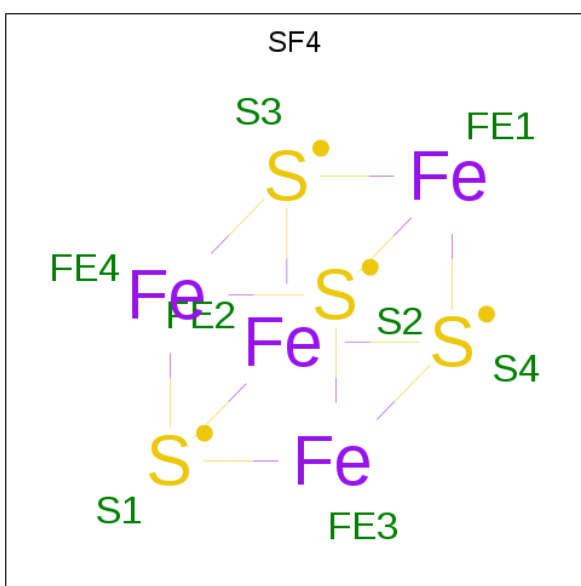
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	1Y	1	Total	Zn	0	0
			1	1		
57	14	1	Total	Zn	0	0
			1	1		
57	1n	1	Total	Zn	0	0
			1	1		
57	15	1	Total	Zn	0	0
			1	1		
57	29	1	Total	Zn	0	0
			1	1		
57	19	1	Total	Zn	0	0
			1	1		
57	26	1	Total	Zn	0	0
			1	1		
57	25	1	Total	Zn	0	0
			1	1		
57	24	1	Total	Zn	0	0
			1	1		
57	2n	1	Total	Zn	0	0
			1	1		
57	2Y	1	Total	Zn	0	0
			1	1		
57	16	1	Total	Zn	0	0
			1	1		

- Molecule 58 is Sarecycline (three-letter code: V7A) (formula: C₂₄H₂₉N₃O₈).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
58	1a	1	Total	C	N	O	0	0
			35	24	3	8		
58	2a	1	Total	C	N	O	0	0
			35	24	3	8		

- Molecule 59 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
59	1d	1	Total 8	Fe 4	S 4	0	0
59	2d	1	Total 8	Fe 4	S 4	0	0

- Molecule 60 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1A	1402	Total 1402	O 1402	0	0
60	1B	54	Total 54	O 54	0	0
60	1D	21	Total 21	O 21	0	0
60	1E	18	Total 18	O 18	0	0
60	1F	9	Total 9	O 9	0	0
60	1G	4	Total 4	O 4	0	0
60	1H	1	Total 1	O 1	0	0
60	1I	1	Total 1	O 1	0	0
60	1N	5	Total 5	O 5	0	0
60	1O	8	Total 8	O 8	0	0
60	1P	18	Total 18	O 18	0	0
60	1Q	7	Total 7	O 7	0	0
60	1R	9	Total 9	O 9	0	0
60	1S	4	Total 4	O 4	0	0
60	1T	4	Total 4	O 4	0	0
60	1U	14	Total 14	O 14	0	0
60	1V	10	Total 10	O 10	0	0
60	1W	8	Total 8	O 8	0	0
60	1X	4	Total 4	O 4	0	0
60	1Y	4	Total 4	O 4	0	0
60	1Z	1	Total 1	O 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	10	11	Total 11	O 11	0	0
60	11	8	Total 8	O 8	0	0
60	12	3	Total 3	O 3	0	0
60	13	3	Total 3	O 3	0	0
60	14	1	Total 1	O 1	0	0
60	15	6	Total 6	O 6	0	0
60	16	4	Total 4	O 4	0	0
60	17	10	Total 10	O 10	0	0
60	18	8	Total 8	O 8	0	0
60	1a	211	Total 211	O 211	0	0
60	1b	1	Total 1	O 1	0	0
60	1d	2	Total 2	O 2	0	0
60	1e	1	Total 1	O 1	0	0
60	1i	1	Total 1	O 1	0	0
60	1l	4	Total 4	O 4	0	0
60	1m	1	Total 1	O 1	0	0
60	1q	2	Total 2	O 2	0	0
60	1u	2	Total 2	O 2	0	0
60	1v	3	Total 3	O 3	0	0
60	1x	11	Total 11	O 11	0	0
60	2A	680	Total 680	O 680	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	2B	24	Total 24	O 24	0	0
60	2D	12	Total 12	O 12	0	0
60	2E	13	Total 13	O 13	0	0
60	2F	10	Total 10	O 10	0	0
60	2I	1	Total 1	O 1	0	0
60	2O	2	Total 2	O 2	0	0
60	2P	4	Total 4	O 4	0	0
60	2Q	2	Total 2	O 2	0	0
60	2R	3	Total 3	O 3	0	0
60	2T	4	Total 4	O 4	0	0
60	2U	1	Total 1	O 1	0	0
60	2W	2	Total 2	O 2	0	0
60	2X	2	Total 2	O 2	0	0
60	2Y	1	Total 1	O 1	0	0
60	2Z	3	Total 3	O 3	0	0
60	21	10	Total 10	O 10	0	0
60	23	1	Total 1	O 1	0	0
60	27	1	Total 1	O 1	0	0
60	28	2	Total 2	O 2	0	0
60	29	1	Total 1	O 1	0	0
60	2a	173	Total 173	O 173	0	0

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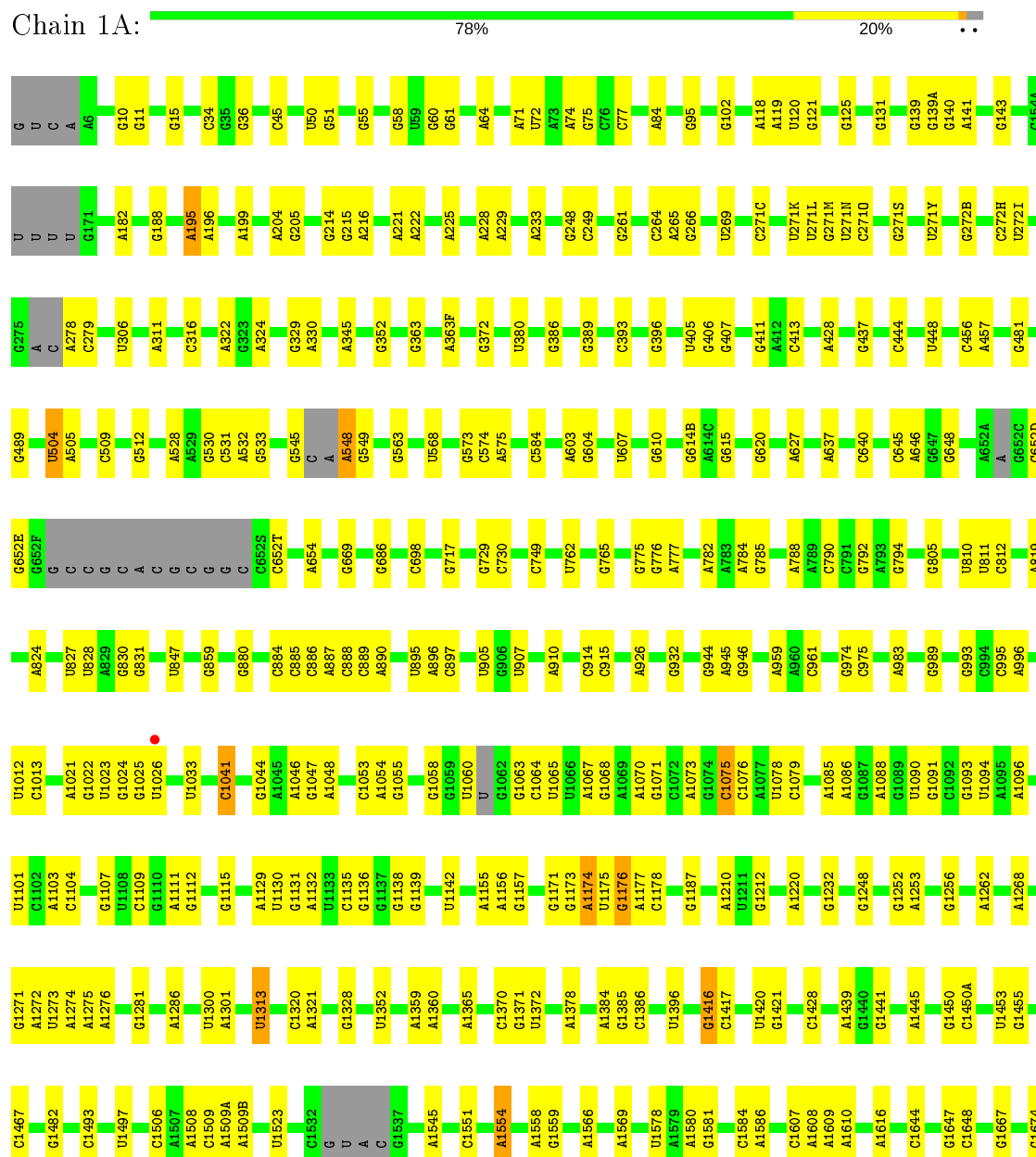
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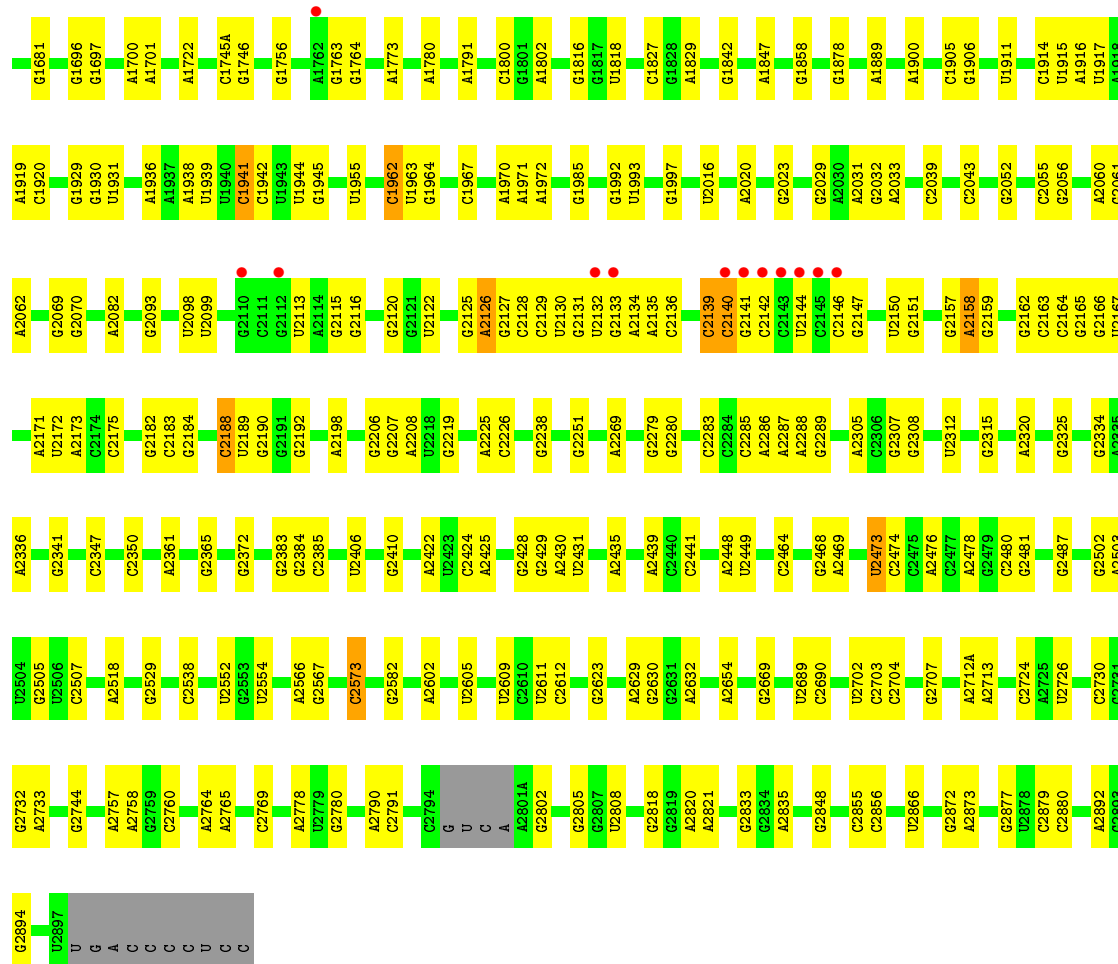
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	2e	2	Total	O	0	0
			2	2		
60	2g	1	Total	O	0	0
			1	1		
60	2i	1	Total	O	0	0
			1	1		
60	2j	4	Total	O	0	0
			4	4		
60	2l	3	Total	O	0	0
			3	3		
60	2n	1	Total	O	0	0
			1	1		
60	2t	3	Total	O	0	0
			3	3		
60	2v	1	Total	O	0	0
			1	1		
60	2x	5	Total	O	0	0
			5	5		

3 Residue-property plots

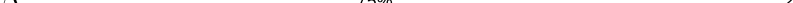
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

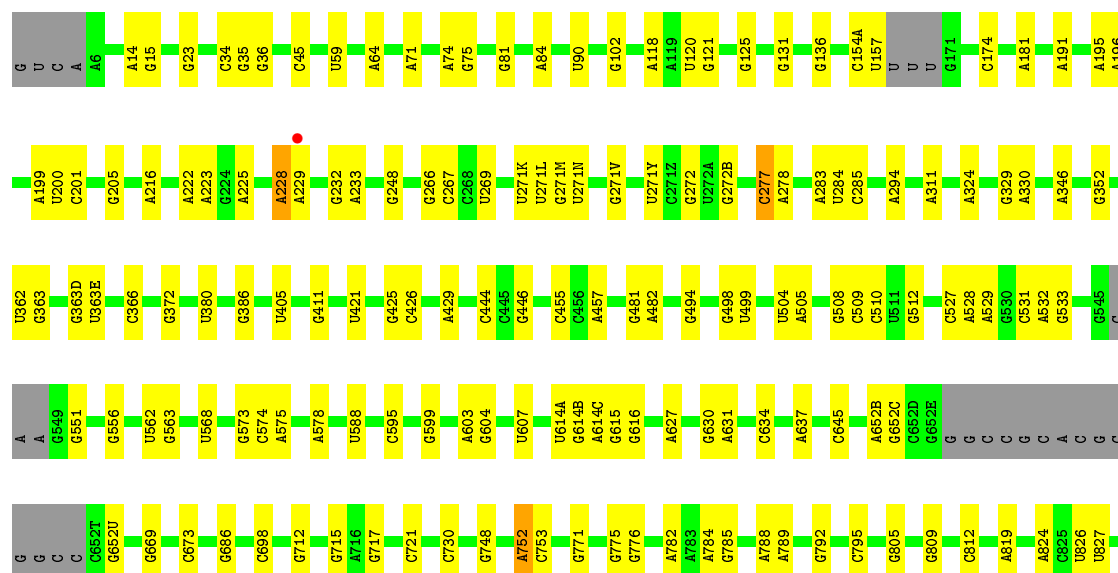
• Molecule 1: 23S Ribosomal RNA





- Molecule 1: 23S Ribosomal RNA

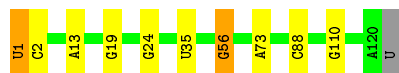
Chain 2A:  75% 21% •



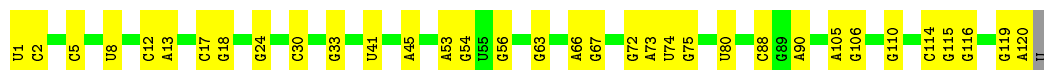
A2764	C2394	C2226	G2121	U1955	U1779	C1588	A1460	G1271	A126	U	A960	G832
A2765	C2395	G2238	U2122	C1962	A1780	G1593	A1461	A1272	A126	U	C961	G843
G2766	G2396	G2239	G2123	U1963	A1791	A1608	C1467	A1273	A1129	G	C964	C857
C2767	C2402	G2251	A2126	G1967	C1800	A1609	A1471	A1275	G1131	U	C965	C856
A2778	U2406	A2274	C2128	A1970	G1801	A1616	A1475	C1298	A1132	U	G968	U858
G2779	G2407	C2275	C2129	A1971	C1804	G1622	G1479	G1299	U1133	A	G972	G859
C2780	U2408	G2279	U2130	A1972	G1816	G1626	G1482	A1301	U1135	G	A973	C865
A	G2410	G2283	G2132	G1982	U1833	G1638	G1486	G1309	G1136	A	G974	A866
C	A2422	A2287	G2133	U1993	U1834	U1639	A1490	G1352	G1139	C	C975	G869
G2782	A2425	A2288	A2134	G1997	U1835	C1638	A1495	U1313	A1142A	A	A980	G874
U	G2429	C2297	A2135	G1998	G1836	C1640	A1496	C1314	A1143	G	A981	C982
C	A2430	G2308	C2136	A2001	A1847	C1648	U1497	G1319	G1144	C	A983	U877
A	A2435	A2305	G2137	A2002	A1848	G1653	C1493	A1321	G1151	A	A996	G880
G2801A	A2440	G2311	C2138	G2021	G1861	A1654	A1494	U1352	A1155	C	C1006	C884
G2802	A2441	U2311	C2139	U2022	U1864	G1661	A1496	G1362	G1164	U	U1012	C885
G2803	G2442	G2308	U2144	G2023	G1865	C1662	U1497	U1341	G1170	U	C1013	C886
G2807	G2446	A2311	C2145	A2031	C1866	C1663	U1503	U1352	G1171	A	U1014	A887
A2820	G2447	U2312	G2146	G2032	G1878	A1664	A1508	A1359	G	A	G1015	C888
A2821	A2448	G2318	G2148	C2043	A1890	C1670	C1509	A1360	A	G	A1020	G892
A2822	U2449	G2319	C2149	G1899	G1899	G1674	A1509A	A1365	U	A	A1021	C893
A2823	G2458	A2320	G2155	G2052	A1900	C1675	U1509A	A1366	A	G	G1022	C894
A2835	G2461	G2321	G2156	C2055	G1906	A1676	C1530	A1369	C1178	U	U1023	U896
C2855	U2473	G2325	G2160	G2056	G1910	G1696	C1531	G1368	G1192	C	G1024	A896
A2868	A2476	A2327	C2161	A2060	U1911	A1700	U	G1369	G1192	C	G1025	C897
G2872	G2481	A2333	C2162	G2061	A1912	A1701	A1536	C1370	A1204	U	U1026	C898
C2879	C2498	A2336	C2163	A2062	A1913	G1702	G1537	A1379	U1205	A	A900	A901
G2880	G2502	G2337	C2164	C2063	A1914	G1703	G1538	G1380	G1206	U	U1033	
U2884	U2503	G2340	U2172	U2068	A1915	G1721	G1588	A1384	A1210	A	C1038	A910
C2885	U2504	G2345	G2181	G2069	U1917	A1722	A1542	G1385	U1211	G	G1039	A917
G2886	G2505	A2346	G2182	G2101	C1920	U1739	A1543	U1406	C1221	C	G1040	C925
A2892	U2506	C2347	C2183	C2107	A1927	G1740	A1544	G1416	G1227	A	C1043	G928
G2893	C2507	C2350	C2185	C2108	A1928	G1746	A1588	C1417	G1232	U	A	G932
U2895	G2518	A2366	C2188	U2109	G1929	G1750	G1559	G1420	A1237	G	A	A933
C2896	G2525	A2376	U2189	G2111	G1930	G1756	A1566	G1421	U1240	U	A	G934
U	G2529	A2379	G2192	G2112	A1936	U1757	A1569	A1427	A1241	C	C	G938
G	U2554	G2379	G2206	U2113	A1937	A1762	A1578	C1428	A1247	A	G	A941
A	A2733	G2383	G2207	G2115	U1938	G1763	A1579	G1429	U1248	C	C	A945
C	A2566	G2384	C2207	G2116	U1940	G1764	A1580	C1437	U1249	A	A	G946
C	G2751	C2385	A2117	A2117	C1942	A1773	C1584	A1445	A1253	G	G	A953
C	A2758	G2391	U2218	U2119	U1944	G1776	A1586	A1449	G1256	A	A	A959
U			A2225	G2120			A1587	A1450		C	G	

6

- Molecule 2: 5S Ribosomal RNA

Chain 1B:  91% 7% ..

- Molecule 2: 5S Ribosomal RNA

Chain 2B:  71% 28% .

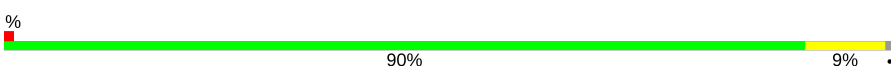
- Molecule 3: 50S ribosomal protein L2

Chain 1D:  91% 9%

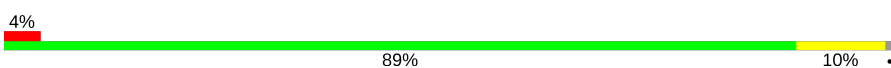
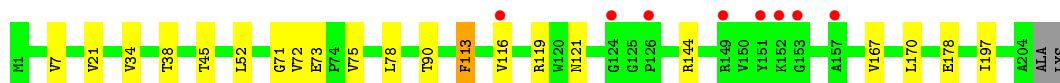
- Molecule 3: 50S ribosomal protein L2

Chain 2D:  93% 7%

- Molecule 4: 50S ribosomal protein L3

Chain 1E:  90% 9%

- Molecule 4: 50S ribosomal protein L3

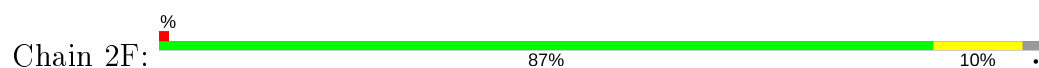
Chain 2E:  89% 10%

- Molecule 5: 50S ribosomal protein L4

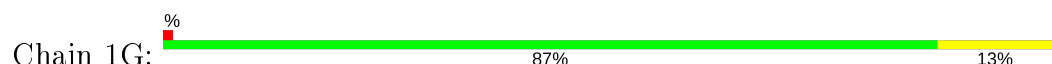
Chain 1F:  88% 9%



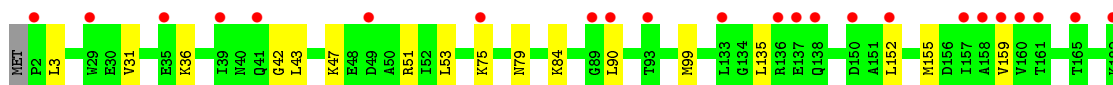
- Molecule 5: 50S ribosomal protein L4



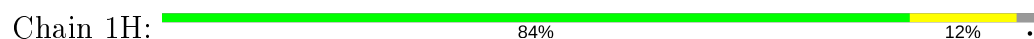
- Molecule 6: 50S ribosomal protein L5



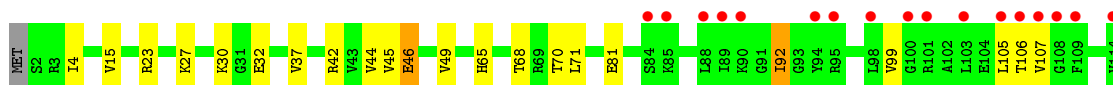
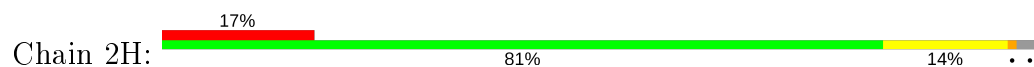
- Molecule 6: 50S ribosomal protein L5



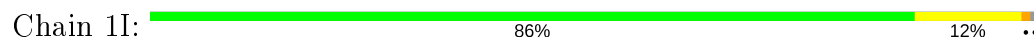
- Molecule 7: 50S ribosomal protein L6



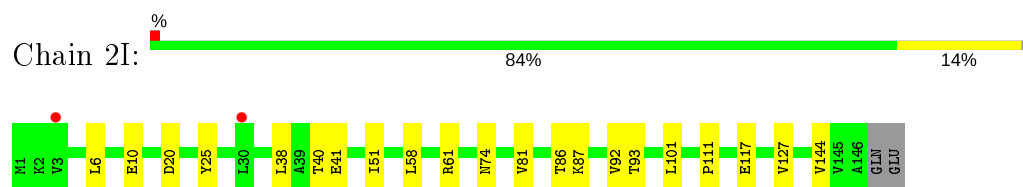
- Molecule 7: 50S ribosomal protein L6



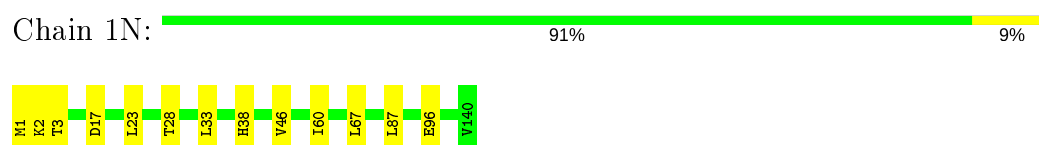
- Molecule 8: 50S ribosomal protein L9



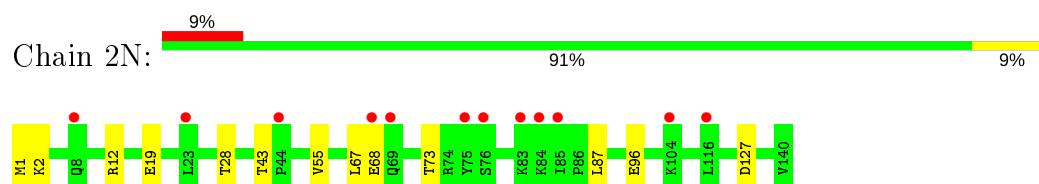
- Molecule 8: 50S ribosomal protein L9



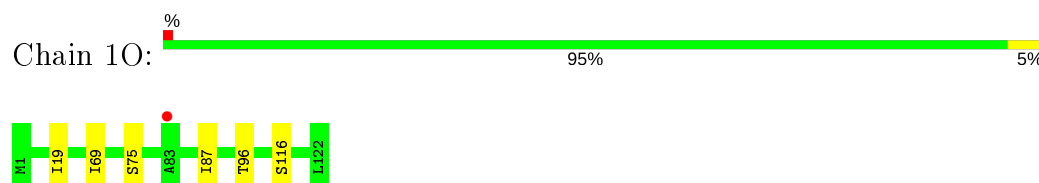
- Molecule 9: 50S ribosomal protein L13



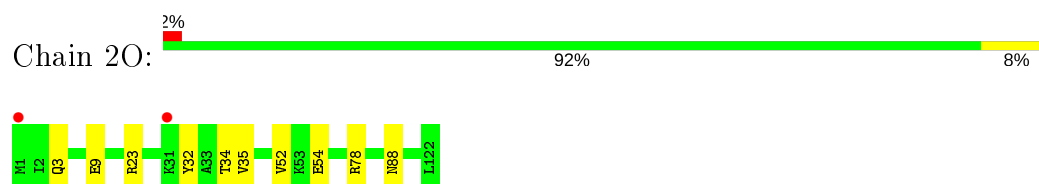
- Molecule 9: 50S ribosomal protein L13



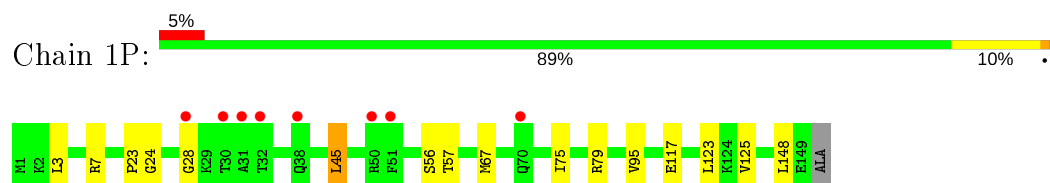
- Molecule 10: 50S ribosomal protein L14



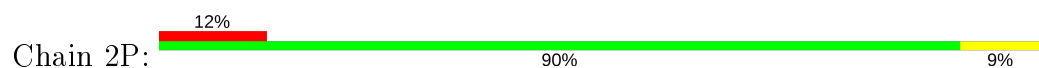
- Molecule 10: 50S ribosomal protein L14

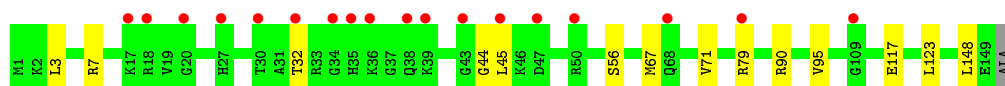


- Molecule 11: 50S ribosomal protein L15



- Molecule 11: 50S ribosomal protein L15





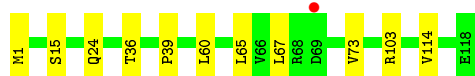
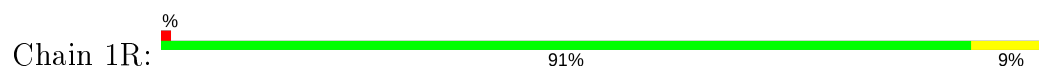
- Molecule 12: 50S ribosomal protein L16



- Molecule 12: 50S ribosomal protein L16



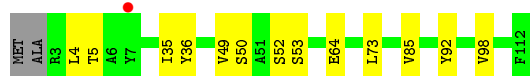
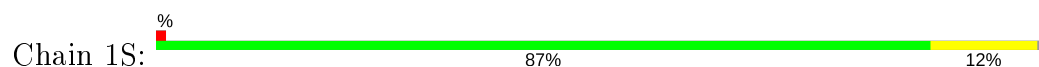
- Molecule 13: 50S ribosomal protein L17



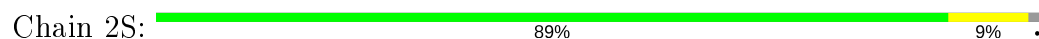
- Molecule 13: 50S ribosomal protein L17




- Molecule 14: 50S ribosomal protein L18

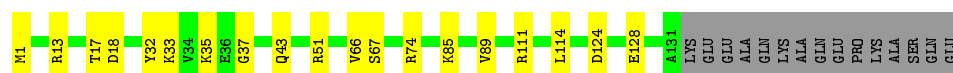


- Molecule 14: 50S ribosomal protein L18




- Molecule 15: 50S ribosomal protein L19

Chain 1T:  77% 13% 10%



- Molecule 15: 50S ribosomal protein L19

Chain 2T:  84% 5% 10%



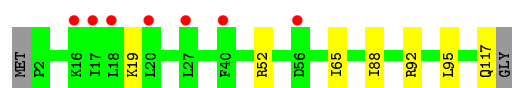
- Molecule 16: 50S ribosomal protein L20

Chain 1U:  96% . .



- Molecule 16: 50S ribosomal protein L20

Chain 2U:  92% 6% .



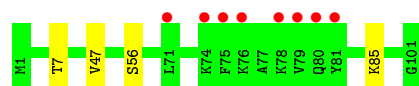
- Molecule 17: 50S ribosomal protein L21

Chain 1V:  91% 9%



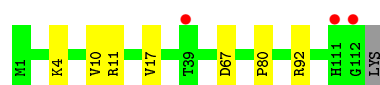
- Molecule 17: 50S ribosomal protein L21

Chain 2V:  96% .

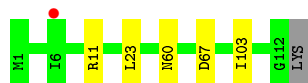


- Molecule 18: 50S ribosomal protein L22

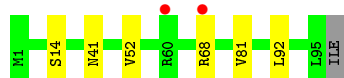
Chain 1W:  93% 6% .



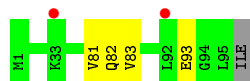
- Molecule 18: 50S ribosomal protein L22



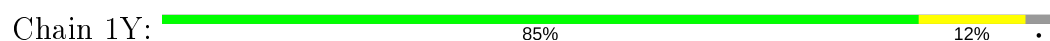
- Molecule 19: 50S ribosomal protein L23



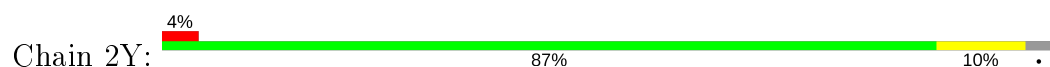
- Molecule 19: 50S ribosomal protein L23



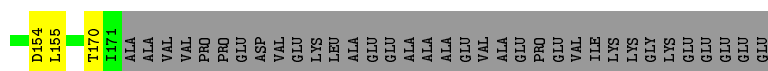
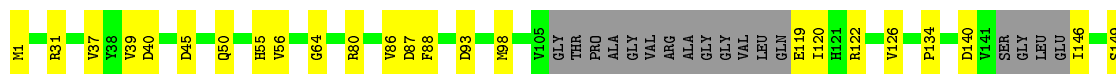
- Molecule 20: 50S ribosomal protein L24



- Molecule 20: 50S ribosomal protein L24

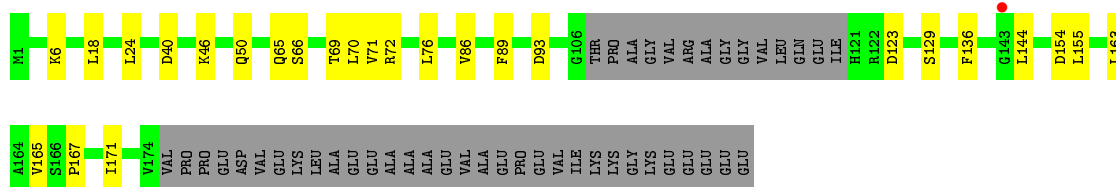


- Molecule 21: 50S ribosomal protein L25

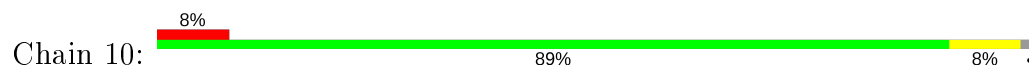


- Molecule 21: 50S ribosomal protein L25

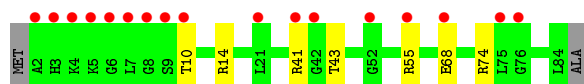
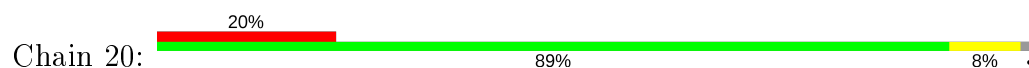




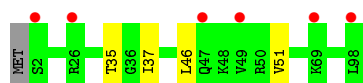
- Molecule 22: 50S ribosomal protein L27



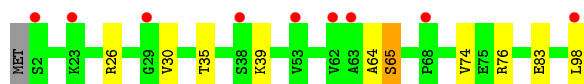
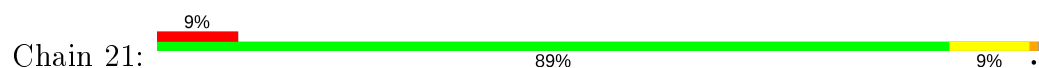
- Molecule 22: 50S ribosomal protein L27



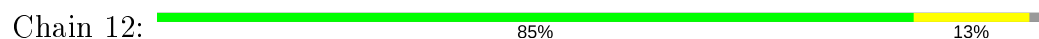
- Molecule 23: 50S ribosomal protein L28



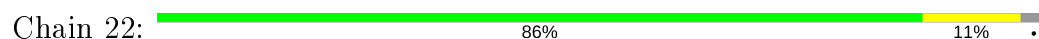
- Molecule 23: 50S ribosomal protein L28




- Molecule 24: 50S ribosomal protein L29



- Molecule 24: 50S ribosomal protein L29




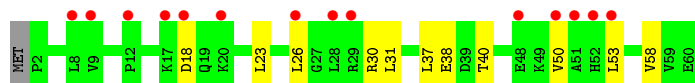
- Molecule 25: 50S ribosomal protein L30

Chain 13:  83% 15% .




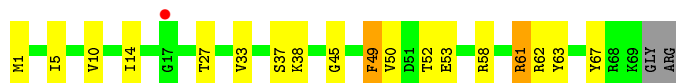
- Molecule 25: 50S ribosomal protein L30

Chain 23:  23% 80% 18% .




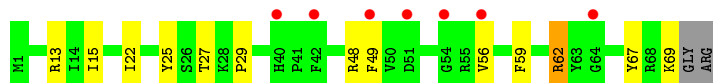
- Molecule 26: 50S ribosomal protein L31

Chain 14:  % 72% 23% . .




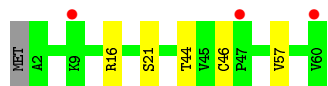
- Molecule 26: 50S ribosomal protein L31

Chain 24:  10% 79% 17% . .



- Molecule 27: 50S ribosomal protein L32

Chain 15:  5% 90% 8% .



- Molecule 27: 50S ribosomal protein L32

Chain 25:  3% 95% . .



- Molecule 28: 50S ribosomal protein L33

Chain 16:  89% 9% .



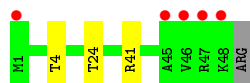
- Molecule 28: 50S ribosomal protein L33

Chain 26:  70% 28%

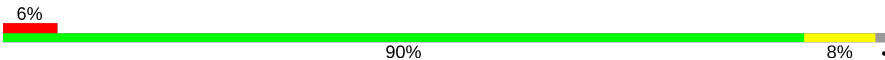


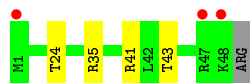
- Molecule 29: 50S ribosomal protein L34

Chain 17:  10% 92% 6%



- Molecule 29: 50S ribosomal protein L34

Chain 27:  6% 90% 8%




- Molecule 30: 50S ribosomal protein L35

Chain 18:  8% 94% 5%



- Molecule 30: 50S ribosomal protein L35

Chain 28:  31% 91% 8%

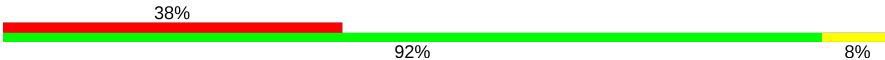


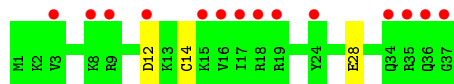
- Molecule 31: 50S ribosomal protein L36

Chain 19:  95% 5%

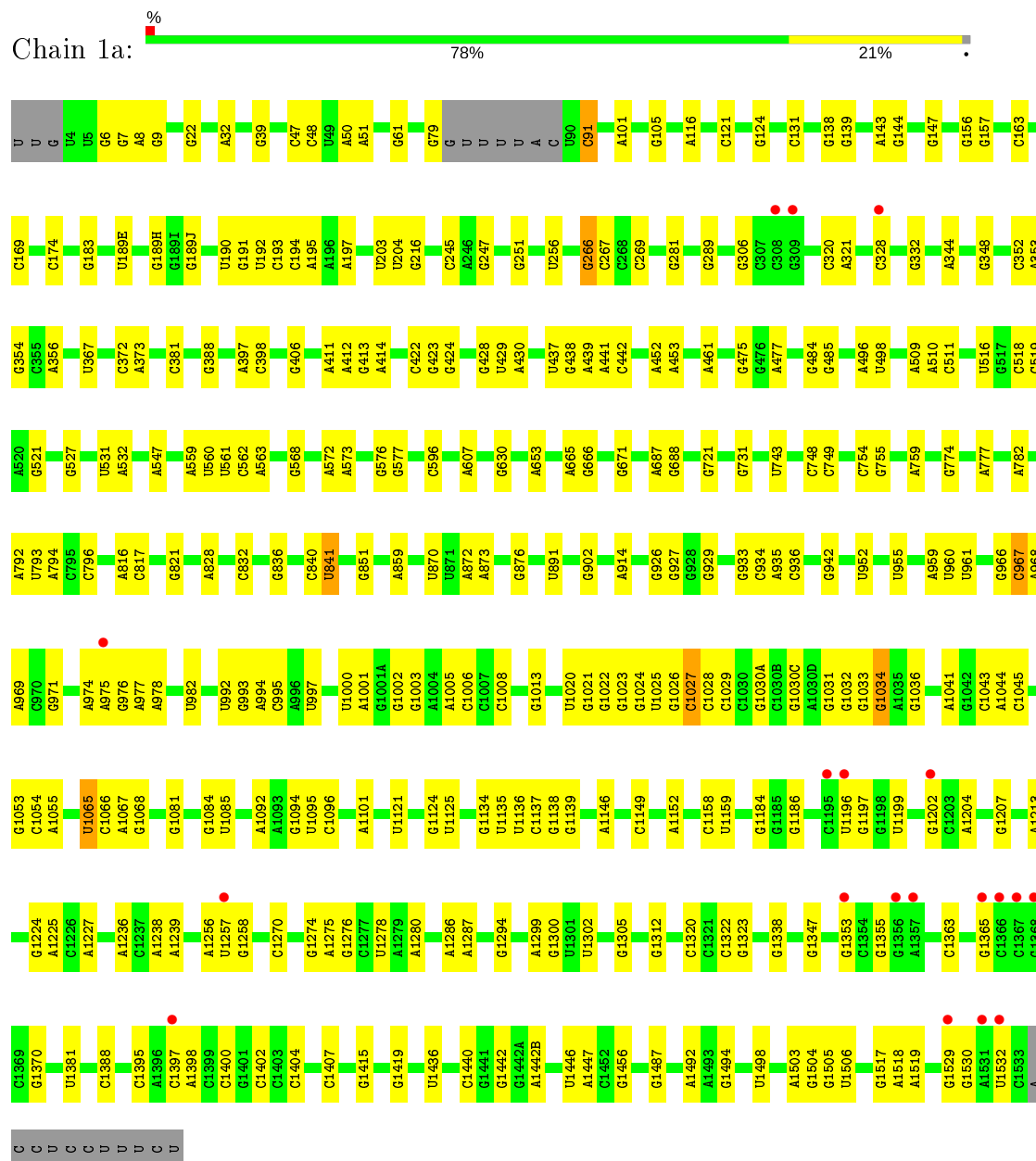


- Molecule 31: 50S ribosomal protein L36

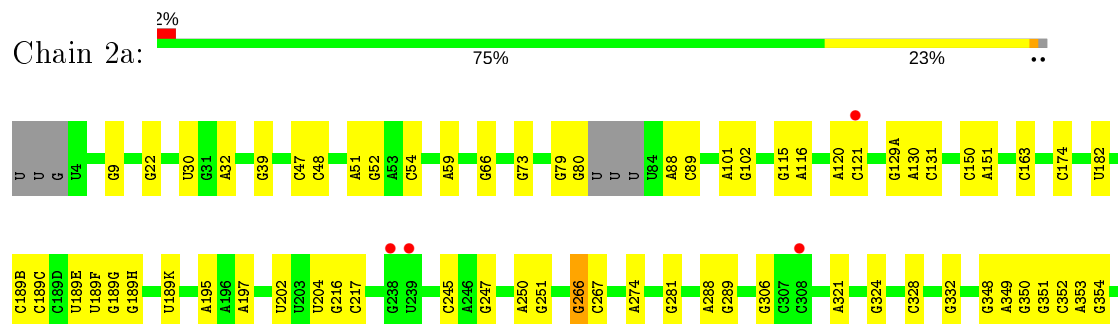
Chain 29:  38% 92% 8%

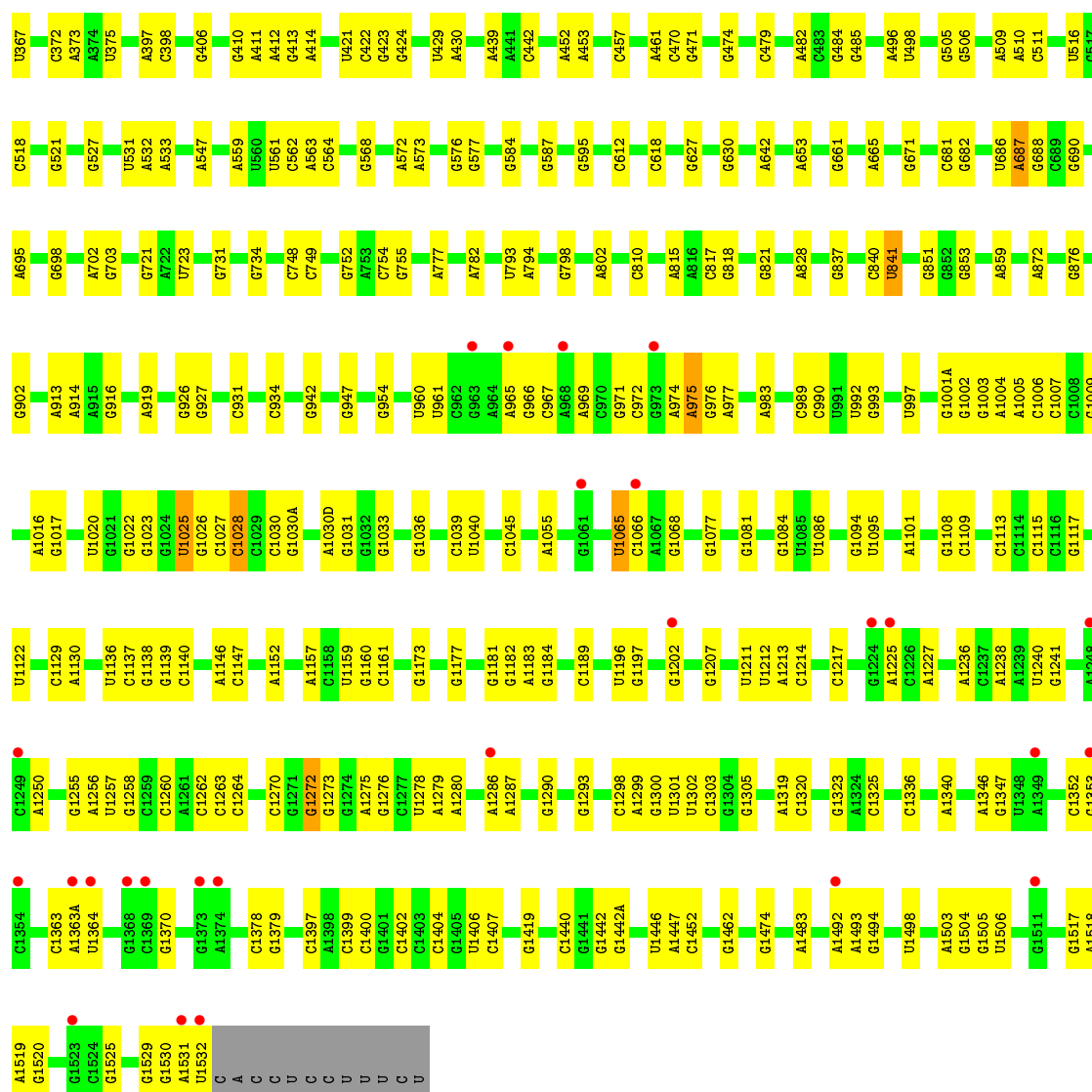


- Molecule 32: 16S Ribosomal RNA

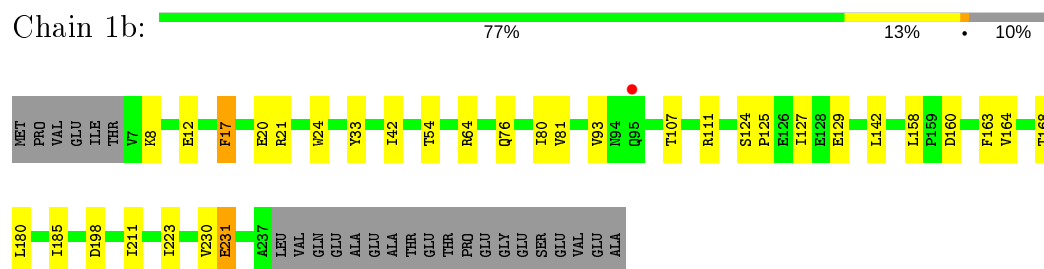


- Molecule 32: 16S Ribosomal RNA

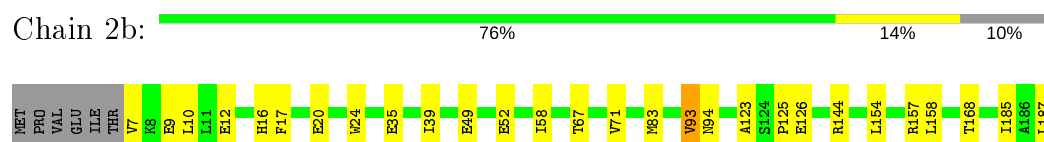


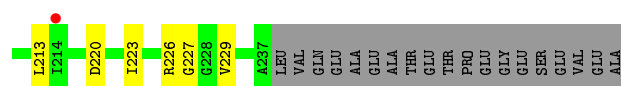


• Molecule 33: 30S ribosomal protein S2

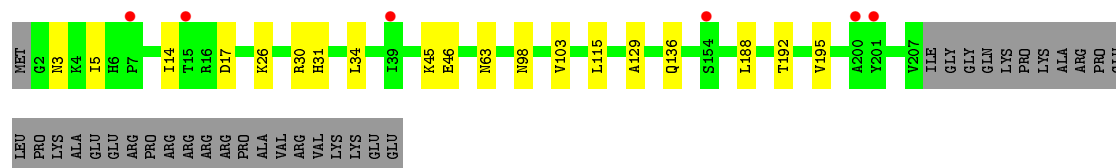
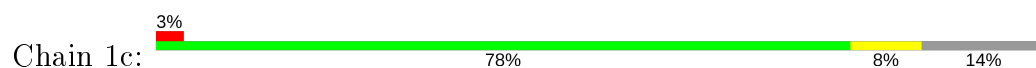


• Molecule 33: 30S ribosomal protein S2

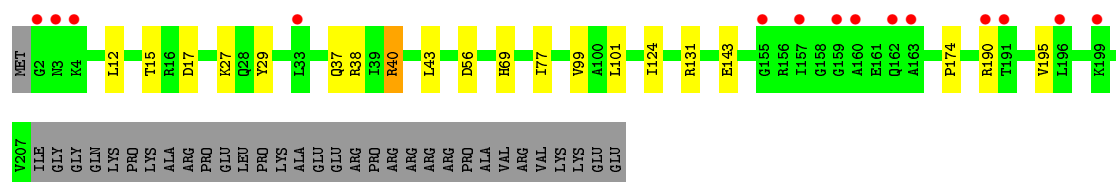
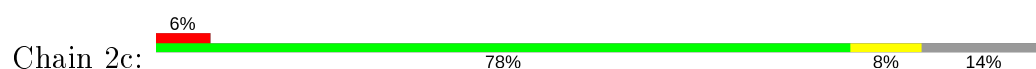




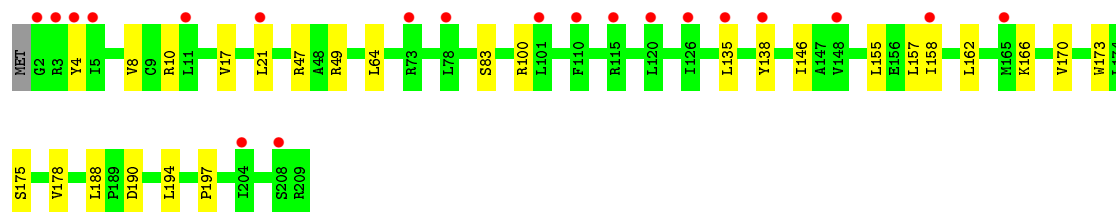
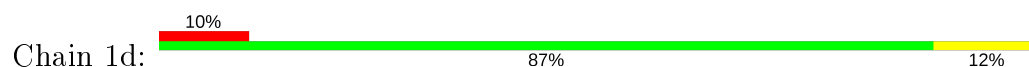
- Molecule 34: 30S ribosomal protein S3



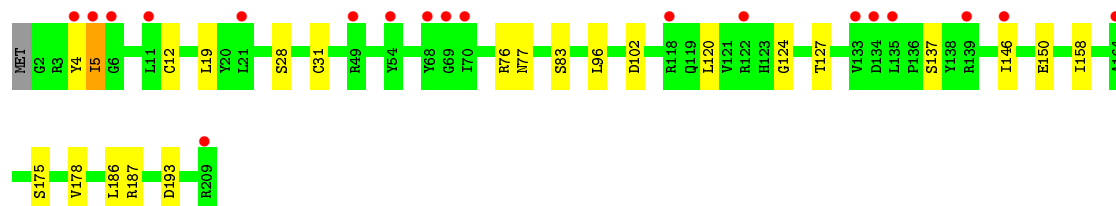
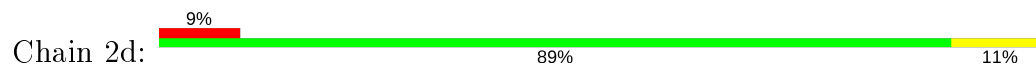
- Molecule 34: 30S ribosomal protein S3



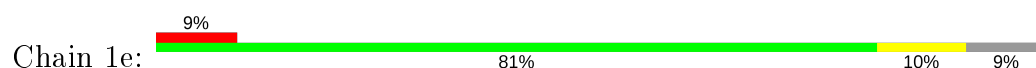
- Molecule 35: 30S ribosomal protein S4

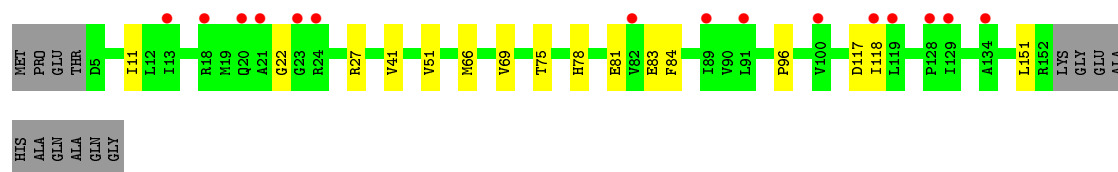


- Molecule 35: 30S ribosomal protein S4

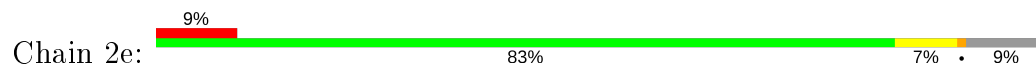


- Molecule 36: 30S ribosomal protein S5





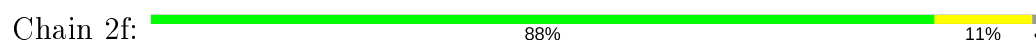
- Molecule 36: 30S ribosomal protein S5



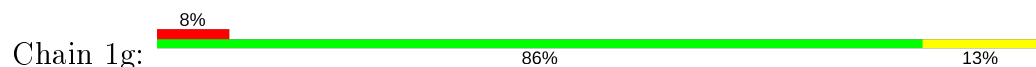
- Molecule 37: 30S ribosomal protein S6



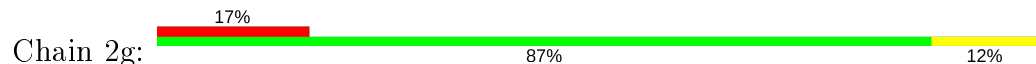
- Molecule 37: 30S ribosomal protein S6



- Molecule 38: 30S ribosomal protein S7



- Molecule 38: 30S ribosomal protein S7

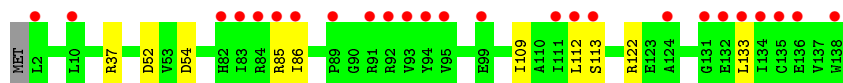


- Molecule 39: 30S ribosomal protein S8

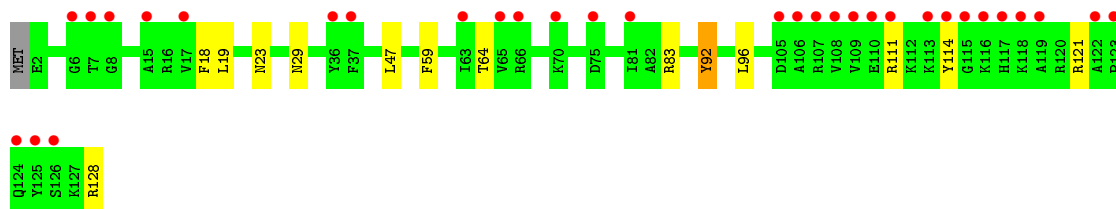
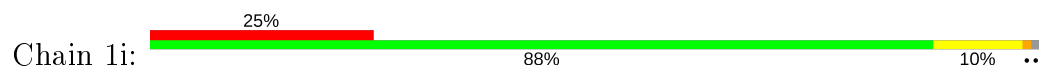




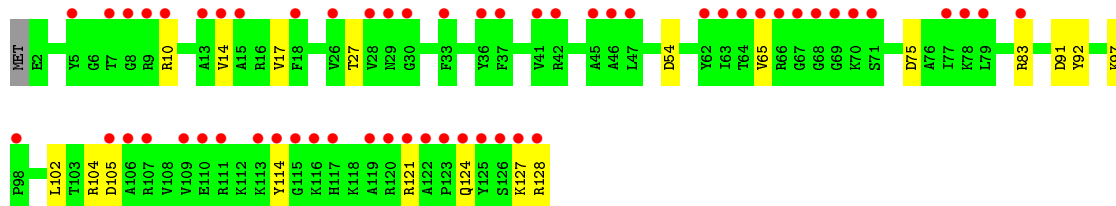
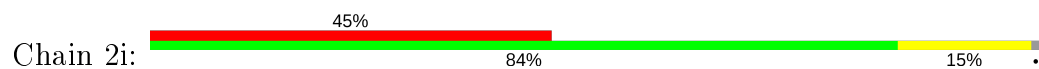
- Molecule 39: 30S ribosomal protein S8



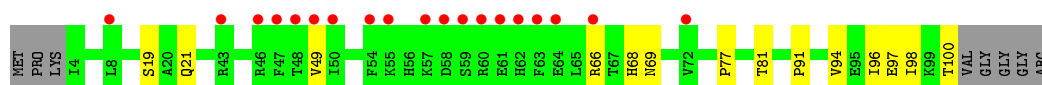
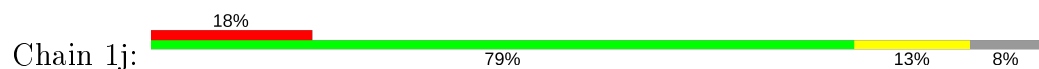
- Molecule 40: 30S ribosomal protein S9



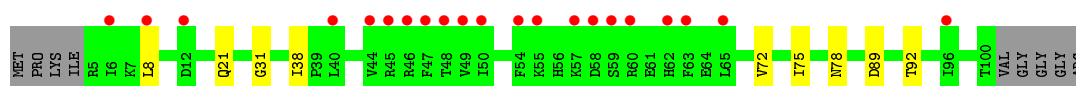
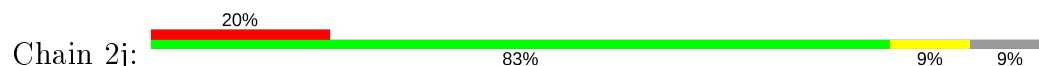
- Molecule 40: 30S ribosomal protein S9



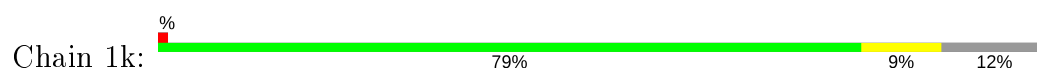
- Molecule 41: 30S ribosomal protein S10



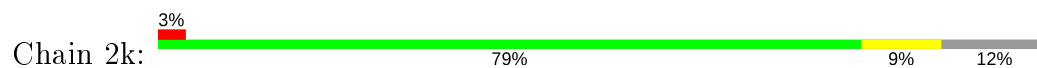
- Molecule 41: 30S ribosomal protein S10



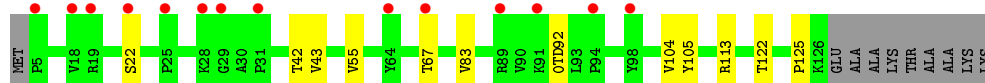
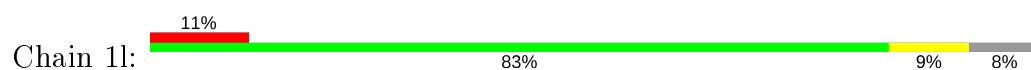
- Molecule 42: 30S ribosomal protein S11



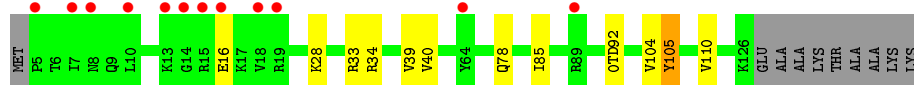
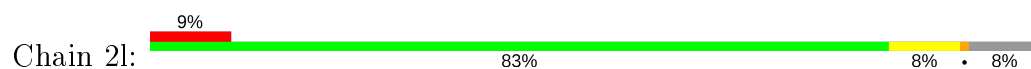
- Molecule 42: 30S ribosomal protein S11



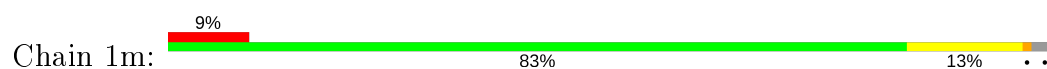
- Molecule 43: 30S ribosomal protein S12



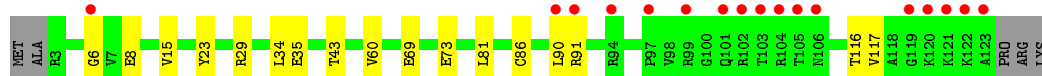
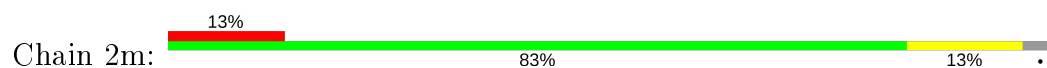
- Molecule 43: 30S ribosomal protein S12



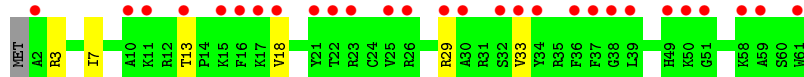
- Molecule 44: 30S ribosomal protein S13



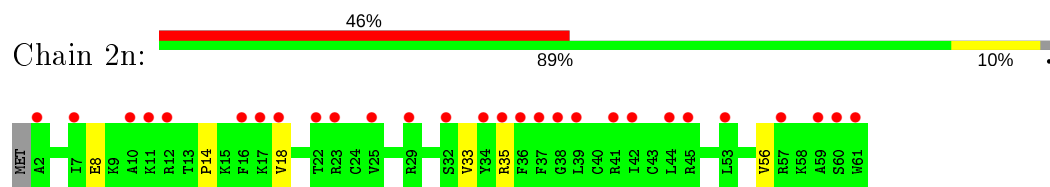
- Molecule 44: 30S ribosomal protein S13



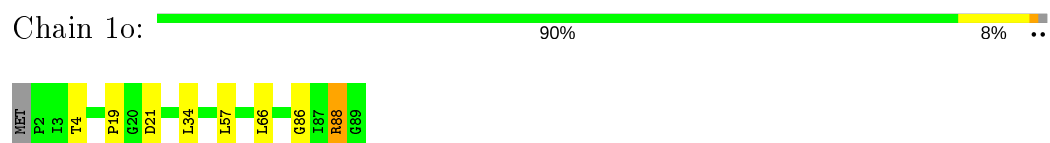
- Molecule 45: 30S ribosomal protein S14 type Z



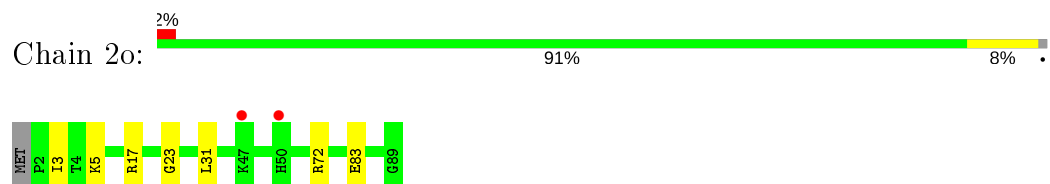
- Molecule 45: 30S ribosomal protein S14 type Z



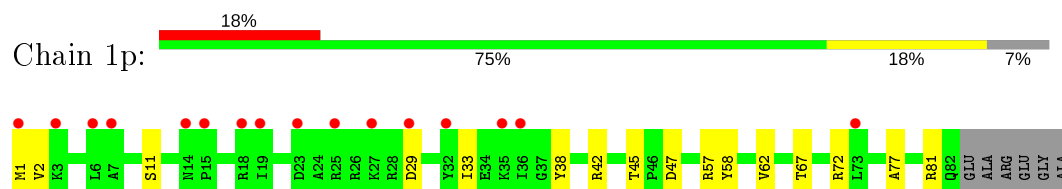
- Molecule 46: 30S ribosomal protein S15



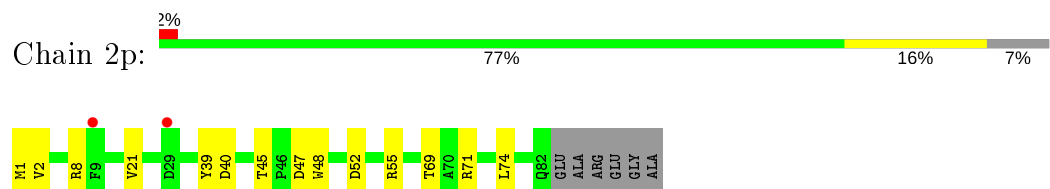
- Molecule 46: 30S ribosomal protein S15



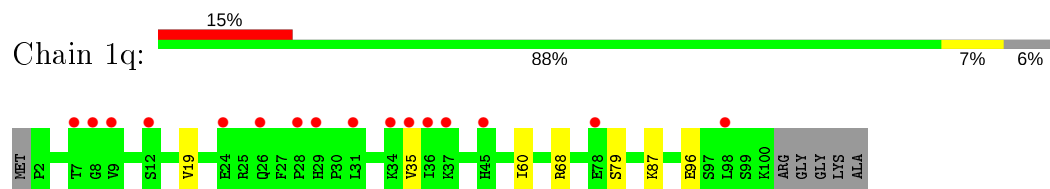
- Molecule 47: 30S ribosomal protein S16



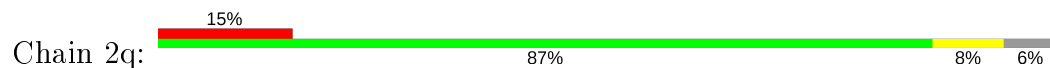
- Molecule 47: 30S ribosomal protein S16



- Molecule 48: 30S ribosomal protein S17

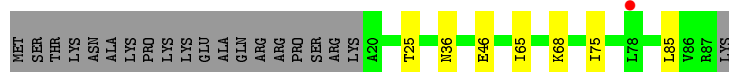


- Molecule 48: 30S ribosomal protein S17

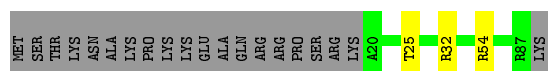




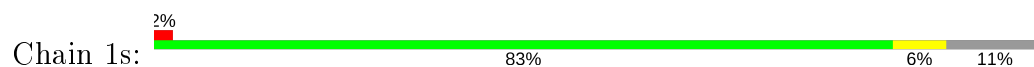
- Molecule 49: 30S ribosomal protein S18



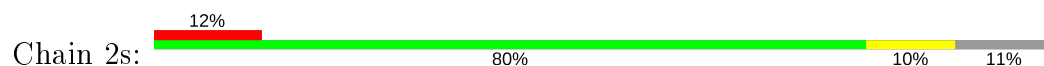
- Molecule 49: 30S ribosomal protein S18



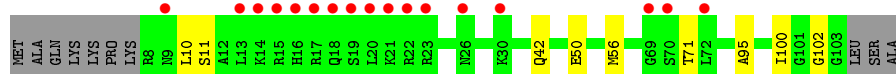
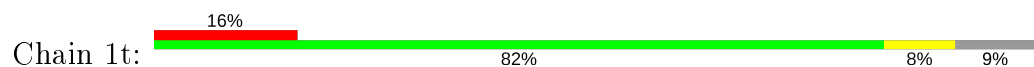
- Molecule 50: 30S ribosomal protein S19



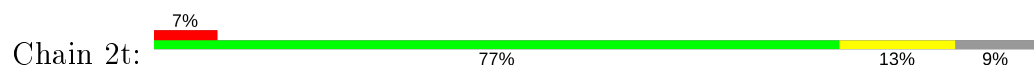
- Molecule 50: 30S ribosomal protein S19



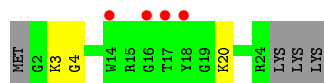
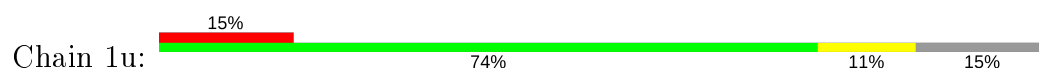
- Molecule 51: 30S ribosomal protein S20



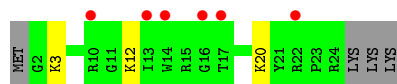
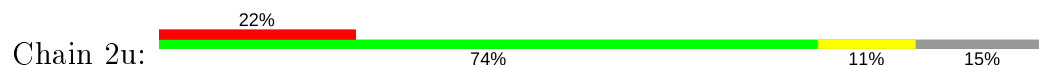
- Molecule 51: 30S ribosomal protein S20



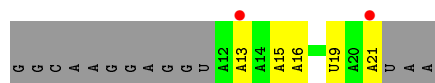
- Molecule 52: 30S ribosomal protein Thx



- Molecule 52: 30S ribosomal protein Thx



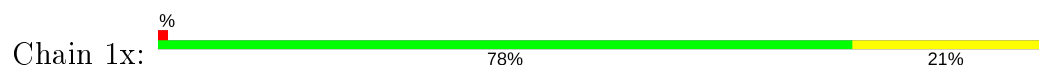
- Molecule 53: mRNA



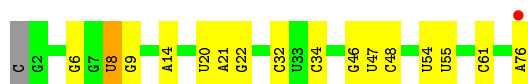
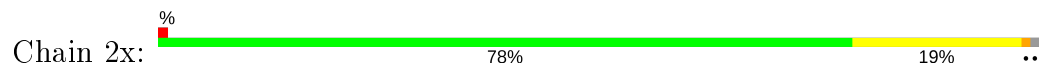
- Molecule 53: mRNA



- Molecule 54: P-site tRNA



- Molecule 54: P-site tRNA



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.13Å 448.15Å 621.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	86.77 – 3.00 310.97 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.0 (86.77-3.00) 99.0 (310.97-3.00)	Depositor EDS
R_{merge}	0.30	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.21 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.246 , 0.311 0.246 , 0.310	Depositor DCC
R_{free} test set	57107 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	58.0	Xtriage
Anisotropy	0.166	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 57.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.36$, $\langle L^2 \rangle = 0.19$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.79	EDS
Total number of atoms	292071	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.60% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, ZN, M2G, OMG, MA6, SF4, 0TD, MG, V7A, 2MA, 2MU, 2MG, 5MC, UR3, 4OC, 4SU, 7MG, K, PSU

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	0.47	0/69009	0.96	54/107712 (0.1%)
1	2A	0.41	0/67293	0.92	50/105034 (0.0%)
2	1B	0.45	1/2882 (0.0%)	0.93	1/4494 (0.0%)
2	2B	0.41	1/2879 (0.0%)	0.92	1/4487 (0.0%)
3	1D	0.36	0/2186	0.54	0/2944
3	2D	0.33	0/2186	0.53	0/2944
4	1E	0.33	0/1592	0.52	0/2149
4	2E	0.31	0/1592	0.51	0/2149
5	1F	0.35	0/1619	0.52	0/2193
5	2F	0.31	0/1615	0.50	0/2188
6	1G	0.30	0/1448	0.50	0/1957
6	2G	0.28	0/1453	0.48	0/1963
7	1H	0.32	0/1356	0.50	0/1834
7	2H	0.30	0/1356	0.46	0/1834
8	1I	0.29	0/1112	0.49	0/1514
8	2I	0.29	0/1079	0.51	1/1475 (0.1%)
9	1N	0.32	0/1144	0.49	0/1543
9	2N	0.31	0/1144	0.49	0/1543
10	1O	0.34	0/943	0.51	0/1269
10	2O	0.32	0/943	0.53	0/1269
11	1P	0.32	0/1152	0.54	0/1533
11	2P	0.31	0/1152	0.54	0/1533
12	1Q	0.33	0/1143	0.53	0/1527
12	2Q	0.31	0/1143	0.51	0/1527
13	1R	0.30	0/982	0.52	0/1312
13	2R	0.29	0/982	0.48	0/1312
14	1S	0.32	0/883	0.53	0/1176
14	2S	0.31	0/880	0.48	0/1172
15	1T	0.30	0/1105	0.50	0/1477
15	2T	0.31	0/1097	0.48	0/1468
16	1U	0.34	0/977	0.45	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	2U	0.28	0/977	0.42	0/1301
17	1V	0.35	0/782	0.52	0/1049
17	2V	0.28	0/782	0.51	0/1049
18	1W	0.33	0/897	0.50	0/1205
18	2W	0.31	0/897	0.48	0/1205
19	1X	0.37	0/764	0.55	0/1025
19	2X	0.31	0/764	0.50	0/1025
20	1Y	0.35	0/819	0.50	0/1095
20	2Y	0.30	0/819	0.51	0/1095
21	1Z	0.31	0/1267	0.51	0/1717
21	2Z	0.30	0/1299	0.51	0/1763
22	10	0.34	0/662	0.54	0/881
22	20	0.30	0/662	0.49	0/881
23	11	0.31	0/762	0.52	0/1014
23	21	0.31	0/762	0.52	0/1014
24	12	0.31	0/590	0.49	0/781
24	22	0.29	0/590	0.44	0/781
25	13	0.33	0/474	0.48	0/635
25	23	0.28	0/469	0.47	0/630
26	14	0.32	0/565	0.51	0/761
26	24	0.30	0/545	0.52	0/737
27	15	0.29	0/469	0.49	0/635
27	25	0.31	0/469	0.46	0/635
28	16	0.38	0/460	0.54	0/613
28	26	0.34	0/456	0.50	0/608
29	17	0.34	0/426	0.49	0/561
29	27	0.31	0/426	0.49	0/561
30	18	0.33	0/525	0.52	0/691
30	28	0.32	0/525	0.50	0/691
31	19	0.31	0/310	0.49	0/407
31	29	0.29	0/310	0.52	0/407
32	1a	0.37	0/35795	0.91	18/55864 (0.0%)
32	2a	0.37	3/35886 (0.0%)	0.93	42/56005 (0.1%)
33	1b	0.29	0/1881	0.49	0/2542
33	2b	0.30	0/1860	0.50	0/2518
34	1c	0.29	0/1572	0.48	0/2126
34	2c	0.30	0/1566	0.50	0/2119
35	1d	0.30	0/1685	0.48	0/2262
35	2d	0.28	0/1704	0.48	0/2284
36	1e	0.30	0/1145	0.51	0/1543
36	2e	0.32	0/1149	0.52	0/1548
37	1f	0.31	0/823	0.50	0/1115
37	2f	0.30	0/829	0.49	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	1g	0.29	0/1250	0.46	0/1679
38	2g	0.30	0/1254	0.47	0/1683
39	1h	0.28	0/1108	0.47	0/1494
39	2h	0.27	0/1108	0.45	0/1494
40	1i	0.29	0/1002	0.51	0/1346
40	2i	0.28	0/997	0.48	0/1343
41	1j	0.29	0/722	0.48	0/982
41	2j	0.29	0/727	0.51	0/988
42	1k	0.29	0/844	0.50	0/1145
42	2k	0.29	0/848	0.46	0/1149
43	1l	0.30	0/937	0.52	0/1260
43	2l	0.30	0/937	0.53	0/1260
44	1m	0.28	0/961	0.48	0/1290
44	2m	0.30	0/953	0.48	0/1279
45	1n	0.31	0/501	0.46	0/664
45	2n	0.30	0/501	0.47	0/664
46	1o	0.27	0/739	0.46	0/985
46	2o	0.27	0/739	0.47	0/985
47	1p	0.32	0/697	0.51	0/939
47	2p	0.28	0/693	0.47	0/935
48	1q	0.29	0/836	0.48	0/1117
48	2q	0.29	0/836	0.48	0/1117
49	1r	0.27	0/560	0.45	0/746
49	2r	0.27	0/560	0.44	0/746
50	1s	0.28	0/667	0.52	1/900 (0.1%)
50	2s	0.29	0/661	0.56	0/893
51	1t	0.28	0/730	0.45	0/965
51	2t	0.27	0/729	0.45	0/965
52	1u	0.29	0/203	0.52	0/266
52	2u	0.27	0/203	0.47	0/266
53	1v	0.47	0/244	0.95	0/378
53	2v	0.57	0/126	1.13	0/195
54	1x	0.51	1/1725 (0.1%)	1.10	7/2689 (0.3%)
54	2x	0.45	0/1725	1.03	6/2689 (0.2%)
All	All	0.39	6/310069 (0.0%)	0.84	181/463831 (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
20	1Y	0	1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2B	1	U	OP3-P	-10.39	1.48	1.61
2	1B	1	U	OP3-P	-10.19	1.49	1.61
32	2a	1272	G	N1-C2	-7.86	1.31	1.37
32	2a	1272	G	C6-N1	-7.51	1.34	1.39
32	2a	1263	C	N3-C4	-5.84	1.29	1.33
54	1x	14	A	C8-N7	-5.23	1.27	1.31

All (181) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1263	C	N1-C2-O2	19.27	130.46	118.90
32	2a	1272	G	N3-C2-N2	17.88	132.41	119.90
32	2a	1272	G	C5-C6-O6	17.17	138.90	128.60
32	2a	1272	G	N1-C2-N2	-14.94	102.76	116.20
32	2a	1263	C	C2-N3-C4	11.86	125.83	119.90
1	2A	2136	C	N1-C2-O2	11.67	125.90	118.90
32	2a	1263	C	N3-C2-O2	-11.14	114.10	121.90
2	2B	80	U	O4'-C1'-N1	10.23	116.38	108.20
32	2a	1272	G	C6-N1-C2	10.14	131.18	125.10
1	1A	1086	A	N1-C6-N6	-9.87	112.68	118.60
32	2a	1272	G	N1-C6-O6	-9.85	113.99	119.90
32	2a	1263	C	C5-C4-N4	9.76	127.03	120.20
32	2a	1272	G	C4-N9-C1'	9.65	139.04	126.50
32	2a	1263	C	N3-C4-N4	-8.87	111.79	118.00
1	1A	1075	C	N1-C2-O2	8.81	124.19	118.90
32	2a	1272	G	C5-C6-N1	-8.81	107.10	111.50
32	2a	1272	G	C8-N9-C1'	-8.80	115.56	127.00
1	1A	1075	C	C2-N3-C4	8.37	124.08	119.90
32	1a	841	U	C2-N1-C1'	8.29	127.64	117.70
54	1x	14	A	C5-N7-C8	8.21	108.01	103.90
1	2A	2136	C	N3-C2-O2	-8.11	116.22	121.90
54	1x	14	A	C4-C5-C6	8.00	121.00	117.00
1	1A	2167	U	C2-N1-C1'	7.95	127.24	117.70
1	2A	1313	U	C2-N1-C1'	7.75	127.00	117.70
1	2A	1178	C	N1-C2-O2	7.32	123.29	118.90
1	2A	2473	U	C2-N1-C1'	7.27	126.43	117.70
1	1A	2167	U	N3-C2-O2	-7.24	117.13	122.20
54	2x	34	C	N1-C2-O2	7.22	123.23	118.90
1	1A	1063	G	C5-C6-O6	7.08	132.85	128.60
32	1a	841	U	N3-C2-O2	-7.01	117.30	122.20
32	2a	754	C	C2-N1-C1'	6.92	126.42	118.80
1	1A	2704	C	N1-C2-O2	6.90	123.04	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2140	C	N1-C2-O2	6.88	123.03	118.90
1	2A	2188	C	C2-N1-C1'	6.86	126.35	118.80
32	2a	1378	C	C2-N1-C1'	6.86	126.34	118.80
1	1A	504	U	C2-N1-C1'	6.84	125.91	117.70
32	1a	91	C	N1-C2-O2	6.84	123.00	118.90
1	1A	847	U	C2-N1-C1'	6.79	125.85	117.70
1	1A	2167	U	N1-C2-O2	6.77	127.54	122.80
1	2A	2473	U	N3-C2-O2	-6.65	117.55	122.20
1	2A	2155	G	N3-C2-N2	6.60	124.52	119.90
54	1x	14	A	C5-C6-N1	-6.58	114.41	117.70
32	2a	1028	C	C2-N3-C4	6.57	123.19	119.90
1	2A	2473	U	N1-C2-O2	6.55	127.39	122.80
1	2A	928	G	C5-C6-O6	-6.52	124.69	128.60
1	1A	1063	G	C6-N1-C2	6.39	128.94	125.10
1	1A	2188	C	N1-C2-O2	6.38	122.73	118.90
32	2a	563	A	O4'-C1'-N9	6.36	113.29	108.20
1	2A	1178	C	C2-N1-C1'	6.32	125.75	118.80
1	2A	277	C	OP2-P-O3'	6.29	119.03	105.20
32	2a	841	U	C5-C6-N1	6.28	125.84	122.70
32	1a	841	U	N1-C2-O2	6.28	127.19	122.80
1	1A	2704	C	C2-N1-C1'	6.22	125.64	118.80
54	2x	46	G	C6-N1-C2	-6.16	121.41	125.10
32	2a	266	G	P-O3'-C3'	6.15	127.08	119.70
32	2a	1263	C	O4'-C1'-N1	6.12	113.10	108.20
32	2a	1033	G	C6-N1-C2	6.11	128.77	125.10
32	1a	1158	C	C2-N1-C1'	6.10	125.51	118.80
1	2A	1313	U	C5-C6-N1	6.09	125.75	122.70
32	1a	841	U	C6-N1-C2	-6.08	117.35	121.00
1	2A	2155	G	C6-N1-C2	6.08	128.75	125.10
1	2A	2188	C	N1-C2-O2	6.05	122.53	118.90
32	2a	1262	C	N1-C2-O2	6.05	122.53	118.90
1	2A	928	G	C4-C5-N7	6.02	113.21	110.80
32	2a	1033	G	C5-C6-O6	6.00	132.20	128.60
1	1A	1827	C	N1-C2-O2	6.00	122.50	118.90
1	1A	2158	A	P-O3'-C3'	5.96	126.85	119.70
1	1A	2140	C	C2-N3-C4	5.95	122.88	119.90
1	2A	1653	G	P-O3'-C3'	5.93	126.82	119.70
1	1A	1176	G	OP1-P-O3'	5.92	118.23	105.20
54	2x	14	A	C5-N7-C8	5.92	106.86	103.90
32	2a	1272	G	N3-C4-N9	5.87	129.52	126.00
1	1A	2167	U	C6-N1-C2	-5.82	117.51	121.00
32	1a	91	C	C2-N1-C1'	5.81	125.19	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	2x	14	A	C4-C5-C6	5.80	119.90	117.00
2	1B	56	G	C4-N9-C1'	5.80	134.04	126.50
1	1A	1075	C	C5-C4-N4	5.80	124.26	120.20
32	2a	1028	C	C5-C4-N4	5.79	124.25	120.20
1	1A	1313	U	C2-N1-C1'	5.74	124.58	117.70
1	1A	512	G	O4'-C1'-N9	5.71	112.77	108.20
1	2A	269	U	N1-C2-O2	5.71	126.80	122.80
32	1a	841	U	C5-C6-N1	5.71	125.55	122.70
1	1A	1086	A	C5-C6-N6	5.70	128.26	123.70
50	1s	5	LEU	CA-CB-CG	5.67	128.35	115.30
1	2A	2394	C	O4'-C1'-N1	5.67	112.74	108.20
32	1a	952	U	C5-C4-O4	5.67	129.30	125.90
1	2A	1178	C	N3-C2-O2	-5.67	117.93	121.90
1	2A	1992	G	P-O3'-C3'	5.66	126.49	119.70
54	1x	22	G	N1-C6-O6	-5.64	116.52	119.90
1	2A	2313	C	C6-N1-C2	-5.63	118.05	120.30
1	1A	640	C	C6-N1-C2	-5.63	118.05	120.30
1	2A	1022	G	N3-C4-N9	-5.62	122.63	126.00
54	1x	46	G	C6-N1-C2	-5.62	121.73	125.10
32	1a	266	G	P-O3'-C3'	5.62	126.44	119.70
1	1A	2167	U	C5-C6-N1	5.62	125.51	122.70
32	1a	1067	A	P-O3'-C3'	5.61	126.43	119.70
1	1A	2188	C	C2-N3-C4	5.59	122.70	119.90
32	2a	1025	U	C2-N1-C1'	5.57	124.39	117.70
1	2A	928	G	C6-C5-N7	-5.56	127.06	130.40
1	1A	1041	C	C2-N1-C1'	5.56	124.92	118.80
32	2a	754	C	N1-C2-O2	5.56	122.24	118.90
1	1A	1372	U	C5-C4-O4	-5.55	122.57	125.90
32	2a	748	C	P-O3'-C3'	5.55	126.36	119.70
32	2a	1378	C	N1-C2-O2	5.52	122.21	118.90
32	2a	1263	C	N1-C2-N3	-5.51	115.34	119.20
32	1a	563	A	O4'-C1'-N9	5.50	112.60	108.20
32	1a	1034	G	C5-C6-O6	5.50	131.90	128.60
1	2A	2149	G	N3-C4-N9	5.50	129.30	126.00
32	2a	913	A	P-O3'-C3'	5.50	126.30	119.70
1	1A	1941	C	C6-N1-C2	-5.46	118.11	120.30
1	2A	269	U	C2-N1-C1'	5.44	124.23	117.70
32	1a	1034	G	C6-N1-C2	5.44	128.36	125.10
1	2A	982	C	C6-N1-C2	-5.44	118.13	120.30
1	1A	1063	G	N3-C2-N2	5.39	123.67	119.90
1	2A	928	G	N1-C6-O6	5.38	123.13	119.90
32	1a	266	G	C4-N9-C1'	5.37	133.49	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	2136	C	C2-N3-C4	5.37	122.58	119.90
1	1A	1053	C	N1-C2-O2	5.36	122.12	118.90
1	1A	2573	C	N3-C2-O2	-5.35	118.16	121.90
54	2x	22	G	N1-C6-O6	-5.35	116.69	119.90
1	1A	548	A	P-O3'-C3'	5.35	126.12	119.70
1	2A	277	C	P-O3'-C3'	5.33	126.10	119.70
1	1A	2856	C	C2-N1-C1'	5.33	124.66	118.80
32	2a	1065	U	P-O3'-C3'	5.31	126.07	119.70
1	2A	269	U	N3-C2-O2	-5.29	118.50	122.20
32	2a	686	U	O4'-C1'-N1	5.28	112.42	108.20
1	1A	504	U	N1-C2-O2	5.26	126.48	122.80
1	2A	964	C	C6-N1-C2	-5.26	118.20	120.30
1	1A	1559	G	C4-N9-C1'	-5.26	119.67	126.50
1	1A	1041	C	N1-C2-O2	5.26	122.05	118.90
1	1A	195	A	P-O3'-C3'	5.25	126.00	119.70
8	2I	117	GLU	C-N-CA	-5.24	108.60	121.70
1	2A	1437	C	C2-N1-C1'	5.23	124.56	118.80
32	2a	754	C	C6-N1-C1'	-5.23	114.52	120.80
1	2A	897	C	N1-C2-O2	5.22	122.03	118.90
32	2a	115	G	P-O3'-C3'	5.22	125.97	119.70
1	2A	1313	U	N1-C2-O2	5.22	126.45	122.80
1	2A	2896	C	C2-N1-C1'	5.22	124.54	118.80
1	1A	2704	C	C6-N1-C1'	-5.21	114.54	120.80
1	2A	897	C	C2-N1-C1'	5.21	124.53	118.80
1	2A	2318	G	N3-C4-N9	5.21	129.12	126.00
1	2A	1558	A	C2-N3-C4	-5.20	108.00	110.60
1	1A	1644	C	N1-C2-O2	5.20	122.02	118.90
32	2a	1378	C	C6-N1-C1'	-5.20	114.56	120.80
1	1A	1818	U	O5'-P-OP2	-5.20	101.02	105.70
32	1a	1027	C	C6-N1-C1'	5.19	127.03	120.80
1	1A	2507	C	C6-N1-C2	-5.19	118.22	120.30
1	1A	2126	A	O4'-C1'-N9	-5.18	104.05	108.20
1	1A	1328	G	N3-C4-C5	-5.18	126.01	128.60
32	2a	1263	C	C5-C6-N1	5.18	123.59	121.00
1	1A	2623	G	N1-C6-O6	-5.18	116.79	119.90
1	1A	1174	A	OP1-P-O3'	5.17	116.57	105.20
1	1A	2167	U	O4'-C1'-N1	5.17	112.33	108.20
32	2a	1262	C	C2-N3-C4	5.16	122.48	119.90
1	2A	1779	U	C2-N1-C1'	5.16	123.89	117.70
1	1A	1176	G	P-O3'-C3'	5.15	125.88	119.70
32	2a	975	A	O4'-C1'-N9	-5.15	104.08	108.20
1	1A	121	G	C8-N9-C4	-5.15	104.34	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	1x	14	A	C8-N9-C1'	-5.14	118.45	127.70
1	1A	2139	C	C5-C4-N4	-5.13	116.61	120.20
1	2A	1437	C	N1-C2-O2	5.13	121.98	118.90
1	1A	2473	U	C2-N1-C1'	5.12	123.85	117.70
1	2A	1313	U	N3-C2-O2	-5.12	118.61	122.20
32	2a	687	A	P-O3'-C3'	5.11	125.84	119.70
1	1A	1554	A	O4'-C1'-N9	5.10	112.28	108.20
1	2A	512	G	O4'-C1'-N9	5.10	112.28	108.20
54	2x	34	C	N3-C2-O2	-5.09	118.34	121.90
1	2A	228	A	P-O3'-C3'	5.08	125.80	119.70
32	2a	1026	G	N3-C4-C5	-5.07	126.06	128.60
1	2A	1804	C	C6-N1-C2	-5.07	118.27	120.30
1	2A	752	A	P-O3'-C3'	5.05	125.77	119.70
32	1a	1065	U	P-O3'-C3'	5.05	125.76	119.70
1	2A	1379	A	OP2-P-O3'	5.05	116.31	105.20
1	2A	2896	C	N1-C2-O2	5.04	121.93	118.90
1	1A	1416	G	O4'-C1'-N9	5.03	112.23	108.20
1	1A	1075	C	N3-C2-O2	-5.03	118.38	121.90
32	2a	1264	C	N1-C2-O2	5.03	121.92	118.90
1	2A	1022	G	C8-N9-C1'	5.03	133.53	127.00
54	1x	14	A	C4-N9-C1'	5.01	135.33	126.30
32	1a	1505	G	C8-N9-C1'	5.00	133.50	127.00
1	2A	1021	A	C2-N3-C4	-5.00	108.10	110.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
20	1Y	52	SER	Peptide

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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%)	249 (91%)	24 (9%)	0	100	100
3	2D	273/276 (99%)	245 (90%)	26 (10%)	2 (1%)	22	60
4	1E	202/206 (98%)	181 (90%)	19 (9%)	2 (1%)	15	53
4	2E	202/206 (98%)	179 (89%)	19 (9%)	4 (2%)	7	34
5	1F	201/210 (96%)	177 (88%)	21 (10%)	3 (2%)	10	42
5	2F	201/210 (96%)	175 (87%)	19 (10%)	7 (4%)	3	20
6	1G	179/182 (98%)	156 (87%)	19 (11%)	4 (2%)	6	31
6	2G	179/182 (98%)	153 (86%)	24 (13%)	2 (1%)	14	50
7	1H	172/180 (96%)	155 (90%)	12 (7%)	5 (3%)	4	24
7	2H	172/180 (96%)	150 (87%)	18 (10%)	4 (2%)	6	30
8	1I	144/148 (97%)	125 (87%)	18 (12%)	1 (1%)	22	60
8	2I	144/148 (97%)	124 (86%)	18 (12%)	2 (1%)	11	43
9	1N	138/140 (99%)	126 (91%)	11 (8%)	1 (1%)	22	60
9	2N	138/140 (99%)	126 (91%)	10 (7%)	2 (1%)	11	43
10	1O	120/122 (98%)	105 (88%)	15 (12%)	0	100	100
10	2O	120/122 (98%)	106 (88%)	13 (11%)	1 (1%)	19	57
11	1P	147/150 (98%)	122 (83%)	20 (14%)	5 (3%)	3	20
11	2P	147/150 (98%)	128 (87%)	17 (12%)	2 (1%)	11	43
12	1Q	139/141 (99%)	123 (88%)	15 (11%)	1 (1%)	22	60
12	2Q	139/141 (99%)	125 (90%)	10 (7%)	4 (3%)	4	24
13	1R	116/118 (98%)	100 (86%)	14 (12%)	2 (2%)	9	39
13	2R	116/118 (98%)	105 (90%)	11 (10%)	0	100	100
14	1S	108/112 (96%)	94 (87%)	14 (13%)	0	100	100
14	2S	108/112 (96%)	100 (93%)	7 (6%)	1 (1%)	17	55
15	1T	129/146 (88%)	109 (84%)	18 (14%)	2 (2%)	9	40
15	2T	129/146 (88%)	114 (88%)	14 (11%)	1 (1%)	19	57
16	1U	114/118 (97%)	111 (97%)	3 (3%)	0	100	100
16	2U	114/118 (97%)	107 (94%)	7 (6%)	0	100	100
17	1V	99/101 (98%)	84 (85%)	14 (14%)	1 (1%)	15	53
17	2V	99/101 (98%)	95 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	1W	110/113 (97%)	107 (97%)	2 (2%)	1 (1%)	17	55
18	2W	110/113 (97%)	101 (92%)	8 (7%)	1 (1%)	17	55
19	1X	93/96 (97%)	85 (91%)	8 (9%)	0	100	100
19	2X	93/96 (97%)	80 (86%)	12 (13%)	1 (1%)	14	50
20	1Y	105/110 (96%)	92 (88%)	12 (11%)	1 (1%)	15	53
20	2Y	105/110 (96%)	93 (89%)	8 (8%)	4 (4%)	3	18
21	1Z	148/206 (72%)	120 (81%)	23 (16%)	5 (3%)	3	20
21	2Z	156/206 (76%)	118 (76%)	35 (22%)	3 (2%)	8	36
22	10	81/85 (95%)	74 (91%)	6 (7%)	1 (1%)	13	48
22	20	81/85 (95%)	74 (91%)	7 (9%)	0	100	100
23	11	95/98 (97%)	88 (93%)	7 (7%)	0	100	100
23	21	95/98 (97%)	85 (90%)	7 (7%)	3 (3%)	4	22
24	12	68/72 (94%)	61 (90%)	7 (10%)	0	100	100
24	22	68/72 (94%)	66 (97%)	2 (3%)	0	100	100
25	13	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
25	23	57/60 (95%)	52 (91%)	5 (9%)	0	100	100
26	14	67/71 (94%)	50 (75%)	12 (18%)	5 (8%)	1	5
26	24	67/71 (94%)	50 (75%)	14 (21%)	3 (4%)	2	14
27	15	57/60 (95%)	51 (90%)	5 (9%)	1 (2%)	8	37
27	25	57/60 (95%)	52 (91%)	5 (9%)	0	100	100
28	16	51/54 (94%)	46 (90%)	5 (10%)	0	100	100
28	26	51/54 (94%)	43 (84%)	8 (16%)	0	100	100
29	17	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
29	27	46/49 (94%)	43 (94%)	3 (6%)	0	100	100
30	18	62/65 (95%)	59 (95%)	3 (5%)	0	100	100
30	28	62/65 (95%)	57 (92%)	5 (8%)	0	100	100
31	19	35/37 (95%)	32 (91%)	3 (9%)	0	100	100
31	29	35/37 (95%)	30 (86%)	5 (14%)	0	100	100
33	1b	229/256 (90%)	186 (81%)	36 (16%)	7 (3%)	4	23
33	2b	229/256 (90%)	193 (84%)	28 (12%)	8 (4%)	3	20
34	1c	204/239 (85%)	179 (88%)	22 (11%)	3 (2%)	10	42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	2c	204/239 (85%)	171 (84%)	29 (14%)	4 (2%)	7	34
35	1d	206/209 (99%)	173 (84%)	31 (15%)	2 (1%)	15	53
35	2d	206/209 (99%)	185 (90%)	17 (8%)	4 (2%)	8	36
36	1e	146/162 (90%)	127 (87%)	15 (10%)	4 (3%)	5	26
36	2e	146/162 (90%)	129 (88%)	14 (10%)	3 (2%)	7	33
37	1f	98/101 (97%)	91 (93%)	7 (7%)	0	100	100
37	2f	98/101 (97%)	89 (91%)	9 (9%)	0	100	100
38	1g	153/156 (98%)	133 (87%)	17 (11%)	3 (2%)	7	34
38	2g	153/156 (98%)	132 (86%)	18 (12%)	3 (2%)	7	34
39	1h	135/138 (98%)	125 (93%)	10 (7%)	0	100	100
39	2h	135/138 (98%)	124 (92%)	10 (7%)	1 (1%)	22	60
40	1i	125/128 (98%)	102 (82%)	20 (16%)	3 (2%)	6	29
40	2i	125/128 (98%)	106 (85%)	15 (12%)	4 (3%)	4	22
41	1j	95/105 (90%)	78 (82%)	15 (16%)	2 (2%)	7	33
41	2j	94/105 (90%)	75 (80%)	16 (17%)	3 (3%)	4	22
42	1k	112/129 (87%)	90 (80%)	19 (17%)	3 (3%)	5	26
42	2k	112/129 (87%)	95 (85%)	13 (12%)	4 (4%)	3	19
43	1l	119/132 (90%)	103 (87%)	14 (12%)	2 (2%)	9	39
43	2l	119/132 (90%)	99 (83%)	19 (16%)	1 (1%)	19	57
44	1m	120/126 (95%)	96 (80%)	19 (16%)	5 (4%)	3	16
44	2m	119/126 (94%)	99 (83%)	17 (14%)	3 (2%)	5	28
45	1n	58/61 (95%)	52 (90%)	6 (10%)	0	100	100
45	2n	58/61 (95%)	55 (95%)	2 (3%)	1 (2%)	9	39
46	1o	86/89 (97%)	77 (90%)	6 (7%)	3 (4%)	3	20
46	2o	86/89 (97%)	77 (90%)	8 (9%)	1 (1%)	13	48
47	1p	80/88 (91%)	71 (89%)	7 (9%)	2 (2%)	5	28
47	2p	80/88 (91%)	64 (80%)	15 (19%)	1 (1%)	12	45
48	1q	97/105 (92%)	84 (87%)	12 (12%)	1 (1%)	15	53
48	2q	97/105 (92%)	88 (91%)	8 (8%)	1 (1%)	15	53
49	1r	66/88 (75%)	60 (91%)	5 (8%)	1 (2%)	10	42
49	2r	66/88 (75%)	64 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
50	1s	81/93 (87%)	65 (80%)	15 (18%)	1 (1%)	13	48
50	2s	81/93 (87%)	60 (74%)	21 (26%)	0	100	100
51	1t	94/106 (89%)	78 (83%)	13 (14%)	3 (3%)	4	22
51	2t	94/106 (89%)	84 (89%)	8 (8%)	2 (2%)	7	33
52	1u	21/27 (78%)	13 (62%)	6 (29%)	2 (10%)	0	3
52	2u	21/27 (78%)	16 (76%)	4 (19%)	1 (5%)	2	13
All	All	11368/12128 (94%)	9944 (88%)	1244 (11%)	180 (2%)	9	40

All (180) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	1F	130	ALA
7	1H	92	ILE
11	1P	45	LEU
33	1b	17	PHE
33	1b	33	TYR
36	1e	96	PRO
44	1m	67	GLU
44	1m	106	ASN
46	1o	88	ARG
52	1u	3	LYS
6	2G	84	LYS
12	2Q	16	ARG
33	2b	10	LEU
33	2b	17	PHE
35	2d	4	TYR
35	2d	5	ILE
40	2i	54	ASP
42	2k	112	THR
43	2l	105	TYR
51	2t	10	LEU
52	2u	3	LYS
6	1G	44	GLY
6	1G	49	ASP
6	1G	164	GLU
7	1H	126	PRO
11	1P	24	GLY
11	1P	28	GLY
12	1Q	16	ARG
21	1Z	45	ASP

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Mol	Chain	Res	Type
21	1Z	64	GLY
26	14	38	LYS
26	14	49	PHE
26	14	61	ARG
26	14	62	ARG
34	1c	129	ALA
40	1i	83	ARG
42	1k	106	LYS
43	1l	105	TYR
47	1p	81	ARG
48	1q	68	ARG
49	1r	36	ASN
3	2D	160	GLY
4	2E	113	PHE
5	2F	16	GLY
5	2F	130	ALA
5	2F	131	GLY
6	2G	42	GLY
7	2H	46	GLU
7	2H	92	ILE
11	2P	45	LEU
14	2S	84	GLN
26	24	49	PHE
33	2b	9	GLU
35	2d	124	GLY
35	2d	186	LEU
38	2g	55	GLY
41	2j	75	ILE
48	2q	68	ARG
4	1E	71	GLY
7	1H	46	GLU
11	1P	67	MET
13	1R	103	ARG
20	1Y	103	GLY
21	1Z	120	ILE
27	15	21	SER
33	1b	20	GLU
33	1b	129	GLU
34	1c	98	ASN
36	1e	22	GLY
40	1i	29	ASN
41	1j	91	PRO

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Mol	Chain	Res	Type
44	1m	105	THR
47	1p	77	ALA
51	1t	100	ILE
5	2F	120	GLU
5	2F	145	GLU
8	2I	10	GLU
9	2N	19	GLU
10	2O	54	GLU
18	2W	60	ASN
20	2Y	21	LYS
20	2Y	57	GLN
21	2Z	66	SER
33	2b	125	PRO
34	2c	27	LYS
38	2g	80	VAL
39	2h	86	ILE
41	2j	78	ASN
42	2k	106	LYS
44	2m	23	TYR
46	2o	23	GLY
4	1E	52	LEU
9	1N	2	LYS
15	1T	128	GLU
17	1V	97	LYS
38	1g	130	GLY
41	1j	77	PRO
44	1m	8	GLU
51	1t	102	GLY
52	1u	4	GLY
4	2E	52	LEU
4	2E	144	ARG
5	2F	168	ARG
7	2H	65	HIS
9	2N	2	LYS
12	2Q	28	ALA
15	2T	127	ALA
19	2X	93	GLU
21	2Z	65	GLN
33	2b	123	ALA
34	2c	40	ARG
34	2c	99	VAL
34	2c	174	PRO

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Mol	Chain	Res	Type
36	2e	69	VAL
36	2e	77	PRO
38	2g	7	ALA
42	2k	49	GLY
45	2n	14	PRO
47	2p	52	ASP
51	2t	102	GLY
6	1G	84	LYS
7	1H	151	ILE
11	1P	23	PRO
18	1W	80	PRO
35	1d	4	TYR
35	1d	197	PRO
42	1k	49	GLY
51	1t	95	ALA
7	2H	118	PRO
11	2P	44	GLY
12	2Q	22	LYS
23	2I	64	ALA
23	2I	65	SER
26	24	62	ARG
33	2b	20	GLU
40	2i	10	ARG
40	2i	91	ASP
44	2m	6	GLY
7	1H	110	SER
40	1i	92	TYR
42	1k	105	VAL
43	1l	125	PRO
3	2D	203	ASN
4	2E	71	GLY
20	2Y	101	LYS
33	2b	227	GLY
41	2j	31	GLY
44	2m	117	VAL
15	1T	37	GLY
34	1c	14	ILE
38	1g	80	VAL
46	1o	19	PRO
46	1o	86	GLY
8	2I	111	PRO
40	2i	97	LYS

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Mol	Chain	Res	Type
42	2k	118	GLY
5	1F	89	VAL
21	1Z	134	PRO
22	10	6	GLY
33	1b	231	GLU
38	1g	112	PRO
44	1m	60	VAL
50	1s	19	VAL
5	2F	207	GLY
12	2Q	47	ILE
8	1I	145	VAL
21	1Z	39	VAL
36	1e	51	VAL
20	2Y	55	TYR
26	24	29	PRO
5	1F	71	GLY
13	1R	39	PRO
26	14	45	GLY
33	1b	124	SER
21	2Z	167	PRO
33	2b	93	VAL
36	1e	69	VAL
23	21	30	VAL
36	2e	13	ILE
33	1b	125	PRO

5.3.2 Protein sidechains ⓘ

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%)	191 (89%)	24 (11%)	6	24
3	2D	215/218 (99%)	198 (92%)	17 (8%)	12	41
4	1E	164/166 (99%)	148 (90%)	16 (10%)	8	30
4	2E	164/166 (99%)	146 (89%)	18 (11%)	6	25
5	1F	160/166 (96%)	144 (90%)	16 (10%)	7	29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	2F	159/166 (96%)	144 (91%)	15 (9%)	8	32
6	1G	143/156 (92%)	124 (87%)	19 (13%)	4	17
6	2G	143/156 (92%)	128 (90%)	15 (10%)	7	27
7	1H	144/148 (97%)	127 (88%)	17 (12%)	5	22
7	2H	144/148 (97%)	118 (82%)	26 (18%)	1	9
8	1I	113/124 (91%)	94 (83%)	19 (17%)	2	11
8	2I	105/124 (85%)	87 (83%)	18 (17%)	2	10
9	1N	118/119 (99%)	106 (90%)	12 (10%)	7	28
9	2N	118/119 (99%)	107 (91%)	11 (9%)	9	33
10	1O	100/100 (100%)	94 (94%)	6 (6%)	19	53
10	2O	100/100 (100%)	91 (91%)	9 (9%)	9	35
11	1P	115/116 (99%)	103 (90%)	12 (10%)	7	27
11	2P	115/116 (99%)	103 (90%)	12 (10%)	7	27
12	1Q	111/111 (100%)	100 (90%)	11 (10%)	8	30
12	2Q	111/111 (100%)	102 (92%)	9 (8%)	11	40
13	1R	101/101 (100%)	92 (91%)	9 (9%)	9	35
13	2R	101/101 (100%)	91 (90%)	10 (10%)	8	30
14	1S	86/88 (98%)	73 (85%)	13 (15%)	3	14
14	2S	85/88 (97%)	76 (89%)	9 (11%)	6	26
15	1T	115/127 (91%)	98 (85%)	17 (15%)	3	14
15	2T	113/127 (89%)	106 (94%)	7 (6%)	18	52
16	1U	93/94 (99%)	90 (97%)	3 (3%)	39	74
16	2U	93/94 (99%)	86 (92%)	7 (8%)	13	43
17	1V	80/82 (98%)	72 (90%)	8 (10%)	7	29
17	2V	80/82 (98%)	76 (95%)	4 (5%)	24	60
18	1W	90/92 (98%)	84 (93%)	6 (7%)	16	49
18	2W	90/92 (98%)	86 (96%)	4 (4%)	28	65
19	1X	77/78 (99%)	71 (92%)	6 (8%)	12	42
19	2X	77/78 (99%)	74 (96%)	3 (4%)	32	69
20	1Y	85/91 (93%)	74 (87%)	11 (13%)	4	19
20	2Y	85/91 (93%)	78 (92%)	7 (8%)	11	39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	1Z	135/179 (75%)	113 (84%)	22 (16%)	2	11
21	2Z	137/179 (76%)	114 (83%)	23 (17%)	2	11
22	10	65/67 (97%)	59 (91%)	6 (9%)	9	34
22	20	65/67 (97%)	58 (89%)	7 (11%)	6	26
23	11	80/83 (96%)	76 (95%)	4 (5%)	24	60
23	21	80/83 (96%)	72 (90%)	8 (10%)	7	29
24	12	65/67 (97%)	56 (86%)	9 (14%)	3	17
24	22	65/67 (97%)	57 (88%)	8 (12%)	4	21
25	13	51/52 (98%)	42 (82%)	9 (18%)	2	10
25	23	50/52 (96%)	39 (78%)	11 (22%)	1	4
26	14	59/63 (94%)	44 (75%)	15 (25%)	0	3
26	24	53/63 (84%)	42 (79%)	11 (21%)	1	5
27	15	50/52 (96%)	46 (92%)	4 (8%)	12	40
27	25	50/52 (96%)	48 (96%)	2 (4%)	31	68
28	16	51/52 (98%)	46 (90%)	5 (10%)	8	30
28	26	50/52 (96%)	35 (70%)	15 (30%)	0	1
29	17	41/42 (98%)	38 (93%)	3 (7%)	14	44
29	27	41/42 (98%)	37 (90%)	4 (10%)	8	30
30	18	54/55 (98%)	51 (94%)	3 (6%)	21	56
30	28	54/55 (98%)	49 (91%)	5 (9%)	9	33
31	19	34/34 (100%)	32 (94%)	2 (6%)	19	54
31	29	34/34 (100%)	31 (91%)	3 (9%)	10	36
33	1b	192/220 (87%)	162 (84%)	30 (16%)	2	13
33	2b	187/220 (85%)	158 (84%)	29 (16%)	2	13
34	1c	142/188 (76%)	126 (89%)	16 (11%)	6	24
34	2c	140/188 (74%)	123 (88%)	17 (12%)	5	21
35	1d	169/181 (93%)	145 (86%)	24 (14%)	3	16
35	2d	173/181 (96%)	153 (88%)	20 (12%)	5	23
36	1e	113/123 (92%)	101 (89%)	12 (11%)	6	26
36	2e	114/123 (93%)	103 (90%)	11 (10%)	8	32
37	1f	84/90 (93%)	78 (93%)	6 (7%)	14	46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	2f	85/90 (94%)	74 (87%)	11 (13%)	4	19
38	1g	119/127 (94%)	101 (85%)	18 (15%)	3	14
38	2g	120/127 (94%)	104 (87%)	16 (13%)	4	17
39	1h	114/119 (96%)	105 (92%)	9 (8%)	12	41
39	2h	114/119 (96%)	105 (92%)	9 (8%)	12	41
40	1i	90/99 (91%)	78 (87%)	12 (13%)	4	17
40	2i	89/99 (90%)	74 (83%)	15 (17%)	2	11
41	1j	66/92 (72%)	54 (82%)	12 (18%)	1	9
41	2j	69/92 (75%)	63 (91%)	6 (9%)	10	37
42	1k	82/99 (83%)	73 (89%)	9 (11%)	6	25
42	2k	83/99 (84%)	75 (90%)	8 (10%)	8	32
43	1l	96/108 (89%)	87 (91%)	9 (9%)	8	32
43	2l	96/108 (89%)	85 (88%)	11 (12%)	5	24
44	1m	92/101 (91%)	78 (85%)	14 (15%)	3	14
44	2m	91/101 (90%)	77 (85%)	14 (15%)	2	13
45	1n	49/50 (98%)	43 (88%)	6 (12%)	5	21
45	2n	49/50 (98%)	44 (90%)	5 (10%)	7	28
46	1o	78/80 (98%)	72 (92%)	6 (8%)	13	42
46	2o	78/80 (98%)	72 (92%)	6 (8%)	13	42
47	1p	69/74 (93%)	55 (80%)	14 (20%)	1	6
47	2p	68/74 (92%)	55 (81%)	13 (19%)	1	8
48	1q	94/97 (97%)	88 (94%)	6 (6%)	17	51
48	2q	94/97 (97%)	87 (93%)	7 (7%)	13	44
49	1r	59/77 (77%)	53 (90%)	6 (10%)	7	28
49	2r	59/77 (77%)	56 (95%)	3 (5%)	24	60
50	1s	69/80 (86%)	65 (94%)	4 (6%)	20	55
50	2s	67/80 (84%)	58 (87%)	9 (13%)	4	17
51	1t	70/82 (85%)	64 (91%)	6 (9%)	10	37
51	2t	70/82 (85%)	58 (83%)	12 (17%)	2	10
52	1u	18/22 (82%)	17 (94%)	1 (6%)	21	56
52	2u	18/22 (82%)	16 (89%)	2 (11%)	6	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	9301/10064 (92%)	8252 (89%)	1049 (11%)	6 24

All (1049) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	1D	3	VAL
3	1D	12	SER
3	1D	15	PHE
3	1D	50	THR
3	1D	72	LYS
3	1D	73	VAL
3	1D	106	ILE
3	1D	111	LEU
3	1D	113	VAL
3	1D	116	GLN
3	1D	122	ASP
3	1D	127	VAL
3	1D	131	LEU
3	1D	138	VAL
3	1D	140	THR
3	1D	141	VAL
3	1D	193	VAL
3	1D	204	ILE
3	1D	229	VAL
3	1D	230	ASP
3	1D	242	ARG
3	1D	254	THR
3	1D	260	ARG
3	1D	267	SER
4	1E	7	VAL
4	1E	21	VAL
4	1E	34	VAL
4	1E	42	ASP
4	1E	45	THR
4	1E	73	GLU
4	1E	75	VAL
4	1E	82	ARG
4	1E	89	ASP
4	1E	104	VAL
4	1E	105	THR
4	1E	116	VAL
4	1E	121	ASN

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Mol	Chain	Res	Type
4	1E	137	HIS
4	1E	155	LYS
4	1E	184	VAL
5	1F	15	SER
5	1F	32	LEU
5	1F	56	GLU
5	1F	74	ARG
5	1F	88	VAL
5	1F	105	VAL
5	1F	132	VAL
5	1F	136	THR
5	1F	140	LEU
5	1F	156	LEU
5	1F	162	LEU
5	1F	170	LEU
5	1F	175	THR
5	1F	191	ARG
5	1F	192	LEU
5	1F	205	ARG
6	1G	3	LEU
6	1G	5	VAL
6	1G	9	ARG
6	1G	21	ARG
6	1G	28	VAL
6	1G	31	VAL
6	1G	82	LEU
6	1G	88	ILE
6	1G	91	ARG
6	1G	96	ARG
6	1G	124	SER
6	1G	132	ASN
6	1G	133	LEU
6	1G	138	GLN
6	1G	140	ILE
6	1G	148	MET
6	1G	150	ASP
6	1G	159	VAL
6	1G	170	ARG
7	1H	3	ARG
7	1H	13	LYS
7	1H	16	SER
7	1H	18	GLU

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Mol	Chain	Res	Type
7	1H	30	LYS
7	1H	35	VAL
7	1H	45	VAL
7	1H	68	THR
7	1H	71	LEU
7	1H	95	ARG
7	1H	98	LEU
7	1H	107	VAL
7	1H	111	HIS
7	1H	119	GLU
7	1H	136	ILE
7	1H	155	SER
7	1H	169	VAL
8	1I	6	LEU
8	1I	9	LEU
8	1I	10	GLU
8	1I	14	ASP
8	1I	19	VAL
8	1I	35	LEU
8	1I	37	VAL
8	1I	47	LEU
8	1I	74	ASN
8	1I	77	LEU
8	1I	85	GLU
8	1I	92	VAL
8	1I	96	ASP
8	1I	108	THR
8	1I	109	ILE
8	1I	114	LEU
8	1I	117	GLU
8	1I	128	LEU
8	1I	145	VAL
9	1N	1	MET
9	1N	3	THR
9	1N	17	ASP
9	1N	23	LEU
9	1N	28	THR
9	1N	33	LEU
9	1N	38	HIS
9	1N	46	VAL
9	1N	60	ILE
9	1N	67	LEU

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Mol	Chain	Res	Type
9	1N	87	LEU
9	1N	96	GLU
10	1O	19	ILE
10	1O	69	ILE
10	1O	75	SER
10	1O	87	ILE
10	1O	96	THR
10	1O	116	SER
11	1P	3	LEU
11	1P	7	ARG
11	1P	45	LEU
11	1P	56	SER
11	1P	57	THR
11	1P	75	ILE
11	1P	79	ARG
11	1P	95	VAL
11	1P	117	GLU
11	1P	123	LEU
11	1P	125	VAL
11	1P	148	LEU
12	1Q	2	LEU
12	1Q	6	ARG
12	1Q	43	THR
12	1Q	56	ARG
12	1Q	60	ARG
12	1Q	75	THR
12	1Q	89	ASN
12	1Q	110	THR
12	1Q	133	ARG
12	1Q	138	ASP
12	1Q	141	GLN
13	1R	1	MET
13	1R	15	SER
13	1R	24	GLN
13	1R	36	THR
13	1R	60	LEU
13	1R	65	LEU
13	1R	67	LEU
13	1R	73	VAL
13	1R	114	VAL
14	1S	4	LEU
14	1S	5	THR

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Mol	Chain	Res	Type
14	1S	35	ILE
14	1S	36	TYR
14	1S	49	VAL
14	1S	50	SER
14	1S	52	SER
14	1S	53	SER
14	1S	64	GLU
14	1S	73	LEU
14	1S	85	VAL
14	1S	92	TYR
14	1S	98	VAL
15	1T	1	MET
15	1T	13	ARG
15	1T	17	THR
15	1T	18	ASP
15	1T	32	TYR
15	1T	33	LYS
15	1T	35	LYS
15	1T	43	GLN
15	1T	51	ARG
15	1T	66	VAL
15	1T	67	SER
15	1T	74	ARG
15	1T	85	LYS
15	1T	89	VAL
15	1T	111	ARG
15	1T	114	LEU
15	1T	124	ASP
16	1U	52	ARG
16	1U	54	LYS
16	1U	97	ASP
17	1V	7	THR
17	1V	33	VAL
17	1V	51	VAL
17	1V	52	VAL
17	1V	61	VAL
17	1V	85	LYS
17	1V	95	LEU
17	1V	99	ILE
18	1W	4	LYS
18	1W	10	VAL
18	1W	11	ARG

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Mol	Chain	Res	Type
18	1W	17	VAL
18	1W	67	ASP
18	1W	92	ARG
19	1X	14	SER
19	1X	41	ASN
19	1X	52	VAL
19	1X	68	ARG
19	1X	81	VAL
19	1X	92	LEU
20	1Y	8	LYS
20	1Y	11	ASP
20	1Y	19	LYS
20	1Y	30	VAL
20	1Y	39	VAL
20	1Y	45	VAL
20	1Y	67	LEU
20	1Y	90	LEU
20	1Y	91	GLU
20	1Y	99	CYS
20	1Y	106	LEU
21	1Z	1	MET
21	1Z	31	ARG
21	1Z	37	VAL
21	1Z	40	ASP
21	1Z	50	GLN
21	1Z	55	HIS
21	1Z	56	VAL
21	1Z	80	ARG
21	1Z	86	VAL
21	1Z	87	ASP
21	1Z	88	PHE
21	1Z	93	ASP
21	1Z	98	MET
21	1Z	119	GLU
21	1Z	122	ARG
21	1Z	126	VAL
21	1Z	140	ASP
21	1Z	146	ILE
21	1Z	149	SER
21	1Z	154	ASP
21	1Z	155	LEU
21	1Z	170	THR

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Mol	Chain	Res	Type
22	10	3	HIS
22	10	12	ASN
22	10	14	ARG
22	10	37	LEU
22	10	43	THR
22	10	55	ARG
23	11	35	THR
23	11	37	ILE
23	11	46	LEU
23	11	51	VAL
24	12	3	LEU
24	12	4	SER
24	12	9	GLN
24	12	10	LEU
24	12	30	ARG
24	12	40	SER
24	12	41	ILE
24	12	44	LEU
24	12	45	SER
25	13	23	LEU
25	13	37	LEU
25	13	38	GLU
25	13	40	THR
25	13	44	ARG
25	13	54	VAL
25	13	56	VAL
25	13	58	VAL
25	13	60	GLU
26	14	1	MET
26	14	5	ILE
26	14	10	VAL
26	14	14	ILE
26	14	27	THR
26	14	33	VAL
26	14	37	SER
26	14	49	PHE
26	14	50	VAL
26	14	52	THR
26	14	53	GLU
26	14	58	ARG
26	14	61	ARG
26	14	63	TYR

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Mol	Chain	Res	Type
26	14	67	TYR
27	15	16	ARG
27	15	44	THR
27	15	46	CYS
27	15	57	VAL
28	16	6	ARG
28	16	19	ARG
28	16	47	THR
28	16	48	VAL
28	16	51	GLU
29	17	4	THR
29	17	24	THR
29	17	41	ARG
30	18	14	VAL
30	18	29	LYS
30	18	31	HIS
31	19	4	ARG
31	19	28	GLU
33	1b	8	LYS
33	1b	12	GLU
33	1b	17	PHE
33	1b	21	ARG
33	1b	24	TRP
33	1b	42	ILE
33	1b	54	THR
33	1b	64	ARG
33	1b	76	GLN
33	1b	80	ILE
33	1b	81	VAL
33	1b	93	VAL
33	1b	107	THR
33	1b	111	ARG
33	1b	127	ILE
33	1b	142	LEU
33	1b	158	LEU
33	1b	160	ASP
33	1b	163	PHE
33	1b	164	VAL
33	1b	168	THR
33	1b	172	ILE
33	1b	179	LYS
33	1b	180	LEU

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Mol	Chain	Res	Type
33	1b	185	ILE
33	1b	198	ASP
33	1b	211	ILE
33	1b	223	ILE
33	1b	230	VAL
33	1b	231	GLU
34	1c	3	ASN
34	1c	5	ILE
34	1c	17	ASP
34	1c	26	LYS
34	1c	30	ARG
34	1c	31	HIS
34	1c	34	LEU
34	1c	45	LYS
34	1c	46	GLU
34	1c	63	ASN
34	1c	103	VAL
34	1c	115	LEU
34	1c	136	GLN
34	1c	188	LEU
34	1c	192	THR
34	1c	195	VAL
35	1d	8	VAL
35	1d	10	ARG
35	1d	17	VAL
35	1d	21	LEU
35	1d	47	ARG
35	1d	49	ARG
35	1d	64	LEU
35	1d	83	SER
35	1d	100	ARG
35	1d	135	LEU
35	1d	138	TYR
35	1d	146	ILE
35	1d	155	LEU
35	1d	157	LEU
35	1d	158	ILE
35	1d	162	LEU
35	1d	166	LYS
35	1d	170	VAL
35	1d	173	TRP
35	1d	175	SER

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Mol	Chain	Res	Type
35	1d	178	VAL
35	1d	188	LEU
35	1d	190	ASP
35	1d	194	LEU
36	1e	11	ILE
36	1e	27	ARG
36	1e	41	VAL
36	1e	66	MET
36	1e	75	THR
36	1e	78	HIS
36	1e	81	GLU
36	1e	83	GLU
36	1e	84	PHE
36	1e	117	ASP
36	1e	118	ILE
36	1e	151	LEU
37	1f	17	SER
37	1f	40	VAL
37	1f	57	GLN
37	1f	72	VAL
37	1f	77	ARG
37	1f	95	GLU
38	1g	12	LEU
38	1g	13	GLN
38	1g	15	ASP
38	1g	18	TYR
38	1g	22	LEU
38	1g	24	THR
38	1g	27	ILE
38	1g	45	ASP
38	1g	51	GLN
38	1g	56	GLN
38	1g	74	GLU
38	1g	79	ARG
38	1g	113	GLU
38	1g	114	ARG
38	1g	115	ARG
38	1g	135	VAL
38	1g	140	ASP
38	1g	143	ARG
39	1h	3	THR
39	1h	19	VAL

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Mol	Chain	Res	Type
39	1h	26	VAL
39	1h	52	ASP
39	1h	79	VAL
39	1h	107	LEU
39	1h	112	LEU
39	1h	115	SER
39	1h	133	LEU
40	1i	18	PHE
40	1i	19	LEU
40	1i	23	ASN
40	1i	47	LEU
40	1i	59	PHE
40	1i	64	THR
40	1i	92	TYR
40	1i	96	LEU
40	1i	111	ARG
40	1i	114	TYR
40	1i	121	ARG
40	1i	128	ARG
41	1j	19	SER
41	1j	21	GLN
41	1j	49	VAL
41	1j	66	ARG
41	1j	68	HIS
41	1j	69	ASN
41	1j	81	THR
41	1j	94	VAL
41	1j	96	ILE
41	1j	97	GLU
41	1j	98	ILE
41	1j	100	THR
42	1k	34	ASP
42	1k	47	VAL
42	1k	78	GLN
42	1k	81	ASP
42	1k	87	THR
42	1k	99	GLN
42	1k	109	VAL
42	1k	114	VAL
42	1k	116	HIS
43	1l	22	SER
43	1l	42	THR

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Mol	Chain	Res	Type
43	1l	43	VAL
43	1l	55	VAL
43	1l	67	THR
43	1l	83	VAL
43	1l	104	VAL
43	1l	113	ARG
43	1l	122	THR
44	1m	4	ILE
44	1m	20	THR
44	1m	23	TYR
44	1m	32	GLU
44	1m	43	THR
44	1m	49	THR
44	1m	56	LEU
44	1m	59	TYR
44	1m	60	VAL
44	1m	63	THR
44	1m	64	TRP
44	1m	96	LEU
44	1m	102	ARG
44	1m	117	VAL
45	1n	3	ARG
45	1n	7	ILE
45	1n	13	THR
45	1n	18	VAL
45	1n	29	ARG
45	1n	33	VAL
46	1o	4	THR
46	1o	21	ASP
46	1o	34	LEU
46	1o	57	LEU
46	1o	66	LEU
46	1o	88	ARG
47	1p	1	MET
47	1p	2	VAL
47	1p	11	SER
47	1p	29	ASP
47	1p	33	ILE
47	1p	38	TYR
47	1p	42	ARG
47	1p	45	THR
47	1p	47	ASP

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Mol	Chain	Res	Type
47	1p	57	ARG
47	1p	58	TYR
47	1p	62	VAL
47	1p	67	THR
47	1p	72	ARG
48	1q	19	VAL
48	1q	35	VAL
48	1q	60	ILE
48	1q	79	SER
48	1q	87	LYS
48	1q	96	GLU
49	1r	25	THR
49	1r	46	GLU
49	1r	65	ILE
49	1r	68	LYS
49	1r	75	ILE
49	1r	85	LEU
50	1s	23	ASN
50	1s	28	LYS
50	1s	30	LEU
50	1s	37	ARG
51	1t	10	LEU
51	1t	11	SER
51	1t	42	GLN
51	1t	50	GLU
51	1t	56	MET
51	1t	71	THR
52	1u	20	LYS
3	2D	13	ARG
3	2D	23	GLU
3	2D	37	LEU
3	2D	45	ASN
3	2D	71	ASP
3	2D	88	ARG
3	2D	109	ASP
3	2D	113	VAL
3	2D	122	ASP
3	2D	138	VAL
3	2D	147	LEU
3	2D	161	THR
3	2D	162	SER
3	2D	193	VAL

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Mol	Chain	Res	Type
3	2D	229	VAL
3	2D	242	ARG
3	2D	275	LYS
4	2E	7	VAL
4	2E	21	VAL
4	2E	34	VAL
4	2E	38	THR
4	2E	45	THR
4	2E	72	VAL
4	2E	73	GLU
4	2E	75	VAL
4	2E	78	LEU
4	2E	90	THR
4	2E	113	PHE
4	2E	116	VAL
4	2E	119	ARG
4	2E	121	ASN
4	2E	167	VAL
4	2E	170	LEU
4	2E	178	GLU
4	2E	197	ILE
5	2F	15	SER
5	2F	27	GLU
5	2F	50	SER
5	2F	70	THR
5	2F	88	VAL
5	2F	89	VAL
5	2F	106	ARG
5	2F	110	LEU
5	2F	140	LEU
5	2F	145	GLU
5	2F	160	ASN
5	2F	170	LEU
5	2F	188	ARG
5	2F	190	GLU
5	2F	191	ARG
6	2G	3	LEU
6	2G	31	VAL
6	2G	36	LYS
6	2G	43	LEU
6	2G	47	LYS
6	2G	51	ARG

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Mol	Chain	Res	Type
6	2G	53	LEU
6	2G	75	LYS
6	2G	79	ASN
6	2G	90	LEU
6	2G	99	MET
6	2G	135	LEU
6	2G	152	LEU
6	2G	155	MET
6	2G	159	VAL
7	2H	4	ILE
7	2H	15	VAL
7	2H	23	ARG
7	2H	27	LYS
7	2H	30	LYS
7	2H	32	GLU
7	2H	37	VAL
7	2H	42	ARG
7	2H	44	VAL
7	2H	45	VAL
7	2H	46	GLU
7	2H	49	VAL
7	2H	68	THR
7	2H	70	THR
7	2H	71	LEU
7	2H	81	GLU
7	2H	92	ILE
7	2H	99	VAL
7	2H	105	LEU
7	2H	106	THR
7	2H	107	VAL
7	2H	119	GLU
7	2H	127	GLU
7	2H	134	SER
7	2H	139	GLN
7	2H	175	LYS
8	2I	6	LEU
8	2I	20	ASP
8	2I	25	TYR
8	2I	38	LEU
8	2I	40	THR
8	2I	41	GLU
8	2I	51	ILE

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Mol	Chain	Res	Type
8	2I	58	LEU
8	2I	61	ARG
8	2I	74	ASN
8	2I	81	VAL
8	2I	86	THR
8	2I	87	LYS
8	2I	92	VAL
8	2I	93	THR
8	2I	101	LEU
8	2I	127	VAL
8	2I	144	VAL
9	2N	1	MET
9	2N	12	ARG
9	2N	28	THR
9	2N	43	THR
9	2N	55	VAL
9	2N	67	LEU
9	2N	68	GLU
9	2N	73	THR
9	2N	87	LEU
9	2N	96	GLU
9	2N	127	ASP
10	2O	3	GLN
10	2O	9	GLU
10	2O	23	ARG
10	2O	32	TYR
10	2O	34	THR
10	2O	35	VAL
10	2O	52	VAL
10	2O	78	ARG
10	2O	88	ASN
11	2P	3	LEU
11	2P	7	ARG
11	2P	32	THR
11	2P	56	SER
11	2P	67	MET
11	2P	71	VAL
11	2P	79	ARG
11	2P	90	ARG
11	2P	95	VAL
11	2P	117	GLU
11	2P	123	LEU

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Mol	Chain	Res	Type
11	2P	148	LEU
12	2Q	1	MET
12	2Q	5	ARG
12	2Q	7	MET
12	2Q	35	VAL
12	2Q	56	ARG
12	2Q	74	TYR
12	2Q	110	THR
12	2Q	131	ILE
12	2Q	141	GLN
13	2R	1	MET
13	2R	37	THR
13	2R	65	LEU
13	2R	73	VAL
13	2R	91	GLN
13	2R	95	THR
13	2R	96	ARG
13	2R	100	LEU
13	2R	103	ARG
13	2R	105	ARG
14	2S	12	PHE
14	2S	20	ARG
14	2S	27	SER
14	2S	40	ILE
14	2S	48	LEU
14	2S	58	LEU
14	2S	69	VAL
14	2S	85	VAL
14	2S	99	LYS
15	2T	6	LEU
15	2T	17	THR
15	2T	67	SER
15	2T	87	ASP
15	2T	88	ILE
15	2T	96	ARG
15	2T	107	ASP
16	2U	19	LYS
16	2U	52	ARG
16	2U	65	ILE
16	2U	88	ILE
16	2U	92	ARG
16	2U	95	LEU

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Mol	Chain	Res	Type
16	2U	117	GLN
17	2V	7	THR
17	2V	47	VAL
17	2V	56	SER
17	2V	85	LYS
18	2W	11	ARG
18	2W	23	LEU
18	2W	67	ASP
18	2W	103	ILE
19	2X	81	VAL
19	2X	82	GLN
19	2X	83	VAL
20	2Y	6	HIS
20	2Y	51	VAL
20	2Y	61	ILE
20	2Y	67	LEU
20	2Y	70	SER
20	2Y	90	LEU
20	2Y	99	CYS
21	2Z	6	LYS
21	2Z	18	LEU
21	2Z	24	LEU
21	2Z	40	ASP
21	2Z	46	LYS
21	2Z	50	GLN
21	2Z	69	THR
21	2Z	70	LEU
21	2Z	71	VAL
21	2Z	72	ARG
21	2Z	76	LEU
21	2Z	86	VAL
21	2Z	89	PHE
21	2Z	93	ASP
21	2Z	123	ASP
21	2Z	129	SER
21	2Z	136	PHE
21	2Z	144	LEU
21	2Z	154	ASP
21	2Z	155	LEU
21	2Z	163	LEU
21	2Z	165	VAL
21	2Z	171	ILE

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Mol	Chain	Res	Type
22	20	10	THR
22	20	14	ARG
22	20	41	ARG
22	20	43	THR
22	20	55	ARG
22	20	68	GLU
22	20	74	ARG
23	21	26	ARG
23	21	35	THR
23	21	39	LYS
23	21	65	SER
23	21	74	VAL
23	21	76	ARG
23	21	83	GLU
23	21	98	LEU
24	22	3	LEU
24	22	19	VAL
24	22	26	ARG
24	22	28	LYS
24	22	30	ARG
24	22	53	LEU
24	22	62	THR
24	22	66	GLU
25	23	18	ASP
25	23	23	LEU
25	23	26	LEU
25	23	30	ARG
25	23	31	LEU
25	23	37	LEU
25	23	38	GLU
25	23	40	THR
25	23	50	VAL
25	23	53	LEU
25	23	58	VAL
26	24	13	ARG
26	24	15	ILE
26	24	22	ILE
26	24	25	TYR
26	24	27	THR
26	24	48	ARG
26	24	56	VAL
26	24	59	PHE

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Mol	Chain	Res	Type
26	24	62	ARG
26	24	67	TYR
26	24	69	LYS
27	25	6	VAL
27	25	48	GLU
28	26	6	ARG
28	26	9	LEU
28	26	14	THR
28	26	15	GLU
28	26	19	ARG
28	26	20	ASN
28	26	28	ARG
28	26	29	ASN
28	26	34	LEU
28	26	35	GLU
28	26	40	CYS
28	26	45	LYS
28	26	47	THR
28	26	48	VAL
28	26	52	VAL
29	27	24	THR
29	27	35	ARG
29	27	41	ARG
29	27	43	THR
30	28	4	MET
30	28	16	ILE
30	28	31	HIS
30	28	34	TRP
30	28	49	VAL
31	29	12	ASP
31	29	14	CYS
31	29	28	GLU
33	2b	7	VAL
33	2b	12	GLU
33	2b	16	HIS
33	2b	24	TRP
33	2b	35	GLU
33	2b	39	ILE
33	2b	49	GLU
33	2b	52	GLU
33	2b	58	ILE
33	2b	67	THR

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Mol	Chain	Res	Type
33	2b	71	VAL
33	2b	83	MET
33	2b	93	VAL
33	2b	94	ASN
33	2b	126	GLU
33	2b	144	ARG
33	2b	154	LEU
33	2b	157	ARG
33	2b	158	LEU
33	2b	168	THR
33	2b	185	ILE
33	2b	187	LEU
33	2b	198	ASP
33	2b	206	ASP
33	2b	213	LEU
33	2b	220	ASP
33	2b	223	ILE
33	2b	226	ARG
33	2b	229	VAL
34	2c	12	LEU
34	2c	15	THR
34	2c	17	ASP
34	2c	29	TYR
34	2c	37	GLN
34	2c	38	ARG
34	2c	40	ARG
34	2c	43	LEU
34	2c	56	ASP
34	2c	69	HIS
34	2c	77	ILE
34	2c	101	LEU
34	2c	124	ILE
34	2c	131	ARG
34	2c	143	GLU
34	2c	190	ARG
34	2c	195	VAL
35	2d	5	ILE
35	2d	12	CYS
35	2d	19	LEU
35	2d	28	SER
35	2d	31	CYS
35	2d	76	ARG

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Mol	Chain	Res	Type
35	2d	77	ASN
35	2d	83	SER
35	2d	96	LEU
35	2d	102	ASP
35	2d	120	LEU
35	2d	127	THR
35	2d	137	SER
35	2d	146	ILE
35	2d	150	GLU
35	2d	158	ILE
35	2d	175	SER
35	2d	178	VAL
35	2d	187	ARG
35	2d	193	ASP
36	2e	10	MET
36	2e	13	ILE
36	2e	31	LEU
36	2e	33	VAL
36	2e	47	LYS
36	2e	57	LYS
36	2e	60	TYR
36	2e	65	ASN
36	2e	78	HIS
36	2e	91	LEU
36	2e	133	TYR
37	2f	5	GLU
37	2f	10	LEU
37	2f	15	ASP
37	2f	18	GLN
37	2f	30	LEU
37	2f	40	VAL
37	2f	46	ARG
37	2f	59	TYR
37	2f	69	GLU
37	2f	82	ARG
37	2f	83	ASP
38	2g	17	VAL
38	2g	24	THR
38	2g	32	ARG
38	2g	45	ASP
38	2g	52	GLU
38	2g	68	ASN

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Mol	Chain	Res	Type
38	2g	75	VAL
38	2g	79	ARG
38	2g	85	TYR
38	2g	86	GLN
38	2g	90	GLU
38	2g	110	GLN
38	2g	113	GLU
38	2g	115	ARG
38	2g	124	LEU
38	2g	155	ARG
39	2h	37	ARG
39	2h	52	ASP
39	2h	54	ASP
39	2h	85	ARG
39	2h	109	ILE
39	2h	112	LEU
39	2h	113	SER
39	2h	122	ARG
39	2h	133	LEU
40	2i	14	VAL
40	2i	17	VAL
40	2i	27	THR
40	2i	65	VAL
40	2i	75	ASP
40	2i	83	ARG
40	2i	92	TYR
40	2i	102	LEU
40	2i	104	ARG
40	2i	105	ASP
40	2i	114	TYR
40	2i	121	ARG
40	2i	124	GLN
40	2i	127	LYS
40	2i	128	ARG
41	2j	8	LEU
41	2j	21	GLN
41	2j	38	ILE
41	2j	72	VAL
41	2j	89	ASP
41	2j	92	THR
42	2k	18	ARG
42	2k	29	ILE

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Mol	Chain	Res	Type
42	2k	41	THR
42	2k	48	ILE
42	2k	63	LEU
42	2k	107	SER
42	2k	111	ASP
42	2k	116	HIS
43	2l	16	GLU
43	2l	28	LYS
43	2l	33	ARG
43	2l	34	ARG
43	2l	39	VAL
43	2l	40	VAL
43	2l	78	GLN
43	2l	85	ILE
43	2l	104	VAL
43	2l	105	TYR
43	2l	110	VAL
44	2m	8	GLU
44	2m	15	VAL
44	2m	29	ARG
44	2m	34	LEU
44	2m	35	GLU
44	2m	43	THR
44	2m	60	VAL
44	2m	69	GLU
44	2m	73	GLU
44	2m	81	LEU
44	2m	86	CYS
44	2m	90	LEU
44	2m	91	ARG
44	2m	116	THR
45	2n	8	GLU
45	2n	18	VAL
45	2n	33	VAL
45	2n	35	ARG
45	2n	56	VAL
46	2o	3	ILE
46	2o	5	LYS
46	2o	17	ARG
46	2o	31	LEU
46	2o	72	ARG
46	2o	83	GLU

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Mol	Chain	Res	Type
47	2p	1	MET
47	2p	2	VAL
47	2p	8	ARG
47	2p	21	VAL
47	2p	39	TYR
47	2p	40	ASP
47	2p	45	THR
47	2p	47	ASP
47	2p	48	TRP
47	2p	55	ARG
47	2p	69	THR
47	2p	71	ARG
47	2p	74	LEU
48	2q	11	VAL
48	2q	13	ASP
48	2q	14	LYS
48	2q	24	GLU
48	2q	35	VAL
48	2q	73	VAL
48	2q	84	LEU
49	2r	25	THR
49	2r	32	ARG
49	2r	54	ARG
50	2s	4	SER
50	2s	15	LEU
50	2s	18	LYS
50	2s	33	THR
50	2s	39	THR
50	2s	51	VAL
50	2s	66	MET
50	2s	67	VAL
50	2s	81	ARG
51	2t	13	LEU
51	2t	14	LYS
51	2t	24	LEU
51	2t	41	ILE
51	2t	45	GLN
51	2t	54	LYS
51	2t	56	MET
51	2t	70	SER
51	2t	72	LEU
51	2t	86	ARG

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Mol	Chain	Res	Type
51	2t	99	LEU
51	2t	100	ILE
52	2u	12	LYS
52	2u	20	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (115) such sidechains are listed below:

Mol	Chain	Res	Type
3	1D	116	GLN
3	1D	126	GLN
3	1D	164	GLN
4	1E	48	GLN
4	1E	132	HIS
5	1F	8	GLN
5	1F	69	HIS
6	1G	79	ASN
6	1G	123	ASN
7	1H	111	HIS
10	1O	3	GLN
10	1O	5	GLN
10	1O	89	ASN
11	1P	27	HIS
12	1Q	45	GLN
13	1R	13	HIS
13	1R	71	GLN
13	1R	91	GLN
15	1T	58	ASN
20	1Y	6	HIS
21	1Z	50	GLN
22	10	17	GLN
22	10	35	ASN
24	12	48	HIS
24	12	70	GLN
33	1b	16	HIS
33	1b	146	GLN
33	1b	212	GLN
34	1c	37	GLN
34	1c	108	ASN
34	1c	118	GLN
35	1d	116	GLN
35	1d	119	GLN
35	1d	129	ASN

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Mol	Chain	Res	Type
35	1d	161	ASN
37	1f	7	ASN
38	1g	28	ASN
38	1g	51	GLN
38	1g	96	GLN
38	1g	106	GLN
38	1g	148	ASN
39	1h	15	ASN
40	1i	3	GLN
40	1i	23	ASN
40	1i	29	ASN
40	1i	31	GLN
40	1i	34	ASN
40	1i	58	HIS
40	1i	73	GLN
40	1i	124	GLN
41	1j	56	HIS
41	1j	68	HIS
41	1j	69	ASN
42	1k	117	ASN
43	1l	8	ASN
46	1o	28	GLN
49	1r	63	GLN
50	1s	57	HIS
50	1s	69	HIS
3	2D	166	GLN
3	2D	201	HIS
4	2E	55	ASN
4	2E	132	HIS
4	2E	169	ASN
5	2F	69	HIS
6	2G	108	ASN
10	2O	5	GLN
11	2P	9	ASN
11	2P	70	GLN
13	2R	31	HIS
14	2S	38	GLN
15	2T	58	ASN
16	2U	81	HIS
16	2U	94	ASN
18	2W	62	HIS
19	2X	31	HIS

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Mol	Chain	Res	Type
20	2Y	6	HIS
21	2Z	55	HIS
23	21	42	GLN
26	24	40	HIS
28	26	20	ASN
29	27	6	GLN
33	2b	40	HIS
33	2b	94	ASN
33	2b	95	GLN
33	2b	110	GLN
34	2c	37	GLN
34	2c	98	ASN
34	2c	110	ASN
34	2c	123	GLN
34	2c	162	GLN
35	2d	74	GLN
35	2d	77	ASN
35	2d	116	GLN
35	2d	123	HIS
36	2e	130	ASN
37	2f	73	ASN
38	2g	86	GLN
38	2g	153	HIS
40	2i	3	GLN
40	2i	23	ASN
40	2i	38	GLN
40	2i	73	GLN
41	2j	13	HIS
41	2j	21	GLN
41	2j	68	HIS
42	2k	93	GLN
44	2m	77	ASN
45	2n	52	GLN
46	2o	28	GLN
49	2r	63	GLN
50	2s	23	ASN
50	2s	53	ASN
50	2s	69	HIS
51	2t	75	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2861/2915 (98%)	554 (19%)	21 (0%)
1	2A	2788/2915 (95%)	579 (20%)	21 (0%)
2	1B	120/121 (99%)	9 (7%)	1 (0%)
2	2B	118/121 (97%)	32 (27%)	0
32	1a	1494/1521 (98%)	303 (20%)	0
32	2a	1498/1521 (98%)	336 (22%)	0
53	1v	9/24 (37%)	5 (55%)	0
53	2v	4/24 (16%)	1 (25%)	0
54	1x	75/77 (97%)	9 (12%)	0
54	2x	75/77 (97%)	9 (12%)	0
All	All	9042/9316 (97%)	1837 (20%)	43 (0%)

All (1837) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	10	G
1	1A	11	G
1	1A	15	G
1	1A	34	C
1	1A	36	G
1	1A	45	C
1	1A	50	U
1	1A	51	G
1	1A	55	G
1	1A	58	G
1	1A	60	G
1	1A	61	G
1	1A	64	A
1	1A	71	A
1	1A	72	U
1	1A	74	A
1	1A	75	G
1	1A	77	C
1	1A	84	A
1	1A	95	G
1	1A	102	G
1	1A	118	A
1	1A	119	A
1	1A	120	U
1	1A	125	G
1	1A	131	G
1	1A	139	G
1	1A	139(A)	G

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Mol	Chain	Res	Type
1	1A	140	G
1	1A	141	A
1	1A	143	G
1	1A	182	A
1	1A	188	G
1	1A	196	A
1	1A	199	A
1	1A	204	A
1	1A	205	G
1	1A	214	G
1	1A	215	G
1	1A	216	A
1	1A	221	A
1	1A	222	A
1	1A	225	A
1	1A	228	A
1	1A	229	A
1	1A	233	A
1	1A	248	G
1	1A	249	C
1	1A	261	G
1	1A	264	C
1	1A	265	A
1	1A	269	U
1	1A	271(C)	C
1	1A	271(K)	U
1	1A	271(L)	U
1	1A	271(M)	G
1	1A	271(N)	U
1	1A	271(O)	C
1	1A	271(S)	G
1	1A	271(Y)	U
1	1A	272(B)	G
1	1A	272(H)	C
1	1A	272(I)	U
1	1A	279	C
1	1A	306	U
1	1A	311	A
1	1A	316	C
1	1A	322	A
1	1A	324	A
1	1A	329	G

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Mol	Chain	Res	Type
1	1A	330	A
1	1A	345	A
1	1A	352	G
1	1A	363	G
1	1A	363(F)	A
1	1A	372	G
1	1A	380	U
1	1A	386	G
1	1A	389	G
1	1A	393	C
1	1A	396	G
1	1A	405	U
1	1A	406	G
1	1A	407	G
1	1A	411	G
1	1A	413	C
1	1A	428	A
1	1A	437	G
1	1A	444	C
1	1A	448	U
1	1A	456	C
1	1A	457	A
1	1A	481	G
1	1A	489	G
1	1A	504	U
1	1A	505	A
1	1A	509	C
1	1A	528	A
1	1A	530	G
1	1A	531	C
1	1A	532	A
1	1A	533	G
1	1A	545	G
1	1A	549	G
1	1A	563	G
1	1A	568	U
1	1A	573	G
1	1A	574	C
1	1A	575	A
1	1A	584	C
1	1A	603	A
1	1A	604	G

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Mol	Chain	Res	Type
1	1A	607	U
1	1A	610	G
1	1A	614(B)	G
1	1A	615	G
1	1A	620	G
1	1A	627	A
1	1A	637	A
1	1A	645	C
1	1A	646	A
1	1A	648	G
1	1A	652(D)	C
1	1A	652(E)	G
1	1A	652(T)	C
1	1A	654	A
1	1A	669	G
1	1A	686	G
1	1A	698	C
1	1A	717	G
1	1A	729	G
1	1A	730	C
1	1A	749	C
1	1A	762	U
1	1A	765	G
1	1A	775	G
1	1A	776	G
1	1A	777	A
1	1A	782	A
1	1A	784	A
1	1A	785	G
1	1A	788	A
1	1A	790	C
1	1A	792	G
1	1A	794	G
1	1A	805	G
1	1A	810	U
1	1A	811	U
1	1A	812	C
1	1A	819	A
1	1A	824	A
1	1A	827	U
1	1A	828	U
1	1A	830	G

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Mol	Chain	Res	Type
1	1A	831	G
1	1A	859	G
1	1A	880	G
1	1A	884	C
1	1A	885	C
1	1A	886	C
1	1A	887	A
1	1A	888	C
1	1A	889	C
1	1A	890	A
1	1A	895	U
1	1A	896	A
1	1A	897	C
1	1A	905	U
1	1A	907	U
1	1A	910	A
1	1A	914	C
1	1A	915	C
1	1A	926	A
1	1A	932	G
1	1A	944	G
1	1A	945	A
1	1A	946	G
1	1A	959	A
1	1A	961	C
1	1A	974	G
1	1A	975	C
1	1A	983	A
1	1A	989	G
1	1A	993	G
1	1A	995	C
1	1A	996	A
1	1A	1012	U
1	1A	1013	C
1	1A	1021	A
1	1A	1022	G
1	1A	1023	U
1	1A	1024	G
1	1A	1025	G
1	1A	1026	U
1	1A	1033	U
1	1A	1041	C

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Mol	Chain	Res	Type
1	1A	1044	G
1	1A	1046	A
1	1A	1047	G
1	1A	1048	A
1	1A	1054	A
1	1A	1055	G
1	1A	1058	G
1	1A	1060	U
1	1A	1064	C
1	1A	1065	U
1	1A	1068	G
1	1A	1070	A
1	1A	1071	G
1	1A	1073	A
1	1A	1075	C
1	1A	1076	C
1	1A	1078	U
1	1A	1079	C
1	1A	1085	A
1	1A	1088	A
1	1A	1090	U
1	1A	1091	G
1	1A	1093	G
1	1A	1094	U
1	1A	1096	A
1	1A	1101	U
1	1A	1103	A
1	1A	1104	C
1	1A	1107	G
1	1A	1109	C
1	1A	1111	A
1	1A	1112	G
1	1A	1115	G
1	1A	1129	A
1	1A	1130	U
1	1A	1131	G
1	1A	1132	A
1	1A	1135	C
1	1A	1136	G
1	1A	1138	G
1	1A	1139	G
1	1A	1142	U

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Mol	Chain	Res	Type
1	1A	1155	A
1	1A	1156	A
1	1A	1157	G
1	1A	1171	G
1	1A	1173	G
1	1A	1174	A
1	1A	1175	U
1	1A	1176	G
1	1A	1177	A
1	1A	1178	C
1	1A	1187	G
1	1A	1210	A
1	1A	1212	G
1	1A	1220	A
1	1A	1232	G
1	1A	1248	G
1	1A	1252	G
1	1A	1253	A
1	1A	1256	G
1	1A	1262	A
1	1A	1268	A
1	1A	1271	G
1	1A	1272	A
1	1A	1273	U
1	1A	1274	A
1	1A	1276	A
1	1A	1281	G
1	1A	1286	A
1	1A	1300	U
1	1A	1301	A
1	1A	1313	U
1	1A	1320	C
1	1A	1321	A
1	1A	1352	U
1	1A	1359	A
1	1A	1360	A
1	1A	1365	A
1	1A	1370	C
1	1A	1371	G
1	1A	1378	A
1	1A	1384	A
1	1A	1385	G

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Mol	Chain	Res	Type
1	1A	1386	C
1	1A	1396	U
1	1A	1416	G
1	1A	1417	C
1	1A	1420	U
1	1A	1421	G
1	1A	1428	C
1	1A	1439	A
1	1A	1441	G
1	1A	1445	A
1	1A	1450	G
1	1A	1450(A)	C
1	1A	1453	U
1	1A	1455	G
1	1A	1467	C
1	1A	1482	G
1	1A	1493	C
1	1A	1497	U
1	1A	1506	C
1	1A	1509	C
1	1A	1509(A)	A
1	1A	1509(B)	A
1	1A	1523	U
1	1A	1545	A
1	1A	1551	C
1	1A	1554	A
1	1A	1558	A
1	1A	1566	A
1	1A	1569	A
1	1A	1578	U
1	1A	1580	A
1	1A	1581	G
1	1A	1584	C
1	1A	1586	A
1	1A	1607	C
1	1A	1608	A
1	1A	1609	A
1	1A	1610	A
1	1A	1616	A
1	1A	1647	G
1	1A	1648	C
1	1A	1667	G

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Mol	Chain	Res	Type
1	1A	1674	G
1	1A	1681	G
1	1A	1696	G
1	1A	1697	G
1	1A	1700	A
1	1A	1701	A
1	1A	1722	A
1	1A	1745(A)	C
1	1A	1746	G
1	1A	1756	G
1	1A	1763	G
1	1A	1764	G
1	1A	1773	A
1	1A	1780	A
1	1A	1791	A
1	1A	1800	C
1	1A	1802	A
1	1A	1816	G
1	1A	1829	A
1	1A	1842	G
1	1A	1847	A
1	1A	1858	G
1	1A	1878	G
1	1A	1889	A
1	1A	1900	A
1	1A	1905	C
1	1A	1906	G
1	1A	1914	C
1	1A	1916	A
1	1A	1919	A
1	1A	1929	G
1	1A	1930	G
1	1A	1931	U
1	1A	1936	A
1	1A	1938	A
1	1A	1941	C
1	1A	1944	U
1	1A	1945	G
1	1A	1955	U
1	1A	1962	5MC
1	1A	1963	U
1	1A	1964	G

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Mol	Chain	Res	Type
1	1A	1967	C
1	1A	1970	A
1	1A	1971	A
1	1A	1972	A
1	1A	1985	G
1	1A	1993	U
1	1A	1997	G
1	1A	2016	U
1	1A	2020	A
1	1A	2023	G
1	1A	2029	G
1	1A	2031	A
1	1A	2032	G
1	1A	2033	A
1	1A	2039	C
1	1A	2043	C
1	1A	2052	G
1	1A	2055	C
1	1A	2056	G
1	1A	2060	A
1	1A	2061	G
1	1A	2062	A
1	1A	2069	G
1	1A	2070	G
1	1A	2082	A
1	1A	2093	G
1	1A	2098	U
1	1A	2099	U
1	1A	2113	U
1	1A	2115	G
1	1A	2116	G
1	1A	2120	G
1	1A	2122	U
1	1A	2125	G
1	1A	2126	A
1	1A	2127	G
1	1A	2128	C
1	1A	2129	C
1	1A	2130	U
1	1A	2131	G
1	1A	2132	U
1	1A	2133	G

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Mol	Chain	Res	Type
1	1A	2134	A
1	1A	2135	A
1	1A	2136	C
1	1A	2139	C
1	1A	2140	C
1	1A	2141	G
1	1A	2142	C
1	1A	2144	U
1	1A	2146	C
1	1A	2147	G
1	1A	2150	U
1	1A	2151	G
1	1A	2157	G
1	1A	2158	A
1	1A	2159	G
1	1A	2162	G
1	1A	2163	C
1	1A	2164	C
1	1A	2165	G
1	1A	2166	G
1	1A	2171	A
1	1A	2172	U
1	1A	2173	A
1	1A	2175	C
1	1A	2182	G
1	1A	2184	G
1	1A	2188	C
1	1A	2189	U
1	1A	2190	G
1	1A	2192	G
1	1A	2198	A
1	1A	2206	G
1	1A	2207	G
1	1A	2208	A
1	1A	2219	G
1	1A	2225	A
1	1A	2226	C
1	1A	2238	G
1	1A	2269	A
1	1A	2279	G
1	1A	2280	G
1	1A	2283	C

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Mol	Chain	Res	Type
1	1A	2285	C
1	1A	2286	A
1	1A	2287	A
1	1A	2288	A
1	1A	2289	G
1	1A	2305	A
1	1A	2307	G
1	1A	2308	G
1	1A	2312	U
1	1A	2315	G
1	1A	2320	A
1	1A	2325	G
1	1A	2334	G
1	1A	2336	A
1	1A	2341	G
1	1A	2347	C
1	1A	2350	C
1	1A	2361	A
1	1A	2365	G
1	1A	2372	G
1	1A	2383	G
1	1A	2384	G
1	1A	2385	C
1	1A	2406	U
1	1A	2410	G
1	1A	2422	A
1	1A	2424	C
1	1A	2425	A
1	1A	2428	G
1	1A	2429	G
1	1A	2430	A
1	1A	2431	U
1	1A	2435	A
1	1A	2439	A
1	1A	2441	C
1	1A	2448	A
1	1A	2449	U
1	1A	2464	C
1	1A	2468	G
1	1A	2469	A
1	1A	2474	C
1	1A	2476	A

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Mol	Chain	Res	Type
1	1A	2478	A
1	1A	2480	C
1	1A	2481	G
1	1A	2487	G
1	1A	2502	G
1	1A	2505	G
1	1A	2518	A
1	1A	2529	G
1	1A	2538	C
1	1A	2554	U
1	1A	2566	A
1	1A	2567	G
1	1A	2573	C
1	1A	2582	G
1	1A	2602	A
1	1A	2609	U
1	1A	2611	U
1	1A	2612	C
1	1A	2629	A
1	1A	2630	G
1	1A	2632	A
1	1A	2654	A
1	1A	2669	G
1	1A	2689	U
1	1A	2690	C
1	1A	2702	U
1	1A	2703	C
1	1A	2707	G
1	1A	2712(A)	A
1	1A	2713	A
1	1A	2724	C
1	1A	2726	U
1	1A	2730	C
1	1A	2732	G
1	1A	2733	A
1	1A	2744	G
1	1A	2757	A
1	1A	2758	A
1	1A	2760	C
1	1A	2764	A
1	1A	2765	A
1	1A	2769	C

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Mol	Chain	Res	Type
1	1A	2778	A
1	1A	2780	G
1	1A	2790	A
1	1A	2791	C
1	1A	2802	G
1	1A	2805	G
1	1A	2808	U
1	1A	2818	G
1	1A	2820	A
1	1A	2821	A
1	1A	2833	G
1	1A	2835	A
1	1A	2848	G
1	1A	2855	C
1	1A	2866	U
1	1A	2872	G
1	1A	2873	A
1	1A	2877	G
1	1A	2879	C
1	1A	2880	C
1	1A	2892	A
1	1A	2894	G
2	1B	2	C
2	1B	13	A
2	1B	19	G
2	1B	24	G
2	1B	35	U
2	1B	56	G
2	1B	73	A
2	1B	88	C
2	1B	110	G
32	1a	6	G
32	1a	7	G
32	1a	8	A
32	1a	9	G
32	1a	22	G
32	1a	32	A
32	1a	39	G
32	1a	47	C
32	1a	48	C
32	1a	50	A
32	1a	51	A

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Mol	Chain	Res	Type
32	1a	61	G
32	1a	79	G
32	1a	91	C
32	1a	101	A
32	1a	105	G
32	1a	116	A
32	1a	121	C
32	1a	124	G
32	1a	131	C
32	1a	138	G
32	1a	139	G
32	1a	143	A
32	1a	144	G
32	1a	147	G
32	1a	156	G
32	1a	157	G
32	1a	163	C
32	1a	169	C
32	1a	174	C
32	1a	183	G
32	1a	189(E)	U
32	1a	189(H)	G
32	1a	189(J)	G
32	1a	190	U
32	1a	191	G
32	1a	192	U
32	1a	193	C
32	1a	194	C
32	1a	195	A
32	1a	197	A
32	1a	203	U
32	1a	204	U
32	1a	216	G
32	1a	245	C
32	1a	247	G
32	1a	251	G
32	1a	256	U
32	1a	266	G
32	1a	267	C
32	1a	269	C
32	1a	281	G
32	1a	289	G

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Mol	Chain	Res	Type
32	1a	306	G
32	1a	320	C
32	1a	321	A
32	1a	328	C
32	1a	332	G
32	1a	344	A
32	1a	348	G
32	1a	352	C
32	1a	353	A
32	1a	354	G
32	1a	356	A
32	1a	367	U
32	1a	372	C
32	1a	373	A
32	1a	381	C
32	1a	388	G
32	1a	397	A
32	1a	398	C
32	1a	406	G
32	1a	411	A
32	1a	412	A
32	1a	413	G
32	1a	414	A
32	1a	422	C
32	1a	423	G
32	1a	424	G
32	1a	428	G
32	1a	429	U
32	1a	430	A
32	1a	437	U
32	1a	438	G
32	1a	439	A
32	1a	441	A
32	1a	442	C
32	1a	452	A
32	1a	453	A
32	1a	461	A
32	1a	475	G
32	1a	477	A
32	1a	484	G
32	1a	485	G
32	1a	496	A

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Mol	Chain	Res	Type
32	1a	498	U
32	1a	509	A
32	1a	510	A
32	1a	511	C
32	1a	518	C
32	1a	519	C
32	1a	521	G
32	1a	531	U
32	1a	532	A
32	1a	547	A
32	1a	559	A
32	1a	560	U
32	1a	561	U
32	1a	562	C
32	1a	568	G
32	1a	572	A
32	1a	573	A
32	1a	576	G
32	1a	577	G
32	1a	596	C
32	1a	607	A
32	1a	630	G
32	1a	653	A
32	1a	665	A
32	1a	666	G
32	1a	671	G
32	1a	687	A
32	1a	688	G
32	1a	721	G
32	1a	731	G
32	1a	743	U
32	1a	748	C
32	1a	749	C
32	1a	754	C
32	1a	755	G
32	1a	759	A
32	1a	774	G
32	1a	777	A
32	1a	782	A
32	1a	792	A
32	1a	793	U
32	1a	794	A

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Mol	Chain	Res	Type
32	1a	796	C
32	1a	816	A
32	1a	817	C
32	1a	821	G
32	1a	828	A
32	1a	832	C
32	1a	836	G
32	1a	840	C
32	1a	841	U
32	1a	851	G
32	1a	859	A
32	1a	870	U
32	1a	872	A
32	1a	873	A
32	1a	876	G
32	1a	891	U
32	1a	902	G
32	1a	914	A
32	1a	926	G
32	1a	927	G
32	1a	929	G
32	1a	933	G
32	1a	934	C
32	1a	935	A
32	1a	936	C
32	1a	942	G
32	1a	955	U
32	1a	959	A
32	1a	960	U
32	1a	961	U
32	1a	967	5MC
32	1a	968	A
32	1a	969	A
32	1a	971	G
32	1a	974	A
32	1a	975	A
32	1a	976	G
32	1a	977	A
32	1a	978	A
32	1a	982	U
32	1a	992	U
32	1a	993	G

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Mol	Chain	Res	Type
32	1a	994	A
32	1a	995	C
32	1a	997	U
32	1a	1000	U
32	1a	1001	A
32	1a	1002	G
32	1a	1003	G
32	1a	1005	A
32	1a	1006	C
32	1a	1008	C
32	1a	1013	G
32	1a	1020	U
32	1a	1021	G
32	1a	1022	G
32	1a	1023	G
32	1a	1024	G
32	1a	1025	U
32	1a	1026	G
32	1a	1027	C
32	1a	1028	C
32	1a	1029	C
32	1a	1030(A)	G
32	1a	1030(C)	G
32	1a	1031	G
32	1a	1032	G
32	1a	1033	G
32	1a	1034	G
32	1a	1036	G
32	1a	1041	A
32	1a	1043	C
32	1a	1044	A
32	1a	1045	C
32	1a	1053	G
32	1a	1054	C
32	1a	1055	A
32	1a	1065	U
32	1a	1066	C
32	1a	1068	G
32	1a	1081	G
32	1a	1084	G
32	1a	1085	U
32	1a	1092	A

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Mol	Chain	Res	Type
32	1a	1094	G
32	1a	1095	U
32	1a	1096	C
32	1a	1101	A
32	1a	1121	U
32	1a	1124	G
32	1a	1125	U
32	1a	1134	G
32	1a	1135	U
32	1a	1136	U
32	1a	1137	C
32	1a	1138	G
32	1a	1139	G
32	1a	1146	A
32	1a	1149	C
32	1a	1152	A
32	1a	1159	U
32	1a	1184	G
32	1a	1186	G
32	1a	1196	U
32	1a	1197	G
32	1a	1199	U
32	1a	1202	G
32	1a	1204	A
32	1a	1213	A
32	1a	1224	G
32	1a	1225	A
32	1a	1227	A
32	1a	1236	A
32	1a	1238	A
32	1a	1239	A
32	1a	1256	A
32	1a	1257	U
32	1a	1258	G
32	1a	1270	C
32	1a	1274	G
32	1a	1275	A
32	1a	1276	G
32	1a	1278	U
32	1a	1280	A
32	1a	1286	A
32	1a	1287	A

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Mol	Chain	Res	Type
32	1a	1294	G
32	1a	1299	A
32	1a	1300	G
32	1a	1302	U
32	1a	1305	G
32	1a	1312	G
32	1a	1320	C
32	1a	1322	C
32	1a	1323	G
32	1a	1338	G
32	1a	1347	G
32	1a	1353	G
32	1a	1355	G
32	1a	1363	C
32	1a	1365	G
32	1a	1370	G
32	1a	1381	U
32	1a	1388	C
32	1a	1395	C
32	1a	1397	C
32	1a	1398	A
32	1a	1415	G
32	1a	1419	G
32	1a	1436	U
32	1a	1440	C
32	1a	1442	G
32	1a	1442(B)	A
32	1a	1446	U
32	1a	1447	A
32	1a	1456	G
32	1a	1487	G
32	1a	1492	A
32	1a	1494	G
32	1a	1503	A
32	1a	1504	G
32	1a	1506	U
32	1a	1517	G
32	1a	1529	G
32	1a	1530	G
32	1a	1532	U
53	1v	13	A
53	1v	15	A

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Mol	Chain	Res	Type
53	1v	16	A
53	1v	19	U
53	1v	21	A
54	1x	6	G
54	1x	7	G
54	1x	9	G
54	1x	18	G
54	1x	21	A
54	1x	47	U
54	1x	48	C
54	1x	61	C
54	1x	76	A
1	2A	14	A
1	2A	15	G
1	2A	23	G
1	2A	34	C
1	2A	35	G
1	2A	36	G
1	2A	45	C
1	2A	59	U
1	2A	64	A
1	2A	71	A
1	2A	74	A
1	2A	75	G
1	2A	81	G
1	2A	84	A
1	2A	90	U
1	2A	102	G
1	2A	118	A
1	2A	120	U
1	2A	121	G
1	2A	125	G
1	2A	131	G
1	2A	136	G
1	2A	154(A)	C
1	2A	157	U
1	2A	174	C
1	2A	181	A
1	2A	191	A
1	2A	196	A
1	2A	199	A
1	2A	200	U

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Mol	Chain	Res	Type
1	2A	201	C
1	2A	205	G
1	2A	216	A
1	2A	222	A
1	2A	223	A
1	2A	225	A
1	2A	228	A
1	2A	229	A
1	2A	232	G
1	2A	233	A
1	2A	248	G
1	2A	266	G
1	2A	267	C
1	2A	271(K)	U
1	2A	271(L)	U
1	2A	271(M)	G
1	2A	271(N)	U
1	2A	271(V)	G
1	2A	271(Y)	U
1	2A	272	G
1	2A	272(B)	G
1	2A	277	C
1	2A	278	A
1	2A	283	A
1	2A	284	U
1	2A	285	C
1	2A	294	A
1	2A	311	A
1	2A	324	A
1	2A	329	G
1	2A	330	A
1	2A	346	A
1	2A	352	G
1	2A	362	U
1	2A	363	G
1	2A	363(D)	G
1	2A	363(E)	U
1	2A	366	C
1	2A	372	G
1	2A	380	U
1	2A	386	G
1	2A	405	U

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Mol	Chain	Res	Type
1	2A	411	G
1	2A	421	U
1	2A	425	G
1	2A	426	C
1	2A	429	A
1	2A	444	C
1	2A	446	G
1	2A	455	C
1	2A	457	A
1	2A	481	G
1	2A	482	A
1	2A	494	G
1	2A	498	G
1	2A	499	U
1	2A	504	U
1	2A	505	A
1	2A	508	G
1	2A	509	C
1	2A	510	C
1	2A	527	C
1	2A	528	A
1	2A	529	A
1	2A	531	C
1	2A	532	A
1	2A	533	G
1	2A	551	G
1	2A	556	G
1	2A	562	U
1	2A	563	G
1	2A	568	U
1	2A	573	G
1	2A	574	C
1	2A	575	A
1	2A	578	A
1	2A	588	U
1	2A	595	C
1	2A	599	G
1	2A	603	A
1	2A	604	G
1	2A	607	U
1	2A	614(A)	U
1	2A	614(B)	G

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Mol	Chain	Res	Type
1	2A	614(C)	A
1	2A	615	G
1	2A	616	G
1	2A	627	A
1	2A	630	G
1	2A	631	A
1	2A	634	C
1	2A	637	A
1	2A	645	C
1	2A	652(B)	A
1	2A	652(C)	G
1	2A	652(U)	G
1	2A	669	G
1	2A	673	C
1	2A	686	G
1	2A	698	C
1	2A	712	G
1	2A	715	G
1	2A	717	G
1	2A	721	C
1	2A	730	C
1	2A	748	G
1	2A	753	C
1	2A	771	G
1	2A	775	G
1	2A	776	G
1	2A	782	A
1	2A	784	A
1	2A	785	G
1	2A	788	A
1	2A	789	A
1	2A	792	G
1	2A	795	C
1	2A	805	G
1	2A	809	G
1	2A	812	C
1	2A	819	A
1	2A	824	A
1	2A	826	U
1	2A	827	U
1	2A	832	G
1	2A	843	G

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Mol	Chain	Res	Type
1	2A	857	C
1	2A	859	G
1	2A	865	C
1	2A	866	A
1	2A	869	G
1	2A	874	G
1	2A	877	U
1	2A	878	A
1	2A	879	G
1	2A	880	G
1	2A	884	C
1	2A	886	C
1	2A	887	A
1	2A	888	C
1	2A	892	G
1	2A	893	C
1	2A	894	C
1	2A	896	A
1	2A	897	C
1	2A	898	C
1	2A	900	A
1	2A	901	A
1	2A	910	A
1	2A	917	A
1	2A	925	C
1	2A	932	G
1	2A	933	A
1	2A	934	G
1	2A	938	G
1	2A	941	A
1	2A	945	A
1	2A	946	G
1	2A	953	A
1	2A	959	A
1	2A	961	C
1	2A	965	C
1	2A	968	G
1	2A	972	G
1	2A	974	G
1	2A	975	C
1	2A	980	A
1	2A	981	A

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Mol	Chain	Res	Type
1	2A	983	A
1	2A	996	A
1	2A	1006	C
1	2A	1012	U
1	2A	1013	C
1	2A	1015	G
1	2A	1020	A
1	2A	1022	G
1	2A	1023	U
1	2A	1025	G
1	2A	1026	U
1	2A	1027	A
1	2A	1033	U
1	2A	1038	C
1	2A	1039	G
1	2A	1041	C
1	2A	1042	G
1	2A	1043	C
1	2A	1114	G
1	2A	1116	C
1	2A	1117	G
1	2A	1121	C
1	2A	1126	A
1	2A	1129	A
1	2A	1130	U
1	2A	1132	A
1	2A	1135	C
1	2A	1136	G
1	2A	1139	G
1	2A	1142(A)	A
1	2A	1144	G
1	2A	1151	G
1	2A	1155	A
1	2A	1164	G
1	2A	1170	G
1	2A	1171	G
1	2A	1192	G
1	2A	1204	A
1	2A	1205	U
1	2A	1206	G
1	2A	1210	A
1	2A	1211	U

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Mol	Chain	Res	Type
1	2A	1221	C
1	2A	1227	G
1	2A	1232	G
1	2A	1237	A
1	2A	1241	A
1	2A	1247	A
1	2A	1248	G
1	2A	1249	U
1	2A	1253	A
1	2A	1256	G
1	2A	1271	G
1	2A	1272	A
1	2A	1273	U
1	2A	1274	A
1	2A	1275	A
1	2A	1298	C
1	2A	1300	U
1	2A	1301	A
1	2A	1309	G
1	2A	1314	C
1	2A	1319	G
1	2A	1321	A
1	2A	1332	G
1	2A	1341	U
1	2A	1352	U
1	2A	1359	A
1	2A	1360	A
1	2A	1365	A
1	2A	1368	G
1	2A	1370	C
1	2A	1379	A
1	2A	1380	G
1	2A	1384	A
1	2A	1385	G
1	2A	1386	C
1	2A	1406	U
1	2A	1416	G
1	2A	1417	C
1	2A	1420	U
1	2A	1421	G
1	2A	1427	A
1	2A	1428	C

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Mol	Chain	Res	Type
1	2A	1429	G
1	2A	1437	C
1	2A	1445	A
1	2A	1449	A
1	2A	1450	G
1	2A	1460	A
1	2A	1461	G
1	2A	1467	C
1	2A	1471	A
1	2A	1475	G
1	2A	1479	G
1	2A	1482	G
1	2A	1486	A
1	2A	1490	A
1	2A	1493	C
1	2A	1495	A
1	2A	1496	A
1	2A	1497	U
1	2A	1503	U
1	2A	1508	A
1	2A	1509(A)	A
1	2A	1531	C
1	2A	1532	C
1	2A	1538	G
1	2A	1541	G
1	2A	1543	C
1	2A	1544	A
1	2A	1545	A
1	2A	1558	A
1	2A	1559	G
1	2A	1566	A
1	2A	1569	A
1	2A	1578	U
1	2A	1580	A
1	2A	1584	C
1	2A	1586	A
1	2A	1588	C
1	2A	1593	G
1	2A	1608	A
1	2A	1609	A
1	2A	1616	A
1	2A	1622	G

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Mol	Chain	Res	Type
1	2A	1638	C
1	2A	1639	U
1	2A	1640	C
1	2A	1648	C
1	2A	1653	G
1	2A	1654	A
1	2A	1661	G
1	2A	1663	C
1	2A	1664	A
1	2A	1670	C
1	2A	1674	G
1	2A	1675	C
1	2A	1676	A
1	2A	1696	G
1	2A	1700	A
1	2A	1701	A
1	2A	1703	G
1	2A	1721	G
1	2A	1722	A
1	2A	1740	G
1	2A	1746	G
1	2A	1750	G
1	2A	1756	G
1	2A	1757	U
1	2A	1762	A
1	2A	1763	G
1	2A	1764	G
1	2A	1773	A
1	2A	1776	G
1	2A	1780	A
1	2A	1791	A
1	2A	1800	C
1	2A	1801	G
1	2A	1816	G
1	2A	1833	U
1	2A	1835	G
1	2A	1847	A
1	2A	1848	A
1	2A	1861	G
1	2A	1864	U
1	2A	1866	C
1	2A	1878	G

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Mol	Chain	Res	Type
1	2A	1890	A
1	2A	1899	G
1	2A	1900	A
1	2A	1906	G
1	2A	1910	G
1	2A	1914	C
1	2A	1915	5MU
1	2A	1927	A
1	2A	1929	G
1	2A	1930	G
1	2A	1936	A
1	2A	1938	A
1	2A	1941	C
1	2A	1943	U
1	2A	1944	U
1	2A	1955	U
1	2A	1963	U
1	2A	1967	C
1	2A	1970	A
1	2A	1971	A
1	2A	1972	A
1	2A	1993	U
1	2A	1997	G
1	2A	2001	A
1	2A	2020	A
1	2A	2023	G
1	2A	2031	A
1	2A	2032	G
1	2A	2033	A
1	2A	2043	C
1	2A	2052	G
1	2A	2055	C
1	2A	2056	G
1	2A	2060	A
1	2A	2061	G
1	2A	2062	A
1	2A	2063	C
1	2A	2068	U
1	2A	2069	G
1	2A	2101	G
1	2A	2104	G
1	2A	2107	C

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Mol	Chain	Res	Type
1	2A	2109	U
1	2A	2110	G
1	2A	2111	C
1	2A	2112	G
1	2A	2113	U
1	2A	2115	G
1	2A	2116	G
1	2A	2118	U
1	2A	2119	A
1	2A	2120	G
1	2A	2122	U
1	2A	2123	G
1	2A	2126	A
1	2A	2127	G
1	2A	2129	C
1	2A	2131	G
1	2A	2132	U
1	2A	2133	G
1	2A	2134	A
1	2A	2137	C
1	2A	2138	C
1	2A	2140	C
1	2A	2142	C
1	2A	2146	C
1	2A	2148	G
1	2A	2155	G
1	2A	2156	G
1	2A	2160	G
1	2A	2161	C
1	2A	2162	G
1	2A	2163	C
1	2A	2164	C
1	2A	2165	G
1	2A	2166	G
1	2A	2167	U
1	2A	2172	U
1	2A	2181	G
1	2A	2182	G
1	2A	2184	G
1	2A	2185	C
1	2A	2188	C
1	2A	2189	U

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Mol	Chain	Res	Type
1	2A	2192	G
1	2A	2206	G
1	2A	2207	G
1	2A	2208	A
1	2A	2218	U
1	2A	2225	A
1	2A	2226	C
1	2A	2238	G
1	2A	2239	G
1	2A	2274	A
1	2A	2275	C
1	2A	2279	G
1	2A	2283	C
1	2A	2287	A
1	2A	2288	A
1	2A	2297	C
1	2A	2305	A
1	2A	2308	G
1	2A	2311	A
1	2A	2319	G
1	2A	2320	A
1	2A	2321	G
1	2A	2325	G
1	2A	2327	A
1	2A	2333	A
1	2A	2336	A
1	2A	2337	G
1	2A	2340	G
1	2A	2345	G
1	2A	2347	C
1	2A	2350	C
1	2A	2366	A
1	2A	2376	A
1	2A	2379	G
1	2A	2383	G
1	2A	2384	G
1	2A	2385	C
1	2A	2391	G
1	2A	2394	C
1	2A	2396	G
1	2A	2402	C
1	2A	2406	U

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Mol	Chain	Res	Type
1	2A	2408	U
1	2A	2410	G
1	2A	2422	A
1	2A	2425	A
1	2A	2429	G
1	2A	2430	A
1	2A	2435	A
1	2A	2439	A
1	2A	2441	C
1	2A	2446	G
1	2A	2448	A
1	2A	2449	U
1	2A	2468	G
1	2A	2476	A
1	2A	2481	G
1	2A	2498	C
1	2A	2502	G
1	2A	2504	U
1	2A	2505	G
1	2A	2506	U
1	2A	2507	C
1	2A	2518	A
1	2A	2525	G
1	2A	2529	G
1	2A	2554	U
1	2A	2566	A
1	2A	2567	G
1	2A	2569	G
1	2A	2572	A
1	2A	2573	C
1	2A	2574	G
1	2A	2578	G
1	2A	2581	G
1	2A	2582	G
1	2A	2601	C
1	2A	2602	A
1	2A	2609	U
1	2A	2611	U
1	2A	2612	C
1	2A	2617	C
1	2A	2629	A
1	2A	2630	G

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Mol	Chain	Res	Type
1	2A	2632	A
1	2A	2634	G
1	2A	2654	A
1	2A	2661	G
1	2A	2667	C
1	2A	2678	C
1	2A	2679	A
1	2A	2683	C
1	2A	2689	U
1	2A	2690	C
1	2A	2691	C
1	2A	2702	U
1	2A	2703	C
1	2A	2712(A)	A
1	2A	2713	A
1	2A	2714	G
1	2A	2726	U
1	2A	2733	A
1	2A	2751	G
1	2A	2758	A
1	2A	2764	A
1	2A	2765	A
1	2A	2766	G
1	2A	2767	C
1	2A	2778	A
1	2A	2780	G
1	2A	2789	C
1	2A	2793	G
1	2A	2802	G
1	2A	2803	C
1	2A	2807	G
1	2A	2820	A
1	2A	2821	A
1	2A	2823	A
1	2A	2835	A
1	2A	2855	C
1	2A	2868	A
1	2A	2872	G
1	2A	2879	C
1	2A	2880	C
1	2A	2884	U
1	2A	2886	G

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Mol	Chain	Res	Type
1	2A	2892	A
1	2A	2894	G
1	2A	2897	U
2	2B	2	C
2	2B	5	C
2	2B	8	U
2	2B	12	C
2	2B	13	A
2	2B	17	C
2	2B	18	G
2	2B	24	G
2	2B	30	C
2	2B	33	G
2	2B	41	U
2	2B	45	A
2	2B	53	A
2	2B	54	G
2	2B	56	G
2	2B	63	G
2	2B	66	A
2	2B	67	G
2	2B	72	G
2	2B	73	A
2	2B	74	U
2	2B	75	G
2	2B	88	C
2	2B	90	A
2	2B	105	A
2	2B	106	G
2	2B	110	G
2	2B	114	C
2	2B	115	G
2	2B	116	G
2	2B	119	G
2	2B	120	A
32	2a	9	G
32	2a	22	G
32	2a	30	U
32	2a	32	A
32	2a	39	G
32	2a	47	C
32	2a	48	C

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Mol	Chain	Res	Type
32	2a	51	A
32	2a	52	G
32	2a	54	C
32	2a	59	A
32	2a	66	G
32	2a	73	G
32	2a	79	G
32	2a	80	G
32	2a	88	A
32	2a	89	C
32	2a	101	A
32	2a	102	G
32	2a	116	A
32	2a	120	A
32	2a	121	C
32	2a	129(A)	G
32	2a	130	A
32	2a	131	C
32	2a	150	C
32	2a	151	A
32	2a	163	C
32	2a	174	C
32	2a	182	U
32	2a	189(B)	C
32	2a	189(C)	C
32	2a	189(E)	U
32	2a	189(F)	U
32	2a	189(G)	G
32	2a	189(H)	G
32	2a	189(K)	U
32	2a	195	A
32	2a	197	A
32	2a	202	U
32	2a	204	U
32	2a	216	G
32	2a	217	C
32	2a	245	C
32	2a	247	G
32	2a	250	A
32	2a	251	G
32	2a	266	G
32	2a	267	C

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Mol	Chain	Res	Type
32	2a	274	A
32	2a	281	G
32	2a	288	A
32	2a	289	G
32	2a	306	G
32	2a	321	A
32	2a	324	G
32	2a	328	C
32	2a	332	G
32	2a	348	G
32	2a	349	A
32	2a	350	G
32	2a	351	G
32	2a	352	C
32	2a	353	A
32	2a	354	G
32	2a	367	U
32	2a	372	C
32	2a	373	A
32	2a	375	U
32	2a	397	A
32	2a	398	C
32	2a	406	G
32	2a	410	G
32	2a	411	A
32	2a	412	A
32	2a	413	G
32	2a	414	A
32	2a	421	U
32	2a	422	C
32	2a	423	G
32	2a	424	G
32	2a	429	U
32	2a	430	A
32	2a	439	A
32	2a	442	C
32	2a	452	A
32	2a	453	A
32	2a	457	C
32	2a	461	A
32	2a	470	C
32	2a	471	G

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Mol	Chain	Res	Type
32	2a	474	G
32	2a	479	C
32	2a	482	A
32	2a	484	G
32	2a	485	G
32	2a	496	A
32	2a	498	U
32	2a	505	G
32	2a	506	G
32	2a	509	A
32	2a	510	A
32	2a	511	C
32	2a	518	C
32	2a	521	G
32	2a	531	U
32	2a	532	A
32	2a	533	A
32	2a	547	A
32	2a	559	A
32	2a	561	U
32	2a	562	C
32	2a	564	C
32	2a	568	G
32	2a	572	A
32	2a	573	A
32	2a	576	G
32	2a	577	G
32	2a	584	G
32	2a	587	G
32	2a	595	G
32	2a	612	C
32	2a	618	C
32	2a	627	G
32	2a	630	G
32	2a	642	A
32	2a	653	A
32	2a	661	G
32	2a	665	A
32	2a	671	G
32	2a	681	C
32	2a	682	G
32	2a	687	A

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Mol	Chain	Res	Type
32	2a	688	G
32	2a	690	G
32	2a	695	A
32	2a	698	G
32	2a	702	A
32	2a	703	G
32	2a	721	G
32	2a	723	U
32	2a	731	G
32	2a	734	G
32	2a	749	C
32	2a	752	G
32	2a	755	G
32	2a	777	A
32	2a	782	A
32	2a	793	U
32	2a	794	A
32	2a	798	G
32	2a	802	A
32	2a	810	C
32	2a	815	A
32	2a	817	C
32	2a	818	G
32	2a	821	G
32	2a	828	A
32	2a	837	G
32	2a	840	C
32	2a	841	U
32	2a	851	G
32	2a	853	G
32	2a	859	A
32	2a	872	A
32	2a	876	G
32	2a	902	G
32	2a	914	A
32	2a	916	G
32	2a	919	A
32	2a	926	G
32	2a	927	G
32	2a	931	C
32	2a	934	C
32	2a	942	G

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Mol	Chain	Res	Type
32	2a	947	G
32	2a	954	G
32	2a	960	U
32	2a	961	U
32	2a	965	A
32	2a	969	A
32	2a	971	G
32	2a	972	C
32	2a	974	A
32	2a	975	A
32	2a	976	G
32	2a	977	A
32	2a	983	A
32	2a	989	C
32	2a	990	C
32	2a	992	U
32	2a	993	G
32	2a	997	U
32	2a	1001(A)	G
32	2a	1002	G
32	2a	1003	G
32	2a	1004	A
32	2a	1005	A
32	2a	1006	C
32	2a	1007	C
32	2a	1009	G
32	2a	1016	A
32	2a	1017	G
32	2a	1020	U
32	2a	1022	G
32	2a	1023	G
32	2a	1025	U
32	2a	1027	C
32	2a	1028	C
32	2a	1030	C
32	2a	1030(A)	G
32	2a	1030(D)	A
32	2a	1031	G
32	2a	1036	G
32	2a	1039	C
32	2a	1040	U
32	2a	1045	C

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Mol	Chain	Res	Type
32	2a	1055	A
32	2a	1065	U
32	2a	1066	C
32	2a	1068	G
32	2a	1077	G
32	2a	1081	G
32	2a	1084	G
32	2a	1086	U
32	2a	1094	G
32	2a	1095	U
32	2a	1101	A
32	2a	1108	G
32	2a	1109	C
32	2a	1113	C
32	2a	1115	C
32	2a	1117	G
32	2a	1122	U
32	2a	1129	C
32	2a	1130	A
32	2a	1136	U
32	2a	1137	C
32	2a	1138	G
32	2a	1139	G
32	2a	1140	C
32	2a	1146	A
32	2a	1147	C
32	2a	1152	A
32	2a	1157	A
32	2a	1159	U
32	2a	1160	G
32	2a	1161	C
32	2a	1173	G
32	2a	1177	G
32	2a	1181	G
32	2a	1182	G
32	2a	1183	A
32	2a	1184	G
32	2a	1189	C
32	2a	1196	U
32	2a	1197	G
32	2a	1202	G
32	2a	1211	U

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Mol	Chain	Res	Type
32	2a	1212	U
32	2a	1213	A
32	2a	1214	C
32	2a	1217	C
32	2a	1225	A
32	2a	1227	A
32	2a	1236	A
32	2a	1238	A
32	2a	1240	U
32	2a	1241	G
32	2a	1250	A
32	2a	1255	G
32	2a	1256	A
32	2a	1257	U
32	2a	1258	G
32	2a	1260	C
32	2a	1270	C
32	2a	1272	G
32	2a	1273	G
32	2a	1275	A
32	2a	1276	G
32	2a	1278	U
32	2a	1279	A
32	2a	1280	A
32	2a	1286	A
32	2a	1287	A
32	2a	1290	G
32	2a	1293	G
32	2a	1298	C
32	2a	1299	A
32	2a	1300	G
32	2a	1301	U
32	2a	1302	U
32	2a	1303	C
32	2a	1305	G
32	2a	1319	A
32	2a	1320	C
32	2a	1323	G
32	2a	1325	C
32	2a	1336	C
32	2a	1340	A
32	2a	1346	A

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Mol	Chain	Res	Type
32	2a	1347	G
32	2a	1352	C
32	2a	1353	G
32	2a	1363	C
32	2a	1363(A)	A
32	2a	1364	U
32	2a	1370	G
32	2a	1379	G
32	2a	1397	C
32	2a	1399	C
32	2a	1406	U
32	2a	1419	G
32	2a	1440	C
32	2a	1442	G
32	2a	1442(A)	G
32	2a	1446	U
32	2a	1447	A
32	2a	1452	C
32	2a	1462	G
32	2a	1474	G
32	2a	1483	A
32	2a	1492	A
32	2a	1493	A
32	2a	1494	G
32	2a	1503	A
32	2a	1504	G
32	2a	1505	G
32	2a	1506	U
32	2a	1517	G
32	2a	1520	G
32	2a	1525	G
32	2a	1529	G
32	2a	1530	G
32	2a	1531	A
32	2a	1532	U
53	2v	15	A
54	2x	6	G
54	2x	8	4SU
54	2x	9	G
54	2x	20	U
54	2x	21	A
54	2x	47	U

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Mol	Chain	Res	Type
54	2x	48	C
54	2x	61	C
54	2x	76	A

All (43) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	195	A
1	1A	266	G
1	1A	278	A
1	1A	548	A
1	1A	1047	G
1	1A	1065	U
1	1A	1067	A
1	1A	1174	A
1	1A	1175	U
1	1A	1176	G
1	1A	1275	A
1	1A	1508	A
1	1A	1944	U
1	1A	1992	G
1	1A	2134	A
1	1A	2158	A
1	1A	2183	C
1	1A	2288	A
1	1A	2430	A
1	1A	2473	U
1	1A	2689	U
2	1B	1	U
1	2A	195	A
1	2A	228	A
1	2A	266	G
1	2A	271(M)	G
1	2A	277	C
1	2A	528	A
1	2A	669	G
1	2A	752	A
1	2A	784	A
1	2A	856	C
1	2A	900	A
1	2A	1026	U
1	2A	1210	A

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Mol	Chain	Res	Type
1	2A	1240	U
1	2A	1379	A
1	2A	1530	C
1	2A	1653	G
1	2A	1913	A
1	2A	1992	G
1	2A	2022	U
1	2A	2689	U

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

56 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
54	4SU	2x	8	54	14,21,22	1.38	2 (14%)	15,30,33	2.32	2 (13%)
32	5MC	1a	967	32	15,22,23	1.21	1 (6%)	19,32,35	1.28	2 (10%)
54	5MU	1x	54	54	15,22,23	1.04	2 (13%)	16,32,35	2.32	1 (6%)
32	PSU	1a	516	55,32	17,21,22	1.47	3 (17%)	20,30,33	3.19	6 (30%)
1	5MU	1A	1939	1	15,22,23	1.11	2 (13%)	16,32,35	1.82	2 (12%)
32	5MC	2a	967	32	15,22,23	1.33	1 (6%)	19,32,35	1.31	2 (10%)
1	2MA	2A	2503	1,55	17,25,26	1.35	2 (11%)	19,37,40	2.03	3 (15%)
1	5MU	1A	1915	1	15,22,23	1.04	1 (6%)	16,32,35	1.73	2 (12%)
32	5MC	1a	1407	32	15,22,23	1.25	1 (6%)	19,32,35	1.38	2 (10%)
32	UR3	1a	1498	32	14,22,23	0.74	1 (7%)	15,32,35	0.77	1 (6%)
32	5MC	2a	1400	32,54	15,22,23	1.46	1 (6%)	19,32,35	1.40	2 (10%)
32	7MG	1a	527	55,32	22,26,27	1.76	4 (18%)	28,39,42	2.74	8 (28%)
32	2MG	1a	1207	32	19,26,27	1.22	2 (10%)	21,38,41	2.19	8 (38%)
32	MA6	1a	1518	32	19,26,27	0.89	1 (5%)	18,38,41	1.71	4 (22%)
54	5MC	1x	32	54	15,22,23	1.28	1 (6%)	19,32,35	1.48	4 (21%)
1	PSU	1A	2605	1	17,21,22	1.57	3 (17%)	20,30,33	3.06	6 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	2MU	2A	2552	1,55	14,22,24	0.90	0	14,31,36	0.92	0
1	5MC	2A	1942	1,55	15,22,23	1.38	1 (6%)	19,32,35	1.46	3 (15%)
32	MA6	2a	1518	32	19,26,27	0.94	1 (5%)	18,38,41	1.72	4 (22%)
32	5MC	1a	1404	32	15,22,23	1.38	1 (6%)	19,32,35	1.25	3 (15%)
32	UR3	2a	1498	32	14,22,23	0.76	1 (7%)	15,32,35	0.70	0
1	5MU	2A	1939	1	15,22,23	1.18	2 (13%)	16,32,35	1.82	2 (12%)
54	4SU	1x	8	54	14,21,22	1.47	2 (14%)	15,30,33	2.63	2 (13%)
1	PSU	2A	1911	1	17,21,22	1.56	2 (11%)	20,30,33	3.16	6 (30%)
1	4OC	2A	1920	1	15,22,24	0.67	0	17,31,35	1.41	2 (11%)
54	PSU	1x	55	54	17,21,22	1.59	2 (11%)	20,30,33	3.32	6 (30%)
32	4OC	1a	1402	32	16,23,24	0.59	0	17,32,35	1.31	1 (5%)
1	5MC	2A	1962	1,55	15,22,23	1.32	1 (6%)	19,32,35	1.37	2 (10%)
1	5MC	1A	1942	1	15,22,23	1.19	1 (6%)	19,32,35	1.39	3 (15%)
32	5MC	2a	1404	32	15,22,23	1.29	1 (6%)	19,32,35	1.40	2 (10%)
32	MA6	1a	1519	32	19,26,27	1.02	1 (5%)	18,38,41	1.60	3 (16%)
43	0TD	1l	92	43	4,9,10	3.03	1 (25%)	3,11,13	2.20	1 (33%)
32	M2G	2a	966	55,32	20,27,28	1.46	3 (15%)	22,40,43	2.19	6 (27%)
32	PSU	2a	516	32	17,21,22	1.45	3 (17%)	20,30,33	3.18	5 (25%)
1	PSU	1A	1917	1	17,21,22	1.85	4 (23%)	20,30,33	3.28	6 (30%)
32	7MG	2a	527	55,32	22,26,27	1.72	4 (18%)	28,39,42	2.67	9 (32%)
1	PSU	1A	1911	1	17,21,22	1.53	2 (11%)	20,30,33	3.22	6 (30%)
1	5MC	1A	1962	1	15,22,23	1.32	1 (6%)	19,32,35	1.30	2 (10%)
43	0TD	2l	92	43	4,9,10	3.20	1 (25%)	3,11,13	7.91	1 (33%)
1	5MU	2A	1915	1,55	15,22,23	1.16	1 (6%)	16,32,35	1.84	2 (12%)
32	M2G	1a	966	55,32	20,27,28	1.43	3 (15%)	22,40,43	2.17	7 (31%)
54	PSU	2x	55	54	17,21,22	1.66	2 (11%)	20,30,33	3.21	6 (30%)
32	2MG	2a	1207	55,32	19,26,27	1.25	2 (10%)	21,38,41	2.26	7 (33%)
1	OMG	1A	2251	1,55,54	18,26,27	1.28	2 (11%)	20,38,41	2.00	7 (35%)
1	PSU	2A	1917	1	17,21,22	1.57	3 (17%)	20,30,33	3.09	6 (30%)
32	4OC	2a	1402	32	16,23,24	0.66	0	17,32,35	1.36	3 (17%)
1	OMG	2A	2251	1,55,54	18,26,27	1.06	2 (11%)	20,38,41	2.12	5 (25%)
1	PSU	2A	2605	1	17,21,22	1.49	2 (11%)	20,30,33	3.15	6 (30%)
32	5MC	1a	1400	32	15,22,23	1.32	1 (6%)	19,32,35	1.43	2 (10%)
32	MA6	2a	1519	32	19,26,27	1.03	1 (5%)	18,38,41	1.69	5 (27%)
1	2MU	1A	2552	1,55	14,22,24	0.88	0	14,31,36	0.86	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
54	5MU	2x	54	54	15,22,23	1.08	1 (6%)	16,32,35	1.74	2 (12%)
32	5MC	2a	1407	32	15,22,23	1.37	1 (6%)	19,32,35	1.36	2 (10%)
1	2MA	1A	2503	1,55	17,25,26	1.30	2 (11%)	19,37,40	2.30	5 (26%)
54	5MC	2x	32	54	15,22,23	1.36	1 (6%)	19,32,35	1.37	3 (15%)
1	4OC	1A	1920	1	15,22,24	0.67	0	17,31,35	1.38	1 (5%)

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
54	4SU	2x	8	54	-	0/5/25/26	0/2/2/2
32	5MC	1a	967	32	-	2/5/25/26	0/2/2/2
54	5MU	1x	54	54	-	0/5/25/26	0/2/2/2
32	PSU	1a	516	55,32	-	0/7/25/26	0/2/2/2
1	5MU	1A	1939	1	-	0/5/25/26	0/2/2/2
32	5MC	2a	967	32	-	0/5/25/26	0/2/2/2
1	2MA	2A	2503	1,55	-	1/3/25/26	0/3/3/3
1	5MU	1A	1915	1	-	0/5/25/26	0/2/2/2
32	5MC	1a	1407	32	-	0/5/25/26	0/2/2/2
32	UR3	1a	1498	32	-	0/5/25/26	0/2/2/2
32	5MC	2a	1400	32,54	-	0/5/25/26	0/2/2/2
32	7MG	1a	527	55,32	-	2/7/37/38	0/3/3/3
32	2MG	1a	1207	32	-	2/5/27/28	0/3/3/3
32	MA6	1a	1518	32	-	3/7/29/30	0/3/3/3
54	5MC	1x	32	54	-	0/5/25/26	0/2/2/2
1	PSU	1A	2605	1	-	0/7/25/26	0/2/2/2
1	2MU	2A	2552	1,55	-	2/7/27/28	0/2/2/2
1	5MC	2A	1942	1,55	-	0/5/25/26	0/2/2/2
32	MA6	2a	1518	32	-	3/7/29/30	0/3/3/3
32	5MC	1a	1404	32	-	0/5/25/26	0/2/2/2
32	UR3	2a	1498	32	-	0/5/25/26	0/2/2/2
1	5MU	2A	1939	1	-	2/5/25/26	0/2/2/2
54	4SU	1x	8	54	-	0/5/25/26	0/2/2/2
1	PSU	2A	1911	1	-	1/7/25/26	0/2/2/2
1	4OC	2A	1920	1	-	1/7/27/30	0/2/2/2
54	PSU	1x	55	54	-	0/7/25/26	0/2/2/2
32	4OC	1a	1402	32	-	4/9/29/30	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5MC	2A	1962	1,55	-	2/5/25/26	0/2/2/2
1	5MC	1A	1942	1	-	0/5/25/26	0/2/2/2
32	5MC	2a	1404	32	-	0/5/25/26	0/2/2/2
32	MA6	1a	1519	32	-	3/7/29/30	0/3/3/3
43	0TD	1l	92	43	-	2/3/12/14	-
32	M2G	2a	966	55,32	-	0/7/29/30	0/3/3/3
32	PSU	2a	516	32	-	0/7/25/26	0/2/2/2
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
32	7MG	2a	527	55,32	-	2/7/37/38	0/3/3/3
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
1	5MC	1A	1962	1	-	2/5/25/26	0/2/2/2
43	0TD	2l	92	43	-	1/3/12/14	-
1	5MU	2A	1915	1,55	-	1/5/25/26	0/2/2/2
32	M2G	1a	966	55,32	-	1/7/29/30	0/3/3/3
54	PSU	2x	55	54	-	0/7/25/26	0/2/2/2
32	2MG	2a	1207	55,32	-	1/5/27/28	0/3/3/3
1	OMG	1A	2251	1,55,54	-	0/5/27/28	0/3/3/3
1	PSU	2A	1917	1	-	1/7/25/26	0/2/2/2
32	4OC	2a	1402	32	-	4/9/29/30	0/2/2/2
1	OMG	2A	2251	1,55,54	-	0/5/27/28	0/3/3/3
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
32	5MC	1a	1400	32	-	2/5/25/26	0/2/2/2
32	MA6	2a	1519	32	-	4/7/29/30	0/3/3/3
1	2MU	1A	2552	1,55	-	0/7/27/28	0/2/2/2
54	5MU	2x	54	54	-	0/5/25/26	0/2/2/2
32	5MC	2a	1407	32	-	0/5/25/26	0/2/2/2
1	2MA	1A	2503	1,55	-	3/3/25/26	0/3/3/3
54	5MC	2x	32	54	-	0/5/25/26	0/2/2/2
1	4OC	1A	1920	1	-	1/7/27/30	0/2/2/2

All (87) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	2l	92	0TD	CB-SB	-6.10	1.69	1.84
1	1A	1917	PSU	C5-C1'	-5.88	1.47	1.52
43	1l	92	0TD	CB-SB	-5.72	1.70	1.84
32	2a	1400	5MC	C5-C4	5.21	1.49	1.41
1	2A	1942	5MC	C5-C4	4.95	1.49	1.41
54	2x	55	PSU	C5-C1'	-4.94	1.48	1.52
32	1a	1404	5MC	C5-C4	4.93	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	2x	32	5MC	C5-C4	4.89	1.48	1.41
32	1a	527	7MG	C6-C5	4.88	1.48	1.41
32	1a	1400	5MC	C5-C4	4.81	1.48	1.41
32	2a	967	5MC	C5-C4	4.79	1.48	1.41
32	2a	1407	5MC	C5-C4	4.75	1.48	1.41
32	2a	527	7MG	C6-C5	4.71	1.47	1.41
1	2A	1962	5MC	C5-C4	4.67	1.48	1.41
32	2a	1404	5MC	C5-C4	4.55	1.48	1.41
1	1A	1962	5MC	C5-C4	4.54	1.48	1.41
1	2A	2503	2MA	C6-C5	4.52	1.48	1.41
54	1x	32	5MC	C5-C4	4.52	1.48	1.41
1	1A	2503	2MA	C6-C5	4.47	1.48	1.41
54	1x	55	PSU	C5-C1'	-4.39	1.48	1.52
32	1a	1407	5MC	C5-C4	4.39	1.48	1.41
32	2a	1207	2MG	C6-C5	4.37	1.48	1.41
32	2a	966	M2G	C6-C5	4.37	1.48	1.41
1	1A	2251	OMG	C6-C5	4.36	1.48	1.41
32	1a	966	M2G	C6-C5	4.35	1.48	1.41
1	2A	1911	PSU	C5-C1'	-4.33	1.48	1.52
32	1a	1207	2MG	C6-C5	4.28	1.48	1.41
1	2A	1917	PSU	C5-C1'	-4.27	1.48	1.52
32	1a	967	5MC	C5-C4	4.25	1.48	1.41
32	1a	527	7MG	C5-C4	4.25	1.47	1.39
32	2a	527	7MG	C5-C4	4.21	1.47	1.39
1	1A	1942	5MC	C5-C4	4.19	1.47	1.41
1	1A	2605	PSU	C5-C1'	-4.05	1.48	1.52
54	2x	8	4SU	C4-S4	-3.98	1.60	1.67
54	1x	8	4SU	C4-S4	-3.82	1.60	1.67
1	2A	1915	5MU	C4-C5	3.79	1.49	1.41
1	1A	1911	PSU	C5-C1'	-3.74	1.49	1.52
1	1A	1911	PSU	C4-C5	3.71	1.49	1.41
1	2A	2605	PSU	C5-C1'	-3.63	1.49	1.52
32	2a	516	PSU	C4-C5	3.57	1.49	1.41
54	1x	55	PSU	C4-C5	3.55	1.49	1.41
54	1x	8	4SU	C2-N3	-3.53	1.31	1.38
32	1a	516	PSU	C4-C5	3.52	1.49	1.41
32	1a	527	7MG	C5-N7	-3.50	1.33	1.39
32	2a	966	M2G	C2-N2	3.47	1.40	1.34
1	2A	1939	5MU	C4-C5	3.43	1.48	1.41
54	2x	54	5MU	C4-C5	3.41	1.48	1.41
1	2A	1917	PSU	C4-C5	3.41	1.48	1.41
1	1A	2605	PSU	C4-C5	3.41	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	1a	516	PSU	C5-C1'	-3.36	1.49	1.52
1	2A	2605	PSU	C4-C5	3.35	1.48	1.41
1	2A	2251	OMG	C6-C5	3.33	1.47	1.41
1	1A	1915	5MU	C4-C5	3.28	1.48	1.41
1	1A	1939	5MU	C4-C5	3.28	1.48	1.41
32	1a	966	M2G	C2-N2	3.26	1.40	1.34
54	2x	55	PSU	C4-C5	3.22	1.48	1.41
1	2A	1911	PSU	C4-C5	3.20	1.48	1.41
54	1x	54	5MU	C4-C5	3.14	1.48	1.41
32	2a	516	PSU	C5-C1'	-3.13	1.49	1.52
1	1A	1917	PSU	C4-C5	3.03	1.48	1.41
32	2a	527	7MG	C5-N7	-3.00	1.34	1.39
54	2x	8	4SU	C2-N3	-2.90	1.32	1.38
32	2a	527	7MG	C4-N9	-2.74	1.33	1.38
32	1a	966	M2G	C5-C4	2.64	1.47	1.40
1	1A	2251	OMG	C5-C4	2.61	1.47	1.40
32	2a	1519	MA6	C5-C4	2.57	1.47	1.40
32	2a	966	M2G	C5-C4	2.57	1.47	1.40
32	2a	1207	2MG	C5-C4	2.51	1.47	1.40
32	1a	1519	MA6	C5-C4	2.50	1.47	1.40
1	2A	2251	OMG	C5-C4	2.46	1.47	1.40
32	2a	1518	MA6	C5-C4	2.44	1.47	1.40
1	2A	2503	2MA	C5-C4	2.44	1.47	1.40
32	1a	527	7MG	C4-N9	-2.43	1.33	1.38
32	1a	1207	2MG	C5-C4	2.40	1.47	1.40
1	2A	1939	5MU	C2-N3	-2.38	1.33	1.38
32	1a	1518	MA6	C5-C4	2.30	1.47	1.40
32	1a	516	PSU	O4'-C1'	-2.25	1.41	1.44
1	1A	1939	5MU	C2-N3	-2.22	1.33	1.38
32	2a	1498	UR3	C4-N3	2.13	1.41	1.38
1	1A	1917	PSU	O4'-C1'	-2.12	1.41	1.44
32	2a	516	PSU	O4'-C1'	-2.11	1.41	1.44
1	1A	2605	PSU	O4'-C1'	-2.05	1.41	1.44
32	1a	1498	UR3	C4-N3	2.05	1.41	1.38
54	1x	54	5MU	C2-N3	-2.03	1.34	1.38
1	1A	1917	PSU	C2-N3	-2.02	1.34	1.38
1	1A	2503	2MA	C5-C4	2.01	1.46	1.40
1	2A	1917	PSU	O4'-C1'	-2.00	1.41	1.44

All (200) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	2l	92	0TD	CSB-SB-CB	-13.65	75.00	101.85
54	1x	8	4SU	C2-N3-C4	8.99	128.18	115.15
32	2a	516	PSU	N1-C2-N3	-8.95	121.32	128.43
54	1x	54	5MU	C4-N3-C2	8.93	122.68	115.14
32	1a	516	PSU	N1-C2-N3	-8.88	121.37	128.43
1	2A	1911	PSU	N1-C2-N3	-8.85	121.39	128.43
32	1a	527	7MG	N3-C4-N9	8.83	138.25	126.91
1	1A	1911	PSU	N1-C2-N3	-8.60	121.60	128.43
54	1x	55	PSU	N1-C2-N3	-8.53	121.65	128.43
1	2A	2605	PSU	N1-C2-N3	-8.50	121.68	128.43
54	2x	55	PSU	N1-C2-N3	-8.19	121.92	128.43
32	2a	527	7MG	N3-C4-N9	8.14	137.37	126.91
1	1A	2605	PSU	N1-C2-N3	-8.03	122.05	128.43
1	2A	1917	PSU	N1-C2-N3	-8.00	122.07	128.43
1	1A	1917	PSU	N1-C2-N3	-7.98	122.09	128.43
54	2x	8	4SU	C2-N3-C4	7.66	126.25	115.15
1	1A	2503	2MA	C2-N3-C4	7.46	121.58	115.52
32	2a	516	PSU	C4-N3-C2	7.34	121.34	115.14
32	1a	516	PSU	C4-N3-C2	7.31	121.31	115.14
54	1x	55	PSU	C4-N3-C2	7.24	121.26	115.14
1	2A	2605	PSU	C4-N3-C2	6.83	120.91	115.14
1	1A	1911	PSU	C4-N3-C2	6.83	120.91	115.14
1	2A	1911	PSU	C4-N3-C2	6.70	120.80	115.14
54	2x	55	PSU	C4-N3-C2	6.58	120.69	115.14
1	2A	1915	5MU	C4-N3-C2	6.44	120.58	115.14
1	2A	1917	PSU	C4-N3-C2	6.39	120.54	115.14
1	1A	2605	PSU	C4-N3-C2	6.33	120.49	115.14
54	2x	54	5MU	C4-N3-C2	6.20	120.38	115.14
1	1A	1939	5MU	C4-N3-C2	6.19	120.37	115.14
1	1A	1915	5MU	C4-N3-C2	6.16	120.34	115.14
1	2A	2503	2MA	C2-N3-C4	6.07	120.45	115.52
1	1A	1917	PSU	C4-N3-C2	6.07	120.26	115.14
32	2a	527	7MG	N7-C8-N9	-5.93	94.89	103.38
54	1x	55	PSU	C5-C4-N3	-5.89	117.78	125.36
1	1A	1917	PSU	C5-C1'-C2'	-5.63	105.27	115.32
54	2x	55	PSU	C5-C4-N3	-5.55	118.21	125.36
1	2A	1939	5MU	C4-N3-C2	5.50	119.79	115.14
32	1a	516	PSU	C5-C4-N3	-5.49	118.28	125.36
1	1A	1917	PSU	C5-C4-N3	-5.44	118.35	125.36
32	2a	516	PSU	C5-C4-N3	-5.43	118.36	125.36
1	2A	1917	PSU	C5-C4-N3	-5.33	118.49	125.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	966	M2G	C6-N1-C2	5.33	122.53	116.18
32	1a	527	7MG	N7-C8-N9	-5.30	95.79	103.38
1	1A	1911	PSU	C5-C4-N3	-5.27	118.57	125.36
32	2a	966	M2G	C2-N3-C4	5.20	121.19	115.28
1	1A	2605	PSU	C5-C4-N3	-5.15	118.72	125.36
32	1a	527	7MG	C5-C4-N3	-5.14	118.09	126.49
1	2A	1911	PSU	C5-C4-N3	-5.09	118.80	125.36
1	1A	2251	OMG	C2-N3-C4	5.08	121.16	115.36
32	1a	1207	2MG	C2-N3-C4	5.08	121.04	115.28
1	2A	2605	PSU	C5-C4-N3	-5.05	118.85	125.36
32	1a	966	M2G	C2-N3-C4	5.05	121.01	115.28
1	1A	1917	PSU	C5-C6-N1	-5.02	118.27	124.44
32	2a	527	7MG	C6-N1-C2	4.98	123.84	115.93
32	1a	966	M2G	C6-N1-C2	4.92	122.05	116.18
1	2A	2503	2MA	C5-C6-N1	-4.84	117.98	123.06
32	2a	1207	2MG	C5-C6-N1	-4.70	117.01	123.43
1	2A	2251	OMG	C6-N1-C2	4.65	123.32	115.93
1	2A	2251	OMG	C5-C6-N1	-4.61	117.12	123.43
1	1A	1920	4OC	C2-N3-C4	4.55	120.96	116.34
54	2x	55	PSU	C5-C6-N1	-4.55	118.85	124.44
32	1a	527	7MG	C6-N1-C2	4.37	122.88	115.93
54	1x	8	4SU	C5-C4-N3	-4.37	117.98	123.83
32	1a	527	7MG	C6-C5-C4	4.36	119.88	115.20
1	2A	1920	4OC	C2-N3-C4	4.35	120.75	116.34
1	2A	1917	PSU	C5-C6-N1	-4.33	119.12	124.44
54	2x	55	PSU	C5-C1'-C2'	-4.29	107.66	115.32
1	2A	2251	OMG	C2-N3-C4	4.26	120.23	115.36
1	1A	1917	PSU	C6-N1-C2	4.26	122.39	115.36
54	1x	55	PSU	C5-C6-N1	-4.26	119.21	124.44
1	1A	1911	PSU	C6-N1-C2	4.25	122.37	115.36
1	2A	1911	PSU	C6-N1-C2	4.22	122.33	115.36
1	1A	2503	2MA	C5-C6-N1	-4.17	118.69	123.06
32	2a	527	7MG	C5-C4-N3	-4.16	119.70	126.49
32	2a	1207	2MG	C2-N3-C4	4.14	119.98	115.28
54	2x	8	4SU	C5-C4-N3	-4.11	118.33	123.83
54	2x	55	PSU	C6-N1-C2	4.11	122.14	115.36
1	2A	1911	PSU	C5-C6-N1	-4.10	119.40	124.44
32	1a	1407	5MC	C2-N3-C4	4.10	120.97	116.02
32	2a	516	PSU	C6-N1-C2	4.08	122.09	115.36
1	2A	1917	PSU	C6-N1-C2	4.06	122.06	115.36
1	1A	1911	PSU	C5-C1'-C2'	-4.06	108.08	115.32
32	1a	1402	4OC	CM4-N4-C4	-4.06	119.48	122.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	516	PSU	C6-N1-C2	4.05	122.04	115.36
32	1a	1400	5MC	C2-N3-C4	4.05	120.91	116.02
1	2A	2605	PSU	C5-C1'-C2'	-4.03	108.12	115.32
54	1x	55	PSU	C6-N1-C2	4.03	122.00	115.36
32	2a	1207	2MG	C6-N1-C2	4.01	122.36	115.18
32	2a	966	M2G	C5-C6-N1	-4.00	117.96	123.43
32	1a	966	M2G	C5-C6-N1	-4.00	117.96	123.43
54	1x	55	PSU	C5-C1'-C2'	-3.99	108.20	115.32
1	1A	2605	PSU	C6-N1-C2	3.97	121.91	115.36
1	1A	1911	PSU	C5-C6-N1	-3.97	119.56	124.44
1	1A	2605	PSU	C5-C1'-C2'	-3.96	108.26	115.32
1	2A	1939	5MU	C5-C6-N1	-3.94	117.94	122.19
1	2A	2605	PSU	C6-N1-C2	3.92	121.83	115.36
32	2a	1407	5MC	C2-N3-C4	3.88	120.70	116.02
32	2a	1207	2MG	C6-C5-C4	-3.88	117.09	120.80
1	1A	2251	OMG	C5-C6-N1	-3.86	118.15	123.43
32	1a	1207	2MG	C6-N1-C2	3.83	122.04	115.18
32	2a	1518	MA6	C4-C5-N7	-3.83	105.41	109.40
32	2a	1404	5MC	C2-N3-C4	3.82	120.63	116.02
32	2a	527	7MG	C5-C6-N1	-3.82	115.28	123.14
32	1a	527	7MG	C5-C6-N1	-3.78	115.38	123.14
32	1a	1207	2MG	C6-C5-C4	-3.77	117.20	120.80
32	1a	1207	2MG	C5-C6-N1	-3.77	118.28	123.43
1	2A	1917	PSU	C5-C1'-C2'	-3.76	108.61	115.32
1	1A	2605	PSU	C5-C6-N1	-3.76	119.82	124.44
32	2a	1402	4OC	CM4-N4-C4	-3.76	119.74	122.97
32	2a	967	5MC	C2-N3-C4	3.76	120.55	116.02
54	1x	32	5MC	C2-N3-C4	3.69	120.47	116.02
32	1a	967	5MC	C2-N3-C4	3.66	120.43	116.02
32	2a	1519	MA6	C4-C5-N7	-3.65	105.59	109.40
32	1a	516	PSU	C5-C6-N1	-3.63	119.98	124.44
32	1a	1519	MA6	C4-C5-N7	-3.60	105.64	109.40
32	2a	966	M2G	C6-C5-C4	-3.59	117.37	120.80
32	1a	1518	MA6	C9-N6-C6	-3.59	108.64	119.51
1	2A	1962	5MC	C2-N3-C4	3.59	120.35	116.02
54	2x	32	5MC	C2-N3-C4	3.57	120.33	116.02
32	2a	516	PSU	C5-C6-N1	-3.55	120.08	124.44
43	1l	92	0TD	CSB-SB-CB	3.54	108.83	101.85
32	2a	1518	MA6	N3-C2-N1	-3.51	123.19	128.68
1	2A	2605	PSU	C5-C6-N1	-3.50	120.14	124.44
1	2A	1942	5MC	C5-C6-N1	-3.46	118.46	122.19
32	1a	1404	5MC	C2-N3-C4	3.46	120.19	116.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1518	MA6	C9-N6-C6	-3.45	109.06	119.51
32	1a	1518	MA6	N3-C2-N1	-3.44	123.29	128.68
32	1a	1518	MA6	C4-C5-N7	-3.43	105.82	109.40
1	1A	1962	5MC	C2-N3-C4	3.43	120.16	116.02
32	2a	1207	2MG	C4-C5-N7	-3.40	105.85	109.40
32	1a	1207	2MG	CM2-N2-C2	-3.37	119.53	123.59
32	2a	1400	5MC	C2-N3-C4	3.36	120.07	116.02
1	1A	1942	5MC	C2-N3-C4	3.35	120.06	116.02
1	1A	2251	OMG	C6-N1-C2	3.32	121.21	115.93
1	2A	2251	OMG	N3-C2-N1	-3.30	122.82	127.22
32	2a	1519	MA6	N3-C2-N1	-3.27	123.57	128.68
32	2a	1207	2MG	CM2-N2-C2	-3.23	119.69	123.59
32	2a	527	7MG	C6-C5-C4	3.22	118.65	115.20
32	2a	1519	MA6	C9-N6-C6	-3.18	109.89	119.51
1	2A	1962	5MC	N4-C4-N3	3.12	121.45	117.03
32	1a	1519	MA6	N3-C2-N1	-3.05	123.91	128.68
1	2A	1942	5MC	C2-N3-C4	3.03	119.67	116.02
32	1a	966	M2G	C4-C5-N7	-3.01	106.26	109.40
1	2A	2503	2MA	C4-C5-N7	-2.92	106.35	109.40
32	1a	966	M2G	C6-C5-C4	-2.92	118.01	120.80
1	1A	1939	5MU	C5-C6-N1	-2.89	119.08	122.19
32	1a	1400	5MC	N4-C4-N3	2.88	121.11	117.03
32	2a	1404	5MC	N4-C4-N3	2.87	121.09	117.03
1	1A	1942	5MC	N4-C4-N3	2.85	121.06	117.03
1	2A	1911	PSU	C5-C1'-C2'	-2.83	110.28	115.32
32	1a	1519	MA6	C9-N6-C6	-2.81	111.00	119.51
1	2A	2251	OMG	C6-C5-C4	-2.81	118.12	120.80
1	2A	1915	5MU	C5-C6-N1	-2.78	119.19	122.19
1	1A	2251	OMG	C4-C5-N7	-2.77	106.51	109.40
32	2a	1207	2MG	N2-C2-N1	2.77	119.62	116.96
32	2a	1400	5MC	C5-C6-N1	-2.77	119.21	122.19
32	1a	1207	2MG	C4-C5-N7	-2.76	106.53	109.40
32	1a	527	7MG	C8-N7-C5	2.73	116.05	108.94
32	2a	527	7MG	C8-N7-C5	2.73	116.04	108.94
32	1a	1518	MA6	C10-N6-C9	-2.73	107.33	116.12
1	1A	1962	5MC	C5-C6-N1	-2.70	119.28	122.19
32	1a	967	5MC	N4-C4-N3	2.68	120.83	117.03
1	1A	2251	OMG	C1'-N9-C4	2.68	131.36	126.64
32	2a	966	M2G	N3-C2-N2	2.67	119.89	117.18
1	1A	2503	2MA	C4-C5-N7	-2.67	106.62	109.40
32	2a	966	M2G	C4-C5-N7	-2.65	106.63	109.40
54	1x	32	5MC	N4-C4-N3	2.60	120.71	117.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	966	M2G	N3-C2-N2	2.57	119.79	117.18
1	1A	1942	5MC	C5-C6-N1	-2.57	119.42	122.19
32	1a	966	M2G	CM2-N2-C2	-2.56	118.85	121.29
32	2a	527	7MG	C5-C4-N9	-2.53	102.90	106.44
32	2a	1407	5MC	N4-C4-N3	2.49	120.56	117.03
32	1a	1407	5MC	N4-C4-N3	2.48	120.54	117.03
54	2x	32	5MC	C5-C6-N1	-2.47	119.54	122.19
32	1a	1404	5MC	N4-C4-N3	2.45	120.49	117.03
1	2A	1920	4OC	N4-C4-N3	2.35	120.20	116.49
54	2x	54	5MU	C5-C6-N1	-2.34	119.67	122.19
1	1A	2251	OMG	N3-C2-N1	-2.32	124.12	127.22
54	1x	32	5MC	C5-C6-N1	-2.32	119.69	122.19
32	2a	967	5MC	N4-C4-N3	2.31	120.30	117.03
54	1x	32	5MC	CM5-C5-C4	-2.31	119.38	121.72
32	1a	516	PSU	O4'-C1'-C2'	2.30	108.39	104.66
1	1A	2251	OMG	C6-C5-C4	-2.29	118.61	120.80
1	2A	1942	5MC	N4-C4-N3	2.28	120.26	117.03
1	1A	2552	2MU	C5-C4-N3	-2.28	118.29	123.31
54	2x	32	5MC	N4-C4-N3	2.28	120.25	117.03
32	2a	1402	4OC	C5-C4-N3	-2.26	119.35	123.16
32	2a	1518	MA6	C10-N6-C9	-2.23	108.94	116.12
32	2a	1519	MA6	N1-C6-N6	2.21	119.38	117.06
32	1a	527	7MG	C2-N3-C4	2.19	119.95	113.89
1	1A	1915	5MU	C5-C6-N1	-2.16	119.87	122.19
32	2a	1519	MA6	C10-N6-C6	-2.15	113.00	119.51
1	1A	2503	2MA	N3-C2-N1	-2.05	121.94	125.72
32	1a	1498	UR3	C3U-N3-C4	2.04	120.82	118.12
32	1a	1404	5MC	C5-C6-N1	-2.04	120.00	122.19
32	1a	1207	2MG	N2-C2-N3	2.04	118.92	116.96
32	2a	527	7MG	CM7-N7-C5	2.04	131.83	124.01
1	1A	2503	2MA	C1'-N9-C4	-2.03	123.08	126.64
32	2a	1402	4OC	N4-C4-N3	2.01	121.50	116.37
32	1a	1207	2MG	N3-C2-N1	-2.00	123.07	126.23

There are no chirality outliers.

All (53) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	1a	1207	2MG	N1-C2-N2-CM2
32	1a	1207	2MG	N3-C2-N2-CM2
32	1a	1518	MA6	C5-C6-N6-C9
32	1a	1518	MA6	C5-C6-N6-C10

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Mol	Chain	Res	Type	Atoms
32	2a	1518	MA6	C5-C6-N6-C9
1	2A	1939	5MU	C2'-C1'-N1-C6
1	2A	1939	5MU	O4'-C1'-N1-C6
32	1a	1402	4OC	N3-C4-N4-CM4
32	1a	1402	4OC	C5-C4-N4-CM4
32	1a	1519	MA6	C5-C6-N6-C10
43	1l	92	0TD	CA-CB-SB-CSB
1	2A	1962	5MC	O4'-C1'-N1-C6
1	2A	1962	5MC	C2'-C1'-N1-C6
1	1A	1962	5MC	O4'-C1'-N1-C6
1	1A	1962	5MC	C2'-C1'-N1-C6
32	2a	1402	4OC	O4'-C4'-C5'-O5'
32	2a	1402	4OC	N3-C4-N4-CM4
32	2a	1402	4OC	C5-C4-N4-CM4
32	2a	1519	MA6	C5-C6-N6-C10
1	1A	1920	4OC	C2'-C1'-N1-C6
32	1a	1519	MA6	O4'-C4'-C5'-O5'
32	2a	527	7MG	C3'-C4'-C5'-O5'
32	2a	1402	4OC	C3'-C4'-C5'-O5'
32	2a	1519	MA6	O4'-C4'-C5'-O5'
32	1a	967	5MC	O4'-C4'-C5'-O5'
1	2A	2552	2MU	O4'-C4'-C5'-O5'
32	1a	1402	4OC	O4'-C4'-C5'-O5'
32	1a	1519	MA6	C3'-C4'-C5'-O5'
32	2a	1519	MA6	C3'-C4'-C5'-O5'
32	1a	1518	MA6	N1-C6-N6-C9
32	2a	1518	MA6	N1-C6-N6-C9
32	1a	1402	4OC	C3'-C4'-C5'-O5'
32	2a	527	7MG	O4'-C4'-C5'-O5'
32	2a	1518	MA6	C5-C6-N6-C10
32	1a	527	7MG	C3'-C4'-C5'-O5'
1	2A	1915	5MU	O4'-C4'-C5'-O5'
32	1a	1400	5MC	O4'-C4'-C5'-O5'
43	1l	92	0TD	CG-CB-SB-CSB
32	1a	967	5MC	C3'-C4'-C5'-O5'
1	2A	1911	PSU	O4'-C4'-C5'-O5'
1	2A	1917	PSU	O4'-C4'-C5'-O5'
1	1A	2503	2MA	O4'-C4'-C5'-O5'
32	1a	966	M2G	C4'-C5'-O5'-P
32	1a	527	7MG	O4'-C4'-C5'-O5'
1	1A	2503	2MA	C4'-C5'-O5'-P
1	2A	2503	2MA	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
32	2a	1519	MA6	C4'-C5'-O5'-P
32	1a	1400	5MC	C3'-C4'-C5'-O5'
1	2A	2552	2MU	C3'-C4'-C5'-O5'
32	2a	1207	2MG	O4'-C4'-C5'-O5'
43	2l	92	0TD	CG-CB-SB-CSB
1	2A	1920	4OC	C3'-C2'-O2'-CM2
1	1A	2503	2MA	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2656 ligands modelled in this entry, 2652 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
59	SF4	1d	302	35	0,12,12	0.00	-	-		
59	SF4	2d	303	35	0,12,12	0.00	-	-		
58	V7A	1a	3213	55	36,38,38	4.06	12 (33%)	40,60,60	2.03	10 (25%)
58	V7A	2a	1817	55	36,38,38	4.08	12 (33%)	40,60,60	2.01	10 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	SF4	1d	302	35	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	SF4	2d	303	35	-	-	0/6/5/5
58	V7A	1a	3213	55	-	4/13/72/72	0/4/4/4
58	V7A	2a	1817	55	-	3/13/72/72	0/4/4/4

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	2a	1817	V7A	CAM-CAL	-13.28	1.40	1.52
58	1a	3213	V7A	CAM-CAL	-12.63	1.41	1.52
58	1a	3213	V7A	CAM-CAP	-11.44	1.39	1.55
58	2a	1817	V7A	CAM-CAP	-10.90	1.40	1.55
58	1a	3213	V7A	CAJ-CAI	-10.84	1.40	1.51
58	2a	1817	V7A	CAJ-CAI	-10.19	1.40	1.51
58	2a	1817	V7A	CAG-CAF	-7.31	1.39	1.51
58	1a	3213	V7A	CAG-CAF	-7.07	1.40	1.51
58	2a	1817	V7A	CAS-CAA	-7.00	1.39	1.51
58	1a	3213	V7A	CAS-CAA	-6.49	1.40	1.51
58	2a	1817	V7A	CAO-CAR	-5.72	1.40	1.51
58	1a	3213	V7A	CAO-CAR	-5.28	1.41	1.51
58	2a	1817	V7A	CAQ-CBC	-3.85	1.39	1.47
58	1a	3213	V7A	CAQ-CBC	-3.67	1.40	1.47
58	2a	1817	V7A	CAI-CAL	3.39	1.40	1.36
58	1a	3213	V7A	CAI-CAL	3.19	1.40	1.36
58	1a	3213	V7A	CAI-CAH	-3.12	1.39	1.47
58	2a	1817	V7A	CAI-CAH	-3.05	1.39	1.47
58	2a	1817	V7A	CAE-CAH	-2.87	1.39	1.46
58	1a	3213	V7A	CAQ-CAP	-2.80	1.38	1.45
58	1a	3213	V7A	CAE-CAH	-2.76	1.39	1.46
58	2a	1817	V7A	CAQ-CAP	-2.34	1.39	1.45
58	2a	1817	V7A	CAK-CAN	-2.29	1.49	1.53
58	1a	3213	V7A	OAU-NAT	2.15	1.49	1.44

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	1a	3213	V7A	CAV-OAU-NAT	5.69	120.33	108.11
58	1a	3213	V7A	OAZ-CAL-CAI	-5.30	116.65	123.90
58	2a	1817	V7A	CAV-OAU-NAT	5.19	119.24	108.11
58	2a	1817	V7A	CAJ-CAK-CAN	-4.67	102.28	110.49
58	2a	1817	V7A	OAZ-CAL-CAI	-4.50	117.74	123.90
58	1a	3213	V7A	OBI-CAR-CAQ	-3.85	116.20	122.96
58	2a	1817	V7A	CBG-NBF-CAO	-3.67	105.47	114.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	1a	3213	V7A	CAJ-CAK-CAN	-3.65	104.06	110.49
58	1a	3213	V7A	CBG-NBF-CAO	-3.65	105.53	114.09
58	2a	1817	V7A	OBI-CAR-CAQ	-3.45	116.90	122.96
58	1a	3213	V7A	CAM-CAP-CAQ	3.29	120.97	115.75
58	1a	3213	V7A	OAZ-CAL-CAM	3.06	117.80	113.37
58	2a	1817	V7A	OAZ-CAL-CAM	2.85	117.50	113.37
58	2a	1817	V7A	CAM-CAP-CAQ	2.70	120.05	115.75
58	2a	1817	V7A	OAX-CAD-CAE	-2.58	116.32	121.14
58	1a	3213	V7A	OAX-CAD-CAE	-2.49	116.47	121.14
58	1a	3213	V7A	CAM-CAL-CAI	2.39	125.49	123.06
58	1a	3213	V7A	OBB-CAP-CAQ	-2.33	118.66	123.55
58	2a	1817	V7A	OBA-CAM-CAN	-2.23	107.35	110.09
58	2a	1817	V7A	CAP-CAM-CAL	2.11	112.36	109.88

There are no chirality outliers.

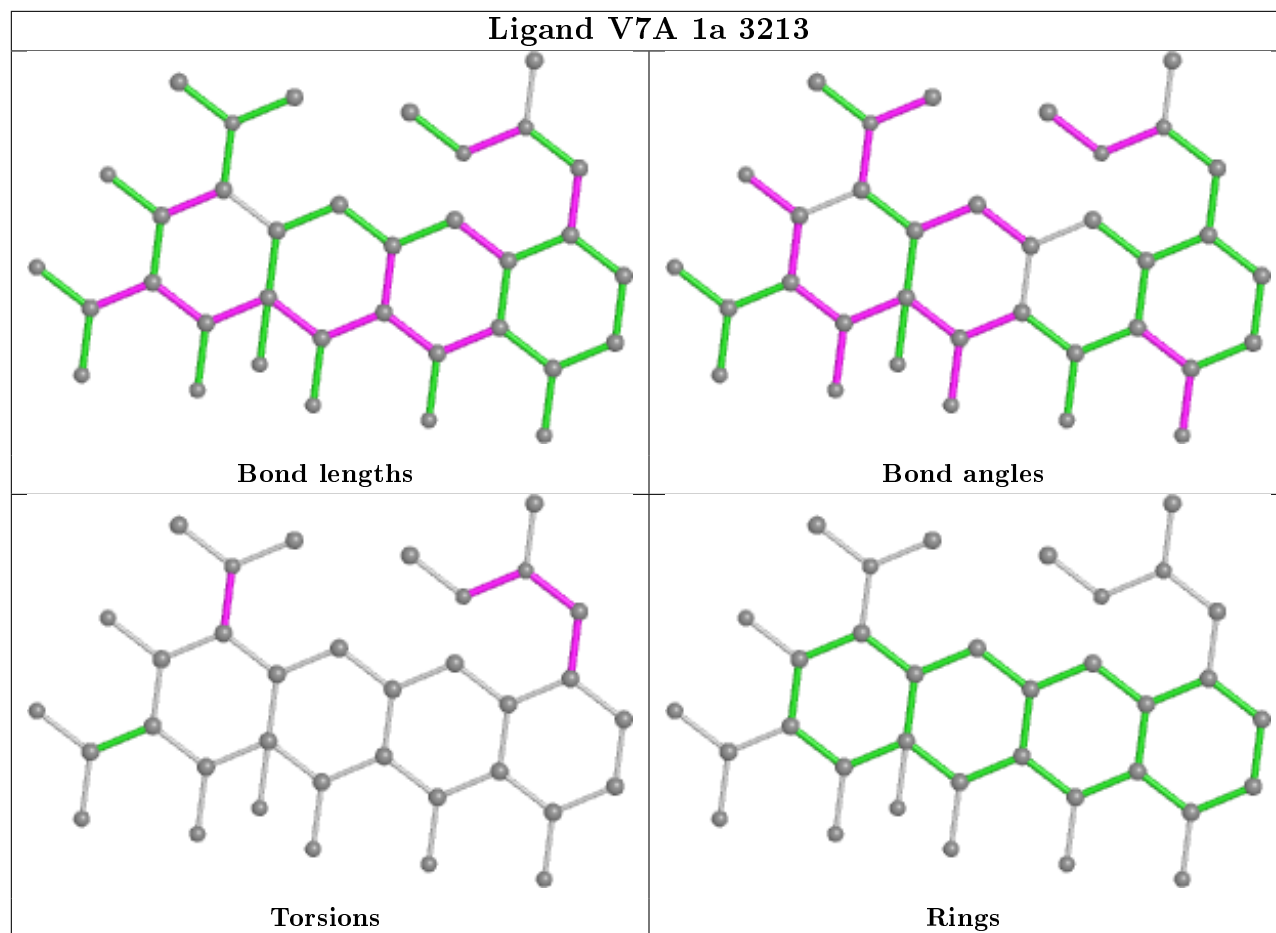
All (7) torsion outliers are listed below:

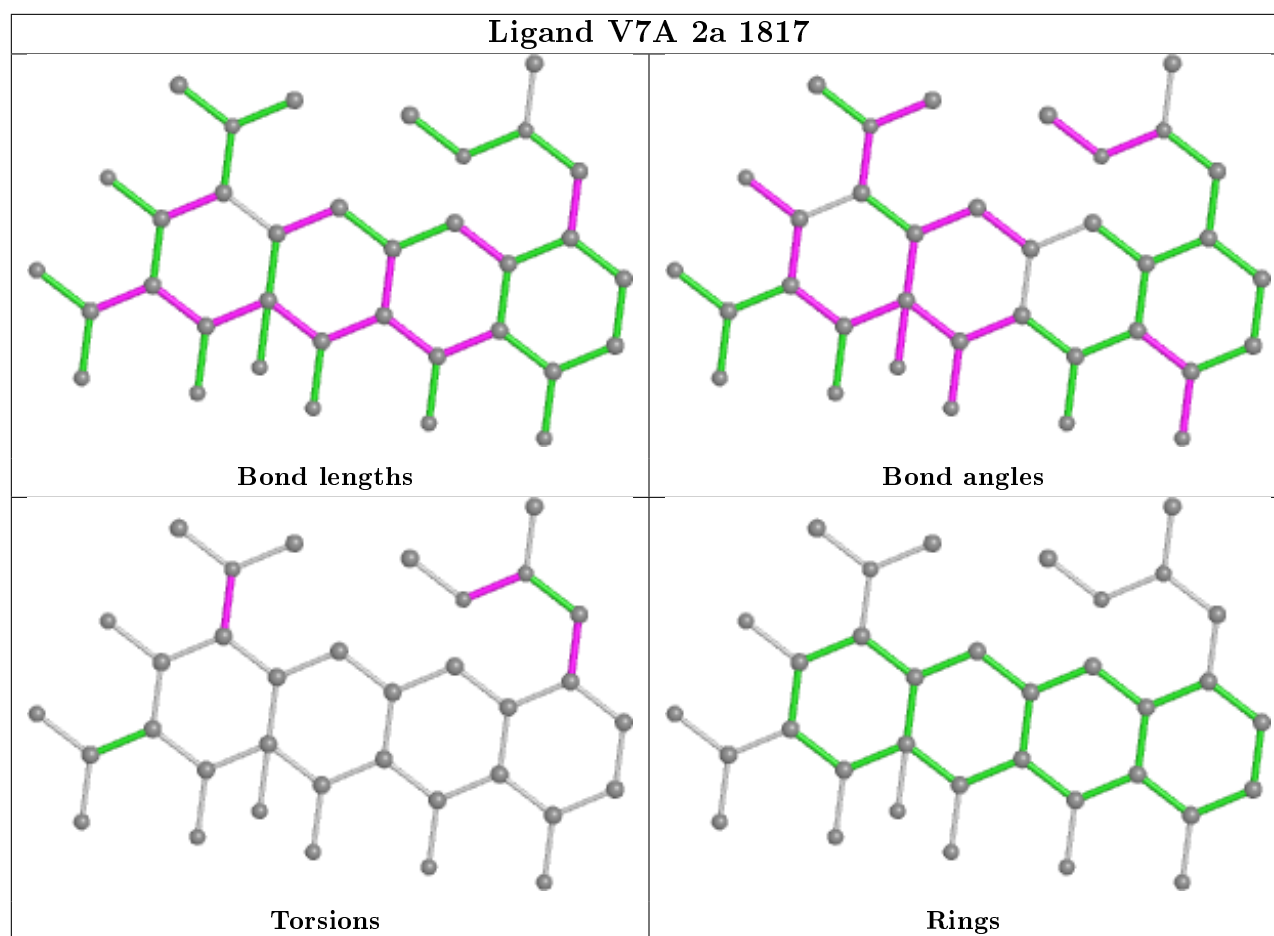
Mol	Chain	Res	Type	Atoms
58	1a	3213	V7A	CAN-CAO-NBF-CBH
58	1a	3213	V7A	CAW-NAT-OAU-CAV
58	2a	1817	V7A	CAN-CAO-NBF-CBH
58	2a	1817	V7A	CAW-NAT-OAU-CAV
58	1a	3213	V7A	CAA-CAS-NAT-CAW
58	2a	1817	V7A	CAF-CAA-CAS-NAT
58	1a	3213	V7A	CAF-CAA-CAS-NAT

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	1A	2860/2915 (98%)	0.06	13 (0%) 91 75	11, 36, 96, 112	0
1	2A	2789/2915 (95%)	0.08	12 (0%) 92 79	21, 49, 90, 116	0
2	1B	120/121 (99%)	-0.24	0 100 100	27, 51, 64, 85	0
2	2B	120/121 (99%)	-0.13	0 100 100	49, 68, 83, 95	0
3	1D	275/276 (99%)	0.14	0 100 100	14, 31, 47, 61	0
3	2D	275/276 (99%)	0.30	4 (1%) 73 46	22, 42, 58, 84	0
4	1E	204/206 (99%)	0.03	2 (0%) 82 59	18, 43, 63, 78	0
4	2E	204/206 (99%)	0.23	8 (3%) 39 15	24, 50, 66, 77	0
5	1F	203/210 (96%)	-0.08	1 (0%) 91 75	16, 40, 64, 82	0
5	2F	203/210 (96%)	0.05	3 (1%) 73 46	27, 57, 73, 79	0
6	1G	181/182 (99%)	-0.12	1 (0%) 89 72	37, 53, 70, 83	0
6	2G	181/182 (99%)	0.64	23 (12%) 3 1	53, 68, 82, 88	0
7	1H	174/180 (96%)	-0.15	0 100 100	33, 51, 64, 71	0
7	2H	174/180 (96%)	0.78	31 (17%) 1 0	50, 75, 84, 88	0
8	1I	146/148 (98%)	-0.34	0 100 100	40, 64, 75, 81	0
8	2I	146/148 (98%)	-0.14	2 (1%) 75 49	42, 68, 80, 87	0
9	1N	140/140 (100%)	0.01	0 100 100	22, 42, 60, 68	0
9	2N	140/140 (100%)	0.51	12 (8%) 10 3	35, 58, 75, 82	0
10	1O	122/122 (100%)	0.22	1 (0%) 86 65	23, 37, 55, 65	0
10	2O	122/122 (100%)	-0.00	2 (1%) 72 44	30, 44, 60, 71	0
11	1P	149/150 (99%)	0.24	8 (5%) 25 9	17, 43, 65, 72	0
11	2P	149/150 (99%)	0.56	18 (12%) 4 1	30, 59, 74, 85	0
12	1Q	141/141 (100%)	0.17	1 (0%) 87 69	25, 41, 53, 61	0
12	2Q	141/141 (100%)	0.46	3 (2%) 63 34	38, 52, 65, 70	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	1R	118/118 (100%)	0.15	1 (0%) 86 65	22, 39, 53, 62	0
13	2R	118/118 (100%)	0.17	2 (1%) 70 41	31, 44, 57, 67	0
14	1S	110/112 (98%)	-0.17	1 (0%) 84 63	33, 45, 57, 65	0
14	2S	110/112 (98%)	-0.07	0 100 100	48, 60, 71, 79	0
15	1T	131/146 (89%)	-0.01	0 100 100	27, 48, 67, 79	0
15	2T	131/146 (89%)	-0.01	1 (0%) 86 65	36, 49, 67, 79	0
16	1U	116/118 (98%)	0.19	0 100 100	22, 37, 56, 63	0
16	2U	116/118 (98%)	0.44	7 (6%) 21 7	37, 54, 66, 82	0
17	1V	101/101 (100%)	-0.11	0 100 100	22, 48, 61, 69	0
17	2V	101/101 (100%)	0.07	8 (7%) 12 4	39, 63, 73, 80	0
18	1W	112/113 (99%)	0.42	3 (2%) 54 26	22, 37, 56, 88	0
18	2W	112/113 (99%)	0.35	1 (0%) 84 63	29, 44, 60, 78	0
19	1X	95/96 (98%)	0.11	2 (2%) 63 34	21, 34, 50, 73	0
19	2X	95/96 (98%)	0.33	2 (2%) 63 34	34, 50, 65, 74	0
20	1Y	107/110 (97%)	-0.16	0 100 100	31, 47, 64, 71	0
20	2Y	107/110 (97%)	0.49	4 (3%) 41 17	49, 64, 77, 84	0
21	1Z	154/206 (74%)	-0.29	0 100 100	38, 56, 70, 85	0
21	2Z	160/206 (77%)	-0.25	1 (0%) 89 72	50, 66, 85, 96	0
22	10	83/85 (97%)	0.72	7 (8%) 11 3	26, 34, 68, 92	0
22	20	83/85 (97%)	1.32	17 (20%) 1 0	37, 51, 73, 87	0
23	11	97/98 (98%)	0.68	6 (6%) 20 7	17, 39, 63, 67	0
23	21	97/98 (98%)	0.84	9 (9%) 8 3	27, 50, 67, 75	0
24	12	70/72 (97%)	-0.30	0 100 100	26, 41, 56, 62	0
24	22	70/72 (97%)	-0.13	0 100 100	43, 59, 71, 77	0
25	13	59/60 (98%)	0.13	0 100 100	27, 39, 59, 63	0
25	23	59/60 (98%)	1.26	14 (23%) 0 0	47, 56, 72, 75	0
26	14	69/71 (97%)	-0.23	1 (1%) 75 49	53, 74, 87, 101	0
26	24	69/71 (97%)	0.27	7 (10%) 7 2	61, 82, 95, 102	0
27	15	59/60 (98%)	0.44	3 (5%) 28 10	23, 44, 75, 81	0
27	25	59/60 (98%)	0.27	2 (3%) 45 19	28, 48, 77, 89	0
28	16	53/54 (98%)	-0.30	0 100 100	30, 39, 51, 56	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	26	53/54 (98%)	-0.16	0 100 100	40, 48, 59, 61	0
29	17	48/49 (97%)	0.74	5 (10%) 6 2	16, 24, 49, 53	0
29	27	48/49 (97%)	0.65	3 (6%) 20 6	26, 33, 51, 67	0
30	18	64/65 (98%)	0.60	5 (7%) 13 4	23, 30, 39, 58	0
30	28	64/65 (98%)	1.58	20 (31%) 0 0	35, 45, 56, 73	0
31	19	37/37 (100%)	0.21	0 100 100	31, 45, 54, 65	0
31	29	37/37 (100%)	1.80	14 (37%) 0 0	46, 61, 74, 76	0
32	1a	1488/1521 (97%)	0.08	19 (1%) 77 51	27, 65, 93, 112	0
32	2a	1491/1521 (98%)	0.13	30 (2%) 65 36	43, 69, 93, 110	0
33	1b	231/256 (90%)	-0.21	1 (0%) 92 79	55, 73, 86, 101	0
33	2b	231/256 (90%)	-0.39	1 (0%) 92 79	61, 79, 86, 93	0
34	1c	206/239 (86%)	0.22	6 (2%) 51 23	51, 66, 79, 90	0
34	2c	206/239 (86%)	0.24	14 (6%) 17 5	60, 76, 84, 91	0
35	1d	208/209 (99%)	0.66	20 (9%) 8 2	49, 67, 79, 85	0
35	2d	208/209 (99%)	0.60	19 (9%) 9 3	51, 66, 75, 82	0
36	1e	148/162 (91%)	0.64	15 (10%) 7 2	43, 57, 68, 71	0
36	2e	148/162 (91%)	0.67	15 (10%) 7 2	47, 67, 77, 81	0
37	1f	100/101 (99%)	-0.16	0 100 100	42, 61, 71, 75	0
37	2f	100/101 (99%)	-0.39	0 100 100	53, 66, 74, 80	0
38	1g	155/156 (99%)	0.29	12 (7%) 13 4	53, 66, 83, 104	0
38	2g	155/156 (99%)	0.72	27 (17%) 1 0	63, 73, 83, 91	0
39	1h	137/138 (99%)	0.13	2 (1%) 73 46	50, 61, 71, 74	0
39	2h	137/138 (99%)	0.97	25 (18%) 1 0	54, 69, 77, 84	0
40	1i	127/128 (99%)	1.00	32 (25%) 0 0	54, 69, 80, 85	0
40	2i	127/128 (99%)	2.14	57 (44%) 0 0	66, 80, 88, 94	0
41	1j	97/105 (92%)	0.62	19 (19%) 1 0	53, 68, 81, 85	0
41	2j	96/105 (91%)	0.89	21 (21%) 0 0	60, 77, 87, 97	0
42	1k	114/129 (88%)	0.16	1 (0%) 84 63	37, 60, 75, 79	0
42	2k	114/129 (88%)	0.23	4 (3%) 44 18	51, 65, 74, 81	0
43	1l	121/132 (91%)	0.39	14 (11%) 4 1	42, 52, 64, 73	0
43	2l	121/132 (91%)	0.50	12 (9%) 7 2	45, 58, 68, 78	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	1m	122/126 (96%)	0.16	11 (9%) 9 3	55, 70, 79, 84	0
44	2m	121/126 (96%)	0.59	17 (14%) 2 1	62, 75, 85, 92	0
45	1n	60/61 (98%)	1.85	28 (46%) 0 0	57, 66, 75, 79	0
45	2n	60/61 (98%)	2.01	28 (46%) 0 0	66, 75, 83, 88	0
46	1o	88/89 (98%)	-0.06	0 100 100	43, 58, 70, 82	0
46	2o	88/89 (98%)	-0.20	2 (2%) 60 31	55, 66, 75, 80	0
47	1p	82/88 (93%)	0.94	16 (19%) 1 0	50, 68, 80, 86	0
47	2p	82/88 (93%)	0.25	2 (2%) 59 30	51, 64, 71, 81	0
48	1q	99/105 (94%)	0.95	16 (16%) 1 0	47, 61, 71, 74	0
48	2q	99/105 (94%)	0.90	16 (16%) 1 0	50, 62, 72, 75	0
49	1r	68/88 (77%)	0.03	1 (1%) 73 46	44, 62, 72, 83	0
49	2r	68/88 (77%)	0.03	0 100 100	51, 67, 76, 80	0
50	1s	83/93 (89%)	0.06	2 (2%) 59 30	59, 70, 80, 91	0
50	2s	83/93 (89%)	0.59	11 (13%) 3 1	67, 77, 86, 90	0
51	1t	96/106 (90%)	0.82	17 (17%) 1 0	53, 67, 78, 81	0
51	2t	96/106 (90%)	0.49	7 (7%) 15 4	45, 62, 75, 83	0
52	1u	23/27 (85%)	0.97	4 (17%) 1 0	58, 65, 72, 79	0
52	2u	23/27 (85%)	1.62	6 (26%) 0 0	65, 71, 78, 79	0
53	1v	10/24 (41%)	0.98	2 (20%) 1 0	46, 82, 94, 95	0
53	2v	6/24 (25%)	0.72	2 (33%) 0 0	56, 66, 85, 85	0
54	1x	72/77 (93%)	-0.13	1 (1%) 75 49	34, 52, 70, 87	0
54	2x	72/77 (93%)	-0.16	1 (1%) 75 49	44, 68, 80, 93	0
All	All	20598/21444 (96%)	0.21	847 (4%) 37 14	11, 57, 84, 116	0

All (847) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
22	10	7	LEU	11.9
22	10	6	GLY	10.1
22	20	3	HIS	8.8
44	2m	120	LYS	8.2
44	2m	122	LYS	8.2
44	2m	121	LYS	8.0
32	2a	1532	U	7.2

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Mol	Chain	Res	Type	RSRZ
40	2i	14	VAL	7.1
40	2i	124	GLN	7.0
40	2i	117	HIS	6.9
22	20	7	LEU	6.9
44	2m	6	GLY	6.9
44	2m	123	ALA	6.8
22	10	4	LYS	6.5
40	2i	109	VAL	6.5
40	2i	115	GLY	6.5
41	2j	62	HIS	6.4
44	1m	123	ALA	6.4
40	2i	106	ALA	6.4
40	2i	125	TYR	6.4
45	2n	2	ALA	6.3
52	2u	14	TRP	6.3
22	20	6	GLY	6.1
22	20	5	LYS	6.1
22	20	2	ALA	6.0
51	1t	20	LEU	6.0
3	2D	276	LYS	5.9
22	20	4	LYS	5.9
39	2h	135	CYS	5.8
48	2q	36	ILE	5.8
40	2i	116	LYS	5.6
23	21	2	SER	5.6
51	1t	18	GLN	5.6
40	2i	122	ALA	5.6
22	10	3	HIS	5.5
36	2e	22	GLY	5.5
45	2n	25	VAL	5.5
38	2g	80	VAL	5.5
22	10	5	LYS	5.4
41	2j	46	ARG	5.4
45	1n	11	LYS	5.4
36	2e	13	ILE	5.4
38	1g	82	GLY	5.4
29	17	46	VAL	5.3
7	2H	103	LEU	5.2
41	1j	48	THR	5.0
40	1i	117	HIS	5.0
40	1i	6	GLY	5.0
40	1i	114	TYR	4.9

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Mol	Chain	Res	Type	RSRZ
40	2i	126	SER	4.9
22	10	2	ALA	4.9
40	2i	36	TYR	4.9
41	2j	58	ASP	4.8
39	2h	134	ILE	4.8
40	2i	110	GLU	4.8
22	10	8	GLY	4.8
36	2e	12	LEU	4.8
40	1i	115	GLY	4.8
41	1j	58	ASP	4.8
11	2P	68	GLN	4.7
41	1j	49	VAL	4.7
7	2H	107	VAL	4.7
40	2i	105	ASP	4.7
38	2g	83	ALA	4.7
45	2n	61	TRP	4.7
40	1i	109	VAL	4.7
38	2g	81	GLY	4.6
41	2j	55	LYS	4.6
38	2g	84	ASN	4.5
30	28	65	GLU	4.5
45	2n	37	PHE	4.5
48	1q	35	VAL	4.5
1	2A	2143	C	4.5
41	2j	48	THR	4.5
52	2u	16	GLY	4.5
40	2i	63	ILE	4.4
30	28	62	LEU	4.4
45	1n	34	TYR	4.4
31	29	37	GLY	4.4
1	2A	2146	C	4.4
40	2i	70	LYS	4.4
38	1g	84	ASN	4.4
31	29	15	LYS	4.4
32	1a	1257	U	4.4
40	2i	127	LYS	4.4
40	2i	30	GLY	4.4
29	27	48	LYS	4.4
29	17	47	ARG	4.3
39	2h	91	ARG	4.3
35	1d	4	TYR	4.3
22	20	8	GLY	4.3

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Mol	Chain	Res	Type	RSRZ
7	2H	123	PHE	4.3
22	20	9	SER	4.2
1	1A	2145	C	4.2
32	1a	1367	C	4.2
40	2i	7	THR	4.2
1	2A	2147	G	4.2
38	1g	80	VAL	4.2
41	1j	60	ARG	4.2
40	2i	28	VAL	4.1
40	1i	126	SER	4.1
40	2i	123	PRO	4.1
40	2i	33	PHE	4.1
44	1m	87	TYR	4.1
40	2i	66	ARG	4.1
1	1A	2132	U	4.0
44	2m	119	GLY	4.0
1	2A	2133	G	4.0
32	1a	1368	G	4.0
39	2h	111	ILE	4.0
45	1n	22	THR	4.0
40	2i	128	ARG	4.0
44	2m	101	GLN	4.0
51	1t	69	GLY	4.0
38	1g	85	TYR	4.0
25	23	26	LEU	4.0
38	2g	33	ASP	4.0
34	2c	163	ALA	4.0
22	20	76	GLY	3.9
9	2N	44	PRO	3.9
51	2t	80	ARG	3.9
41	1j	47	PHE	3.9
39	2h	112	LEU	3.9
5	2F	82	ILE	3.9
48	1q	28	PRO	3.9
6	2G	138	GLN	3.9
7	2H	101	ARG	3.9
48	2q	30	PRO	3.9
52	1u	14	TRP	3.9
51	1t	19	SER	3.9
48	2q	32	TYR	3.9
45	2n	42	ILE	3.9
44	2m	90	LEU	3.9

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Mol	Chain	Res	Type	RSRZ
6	2G	157	ILE	3.9
23	21	62	VAL	3.9
40	2i	29	ASN	3.9
40	2i	119	ALA	3.9
45	1n	25	VAL	3.8
41	2j	63	PHE	3.8
4	2E	116	VAL	3.8
6	2G	161	THR	3.8
41	2j	59	SER	3.8
48	2q	29	HIS	3.8
30	28	22	VAL	3.8
6	2G	41	GLN	3.8
23	11	2	SER	3.8
45	1n	29	ARG	3.8
39	2h	133	LEU	3.8
23	11	98	LEU	3.7
31	29	17	ILE	3.7
42	2k	126	ARG	3.7
45	2n	39	LEU	3.7
11	2P	45	LEU	3.7
36	1e	20	GLN	3.7
41	1j	50	ILE	3.7
40	1i	108	VAL	3.7
38	2g	2	ALA	3.7
48	1q	26	GLN	3.7
44	1m	105	THR	3.7
31	29	3	VAL	3.7
40	2i	65	VAL	3.7
41	2j	47	PHE	3.7
38	2g	37	ASN	3.7
45	1n	32	SER	3.6
26	24	51	ASP	3.6
40	2i	120	ARG	3.6
41	2j	45	ARG	3.6
52	2u	13	ILE	3.6
7	2H	84	SER	3.6
30	28	64	TYR	3.6
39	2h	86	ILE	3.6
40	2i	83	ARG	3.6
45	1n	59	ALA	3.6
31	29	18	ARG	3.6
38	2g	82	GLY	3.6

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Mol	Chain	Res	Type	RSRZ
41	1j	62	HIS	3.6
40	2i	64	THR	3.6
30	28	61	LEU	3.6
38	2g	78	ARG	3.5
30	28	59	LYS	3.5
50	2s	49	ILE	3.5
43	2l	15	ARG	3.5
48	1q	36	ILE	3.5
48	1q	29	HIS	3.5
6	2G	39	ILE	3.5
48	2q	33	GLY	3.5
32	2a	1202	G	3.5
11	2P	30	THR	3.5
12	1Q	33	GLY	3.5
40	1i	118	LYS	3.5
29	17	45	ALA	3.5
44	2m	102	ARG	3.5
40	1i	125	TYR	3.5
38	2g	154	TYR	3.5
30	18	52	LYS	3.5
9	2N	76	SER	3.4
48	2q	34	LYS	3.4
45	2n	41	ARG	3.4
51	1t	21	LYS	3.4
32	2a	1286	A	3.4
6	2G	158	ALA	3.4
35	2d	164	ALA	3.4
1	2A	2145	C	3.4
32	1a	1532	U	3.4
52	1u	16	GLY	3.4
11	2P	35	HIS	3.4
40	1i	122	ALA	3.4
32	1a	975	A	3.4
32	1a	1365	G	3.4
47	1p	25	ARG	3.4
47	1p	1	MET	3.4
9	2N	69	GLN	3.4
43	2l	64	TYR	3.4
1	2A	1026	U	3.4
39	2h	93	VAL	3.4
26	24	49	PHE	3.4
45	2n	36	PHE	3.4

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Mol	Chain	Res	Type	RSRZ
3	2D	5	LYS	3.4
44	1m	122	LYS	3.4
7	2H	88	LEU	3.4
21	2Z	143	GLY	3.4
43	2l	19	ARG	3.4
43	1l	28	LYS	3.3
1	1A	2146	C	3.3
35	1d	126	ILE	3.3
45	1n	49	HIS	3.3
51	1t	17	ARG	3.3
7	2H	128	PRO	3.3
40	1i	123	PRO	3.3
35	2d	134	ASP	3.3
44	2m	104	ARG	3.3
51	2t	9	ASN	3.3
12	2Q	80	GLU	3.3
43	1l	18	VAL	3.3
11	2P	109	GLY	3.3
36	1e	100	VAL	3.3
40	2i	114	TYR	3.3
40	2i	47	LEU	3.3
29	17	48	LYS	3.3
43	2l	14	GLY	3.3
34	1c	201	TYR	3.3
41	2j	50	ILE	3.2
38	1g	83	ALA	3.2
35	1d	110	PHE	3.2
45	2n	18	VAL	3.2
40	1i	111	ARG	3.2
41	1j	61	GLU	3.2
32	1a	1366	C	3.2
41	2j	49	VAL	3.2
11	2P	36	LYS	3.2
48	2q	24	GLU	3.2
39	2h	131	GLY	3.2
43	1l	19	ARG	3.2
40	2i	41	VAL	3.2
32	1a	1531	A	3.2
40	2i	111	ARG	3.2
35	1d	120	LEU	3.2
35	2d	70	ILE	3.2
30	28	63	PRO	3.2

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Mol	Chain	Res	Type	RSRZ
30	28	3	LYS	3.2
41	2j	60	ARG	3.2
39	2h	82	HIS	3.2
25	23	12	PRO	3.2
38	2g	79	ARG	3.2
25	23	29	ARG	3.2
34	2c	159	GLY	3.2
41	1j	57	LYS	3.2
9	2N	84	LYS	3.1
23	21	98	LEU	3.1
38	1g	78	ARG	3.1
51	1t	30	LYS	3.1
36	2e	125	SER	3.1
40	2i	69	GLY	3.1
1	2A	2144	U	3.1
25	23	48	GLU	3.1
26	24	56	VAL	3.1
40	1i	110	GLU	3.1
39	2h	92	ARG	3.1
40	2i	10	ARG	3.1
44	2m	99	ARG	3.1
38	2g	36	LYS	3.1
40	1i	37	PHE	3.1
45	1n	51	GLY	3.1
45	1n	30	ALA	3.1
41	1j	8	LEU	3.1
40	2i	37	PHE	3.1
43	2l	8	ASN	3.1
17	2V	81	TYR	3.1
17	2V	71	LEU	3.1
7	2H	114	VAL	3.1
40	2i	121	ARG	3.1
32	2a	1369	C	3.1
1	1A	2142	C	3.0
7	2H	151	ILE	3.0
36	1e	82	VAL	3.0
38	2g	4	ARG	3.0
39	2h	83	ILE	3.0
40	1i	66	ARG	3.0
40	2i	71	SER	3.0
41	1j	46	ARG	3.0
1	1A	2144	U	3.0

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Mol	Chain	Res	Type	RSRZ
7	2H	94	TYR	3.0
40	1i	8	GLY	3.0
43	1l	5	PRO	3.0
38	1g	156	TRP	3.0
48	2q	37	LYS	3.0
32	2a	1531	A	3.0
31	29	24	TYR	3.0
35	2d	118	ARG	3.0
40	2i	62	TYR	3.0
36	1e	119	LEU	3.0
45	1n	61	TRP	3.0
1	2A	229	A	3.0
38	1g	59	LEU	3.0
6	2G	90	LEU	3.0
36	1e	23	GLY	3.0
7	2H	121	ILE	3.0
12	2Q	104	PHE	3.0
45	2n	7	ILE	3.0
7	2H	133	VAL	3.0
43	1l	91	LYS	3.0
47	1p	35	LYS	3.0
38	1g	120	ILE	3.0
45	1n	33	VAL	3.0
30	18	56	GLU	3.0
45	2n	34	TYR	2.9
36	2e	45	PHE	2.9
39	2h	113	SER	2.9
10	2O	1	MET	2.9
34	2c	199	LYS	2.9
31	29	12	ASP	2.9
6	2G	137	GLU	2.9
40	1i	113	LYS	2.9
7	2H	144	VAL	2.9
35	1d	21	LEU	2.9
41	1j	64	GLU	2.9
7	2H	115	VAL	2.9
43	2l	18	VAL	2.9
39	2h	85	ARG	2.9
44	2m	105	THR	2.9
43	1l	64	TYR	2.9
25	23	51	ALA	2.9
45	2n	59	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
32	1a	1196	U	2.9
32	2a	1363(A)	A	2.9
4	2E	153	GLY	2.9
45	2n	35	ARG	2.9
30	18	53	PRO	2.9
40	1i	124	GLN	2.9
1	2A	2118	U	2.8
35	1d	2	GLY	2.8
54	2x	76	A	2.8
17	2V	79	VAL	2.8
48	2q	28	PRO	2.8
43	2l	89	ARG	2.8
44	1m	121	LYS	2.8
30	28	23	VAL	2.8
43	1l	94	PRO	2.8
45	1n	18	VAL	2.8
44	1m	102	ARG	2.8
6	2G	89	GLY	2.8
41	2j	40	LEU	2.8
31	29	36	GLN	2.8
34	1c	200	ALA	2.8
32	2a	1511	G	2.8
45	1n	36	PHE	2.8
44	2m	97	PRO	2.8
39	2h	94	TYR	2.8
6	2G	159	VAL	2.8
26	24	42	PHE	2.8
35	1d	208	SER	2.8
16	2U	20	LEU	2.8
40	2i	113	LYS	2.8
27	15	60	VAL	2.8
45	2n	17	LYS	2.8
40	1i	106	ALA	2.8
40	1i	105	ASP	2.8
40	2i	18	PHE	2.8
48	1q	24	GLU	2.8
35	1d	3	ARG	2.8
41	1j	63	PHE	2.8
48	1q	34	LYS	2.8
33	2b	214	ILE	2.7
6	2G	29	TRP	2.7
18	1W	112	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
31	29	35	ARG	2.7
54	1x	76	A	2.7
35	1d	148	VAL	2.7
11	2P	38	GLN	2.7
20	2Y	1	MET	2.7
40	1i	116	LYS	2.7
39	2h	138	TRP	2.7
44	2m	103	THR	2.7
35	2d	69	GLY	2.7
35	1d	115	ARG	2.7
16	2U	56	ASP	2.7
22	20	42	GLY	2.7
31	29	16	VAL	2.7
36	1e	21	ALA	2.7
7	2H	169	VAL	2.7
40	1i	15	ALA	2.7
50	2s	79	THR	2.7
47	1p	19	ILE	2.7
41	1j	43	ARG	2.7
41	2j	8	LEU	2.7
35	1d	165	MET	2.7
36	2e	14	ARG	2.7
51	2t	30	LYS	2.7
6	2G	165	THR	2.7
11	2P	39	LYS	2.7
35	2d	49	ARG	2.7
34	2c	160	ALA	2.7
6	2G	75	LYS	2.7
19	2X	33	LYS	2.7
30	28	26	LYS	2.7
22	20	55	ARG	2.7
38	2g	32	ARG	2.7
53	1v	13	A	2.7
29	27	47	ARG	2.6
36	1e	24	ARG	2.6
47	1p	6	LEU	2.6
5	2F	79	GLY	2.6
26	14	17	GLY	2.6
40	2i	26	VAL	2.6
11	2P	18	ARG	2.6
11	2P	47	ASP	2.6
45	1n	37	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
11	1P	28	GLY	2.6
36	2e	90	VAL	2.6
45	2n	38	GLY	2.6
41	2j	96	ILE	2.6
32	2a	1492	A	2.6
32	2a	1249	C	2.6
9	2N	104	LYS	2.6
1	1A	1026	U	2.6
30	28	15	LYS	2.6
47	1p	14	ASN	2.6
46	2o	50	HIS	2.6
51	1t	16	HIS	2.6
30	28	5	LYS	2.6
36	2e	88	LYS	2.6
45	1n	50	LYS	2.6
35	1d	135	LEU	2.6
45	1n	23	ARG	2.6
30	28	10	ALA	2.6
41	2j	44	VAL	2.6
45	2n	11	LYS	2.6
52	2u	22	ARG	2.6
34	1c	39	ILE	2.6
38	2g	150	ALA	2.6
50	2s	52	TYR	2.6
7	2H	106	THR	2.6
25	23	52	HIS	2.6
35	2d	5	ILE	2.6
40	1i	63	ILE	2.6
52	1u	17	THR	2.6
40	2i	5	TYR	2.5
1	1A	2141	G	2.5
35	1d	11	LEU	2.5
36	1e	128	PRO	2.5
4	1E	151	TYR	2.5
51	1t	23	ARG	2.5
4	2E	124	GLY	2.5
11	2P	34	GLY	2.5
50	2s	82	GLY	2.5
7	2H	105	LEU	2.5
30	28	21	LYS	2.5
11	1P	50	ARG	2.5
34	2c	33	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
45	2n	44	LEU	2.5
23	21	53	VAL	2.5
48	2q	35	VAL	2.5
16	2U	17	ILE	2.5
20	2Y	5	MET	2.5
40	2i	42	ARG	2.5
41	2j	54	PHE	2.5
42	2k	115	PRO	2.5
38	2g	85	TYR	2.5
39	2h	124	ALA	2.5
16	2U	16	LYS	2.5
38	1g	79	ARG	2.5
1	1A	2133	G	2.5
36	1e	89	ILE	2.5
22	20	68	GLU	2.5
39	2h	136	GLU	2.5
50	2s	35	SER	2.5
38	2g	23	VAL	2.5
29	27	1	MET	2.5
47	1p	7	ALA	2.5
35	2d	135	LEU	2.5
6	2G	93	THR	2.5
48	2q	27	PHE	2.5
39	2h	99	GLU	2.5
16	2U	18	LEU	2.5
23	21	63	ALA	2.5
51	1t	15	ARG	2.5
45	2n	22	THR	2.5
23	11	26	ARG	2.5
45	1n	2	ALA	2.5
50	2s	41	VAL	2.5
6	2G	182	LYS	2.5
11	1P	30	THR	2.5
36	1e	18	ARG	2.5
50	1s	78	ARG	2.5
51	2t	25	ARG	2.5
6	2G	160	VAL	2.5
35	2d	133	VAL	2.5
39	2h	95	VAL	2.5
45	1n	16	PHE	2.5
43	1l	89	ARG	2.5
9	2N	75	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
17	2V	80	GLN	2.4
17	2V	76	LYS	2.4
32	1a	1529	G	2.4
32	2a	1373	G	2.4
40	2i	8	GLY	2.4
32	2a	1364	U	2.4
38	2g	10	ARG	2.4
36	1e	129	ILE	2.4
39	2h	2	LEU	2.4
31	29	19	ARG	2.4
47	1p	18	ARG	2.4
18	2W	6	ILE	2.4
32	1a	1353	G	2.4
6	2G	136	ARG	2.4
41	1j	66	ARG	2.4
40	2i	13	ALA	2.4
30	28	58	ILE	2.4
45	1n	13	THR	2.4
45	2n	29	ARG	2.4
51	1t	72	LEU	2.4
32	2a	973	G	2.4
42	2k	25	TYR	2.4
51	1t	14	LYS	2.4
9	2N	85	ILE	2.4
12	2Q	38	GLU	2.4
30	28	16	ILE	2.4
40	1i	119	ALA	2.4
32	2a	1353	G	2.4
32	2a	1523	G	2.4
13	2R	10	LEU	2.4
31	29	34	GLN	2.4
40	1i	17	VAL	2.4
18	1W	111	HIS	2.4
20	2Y	75	ILE	2.4
8	2I	3	VAL	2.4
17	2V	74	LYS	2.4
17	2V	75	PHE	2.4
35	1d	138	TYR	2.4
48	1q	37	LYS	2.4
11	1P	51	PHE	2.4
34	2c	155	GLY	2.4
25	23	18	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
40	1i	75	ASP	2.4
34	2c	196	LEU	2.4
29	17	1	MET	2.4
17	2V	78	LYS	2.4
36	2e	133	TYR	2.4
35	2d	146	ILE	2.4
26	24	64	GLY	2.4
11	2P	79	ARG	2.4
38	2g	77	SER	2.4
25	23	17	LYS	2.4
25	23	20	LYS	2.4
32	1a	1397	C	2.4
38	2g	25	ALA	2.4
45	1n	15	LYS	2.4
38	2g	16	LEU	2.4
7	2H	142	GLY	2.3
48	1q	8	GLY	2.3
23	11	69	LYS	2.3
32	2a	239	U	2.3
11	2P	32	THR	2.3
6	2G	150	ASP	2.3
7	2H	134	SER	2.3
19	2X	92	LEU	2.3
35	1d	5	ILE	2.3
39	2h	89	PRO	2.3
50	2s	15	LEU	2.3
11	2P	27	HIS	2.3
32	2a	1368	G	2.3
35	2d	11	LEU	2.3
35	2d	209	ARG	2.3
43	2l	7	ILE	2.3
43	2l	10	LEU	2.3
45	1n	21	TYR	2.3
36	2e	24	ARG	2.3
39	2h	84	ARG	2.3
44	2m	91	ARG	2.3
22	20	75	LEU	2.3
42	2k	32	ILE	2.3
47	1p	36	ILE	2.3
50	2s	71	LEU	2.3
47	1p	27	LYS	2.3
1	2A	2585	U	2.3

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Mol	Chain	Res	Type	RSRZ
32	2a	968	A	2.3
53	1v	21	A	2.3
5	1F	51	THR	2.3
44	2m	94	ARG	2.3
25	23	53	LEU	2.3
34	2c	157	ILE	2.3
40	2i	45	ALA	2.3
1	1A	2110	G	2.3
30	28	2	PRO	2.3
43	1l	22	SER	2.3
6	2G	133	LEU	2.3
34	1c	15	THR	2.3
35	2d	4	TYR	2.3
35	2d	21	LEU	2.3
47	1p	32	TYR	2.3
50	2s	50	ALA	2.3
11	2P	43	GLY	2.3
7	2H	85	LYS	2.3
11	1P	31	ALA	2.3
11	2P	20	GLY	2.3
22	20	52	GLY	2.3
51	2t	14	LYS	2.3
36	2e	31	LEU	2.3
48	1q	45	HIS	2.3
22	20	41	ARG	2.3
32	1a	1202	G	2.3
32	2a	1061	G	2.3
36	2e	122	GLU	2.3
47	1p	15	PRO	2.3
7	2H	98	LEU	2.3
7	2H	164	TYR	2.3
52	2u	10	ARG	2.3
1	1A	2143	C	2.3
1	2A	2111	C	2.3
11	2P	17	LYS	2.3
13	2R	69	ASP	2.3
44	1m	106	ASN	2.3
39	2h	10	LEU	2.3
19	1X	60	ARG	2.3
32	1a	309	G	2.3
27	25	9	LYS	2.3
30	28	12	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
46	2o	47	LYS	2.3
43	1l	29	GLY	2.3
47	1p	23	ASP	2.3
31	29	9	ARG	2.3
40	2i	79	LEU	2.3
23	21	23	LYS	2.3
48	2q	71	PHE	2.3
32	2a	965	A	2.3
51	1t	70	SER	2.3
34	2c	2	GLY	2.2
48	2q	31	LEU	2.2
27	15	47	PRO	2.2
33	1b	95	GLN	2.2
7	2H	100	GLY	2.2
40	1i	36	TYR	2.2
4	2E	152	LYS	2.2
32	2a	1224	G	2.2
40	1i	81	ILE	2.2
43	1l	67	THR	2.2
45	2n	16	PHE	2.2
1	1A	2140	C	2.2
6	2G	35	GLU	2.2
11	2P	50	ARG	2.2
19	1X	68	ARG	2.2
34	1c	154	SER	2.2
53	2v	14	A	2.2
4	2E	126	PRO	2.2
23	21	29	GLY	2.2
26	24	54	GLY	2.2
45	2n	10	ALA	2.2
45	2n	45	ARG	2.2
10	2O	31	LYS	2.2
36	2e	92	LYS	2.2
41	2j	57	LYS	2.2
44	1m	115	LYS	2.2
23	21	38	SER	2.2
26	24	40	HIS	2.2
41	2j	65	LEU	2.2
45	2n	32	SER	2.2
50	1s	71	LEU	2.2
7	2H	89	ILE	2.2
48	1q	9	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
23	2l	68	PRO	2.2
35	2d	6	GLY	2.2
50	2s	34	TRP	2.2
51	1t	13	LEU	2.2
32	2a	308	C	2.2
51	1t	22	ARG	2.2
30	18	65	GLU	2.2
43	2l	13	LYS	2.2
47	2p	29	ASP	2.2
22	20	10	THR	2.2
35	2d	54	TYR	2.2
38	2g	40	ALA	2.2
9	2N	23	LEU	2.2
32	2a	1248	A	2.2
7	2H	148	ILE	2.2
38	2g	43	PHE	2.2
23	11	49	VAL	2.2
38	2g	35	LYS	2.2
43	2l	16	GLU	2.2
1	2A	1626	G	2.2
10	1O	83	ALA	2.2
40	2i	46	ALA	2.2
11	1P	32	THR	2.2
48	1q	98	LEU	2.2
51	1t	26	ASN	2.2
35	1d	73	ARG	2.2
9	2N	68	GLU	2.2
45	1n	10	ALA	2.2
35	2d	122	ARG	2.2
45	2n	23	ARG	2.2
47	1p	3	LYS	2.2
52	2u	17	THR	2.2
45	1n	38	GLY	2.2
36	1e	134	ALA	2.2
38	1g	154	TYR	2.2
40	2i	15	ALA	2.2
32	2a	121	C	2.2
44	2m	106	ASN	2.2
50	2s	53	ASN	2.2
40	2i	68	GLY	2.2
36	2e	21	ALA	2.2
13	1R	69	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
25	23	50	VAL	2.2
9	2N	83	LYS	2.2
36	2e	126	ARG	2.2
1	1A	1762	A	2.2
32	2a	1225	A	2.2
32	2a	1349	A	2.2
30	18	3	LYS	2.2
45	2n	53	LEU	2.1
32	1a	308	C	2.1
11	1P	70	GLN	2.1
30	28	35	GLN	2.1
35	1d	158	ILE	2.1
36	1e	118	ILE	2.1
7	2H	90	LYS	2.1
32	2a	963	G	2.1
8	2I	30	LEU	2.1
25	23	8	LEU	2.1
38	1g	151	TYR	2.1
45	1n	39	LEU	2.1
38	2g	39	ALA	2.1
34	1c	7	PRO	2.1
45	1n	58	LYS	2.1
6	2G	49	ASP	2.1
48	2q	22	LEU	2.1
4	2E	157	ALA	2.1
20	2Y	35	TYR	2.1
34	2c	3	ASN	2.1
32	1a	1357	A	2.1
34	2c	4	LYS	2.1
38	2g	112	PRO	2.1
43	1l	31	PRO	2.1
43	1l	98	TYR	2.1
34	2c	191	THR	2.1
35	2d	139	ARG	2.1
40	1i	7	THR	2.1
32	1a	1356	G	2.1
35	1d	101	LEU	2.1
48	1q	12	SER	2.1
53	2v	15	A	2.1
4	2E	151	TYR	2.1
32	1a	1195	C	2.1
32	2a	1066	C	2.1

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Mol	Chain	Res	Type	RSRZ
32	2a	1354	C	2.1
40	1i	70	LYS	2.1
48	1q	7	THR	2.1
6	2G	2	PRO	2.1
40	2i	98	PRO	2.1
39	2h	132	GLU	2.1
40	2i	77	ILE	2.1
4	1E	153	GLY	2.1
9	2N	8	GLN	2.1
11	1P	38	GLN	2.1
15	2T	114	LEU	2.1
40	1i	107	ARG	2.1
44	1m	94	ARG	2.1
16	2U	40	PHE	2.1
7	2H	145	ALA	2.1
52	1u	18	TYR	2.1
48	1q	78	GLU	2.1
48	1q	31	LEU	2.1
43	1l	25	PRO	2.1
43	2l	5	PRO	2.1
3	2D	252	TRP	2.1
41	1j	55	LYS	2.1
51	1t	9	ASN	2.1
6	1G	25	TYR	2.1
32	2a	238	G	2.1
42	1k	25	TYR	2.1
25	23	9	VAL	2.1
40	2i	78	LYS	2.1
45	2n	12	ARG	2.1
51	2t	34	LYS	2.1
48	2q	90	ILE	2.1
9	2N	116	LEU	2.1
38	2g	153	HIS	2.1
41	1j	59	SER	2.1
1	1A	2112	G	2.1
6	2G	152	LEU	2.1
49	1r	78	LEU	2.1
41	1j	54	PHE	2.1
47	2p	9	PHE	2.1
45	1n	17	LYS	2.1
44	1m	103	THR	2.1
45	2n	57	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
36	1e	13	ILE	2.1
7	2H	108	GLY	2.1
16	2U	27	LEU	2.1
32	1a	328	C	2.1
47	1p	29	ASP	2.1
31	29	8	LYS	2.0
14	1S	7	TYR	2.0
27	25	28	PRO	2.0
39	1h	133	LEU	2.0
7	2H	109	PHE	2.0
40	2i	107	ARG	2.0
22	20	21	LEU	2.0
44	1m	97	PRO	2.0
34	2c	190	ARG	2.0
39	1h	91	ARG	2.0
23	11	47	GLN	2.0
34	2c	162	GLN	2.0
45	2n	60	SER	2.0
5	2F	80	ALA	2.0
35	2d	68	TYR	2.0
40	1i	65	VAL	2.0
41	1j	72	VAL	2.0
35	1d	204	ILE	2.0
30	28	57	ARG	2.0
40	2i	9	ARG	2.0
41	2j	12	ASP	2.0
3	2D	35	LYS	2.0
25	23	28	LEU	2.0
27	15	9	LYS	2.0
35	1d	78	LEU	2.0
41	2j	6	ILE	2.0
47	1p	73	LEU	2.0
32	2a	1374	A	2.0
40	2i	67	GLY	2.0
7	2H	124	GLU	2.0
48	2q	10	VAL	2.0
4	2E	149	ARG	2.0
7	2H	95	ARG	2.0
36	1e	91	LEU	2.0
45	1n	26	ARG	2.0
51	2t	22	ARG	2.0
18	1W	39	THR	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	5MU	2A	1915	21/22	0.90	0.18	55,72,85,88	0
54	PSU	2x	55	20/21	0.90	0.15	64,72,80,82	0
32	7MG	2a	527	24/25	0.91	0.22	47,63,71,72	0
32	PSU	1a	516	20/21	0.91	0.16	53,70,76,77	0
54	PSU	1x	55	20/21	0.91	0.15	49,59,66,70	0
32	M2G	2a	966	25/26	0.92	0.36	65,73,80,82	0
32	UR3	2a	1498	21/22	0.93	0.23	31,51,56,64	0
54	4SU	2x	8	20/21	0.93	0.14	63,68,73,78	0
32	5MC	2a	967	21/22	0.93	0.28	65,71,77,81	0
32	2MG	2a	1207	24/25	0.93	0.15	69,74,78,93	0
32	4OC	2a	1402	22/23	0.93	0.23	54,61,66,69	0
54	5MU	2x	54	21/22	0.93	0.16	70,76,87,97	0
54	5MU	1x	54	21/22	0.94	0.14	45,63,65,67	0
43	0TD	2l	92	10/11	0.94	0.35	55,59,62,66	0
54	4SU	1x	8	20/21	0.94	0.17	44,55,61,70	0
1	PSU	2A	1911	20/21	0.94	0.15	51,55,79,79	0
32	5MC	2a	1400	21/22	0.94	0.28	60,73,79,95	0
32	2MG	1a	1207	24/25	0.94	0.13	63,68,73,79	0
1	PSU	1A	1917	20/21	0.94	0.18	48,59,63,65	0
32	PSU	2a	516	20/21	0.94	0.15	61,69,73,76	0
54	5MC	2x	32	21/22	0.94	0.23	57,63,70,71	0
32	MA6	1a	1518	24/25	0.95	0.23	27,35,38,40	0
32	M2G	1a	966	25/26	0.95	0.27	45,52,57,60	0
32	4OC	1a	1402	22/23	0.95	0.25	35,46,53,58	0
32	MA6	2a	1518	24/25	0.95	0.25	44,53,61,64	0
1	5MU	1A	1915	21/22	0.95	0.15	53,60,70,73	0
1	PSU	1A	1911	20/21	0.95	0.17	40,51,56,57	0
32	5MC	1a	1400	21/22	0.95	0.20	43,50,56,59	0
32	MA6	2a	1519	24/25	0.95	0.35	46,53,56,65	0
1	5MC	2A	1962	21/22	0.95	0.17	31,40,49,54	0
32	5MC	1a	967	21/22	0.95	0.34	47,57,63,65	0
1	4OC	1A	1920	21/23	0.95	0.22	27,44,55,57	0
54	5MC	1x	32	21/22	0.96	0.19	37,52,60,64	0
1	5MC	2A	1942	21/22	0.96	0.15	36,49,55,57	0
32	5MC	2a	1404	21/22	0.96	0.24	47,58,62,62	0
32	MA6	1a	1519	24/25	0.96	0.24	29,36,41,42	0
32	UR3	1a	1498	21/22	0.96	0.19	23,37,42,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	PSU	2A	2605	20/21	0.96	0.24	23,31,35,36	0
1	OMG	2A	2251	24/25	0.96	0.24	27,33,36,37	0
1	5MU	2A	1939	21/22	0.96	0.17	30,37,45,48	0
1	2MA	2A	2503	23/24	0.96	0.23	20,26,36,41	0
32	5MC	2a	1407	21/22	0.96	0.22	41,52,56,58	0
32	5MC	1a	1407	21/22	0.96	0.18	32,42,49,52	0
1	4OC	2A	1920	21/23	0.96	0.19	44,56,61,64	0
1	PSU	2A	1917	20/21	0.97	0.13	45,56,60,60	0
1	2MU	2A	2552	21/23	0.97	0.18	25,33,39,42	0
1	5MC	1A	1942	21/22	0.97	0.18	22,36,41,46	0
1	5MC	1A	1962	21/22	0.97	0.19	25,37,42,46	0
32	7MG	1a	527	24/25	0.97	0.21	34,39,51,55	0
1	5MU	1A	1939	21/22	0.97	0.19	19,25,29,32	0
1	2MU	1A	2552	21/23	0.97	0.24	26,37,41,43	0
43	0TD	1l	92	10/11	0.97	0.20	43,49,50,55	0
32	5MC	1a	1404	21/22	0.97	0.18	29,38,43,47	0
1	2MA	1A	2503	23/24	0.97	0.24	12,19,25,31	0
1	PSU	1A	2605	20/21	0.97	0.18	19,24,28,28	0
1	OMG	1A	2251	24/25	0.97	0.25	18,23,30,34	0

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

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(\AA^2)	Q<0.9
55	MG	1A	4012	1/1	0.38	0.28	47,47,47,47	0
55	MG	2A	3272	1/1	0.49	0.21	56,56,56,56	0
55	MG	1a	3102	1/1	0.52	0.18	61,61,61,61	0
55	MG	2V	201	1/1	0.57	0.21	53,53,53,53	0
55	MG	1A	3952	1/1	0.58	0.26	68,68,68,68	0
57	ZN	25	105	1/1	0.59	0.12	164,164,164,164	0
55	MG	1a	3061	1/1	0.60	0.86	61,61,61,61	0
55	MG	1A	3528	1/1	0.62	0.22	59,59,59,59	0
55	MG	1v	102	1/1	0.64	0.09	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	ZN	14	102	1/1	0.64	0.18	159,159,159,159	0
55	MG	2a	1687	1/1	0.65	0.15	44,44,44,44	0
55	MG	2T	203	1/1	0.65	0.23	51,51,51,51	0
55	MG	1A	3249	1/1	0.66	0.19	49,49,49,49	0
55	MG	1A	3296	1/1	0.66	0.28	48,48,48,48	0
55	MG	2A	3115	1/1	0.67	0.20	47,47,47,47	0
55	MG	1a	3066	1/1	0.68	0.18	62,62,62,62	0
55	MG	2a	1790	1/1	0.70	0.88	62,62,62,62	0
55	MG	1A	3354	1/1	0.70	0.21	37,37,37,37	0
55	MG	2A	3027	1/1	0.70	0.23	46,46,46,46	0
55	MG	1Q	205	1/1	0.71	0.53	37,37,37,37	0
55	MG	1A	3079	1/1	0.72	0.21	46,46,46,46	0
55	MG	1F	308	1/1	0.72	0.31	51,51,51,51	0
55	MG	1a	3027	1/1	0.72	0.17	45,45,45,45	0
55	MG	1P	205	1/1	0.72	0.36	56,56,56,56	0
55	MG	2A	3577	1/1	0.72	0.20	69,69,69,69	0
55	MG	1A	3842	1/1	0.74	0.86	28,28,28,28	0
55	MG	1A	3290	1/1	0.74	0.19	39,39,39,39	0
55	MG	2A	3294	1/1	0.74	0.82	33,33,33,33	0
55	MG	2A	3200	1/1	0.74	0.13	57,57,57,57	0
55	MG	2A	3787	1/1	0.74	0.29	57,57,57,57	0
55	MG	2A	3187	1/1	0.74	0.25	62,62,62,62	0
55	MG	1A	3884	1/1	0.75	0.30	68,68,68,68	0
55	MG	1A	3217	1/1	0.75	0.21	48,48,48,48	0
55	MG	2A	3751	1/1	0.75	0.21	50,50,50,50	0
55	MG	1A	3553	1/1	0.75	0.17	27,27,27,27	0
55	MG	1A	3883	1/1	0.75	0.15	55,55,55,55	0
55	MG	13	102	1/1	0.75	0.29	59,59,59,59	0
55	MG	2d	301	1/1	0.75	0.13	38,38,38,38	0
55	MG	2A	3242	1/1	0.75	0.17	62,62,62,62	0
55	MG	1A	3815	1/1	0.76	0.37	31,31,31,31	0
55	MG	2a	1650	1/1	0.76	0.21	49,49,49,49	0
55	MG	1A	3370	1/1	0.76	0.57	35,35,35,35	0
55	MG	2a	1665	1/1	0.76	0.20	57,57,57,57	0
55	MG	2B	207	1/1	0.76	0.21	60,60,60,60	0
55	MG	2a	1714	1/1	0.76	0.27	50,50,50,50	0
55	MG	1E	301	1/1	0.76	0.32	57,57,57,57	0
55	MG	2A	3558	1/1	0.76	0.12	28,28,28,28	0
55	MG	1A	3996	1/1	0.77	0.13	51,51,51,51	0
55	MG	2a	1795	1/1	0.77	0.29	65,65,65,65	0
55	MG	2A	3262	1/1	0.77	0.17	50,50,50,50	0
55	MG	2q	202	1/1	0.77	0.18	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	ZN	24	501	1/1	0.77	0.09	147,147,147,147	0
55	MG	2A	3225	1/1	0.77	0.35	42,42,42,42	0
55	MG	2A	3232	1/1	0.77	0.77	43,43,43,43	0
55	MG	1x	103	1/1	0.77	0.14	50,50,50,50	0
55	MG	2a	1653	1/1	0.77	0.11	42,42,42,42	0
55	MG	1a	3058	1/1	0.77	0.18	48,48,48,48	0
55	MG	1A	3048	1/1	0.77	0.24	33,33,33,33	0
55	MG	1A	3813	1/1	0.77	0.12	44,44,44,44	0
55	MG	1A	3304	1/1	0.77	0.43	35,35,35,35	0
55	MG	1a	3050	1/1	0.77	0.33	25,25,25,25	0
55	MG	1B	226	1/1	0.78	0.16	53,53,53,53	0
55	MG	1A	3887	1/1	0.78	0.23	55,55,55,55	0
55	MG	1a	3177	1/1	0.78	0.28	69,69,69,69	0
55	MG	1D	303	1/1	0.78	0.17	31,31,31,31	0
55	MG	1A	3418	1/1	0.78	0.15	36,36,36,36	0
55	MG	2a	1717	1/1	0.78	0.24	68,68,68,68	0
55	MG	2a	1746	1/1	0.78	0.20	40,40,40,40	0
55	MG	2A	3160	1/1	0.78	0.10	58,58,58,58	0
55	MG	2A	3132	1/1	0.78	0.38	38,38,38,38	0
55	MG	2a	1723	1/1	0.79	0.13	65,65,65,65	0
55	MG	2A	3539	1/1	0.79	0.57	41,41,41,41	0
55	MG	2A	3278	1/1	0.79	0.53	36,36,36,36	0
55	MG	1n	102	1/1	0.79	0.39	55,55,55,55	0
55	MG	2A	3361	1/1	0.79	0.15	50,50,50,50	0
55	MG	1a	3176	1/1	0.79	0.09	71,71,71,71	0
55	MG	1A	3582	1/1	0.79	0.11	45,45,45,45	0
55	MG	1x	102	1/1	0.79	0.56	80,80,80,80	0
55	MG	1a	3193	1/1	0.79	0.16	62,62,62,62	0
55	MG	1a	3172	1/1	0.79	0.48	67,67,67,67	0
55	MG	2a	1806	1/1	0.79	0.45	55,55,55,55	0
55	MG	1O	203	1/1	0.79	0.40	58,58,58,58	0
55	MG	1a	3032	1/1	0.79	0.21	57,57,57,57	0
55	MG	2a	1704	1/1	0.79	0.22	47,47,47,47	0
55	MG	2A	3380	1/1	0.79	0.21	49,49,49,49	0
55	MG	2A	3195	1/1	0.79	0.71	42,42,42,42	0
55	MG	2A	3676	1/1	0.79	0.12	65,65,65,65	0
55	MG	2A	3048	1/1	0.80	0.26	57,57,57,57	0
55	MG	2A	3851	1/1	0.80	0.69	47,47,47,47	0
55	MG	2a	1622	1/1	0.80	0.13	63,63,63,63	0
55	MG	1A	3881	1/1	0.80	0.20	44,44,44,44	0
55	MG	2A	3673	1/1	0.80	0.17	56,56,56,56	0
55	MG	1A	3722	1/1	0.80	0.13	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	2A	3541	1/1	0.80	0.15	39,39,39,39	0
55	MG	2a	1730	1/1	0.80	0.17	59,59,59,59	0
55	MG	2A	3246	1/1	0.80	0.46	48,48,48,48	0
55	MG	2A	3171	1/1	0.80	0.13	35,35,35,35	0
55	MG	2A	3576	1/1	0.80	0.20	48,48,48,48	0
55	MG	2A	3158	1/1	0.80	0.20	38,38,38,38	0
55	MG	1A	3312	1/1	0.80	0.48	40,40,40,40	0
55	MG	2A	3717	1/1	0.80	0.17	28,28,28,28	0
55	MG	1A	3655	1/1	0.81	0.48	41,41,41,41	0
55	MG	1A	3015	1/1	0.81	0.12	36,36,36,36	0
55	MG	1A	3695	1/1	0.81	0.12	10,10,10,10	0
55	MG	1A	3166	1/1	0.81	0.25	36,36,36,36	0
55	MG	2a	1662	1/1	0.81	0.62	52,52,52,52	0
55	MG	2A	3663	1/1	0.81	0.46	43,43,43,43	0
55	MG	1A	3935	1/1	0.81	0.13	56,56,56,56	0
55	MG	2A	3234	1/1	0.81	0.18	53,53,53,53	0
55	MG	2A	3418	1/1	0.81	0.11	46,46,46,46	0
55	MG	1a	3198	1/1	0.81	0.14	56,56,56,56	0
55	MG	2A	3455	1/1	0.81	0.14	32,32,32,32	0
55	MG	2A	3502	1/1	0.81	0.21	56,56,56,56	0
55	MG	2A	3381	1/1	0.81	0.78	68,68,68,68	0
55	MG	2A	3814	1/1	0.81	0.26	44,44,44,44	0
55	MG	1A	3962	1/1	0.81	0.45	53,53,53,53	0
55	MG	2a	1641	1/1	0.81	0.32	51,51,51,51	0
55	MG	2a	1604	1/1	0.81	0.14	47,47,47,47	0
55	MG	2a	1659	1/1	0.81	0.14	45,45,45,45	0
55	MG	1B	218	1/1	0.81	0.13	41,41,41,41	0
55	MG	2A	3722	1/1	0.82	0.17	25,25,25,25	0
55	MG	1A	3840	1/1	0.82	0.31	28,28,28,28	0
55	MG	2a	1610	1/1	0.82	0.13	55,55,55,55	0
55	MG	2A	3150	1/1	0.82	0.22	45,45,45,45	0
55	MG	1A	3162	1/1	0.82	0.14	36,36,36,36	0
55	MG	2a	1739	1/1	0.82	0.23	83,83,83,83	0
55	MG	1A	3612	1/1	0.82	0.17	14,14,14,14	0
55	MG	2a	1774	1/1	0.82	0.13	29,29,29,29	0
55	MG	1A	3173	1/1	0.82	0.33	28,28,28,28	0
55	MG	1A	3650	1/1	0.82	0.14	60,60,60,60	0
55	MG	14	101	1/1	0.82	0.18	40,40,40,40	0
55	MG	2A	3137	1/1	0.82	0.83	39,39,39,39	0
55	MG	1A	3423	1/1	0.82	0.16	34,34,34,34	0
55	MG	2A	3289	1/1	0.82	0.30	49,49,49,49	0
55	MG	2a	1740	1/1	0.82	0.26	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	1A	3793	1/1	0.82	1.61	48,48,48,48	0
55	MG	1A	3421	1/1	0.82	0.20	33,33,33,33	0
55	MG	2A	3321	1/1	0.82	0.51	37,37,37,37	0
55	MG	2A	3214	1/1	0.82	0.29	33,33,33,33	0
55	MG	1A	3740	1/1	0.82	0.11	39,39,39,39	0
55	MG	1A	3356	1/1	0.82	0.39	29,29,29,29	0
55	MG	2A	3569	1/1	0.82	0.12	35,35,35,35	0
55	MG	2A	3718	1/1	0.82	0.17	62,62,62,62	0
55	MG	2A	3169	1/1	0.82	0.20	40,40,40,40	0
55	MG	2A	3396	1/1	0.82	0.18	51,51,51,51	0
55	MG	1A	3471	1/1	0.82	0.48	47,47,47,47	0
55	MG	2a	1617	1/1	0.82	0.18	46,46,46,46	0
55	MG	2A	3662	1/1	0.82	0.26	39,39,39,39	0
55	MG	1a	3071	1/1	0.83	0.15	37,37,37,37	0
55	MG	2A	3277	1/1	0.83	0.43	42,42,42,42	0
55	MG	1B	208	1/1	0.83	0.13	43,43,43,43	0
55	MG	1A	3841	1/1	0.83	0.25	41,41,41,41	0
55	MG	2B	211	1/1	0.83	0.24	35,35,35,35	0
55	MG	1a	3096	1/1	0.83	0.19	42,42,42,42	0
55	MG	1B	224	1/1	0.83	0.16	40,40,40,40	0
55	MG	1P	203	1/1	0.83	0.41	44,44,44,44	0
55	MG	2A	3493	1/1	0.83	0.41	42,42,42,42	0
55	MG	2A	3151	1/1	0.83	0.23	56,56,56,56	0
55	MG	2A	3646	1/1	0.83	0.18	54,54,54,54	0
55	MG	2A	3350	1/1	0.83	0.34	38,38,38,38	0
55	MG	2A	3061	1/1	0.83	0.12	50,50,50,50	0
55	MG	2A	3377	1/1	0.83	0.15	49,49,49,49	0
55	MG	2A	3264	1/1	0.83	0.34	52,52,52,52	0
55	MG	1b	301	1/1	0.83	0.12	54,54,54,54	0
55	MG	25	104	1/1	0.83	0.38	34,34,34,34	0
55	MG	1A	3059	1/1	0.83	0.24	35,35,35,35	0
55	MG	1B	203	1/1	0.83	0.18	51,51,51,51	0
55	MG	2A	3707	1/1	0.83	0.13	44,44,44,44	0
55	MG	17	103	1/1	0.83	0.53	41,41,41,41	0
55	MG	1A	3914	1/1	0.83	0.46	62,62,62,62	0
55	MG	23	102	1/1	0.83	0.62	52,52,52,52	0
55	MG	2a	1608	1/1	0.83	0.67	53,53,53,53	0
55	MG	2A	3327	1/1	0.83	0.26	43,43,43,43	0
55	MG	2A	3068	1/1	0.83	0.67	32,32,32,32	0
55	MG	2A	3075	1/1	0.84	0.12	30,30,30,30	0
55	MG	1B	229	1/1	0.84	0.18	75,75,75,75	0
55	MG	1O	201	1/1	0.84	0.55	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	2f	202	1/1	0.84	0.15	52,52,52,52	0
55	MG	2A	3471	1/1	0.84	0.14	43,43,43,43	0
55	MG	1A	3317	1/1	0.84	0.55	24,24,24,24	0
55	MG	1a	3171	1/1	0.84	0.31	59,59,59,59	0
55	MG	2a	1632	1/1	0.84	0.21	51,51,51,51	0
55	MG	1a	3051	1/1	0.84	0.15	78,78,78,78	0
55	MG	1A	3308	1/1	0.84	0.15	45,45,45,45	0
55	MG	1A	3310	1/1	0.84	0.19	36,36,36,36	0
55	MG	1a	3210	1/1	0.84	0.18	34,34,34,34	0
55	MG	1A	3145	1/1	0.84	0.43	45,45,45,45	0
55	MG	2A	3215	1/1	0.84	0.18	24,24,24,24	0
55	MG	2A	3126	1/1	0.84	0.24	46,46,46,46	0
55	MG	2A	3566	1/1	0.84	0.19	25,25,25,25	0
55	MG	2A	3540	1/1	0.84	0.16	32,32,32,32	0
55	MG	1A	3164	1/1	0.84	0.54	31,31,31,31	0
55	MG	25	102	1/1	0.84	0.32	28,28,28,28	0
55	MG	1A	3512	1/1	0.84	0.16	23,23,23,23	0
55	MG	2A	3255	1/1	0.84	1.19	51,51,51,51	0
57	ZN	2Y	203	1/1	0.84	0.08	98,98,98,98	0
55	MG	2A	3422	1/1	0.84	0.22	52,52,52,52	0
55	MG	2A	3619	1/1	0.84	0.17	42,42,42,42	0
55	MG	2A	3572	1/1	0.84	0.47	50,50,50,50	0
55	MG	1A	3359	1/1	0.84	0.18	33,33,33,33	0
55	MG	1a	3028	1/1	0.84	0.26	52,52,52,52	0
55	MG	2A	3549	1/1	0.84	0.47	61,61,61,61	0
55	MG	2A	3341	1/1	0.84	0.13	43,43,43,43	0
55	MG	2A	3546	1/1	0.84	0.33	54,54,54,54	0
55	MG	2A	3267	1/1	0.84	0.16	54,54,54,54	0
55	MG	1A	3910	1/1	0.84	0.13	35,35,35,35	0
55	MG	1A	3569	1/1	0.85	0.14	28,28,28,28	0
55	MG	2D	301	1/1	0.85	0.51	42,42,42,42	0
55	MG	1A	3969	1/1	0.85	0.11	45,45,45,45	0
55	MG	2A	3489	1/1	0.85	0.14	17,17,17,17	0
55	MG	1A	3332	1/1	0.85	0.32	47,47,47,47	0
55	MG	1A	3865	1/1	0.85	0.17	49,49,49,49	0
55	MG	2A	3600	1/1	0.85	0.15	37,37,37,37	0
55	MG	2A	3199	1/1	0.85	0.14	38,38,38,38	0
55	MG	1a	3060	1/1	0.85	0.10	44,44,44,44	0
55	MG	1A	3662	1/1	0.85	0.13	72,72,72,72	0
55	MG	2A	3301	1/1	0.85	0.24	44,44,44,44	0
55	MG	1A	3912	1/1	0.85	0.69	39,39,39,39	0
55	MG	1A	3530	1/1	0.85	0.15	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	1a	3155	1/1	0.85	0.11	49,49,49,49	0
55	MG	10	104	1/1	0.85	0.21	46,46,46,46	0
55	MG	1B	233	1/1	0.85	0.11	42,42,42,42	0
55	MG	2A	3292	1/1	0.85	0.48	48,48,48,48	0
55	MG	2a	1605	1/1	0.85	0.47	42,42,42,42	0
55	MG	2A	3649	1/1	0.85	0.13	47,47,47,47	0
55	MG	1E	309	1/1	0.85	0.49	36,36,36,36	0
55	MG	1A	3262	1/1	0.85	0.15	27,27,27,27	0
55	MG	2A	3625	1/1	0.85	0.12	24,24,24,24	0
55	MG	1A	3182	1/1	0.85	0.27	42,42,42,42	0
55	MG	2A	3618	1/1	0.85	0.17	22,22,22,22	0
55	MG	2A	3088	1/1	0.85	0.15	45,45,45,45	0
55	MG	2a	1611	1/1	0.85	0.19	47,47,47,47	0
55	MG	1A	3362	1/1	0.85	0.56	44,44,44,44	0
55	MG	2a	1607	1/1	0.85	0.25	31,31,31,31	0
55	MG	2A	3202	1/1	0.85	0.18	45,45,45,45	0
55	MG	1A	3618	1/1	0.85	0.12	46,46,46,46	0
55	MG	2A	3312	1/1	0.85	0.58	52,52,52,52	0
55	MG	2A	3840	1/1	0.85	0.18	51,51,51,51	0
55	MG	1A	3250	1/1	0.85	0.32	46,46,46,46	0
55	MG	2A	3482	1/1	0.85	0.16	35,35,35,35	0
55	MG	2A	3838	1/1	0.85	0.13	49,49,49,49	0
55	MG	1B	219	1/1	0.85	0.22	40,40,40,40	0
55	MG	2A	3224	1/1	0.85	0.22	34,34,34,34	0
55	MG	2A	3497	1/1	0.85	0.11	51,51,51,51	0
55	MG	2a	1618	1/1	0.85	0.15	40,40,40,40	0
55	MG	27	101	1/1	0.86	0.15	31,31,31,31	0
55	MG	1A	3567	1/1	0.86	0.16	27,27,27,27	0
55	MG	2A	3008	1/1	0.86	0.43	24,24,24,24	0
55	MG	2a	1614	1/1	0.86	0.23	53,53,53,53	0
55	MG	2f	201	1/1	0.86	0.10	44,44,44,44	0
55	MG	2A	3411	1/1	0.86	0.10	43,43,43,43	0
55	MG	2A	3819	1/1	0.86	0.14	21,21,21,21	0
55	MG	2A	3367	1/1	0.86	0.31	27,27,27,27	0
55	MG	2A	3265	1/1	0.86	0.14	37,37,37,37	0
55	MG	2a	1791	1/1	0.86	0.09	66,66,66,66	0
55	MG	1A	3306	1/1	0.86	0.13	38,38,38,38	0
55	MG	2A	3769	1/1	0.86	0.18	69,69,69,69	0
55	MG	2a	1710	1/1	0.86	0.21	57,57,57,57	0
55	MG	1A	3436	1/1	0.86	0.11	53,53,53,53	0
55	MG	2A	3737	1/1	0.86	0.20	51,51,51,51	0
55	MG	2a	1670	1/1	0.86	0.16	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	1W	208	1/1	0.86	0.45	27,27,27,27	0
55	MG	1A	3371	1/1	0.86	0.15	45,45,45,45	0
55	MG	1a	3065	1/1	0.86	0.18	51,51,51,51	0
55	MG	2A	3835	1/1	0.86	0.11	42,42,42,42	0
55	MG	1E	312	1/1	0.86	1.08	54,54,54,54	0
55	MG	2a	1815	1/1	0.86	0.23	53,53,53,53	0
55	MG	19	101	1/1	0.86	0.16	58,58,58,58	0
55	MG	2A	3434	1/1	0.86	0.09	15,15,15,15	0
55	MG	2A	3141	1/1	0.86	0.17	31,31,31,31	0
55	MG	1a	3197	1/1	0.86	0.46	61,61,61,61	0
55	MG	1A	3083	1/1	0.86	0.20	42,42,42,42	0
55	MG	2A	3412	1/1	0.86	0.36	45,45,45,45	0
55	MG	1A	3458	1/1	0.86	0.25	25,25,25,25	0
55	MG	1A	3443	1/1	0.86	0.14	39,39,39,39	0
55	MG	2a	1609	1/1	0.86	0.15	39,39,39,39	0
55	MG	1A	3190	1/1	0.86	0.25	41,41,41,41	0
55	MG	1A	3516	1/1	0.86	0.35	31,31,31,31	0
55	MG	1a	3184	1/1	0.86	0.26	55,55,55,55	0
55	MG	2A	3145	1/1	0.86	0.09	51,51,51,51	0
55	MG	2a	1802	1/1	0.86	0.10	58,58,58,58	0
55	MG	2A	3607	1/1	0.86	0.28	44,44,44,44	0
55	MG	2A	3286	1/1	0.86	0.45	33,33,33,33	0
55	MG	2a	1699	1/1	0.86	0.16	36,36,36,36	0
55	MG	2a	1703	1/1	0.86	0.15	38,38,38,38	0
55	MG	1A	3919	1/1	0.86	0.19	33,33,33,33	0
55	MG	2A	3347	1/1	0.86	0.17	48,48,48,48	0
55	MG	2A	3683	1/1	0.86	0.19	47,47,47,47	0
55	MG	2A	3487	1/1	0.86	0.17	44,44,44,44	0
55	MG	1A	4005	1/1	0.86	0.14	47,47,47,47	0
55	MG	2P	201	1/1	0.86	0.43	40,40,40,40	0
55	MG	2a	1698	1/1	0.86	0.40	40,40,40,40	0
55	MG	1A	3591	1/1	0.86	0.10	29,29,29,29	0
55	MG	1A	3903	1/1	0.86	0.88	37,37,37,37	0
55	MG	2A	3316	1/1	0.86	0.13	36,36,36,36	0
55	MG	2a	1705	1/1	0.87	0.29	54,54,54,54	0
55	MG	1A	3853	1/1	0.87	0.14	39,39,39,39	0
55	MG	2a	1725	1/1	0.87	0.14	59,59,59,59	0
55	MG	1A	3268	1/1	0.87	0.14	42,42,42,42	0
55	MG	2A	3738	1/1	0.87	0.17	27,27,27,27	0
55	MG	2A	3407	1/1	0.87	0.14	50,50,50,50	0
55	MG	1A	3473	1/1	0.87	0.67	27,27,27,27	0
55	MG	1A	3094	1/1	0.87	1.01	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	1A	4031	1/1	0.87	0.21	21,21,21,21	0
55	MG	1A	3297	1/1	0.87	0.44	40,40,40,40	0
55	MG	1A	3236	1/1	0.87	0.74	28,28,28,28	0
55	MG	2a	1628	1/1	0.87	0.16	41,41,41,41	0
55	MG	2a	1761	1/1	0.87	0.16	49,49,49,49	0
55	MG	1E	313	1/1	0.87	0.17	43,43,43,43	0
55	MG	1A	3040	1/1	0.87	0.28	36,36,36,36	0
55	MG	2A	3249	1/1	0.87	0.13	25,25,25,25	0
55	MG	1A	3439	1/1	0.87	0.21	26,26,26,26	0
55	MG	1A	3121	1/1	0.87	0.32	27,27,27,27	0
55	MG	2A	3680	1/1	0.87	0.12	46,46,46,46	0
55	MG	1A	3972	1/1	0.87	0.81	37,37,37,37	0
55	MG	2a	1733	1/1	0.87	0.08	44,44,44,44	0
55	MG	1a	3100	1/1	0.87	0.18	31,31,31,31	0
55	MG	2A	3849	1/1	0.87	0.26	50,50,50,50	0
55	MG	1A	3358	1/1	0.87	0.99	35,35,35,35	0
55	MG	1A	3523	1/1	0.87	0.14	42,42,42,42	0
55	MG	2A	3660	1/1	0.87	0.34	38,38,38,38	0
55	MG	2A	3168	1/1	0.87	0.24	47,47,47,47	0
55	MG	2A	3288	1/1	0.87	0.20	30,30,30,30	0
55	MG	13	103	1/1	0.87	0.41	53,53,53,53	0
55	MG	2A	3236	1/1	0.87	0.61	38,38,38,38	0
55	MG	2A	3058	1/1	0.87	0.17	47,47,47,47	0
55	MG	1a	3035	1/1	0.87	0.19	52,52,52,52	0
55	MG	2a	1625	1/1	0.87	0.58	43,43,43,43	0
55	MG	1a	3075	1/1	0.87	0.45	43,43,43,43	0
55	MG	2A	3730	1/1	0.87	0.65	54,54,54,54	0
55	MG	2A	3332	1/1	0.87	0.10	33,33,33,33	0
55	MG	2F	301	1/1	0.87	0.15	28,28,28,28	0
55	MG	1a	3191	1/1	0.87	0.12	62,62,62,62	0
55	MG	1A	4014	1/1	0.87	0.79	51,51,51,51	0
55	MG	2A	3308	1/1	0.87	0.60	44,44,44,44	0
55	MG	2A	3078	1/1	0.87	0.84	41,41,41,41	0
55	MG	2A	3186	1/1	0.87	0.17	43,43,43,43	0
55	MG	1G	202	1/1	0.87	0.48	40,40,40,40	0
55	MG	1A	3849	1/1	0.87	0.65	22,22,22,22	0
55	MG	2A	3420	1/1	0.87	0.12	38,38,38,38	0
55	MG	1A	3623	1/1	0.87	0.13	15,15,15,15	0
55	MG	1A	3226	1/1	0.87	0.17	46,46,46,46	0
55	MG	2A	3406	1/1	0.87	0.16	30,30,30,30	0
55	MG	1A	3889	1/1	0.87	0.08	45,45,45,45	0
55	MG	1A	3746	1/1	0.87	0.33	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	1a	3076	1/1	0.87	0.38	59,59,59,59	0
55	MG	1a	3029	1/1	0.87	0.11	30,30,30,30	0
55	MG	1A	3861	1/1	0.87	0.23	28,28,28,28	0
55	MG	1A	3323	1/1	0.87	0.16	30,30,30,30	0
55	MG	2A	3323	1/1	0.87	0.35	38,38,38,38	0
55	MG	1a	3041	1/1	0.88	0.14	45,45,45,45	0
55	MG	2A	3435	1/1	0.88	0.09	24,24,24,24	0
55	MG	2A	3805	1/1	0.88	0.15	46,46,46,46	0
55	MG	2A	3727	1/1	0.88	0.31	40,40,40,40	0
55	MG	1A	3376	1/1	0.88	0.17	24,24,24,24	0
55	MG	1A	3326	1/1	0.88	0.35	26,26,26,26	0
55	MG	2A	3207	1/1	0.88	0.41	48,48,48,48	0
55	MG	1A	3406	1/1	0.88	0.25	31,31,31,31	0
55	MG	1a	3093	1/1	0.88	0.20	53,53,53,53	0
55	MG	1a	3187	1/1	0.88	0.34	76,76,76,76	0
55	MG	2A	3074	1/1	0.88	0.21	44,44,44,44	0
55	MG	1A	3762	1/1	0.88	0.15	30,30,30,30	0
55	MG	1A	3133	1/1	0.88	0.10	27,27,27,27	0
55	MG	2a	1624	1/1	0.88	0.18	38,38,38,38	0
55	MG	1A	3026	1/1	0.88	0.12	52,52,52,52	0
55	MG	2A	3345	1/1	0.88	0.60	41,41,41,41	0
55	MG	1a	3047	1/1	0.88	0.11	55,55,55,55	0
55	MG	2a	1645	1/1	0.88	0.47	46,46,46,46	0
55	MG	1A	3943	1/1	0.88	0.19	41,41,41,41	0
55	MG	2A	3728	1/1	0.88	0.15	57,57,57,57	0
55	MG	1A	3587	1/1	0.88	0.11	37,37,37,37	0
55	MG	2a	1616	1/1	0.88	0.13	52,52,52,52	0
55	MG	2A	3759	1/1	0.88	0.18	43,43,43,43	0
55	MG	2A	3319	1/1	0.88	0.32	38,38,38,38	0
55	MG	2A	3349	1/1	0.88	0.18	49,49,49,49	0
55	MG	1A	3104	1/1	0.88	0.91	32,32,32,32	0
55	MG	2A	3201	1/1	0.88	0.20	51,51,51,51	0
55	MG	1x	106	1/1	0.88	0.21	39,39,39,39	0
55	MG	1a	3166	1/1	0.88	0.13	84,84,84,84	0
55	MG	2A	3587	1/1	0.88	0.25	60,60,60,60	0
55	MG	1A	3898	1/1	0.88	0.20	54,54,54,54	0
55	MG	2A	3340	1/1	0.88	0.21	43,43,43,43	0
55	MG	1Q	203	1/1	0.88	0.19	45,45,45,45	0
55	MG	2A	3172	1/1	0.88	0.28	43,43,43,43	0
55	MG	2A	3774	1/1	0.88	0.20	58,58,58,58	0
55	MG	17	102	1/1	0.88	0.33	18,18,18,18	0
55	MG	1A	4036	1/1	0.88	0.17	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	1A	3281	1/1	0.88	0.12	12,12,12,12	0
55	MG	2B	212	1/1	0.88	0.21	60,60,60,60	0
55	MG	1A	3967	1/1	0.88	0.14	38,38,38,38	0
55	MG	1A	3143	1/1	0.88	0.38	28,28,28,28	0
55	MG	2a	1776	1/1	0.88	0.11	55,55,55,55	0
55	MG	2a	1762	1/1	0.88	0.13	55,55,55,55	0
55	MG	1B	230	1/1	0.88	0.32	44,44,44,44	0
55	MG	2A	3336	1/1	0.88	0.71	59,59,59,59	0
55	MG	2A	3544	1/1	0.88	0.28	48,48,48,48	0
55	MG	2A	3304	1/1	0.88	0.52	39,39,39,39	0
55	MG	2a	1691	1/1	0.88	0.20	53,53,53,53	0
55	MG	2A	3705	1/1	0.88	0.13	55,55,55,55	0
55	MG	1a	3104	1/1	0.88	0.49	48,48,48,48	0
55	MG	2A	3850	1/1	0.88	0.34	54,54,54,54	0
55	MG	1D	309	1/1	0.88	0.45	21,21,21,21	0
55	MG	1x	104	1/1	0.88	0.12	46,46,46,46	0
55	MG	2A	3428	1/1	0.88	0.35	58,58,58,58	0
55	MG	1a	3004	1/1	0.88	0.25	57,57,57,57	0
55	MG	1A	3820	1/1	0.88	0.15	14,14,14,14	0
55	MG	1A	3518	1/1	0.88	0.72	45,45,45,45	0
55	MG	2a	1782	1/1	0.88	0.16	40,40,40,40	0
55	MG	2A	3409	1/1	0.88	0.12	28,28,28,28	0
55	MG	1B	231	1/1	0.88	0.13	39,39,39,39	0
55	MG	2A	3051	1/1	0.88	0.10	42,42,42,42	0
55	MG	1A	3506	1/1	0.88	0.16	23,23,23,23	0
55	MG	2a	1651	1/1	0.88	0.10	58,58,58,58	0
55	MG	2A	3732	1/1	0.88	0.16	28,28,28,28	0
55	MG	1A	3198	1/1	0.88	0.22	29,29,29,29	0
55	MG	2A	3251	1/1	0.88	0.41	21,21,21,21	0
55	MG	1A	3200	1/1	0.88	0.26	37,37,37,37	0
55	MG	1A	3475	1/1	0.88	0.62	27,27,27,27	0
55	MG	1a	3016	1/1	0.88	0.53	46,46,46,46	0
55	MG	2A	3243	1/1	0.88	0.32	51,51,51,51	0
55	MG	2B	216	1/1	0.88	0.15	57,57,57,57	0
55	MG	2A	3836	1/1	0.88	0.21	39,39,39,39	0
55	MG	2A	3545	1/1	0.88	0.20	57,57,57,57	0
55	MG	2a	1749	1/1	0.88	0.21	53,53,53,53	0
55	MG	1a	3094	1/1	0.88	0.66	41,41,41,41	0
55	MG	2A	3504	1/1	0.88	0.27	37,37,37,37	0
55	MG	1A	3752	1/1	0.88	0.48	24,24,24,24	0
55	MG	1A	3822	1/1	0.88	0.11	26,26,26,26	0
55	MG	2a	1603	1/1	0.88	0.10	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	2t	201	1/1	0.88	0.14	36,36,36,36	0
55	MG	2F	304	1/1	0.88	0.17	54,54,54,54	0
55	MG	1a	3142	1/1	0.88	0.37	44,44,44,44	0
55	MG	2a	1649	1/1	0.88	0.19	62,62,62,62	0
55	MG	1A	3726	1/1	0.88	0.08	18,18,18,18	0
55	MG	1a	3009	1/1	0.88	0.20	28,28,28,28	0
55	MG	2A	3101	1/1	0.89	0.19	30,30,30,30	0
55	MG	1A	3602	1/1	0.89	0.12	28,28,28,28	0
55	MG	1A	3714	1/1	0.89	0.12	11,11,11,11	0
55	MG	2a	1789	1/1	0.89	0.07	44,44,44,44	0
55	MG	1A	3228	1/1	0.89	0.24	30,30,30,30	0
55	MG	1A	4003	1/1	0.89	0.20	42,42,42,42	0
55	MG	1B	235	1/1	0.89	0.10	38,38,38,38	0
55	MG	2A	3453	1/1	0.89	0.11	31,31,31,31	0
55	MG	1R	207	1/1	0.89	0.43	55,55,55,55	0
55	MG	1A	3184	1/1	0.89	0.45	43,43,43,43	0
55	MG	1a	3054	1/1	0.89	0.23	46,46,46,46	0
55	MG	1A	3030	1/1	0.89	0.68	21,21,21,21	0
55	MG	2a	1794	1/1	0.89	0.12	51,51,51,51	0
55	MG	2A	3155	1/1	0.89	0.13	54,54,54,54	0
55	MG	2A	3113	1/1	0.89	0.11	50,50,50,50	0
55	MG	2A	3764	1/1	0.89	0.17	37,37,37,37	0
55	MG	1A	3498	1/1	0.89	0.12	25,25,25,25	0
55	MG	1a	3062	1/1	0.89	0.14	51,51,51,51	0
55	MG	2A	3087	1/1	0.89	0.13	31,31,31,31	0
55	MG	1A	3189	1/1	0.89	0.43	22,22,22,22	0
55	MG	1A	3957	1/1	0.89	0.50	63,63,63,63	0
55	MG	1A	3965	1/1	0.89	0.20	27,27,27,27	0
55	MG	2A	3658	1/1	0.89	0.42	52,52,52,52	0
55	MG	2A	3584	1/1	0.89	0.11	40,40,40,40	0
55	MG	1W	204	1/1	0.89	0.43	43,43,43,43	0
55	MG	1A	3293	1/1	0.89	0.17	41,41,41,41	0
55	MG	1A	3737	1/1	0.89	0.10	33,33,33,33	0
55	MG	1A	3615	1/1	0.89	0.15	15,15,15,15	0
55	MG	1A	3760	1/1	0.89	0.13	22,22,22,22	0
55	MG	1A	4034	1/1	0.89	0.41	54,54,54,54	0
55	MG	1A	3199	1/1	0.89	0.15	43,43,43,43	0
55	MG	2A	3237	1/1	0.89	0.68	40,40,40,40	0
55	MG	2A	3672	1/1	0.89	0.20	39,39,39,39	0
55	MG	2A	3765	1/1	0.89	0.16	54,54,54,54	0
55	MG	1B	225	1/1	0.89	0.13	49,49,49,49	0
55	MG	1a	3189	1/1	0.89	0.14	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	1a	3116	1/1	0.89	0.18	32,32,32,32	0
55	MG	1A	3167	1/1	0.89	0.75	30,30,30,30	0
55	MG	1A	3601	1/1	0.89	0.13	47,47,47,47	0
55	MG	1A	3524	1/1	0.89	0.12	35,35,35,35	0
55	MG	2a	1751	1/1	0.89	0.08	34,34,34,34	0
55	MG	2A	3466	1/1	0.89	0.14	45,45,45,45	0
55	MG	1A	3348	1/1	0.89	0.20	28,28,28,28	0
55	MG	1A	3355	1/1	0.89	0.45	37,37,37,37	0
55	MG	1A	3070	1/1	0.89	0.15	41,41,41,41	0
55	MG	2A	3217	1/1	0.89	0.21	50,50,50,50	0
55	MG	1A	3702	1/1	0.89	0.13	21,21,21,21	0
55	MG	2A	3456	1/1	0.89	0.16	38,38,38,38	0
55	MG	2Q	202	1/1	0.89	0.21	38,38,38,38	0
55	MG	2A	3425	1/1	0.89	0.29	42,42,42,42	0
55	MG	2E	305	1/1	0.89	0.15	27,27,27,27	0
55	MG	1A	3433	1/1	0.89	0.21	28,28,28,28	0
55	MG	2X	101	1/1	0.89	0.15	34,34,34,34	0
55	MG	1a	3088	1/1	0.89	0.19	51,51,51,51	0
55	MG	2A	3091	1/1	0.89	0.16	58,58,58,58	0
55	MG	2a	1626	1/1	0.89	0.66	46,46,46,46	0
55	MG	2A	3675	1/1	0.89	0.09	42,42,42,42	0
55	MG	2A	3403	1/1	0.89	0.17	35,35,35,35	0
55	MG	2a	1673	1/1	0.89	0.25	50,50,50,50	0
55	MG	1A	3179	1/1	0.89	0.15	44,44,44,44	0
55	MG	2a	1656	1/1	0.89	0.14	44,44,44,44	0
55	MG	1v	103	1/1	0.89	0.14	55,55,55,55	0
55	MG	1a	3089	1/1	0.89	0.15	49,49,49,49	0
55	MG	2A	3711	1/1	0.89	0.18	47,47,47,47	0
55	MG	1A	3680	1/1	0.89	0.11	37,37,37,37	0
58	V7A	2a	1817	35/35	0.89	0.51	61,80,87,88	0
55	MG	2A	3775	1/1	0.89	0.14	30,30,30,30	0
55	MG	1A	3611	1/1	0.89	0.14	59,59,59,59	0
55	MG	2a	1709	1/1	0.89	0.11	44,44,44,44	0
55	MG	16	103	1/1	0.89	0.56	42,42,42,42	0
57	ZN	15	105	1/1	0.89	0.35	155,155,155,155	0
55	MG	2A	3613	1/1	0.89	0.23	28,28,28,28	0
55	MG	2A	3364	1/1	0.89	0.21	33,33,33,33	0
55	MG	1B	211	1/1	0.89	0.35	39,39,39,39	0
55	MG	1a	3122	1/1	0.89	0.12	42,42,42,42	0
55	MG	2A	3314	1/1	0.89	0.11	39,39,39,39	0
55	MG	1A	3025	1/1	0.89	0.27	51,51,51,51	0
55	MG	2A	3376	1/1	0.89	0.18	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	2A	3356	1/1	0.90	0.20	36,36,36,36	0
55	MG	2A	3279	1/1	0.90	0.14	33,33,33,33	0
55	MG	2A	3659	1/1	0.90	0.14	41,41,41,41	0
55	MG	2a	1640	1/1	0.90	0.13	42,42,42,42	0
55	MG	2A	3015	1/1	0.90	0.14	55,55,55,55	0
55	MG	2A	3291	1/1	0.90	0.15	39,39,39,39	0
55	MG	2A	3424	1/1	0.90	0.11	40,40,40,40	0
55	MG	2A	3090	1/1	0.90	0.16	40,40,40,40	0
55	MG	2A	3162	1/1	0.90	0.23	37,37,37,37	0
55	MG	1A	3125	1/1	0.90	0.14	29,29,29,29	0
55	MG	1A	3704	1/1	0.90	0.10	41,41,41,41	0
55	MG	2A	3398	1/1	0.90	0.18	38,38,38,38	0
55	MG	1A	3314	1/1	0.90	0.19	29,29,29,29	0
55	MG	2a	1666	1/1	0.90	0.07	44,44,44,44	0
55	MG	1A	3158	1/1	0.90	0.21	58,58,58,58	0
55	MG	2a	1642	1/1	0.90	0.12	43,43,43,43	0
55	MG	1x	112	1/1	0.90	0.12	51,51,51,51	0
55	MG	1a	3149	1/1	0.90	0.18	56,56,56,56	0
55	MG	2A	3560	1/1	0.90	0.10	23,23,23,23	0
55	MG	2a	1748	1/1	0.90	0.11	61,61,61,61	0
55	MG	1A	3583	1/1	0.90	0.11	43,43,43,43	0
55	MG	2A	3039	1/1	0.90	0.11	32,32,32,32	0
55	MG	2a	1685	1/1	0.90	0.75	51,51,51,51	0
55	MG	1A	3590	1/1	0.90	0.14	21,21,21,21	0
55	MG	2A	3817	1/1	0.90	0.13	55,55,55,55	0
55	MG	1A	3287	1/1	0.90	0.20	48,48,48,48	0
55	MG	1A	3497	1/1	0.90	0.14	37,37,37,37	0
55	MG	1a	3049	1/1	0.90	0.12	63,63,63,63	0
55	MG	2A	3346	1/1	0.90	0.26	47,47,47,47	0
55	MG	1A	3447	1/1	0.90	0.24	33,33,33,33	0
55	MG	2A	3143	1/1	0.90	0.51	44,44,44,44	0
55	MG	2A	3531	1/1	0.90	0.10	43,43,43,43	0
55	MG	2A	3042	1/1	0.90	0.30	42,42,42,42	0
55	MG	1A	3270	1/1	0.90	0.14	41,41,41,41	0
55	MG	2A	3028	1/1	0.90	0.18	35,35,35,35	0
55	MG	1A	3057	1/1	0.90	0.16	18,18,18,18	0
55	MG	1A	3481	1/1	0.90	0.80	31,31,31,31	0
55	MG	1a	3012	1/1	0.90	0.17	43,43,43,43	0
55	MG	2A	3359	1/1	0.90	0.21	33,33,33,33	0
55	MG	1e	201	1/1	0.90	0.17	54,54,54,54	0
55	MG	2A	3697	1/1	0.90	0.06	30,30,30,30	0
55	MG	1A	3735	1/1	0.90	0.32	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	2a	1727	1/1	0.90	0.15	44,44,44,44	0
55	MG	2A	3709	1/1	0.90	0.09	42,42,42,42	0
55	MG	1A	3004	1/1	0.90	0.59	25,25,25,25	0
55	MG	2A	3218	1/1	0.90	0.41	43,43,43,43	0
55	MG	1A	3193	1/1	0.90	0.11	15,15,15,15	0
55	MG	2a	1778	1/1	0.90	0.32	61,61,61,61	0
55	MG	2A	3282	1/1	0.90	0.40	49,49,49,49	0
55	MG	2a	1755	1/1	0.90	0.11	44,44,44,44	0
55	MG	2A	3689	1/1	0.90	0.19	51,51,51,51	0
55	MG	1A	3448	1/1	0.90	0.08	37,37,37,37	0
55	MG	2A	3244	1/1	0.90	0.09	35,35,35,35	0
55	MG	2A	3098	1/1	0.90	0.10	42,42,42,42	0
55	MG	2A	3111	1/1	0.90	0.11	56,56,56,56	0
55	MG	1a	3181	1/1	0.90	0.19	48,48,48,48	0
55	MG	1A	3006	1/1	0.90	0.52	25,25,25,25	0
55	MG	1A	3172	1/1	0.90	0.45	22,22,22,22	0
55	MG	2A	3778	1/1	0.90	0.20	50,50,50,50	0
55	MG	2A	3057	1/1	0.90	0.12	38,38,38,38	0
55	MG	2A	3460	1/1	0.90	0.09	32,32,32,32	0
55	MG	2a	1702	1/1	0.90	0.16	55,55,55,55	0
55	MG	2A	3768	1/1	0.90	0.22	35,35,35,35	0
55	MG	2A	3005	1/1	0.90	0.12	45,45,45,45	0
55	MG	1B	215	1/1	0.90	0.23	56,56,56,56	0
55	MG	2A	3494	1/1	0.90	0.47	50,50,50,50	0
55	MG	1A	3600	1/1	0.90	0.21	33,33,33,33	0
55	MG	2A	3701	1/1	0.90	0.23	48,48,48,48	0
55	MG	2A	3161	1/1	0.90	0.14	51,51,51,51	0
55	MG	2A	3621	1/1	0.90	0.15	21,21,21,21	0
55	MG	2a	1792	1/1	0.90	0.16	72,72,72,72	0
55	MG	2A	3235	1/1	0.90	0.29	34,34,34,34	0
55	MG	2A	3414	1/1	0.90	0.40	28,28,28,28	0
55	MG	2I	101	1/1	0.90	0.14	37,37,37,37	0
55	MG	2F	306	1/1	0.90	0.11	54,54,54,54	0
55	MG	2A	3326	1/1	0.90	0.11	34,34,34,34	0
55	MG	2A	3442	1/1	0.90	0.14	33,33,33,33	0
55	MG	1A	3933	1/1	0.90	0.17	51,51,51,51	0
55	MG	2a	1721	1/1	0.90	0.09	57,57,57,57	0
55	MG	1A	3252	1/1	0.90	0.59	35,35,35,35	0
55	MG	1A	3493	1/1	0.90	0.15	37,37,37,37	0
55	MG	2P	203	1/1	0.90	0.38	46,46,46,46	0
55	MG	1A	3691	1/1	0.90	0.14	26,26,26,26	0
55	MG	2A	3135	1/1	0.90	0.28	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	2A	3634	1/1	0.90	0.24	40,40,40,40	0
55	MG	2A	3156	1/1	0.90	0.74	32,32,32,32	0
55	MG	1V	203	1/1	0.90	0.17	22,22,22,22	0
55	MG	2A	3014	1/1	0.90	0.26	21,21,21,21	0
55	MG	2A	3112	1/1	0.90	0.19	42,42,42,42	0
55	MG	2a	1676	1/1	0.90	0.12	40,40,40,40	0
55	MG	2A	3092	1/1	0.91	0.17	44,44,44,44	0
55	MG	1A	3908	1/1	0.91	0.12	29,29,29,29	0
55	MG	1A	3479	1/1	0.91	0.17	48,48,48,48	0
55	MG	2a	1813	1/1	0.91	0.40	63,63,63,63	0
55	MG	2a	1621	1/1	0.91	0.23	40,40,40,40	0
55	MG	1A	3169	1/1	0.91	0.08	38,38,38,38	0
55	MG	2A	3045	1/1	0.91	0.17	45,45,45,45	0
55	MG	2g	201	1/1	0.91	0.11	65,65,65,65	0
55	MG	1A	4010	1/1	0.91	0.13	54,54,54,54	0
55	MG	1A	3013	1/1	0.91	0.28	20,20,20,20	0
55	MG	2A	3122	1/1	0.91	0.14	49,49,49,49	0
55	MG	1a	3081	1/1	0.91	0.14	41,41,41,41	0
55	MG	1a	3212	1/1	0.91	0.12	66,66,66,66	0
55	MG	2A	3222	1/1	0.91	0.24	47,47,47,47	0
55	MG	2A	3392	1/1	0.91	0.23	25,25,25,25	0
55	MG	1A	3606	1/1	0.91	0.09	28,28,28,28	0
55	MG	1a	3042	1/1	0.91	0.16	53,53,53,53	0
55	MG	2A	3612	1/1	0.91	0.15	26,26,26,26	0
55	MG	2A	3763	1/1	0.91	0.13	60,60,60,60	0
55	MG	2A	3740	1/1	0.91	0.11	42,42,42,42	0
55	MG	1A	3875	1/1	0.91	0.12	39,39,39,39	0
55	MG	2A	3595	1/1	0.91	0.13	45,45,45,45	0
55	MG	1A	3295	1/1	0.91	0.16	26,26,26,26	0
55	MG	2a	1647	1/1	0.91	0.10	60,60,60,60	0
55	MG	1a	3085	1/1	0.91	0.20	38,38,38,38	0
55	MG	2W	201	1/1	0.91	0.48	45,45,45,45	0
55	MG	2j	202	1/1	0.91	0.28	49,49,49,49	0
55	MG	2A	3223	1/1	0.91	0.67	51,51,51,51	0
55	MG	2A	3317	1/1	0.91	0.25	49,49,49,49	0
55	MG	1A	3324	1/1	0.91	0.16	31,31,31,31	0
55	MG	1a	3101	1/1	0.91	0.15	45,45,45,45	0
55	MG	2A	3461	1/1	0.91	0.10	51,51,51,51	0
55	MG	2A	3016	1/1	0.91	0.34	33,33,33,33	0
55	MG	2A	3252	1/1	0.91	0.30	36,36,36,36	0
55	MG	2A	3250	1/1	0.91	0.11	44,44,44,44	0
55	MG	2a	1667	1/1	0.91	0.12	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	V7A	1a	3213	35/35	0.91	0.31	47,61,72,74	0
55	MG	1A	4037	1/1	0.91	0.27	33,33,33,33	0
55	MG	2A	3429	1/1	0.91	0.25	32,32,32,32	0
55	MG	1A	3313	1/1	0.91	0.12	21,21,21,21	0
55	MG	1A	3697	1/1	0.91	0.18	32,32,32,32	0
55	MG	1a	3003	1/1	0.91	0.11	54,54,54,54	0
55	MG	2A	3064	1/1	0.91	0.13	33,33,33,33	0
55	MG	2a	1639	1/1	0.91	0.13	34,34,34,34	0
55	MG	1A	3707	1/1	0.91	0.25	24,24,24,24	0
55	MG	1A	3339	1/1	0.91	1.00	33,33,33,33	0
55	MG	2a	1606	1/1	0.91	0.15	30,30,30,30	0
55	MG	1A	3492	1/1	0.91	0.12	47,47,47,47	0
55	MG	1A	3330	1/1	0.91	0.47	33,33,33,33	0
55	MG	1A	3683	1/1	0.91	0.13	39,39,39,39	0
55	MG	1A	3720	1/1	0.91	0.09	56,56,56,56	0
55	MG	1A	3767	1/1	0.91	0.10	40,40,40,40	0
55	MG	2A	3643	1/1	0.91	0.16	43,43,43,43	0
55	MG	2A	3128	1/1	0.91	0.34	36,36,36,36	0
55	MG	2B	217	1/1	0.91	0.20	53,53,53,53	0
55	MG	1a	3059	1/1	0.91	0.25	41,41,41,41	0
55	MG	1A	3062	1/1	0.91	0.13	36,36,36,36	0
55	MG	1A	3502	1/1	0.91	0.10	24,24,24,24	0
55	MG	1A	3750	1/1	0.91	0.13	58,58,58,58	0
55	MG	1A	3161	1/1	0.91	0.52	29,29,29,29	0
55	MG	28	101	1/1	0.91	0.16	31,31,31,31	0
55	MG	2A	3256	1/1	0.91	0.29	55,55,55,55	0
55	MG	1a	3048	1/1	0.91	0.16	64,64,64,64	0
55	MG	2A	3280	1/1	0.91	0.12	39,39,39,39	0
55	MG	1a	3148	1/1	0.91	0.16	40,40,40,40	0
55	MG	1A	3932	1/1	0.91	0.19	15,15,15,15	0
55	MG	1A	3608	1/1	0.91	0.24	19,19,19,19	0
55	MG	1A	3588	1/1	0.91	0.24	35,35,35,35	0
55	MG	2A	3770	1/1	0.91	0.38	45,45,45,45	0
55	MG	2a	1756	1/1	0.91	0.16	33,33,33,33	0
55	MG	2A	3170	1/1	0.91	0.21	47,47,47,47	0
55	MG	1A	3063	1/1	0.91	0.15	21,21,21,21	0
55	MG	1B	234	1/1	0.91	0.20	48,48,48,48	0
55	MG	2A	3055	1/1	0.91	0.08	48,48,48,48	0
55	MG	1Y	201	1/1	0.91	0.25	33,33,33,33	0
55	MG	1A	3507	1/1	0.91	0.12	37,37,37,37	0
55	MG	1A	3610	1/1	0.91	0.34	24,24,24,24	0
55	MG	1X	102	1/1	0.91	0.67	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	1A	3411	1/1	0.91	0.19	29,29,29,29	0
55	MG	2A	3693	1/1	0.91	0.15	20,20,20,20	0
55	MG	1a	3030	1/1	0.91	0.21	50,50,50,50	0
55	MG	1A	3315	1/1	0.91	0.29	21,21,21,21	0
55	MG	1a	3067	1/1	0.91	0.12	34,34,34,34	0
55	MG	1A	3364	1/1	0.91	0.20	43,43,43,43	0
55	MG	1A	3271	1/1	0.91	0.23	32,32,32,32	0
55	MG	2A	3054	1/1	0.91	0.14	43,43,43,43	0
55	MG	1A	3069	1/1	0.91	0.21	29,29,29,29	0
55	MG	1P	206	1/1	0.91	0.55	34,34,34,34	0
55	MG	1A	3227	1/1	0.91	0.11	37,37,37,37	0
55	MG	2A	3480	1/1	0.91	0.13	38,38,38,38	0
55	MG	1A	3986	1/1	0.91	0.14	23,23,23,23	0
55	MG	2A	3848	1/1	0.91	0.13	31,31,31,31	0
55	MG	2A	3180	1/1	0.91	0.47	38,38,38,38	0
55	MG	1A	3496	1/1	0.91	0.25	26,26,26,26	0
55	MG	1A	3405	1/1	0.91	0.34	32,32,32,32	0
55	MG	1A	3401	1/1	0.91	0.15	37,37,37,37	0
55	MG	1A	3360	1/1	0.91	0.56	28,28,28,28	0
55	MG	2A	3630	1/1	0.91	0.20	32,32,32,32	0
55	MG	2A	3526	1/1	0.91	0.09	27,27,27,27	0
55	MG	1A	3322	1/1	0.91	0.15	20,20,20,20	0
55	MG	2A	3582	1/1	0.91	0.18	33,33,33,33	0
55	MG	1A	3113	1/1	0.91	0.13	36,36,36,36	0
55	MG	1D	305	1/1	0.91	0.42	20,20,20,20	0
55	MG	2A	3766	1/1	0.91	0.26	37,37,37,37	0
55	MG	1A	3320	1/1	0.91	0.52	28,28,28,28	0
55	MG	1a	3202	1/1	0.91	0.17	47,47,47,47	0
55	MG	2A	3593	1/1	0.91	0.16	50,50,50,50	0
55	MG	2A	3240	1/1	0.91	0.14	29,29,29,29	0
55	MG	1A	3463	1/1	0.91	0.32	45,45,45,45	0
55	MG	2A	3184	1/1	0.91	0.16	29,29,29,29	0
55	MG	2a	1724	1/1	0.91	0.11	49,49,49,49	0
55	MG	1U	202	1/1	0.91	0.17	28,28,28,28	0
55	MG	1A	3586	1/1	0.91	0.17	31,31,31,31	0
55	MG	2A	3178	1/1	0.91	0.14	42,42,42,42	0
55	MG	1A	3924	1/1	0.91	0.49	47,47,47,47	0
55	MG	1A	3080	1/1	0.91	0.53	41,41,41,41	0
55	MG	2A	3263	1/1	0.91	0.09	33,33,33,33	0
55	MG	1A	3427	1/1	0.91	0.10	22,22,22,22	0
55	MG	1A	3521	1/1	0.91	0.17	25,25,25,25	0
55	MG	1A	4039	1/1	0.91	0.53	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	2A	3379	1/1	0.91	0.17	43,43,43,43	0
55	MG	1A	3468	1/1	0.91	0.24	34,34,34,34	0
55	MG	2A	3629	1/1	0.91	0.51	39,39,39,39	0
55	MG	1A	3192	1/1	0.91	0.74	39,39,39,39	0
55	MG	2A	3528	1/1	0.91	0.15	24,24,24,24	0
55	MG	2A	3131	1/1	0.91	0.09	49,49,49,49	0
55	MG	1A	3852	1/1	0.91	0.10	62,62,62,62	0
55	MG	2a	1716	1/1	0.91	0.08	47,47,47,47	0
55	MG	1O	205	1/1	0.91	0.25	31,31,31,31	0
55	MG	2A	3149	1/1	0.91	0.20	43,43,43,43	0
55	MG	1A	3706	1/1	0.91	0.12	39,39,39,39	0
55	MG	2A	3550	1/1	0.91	0.12	10,10,10,10	0
55	MG	1A	3568	1/1	0.91	0.24	31,31,31,31	0
55	MG	2a	1601	1/1	0.91	0.29	23,23,23,23	0
55	MG	1A	3147	1/1	0.91	0.10	41,41,41,41	0
55	MG	1A	3529	1/1	0.91	0.25	38,38,38,38	0
55	MG	1A	3938	1/1	0.91	0.17	18,18,18,18	0
55	MG	1A	3066	1/1	0.91	0.23	23,23,23,23	0
55	MG	1A	4024	1/1	0.91	0.16	35,35,35,35	0
55	MG	1t	201	1/1	0.91	0.21	42,42,42,42	0
55	MG	2A	3351	1/1	0.91	0.10	38,38,38,38	0
55	MG	1A	3589	1/1	0.91	0.13	25,25,25,25	0
55	MG	2a	1805	1/1	0.91	0.30	50,50,50,50	0
55	MG	1A	3736	1/1	0.91	0.10	33,33,33,33	0
55	MG	1E	306	1/1	0.91	0.18	33,33,33,33	0
55	MG	2A	3714	1/1	0.91	0.11	56,56,56,56	0
55	MG	1a	3105	1/1	0.91	0.15	35,35,35,35	0
55	MG	2l	201	1/1	0.91	0.76	47,47,47,47	0
55	MG	1A	3994	1/1	0.91	0.13	10,10,10,10	0
55	MG	2A	3362	1/1	0.91	0.11	42,42,42,42	0
55	MG	1A	3678	1/1	0.91	0.13	16,16,16,16	0
55	MG	1a	3144	1/1	0.91	0.12	56,56,56,56	0
55	MG	1A	3027	1/1	0.92	0.40	28,28,28,28	0
55	MG	1A	3055	1/1	0.92	0.15	29,29,29,29	0
55	MG	2A	3258	1/1	0.92	0.14	23,23,23,23	0
55	MG	2a	1787	1/1	0.92	0.13	49,49,49,49	0
55	MG	2A	3205	1/1	0.92	0.14	54,54,54,54	0
55	MG	2A	3645	1/1	0.92	0.20	49,49,49,49	0
55	MG	1E	311	1/1	0.92	0.24	48,48,48,48	0
55	MG	1A	3998	1/1	0.92	0.10	44,44,44,44	0
55	MG	1a	3162	1/1	0.92	0.35	47,47,47,47	0
55	MG	1a	3200	1/1	0.92	0.13	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	2A	3733	1/1	0.92	0.20	15,15,15,15	0
55	MG	2A	3174	1/1	0.92	0.31	33,33,33,33	0
55	MG	1a	3121	1/1	0.92	0.12	54,54,54,54	0
55	MG	1A	3240	1/1	0.92	0.20	31,31,31,31	0
55	MG	1A	3787	1/1	0.92	0.10	58,58,58,58	0
55	MG	1A	3734	1/1	0.92	0.20	12,12,12,12	0
55	MG	2A	3076	1/1	0.92	0.24	30,30,30,30	0
55	MG	2A	3720	1/1	0.92	0.18	44,44,44,44	0
55	MG	2A	3134	1/1	0.92	0.15	40,40,40,40	0
55	MG	1A	3280	1/1	0.92	0.20	19,19,19,19	0
55	MG	1A	3644	1/1	0.92	0.18	28,28,28,28	0
55	MG	2A	3651	1/1	0.92	0.14	48,48,48,48	0
55	MG	1A	3009	1/1	0.92	0.10	32,32,32,32	0
55	MG	1A	3215	1/1	0.92	0.11	44,44,44,44	0
55	MG	2A	3841	1/1	0.92	0.48	53,53,53,53	0
55	MG	1A	3751	1/1	0.92	0.15	44,44,44,44	0
55	MG	1a	3170	1/1	0.92	0.11	36,36,36,36	0
55	MG	2a	1706	1/1	0.92	0.17	30,30,30,30	0
55	MG	2A	3059	1/1	0.92	0.18	32,32,32,32	0
55	MG	2A	3444	1/1	0.92	1.16	36,36,36,36	0
55	MG	1A	3284	1/1	0.92	0.13	14,14,14,14	0
55	MG	2a	1775	1/1	0.92	0.12	68,68,68,68	0
55	MG	2A	3191	1/1	0.92	0.11	50,50,50,50	0
55	MG	1a	3007	1/1	0.92	0.18	27,27,27,27	0
55	MG	1A	3715	1/1	0.92	0.09	21,21,21,21	0
55	MG	1A	3877	1/1	0.92	0.12	37,37,37,37	0
55	MG	1A	3180	1/1	0.92	0.30	56,56,56,56	0
55	MG	2A	3514	1/1	0.92	0.10	51,51,51,51	0
55	MG	2A	3716	1/1	0.92	0.09	45,45,45,45	0
55	MG	2a	1780	1/1	0.92	0.47	62,62,62,62	0
55	MG	1A	3336	1/1	0.92	0.57	32,32,32,32	0
55	MG	1A	3472	1/1	0.92	0.14	30,30,30,30	0
55	MG	1A	3915	1/1	0.92	0.22	53,53,53,53	0
55	MG	2A	3416	1/1	0.92	0.12	33,33,33,33	0
55	MG	2B	220	1/1	0.92	0.20	50,50,50,50	0
55	MG	1A	3412	1/1	0.92	0.12	27,27,27,27	0
55	MG	2A	3832	1/1	0.92	0.18	36,36,36,36	0
55	MG	2a	1712	1/1	0.92	0.15	41,41,41,41	0
55	MG	1a	3090	1/1	0.92	0.23	46,46,46,46	0
55	MG	1A	3159	1/1	0.92	0.13	28,28,28,28	0
55	MG	1G	201	1/1	0.92	0.13	30,30,30,30	0
55	MG	1B	214	1/1	0.92	0.26	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	2A	3041	1/1	0.92	0.14	29,29,29,29	0
55	MG	1a	3072	1/1	0.92	0.17	60,60,60,60	0
55	MG	2a	1798	1/1	0.92	0.15	53,53,53,53	0
55	MG	1A	3288	1/1	0.92	0.31	27,27,27,27	0
55	MG	2A	3094	1/1	0.92	0.31	49,49,49,49	0
55	MG	2A	3794	1/1	0.92	0.11	37,37,37,37	0
55	MG	1A	3333	1/1	0.92	0.41	30,30,30,30	0
55	MG	2A	3194	1/1	0.92	0.29	26,26,26,26	0
55	MG	2A	3241	1/1	0.92	0.68	32,32,32,32	0
55	MG	1A	3311	1/1	0.92	0.55	41,41,41,41	0
55	MG	1A	3400	1/1	0.92	0.15	27,27,27,27	0
55	MG	2a	1814	1/1	0.92	0.24	46,46,46,46	0
55	MG	1A	3744	1/1	0.92	0.82	21,21,21,21	0
55	MG	1A	4001	1/1	0.92	0.12	41,41,41,41	0
55	MG	1A	3868	1/1	0.92	0.11	29,29,29,29	0
55	MG	2A	3731	1/1	0.92	0.28	46,46,46,46	0
55	MG	1a	3079	1/1	0.92	0.16	41,41,41,41	0
55	MG	1A	3897	1/1	0.92	0.24	42,42,42,42	0
55	MG	2A	3762	1/1	0.92	0.46	67,67,67,67	0
55	MG	2A	3589	1/1	0.92	0.14	42,42,42,42	0
55	MG	2a	1743	1/1	0.92	0.14	38,38,38,38	0
55	MG	2A	3614	1/1	0.92	0.20	13,13,13,13	0
55	MG	2A	3495	1/1	0.92	0.11	17,17,17,17	0
55	MG	2A	3616	1/1	0.92	0.21	44,44,44,44	0
55	MG	2A	3310	1/1	0.92	0.25	28,28,28,28	0
55	MG	2A	3536	1/1	0.92	0.17	15,15,15,15	0
55	MG	2A	3108	1/1	0.92	0.31	41,41,41,41	0
55	MG	2A	3095	1/1	0.92	0.12	37,37,37,37	0
55	MG	2a	1680	1/1	0.92	0.20	40,40,40,40	0
55	MG	1A	3904	1/1	0.92	0.12	32,32,32,32	0
55	MG	1A	3307	1/1	0.92	0.17	39,39,39,39	0
55	MG	1a	3107	1/1	0.92	0.25	36,36,36,36	0
55	MG	2A	3248	1/1	0.92	0.12	33,33,33,33	0
55	MG	1A	3435	1/1	0.92	0.10	54,54,54,54	0
55	MG	2A	3824	1/1	0.92	0.48	53,53,53,53	0
55	MG	2A	3655	1/1	0.92	0.43	26,26,26,26	0
55	MG	1A	3595	1/1	0.92	0.18	24,24,24,24	0
55	MG	2A	3511	1/1	0.92	0.10	27,27,27,27	0
55	MG	1a	3017	1/1	0.92	0.13	48,48,48,48	0
55	MG	2B	203	1/1	0.92	0.14	52,52,52,52	0
55	MG	2a	1718	1/1	0.92	0.18	38,38,38,38	0
55	MG	1G	204	1/1	0.92	0.14	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	1A	3205	1/1	0.92	0.16	18,18,18,18	0
55	MG	1A	3597	1/1	0.92	0.10	34,34,34,34	0
55	MG	2a	1646	1/1	0.92	0.07	58,58,58,58	0
55	MG	2A	3181	1/1	0.92	0.09	10,10,10,10	0
55	MG	2A	3752	1/1	0.92	0.07	30,30,30,30	0
55	MG	1B	228	1/1	0.92	0.11	33,33,33,33	0
55	MG	2A	3736	1/1	0.92	0.17	54,54,54,54	0
55	MG	1a	3005	1/1	0.92	0.23	51,51,51,51	0
55	MG	1A	3893	1/1	0.92	0.13	35,35,35,35	0
55	MG	1A	3622	1/1	0.92	0.24	39,39,39,39	0
55	MG	1A	3208	1/1	0.92	0.57	28,28,28,28	0
55	MG	2a	1759	1/1	0.92	0.19	50,50,50,50	0
55	MG	1U	208	1/1	0.92	0.38	36,36,36,36	0
55	MG	2A	3440	1/1	0.92	0.35	40,40,40,40	0
55	MG	2a	1767	1/1	0.92	0.20	52,52,52,52	0
55	MG	2A	3209	1/1	0.92	0.17	24,24,24,24	0
55	MG	2A	3302	1/1	0.92	0.40	40,40,40,40	0
55	MG	2A	3183	1/1	0.92	0.30	39,39,39,39	0
55	MG	1A	3684	1/1	0.92	0.13	52,52,52,52	0
55	MG	1A	4040	1/1	0.92	0.19	33,33,33,33	0
55	MG	2A	3213	1/1	0.92	0.40	32,32,32,32	0
55	MG	1A	3807	1/1	0.92	0.34	31,31,31,31	0
55	MG	2A	3193	1/1	0.92	0.29	52,52,52,52	0
55	MG	2a	1643	1/1	0.92	0.18	49,49,49,49	0
55	MG	2a	1671	1/1	0.92	0.12	42,42,42,42	0
55	MG	2a	1688	1/1	0.92	0.39	33,33,33,33	0
55	MG	1f	202	1/1	0.92	0.19	38,38,38,38	0
55	MG	2a	1741	1/1	0.92	0.16	59,59,59,59	0
55	MG	2A	3296	1/1	0.92	0.28	35,35,35,35	0
55	MG	2A	3785	1/1	0.92	0.21	43,43,43,43	0
55	MG	2A	3006	1/1	0.92	0.17	38,38,38,38	0
55	MG	2a	1768	1/1	0.92	0.19	36,36,36,36	0
55	MG	1a	3112	1/1	0.92	0.11	54,54,54,54	0
55	MG	2A	3530	1/1	0.92	0.19	45,45,45,45	0
55	MG	2k	201	1/1	0.92	0.11	54,54,54,54	0
55	MG	1a	3174	1/1	0.92	0.10	49,49,49,49	0
55	MG	2A	3457	1/1	0.92	0.10	54,54,54,54	0
55	MG	2T	202	1/1	0.92	0.14	39,39,39,39	0
55	MG	2B	213	1/1	0.92	0.26	50,50,50,50	0
55	MG	2a	1757	1/1	0.92	0.23	44,44,44,44	0
55	MG	1A	3437	1/1	0.92	0.21	29,29,29,29	0
55	MG	2A	3086	1/1	0.92	0.17	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	2A	3142	1/1	0.92	0.24	37,37,37,37	0
55	MG	1a	3169	1/1	0.92	0.10	55,55,55,55	0
55	MG	2A	3839	1/1	0.92	0.14	30,30,30,30	0
55	MG	2a	1744	1/1	0.92	0.58	72,72,72,72	0
55	MG	1A	3366	1/1	0.92	0.17	43,43,43,43	0
55	MG	2A	3275	1/1	0.92	0.13	45,45,45,45	0
55	MG	1V	202	1/1	0.92	0.78	35,35,35,35	0
55	MG	1A	3419	1/1	0.92	0.28	49,49,49,49	0
55	MG	2a	1654	1/1	0.92	0.09	35,35,35,35	0
55	MG	1A	3204	1/1	0.92	1.09	25,25,25,25	0
55	MG	2A	3067	1/1	0.92	0.16	27,27,27,27	0
55	MG	1A	3430	1/1	0.92	0.10	32,32,32,32	0
55	MG	27	102	1/1	0.92	0.51	36,36,36,36	0
55	MG	1A	3835	1/1	0.92	0.74	24,24,24,24	0
55	MG	1A	3012	1/1	0.92	0.74	27,27,27,27	0
55	MG	1A	3218	1/1	0.93	0.24	22,22,22,22	0
55	MG	1A	3273	1/1	0.93	0.10	26,26,26,26	0
55	MG	1P	204	1/1	0.93	1.23	19,19,19,19	0
55	MG	1A	3508	1/1	0.93	0.12	33,33,33,33	0
55	MG	1A	3780	1/1	0.93	0.20	41,41,41,41	0
55	MG	1A	3274	1/1	0.93	0.13	40,40,40,40	0
55	MG	1A	3570	1/1	0.93	0.38	43,43,43,43	0
55	MG	2A	3320	1/1	0.93	0.14	30,30,30,30	0
55	MG	2a	1613	1/1	0.93	0.10	45,45,45,45	0
55	MG	1A	3146	1/1	0.93	0.31	49,49,49,49	0
55	MG	2a	1810	1/1	0.93	0.08	66,66,66,66	0
55	MG	2a	1681	1/1	0.93	0.79	54,54,54,54	0
55	MG	1A	3911	1/1	0.93	0.25	47,47,47,47	0
55	MG	2A	3436	1/1	0.93	0.64	33,33,33,33	0
55	MG	2A	3449	1/1	0.93	0.15	32,32,32,32	0
55	MG	2a	1770	1/1	0.93	0.12	40,40,40,40	0
55	MG	1A	3001	1/1	0.93	0.28	26,26,26,26	0
55	MG	2A	3331	1/1	0.93	0.21	45,45,45,45	0
55	MG	1A	3532	1/1	0.93	0.18	40,40,40,40	0
55	MG	2A	3443	1/1	0.93	0.67	46,46,46,46	0
55	MG	2A	3754	1/1	0.93	0.25	43,43,43,43	0
55	MG	1A	3719	1/1	0.93	0.15	19,19,19,19	0
55	MG	1A	3808	1/1	0.93	0.47	22,22,22,22	0
55	MG	1A	3687	1/1	0.93	0.13	59,59,59,59	0
55	MG	2A	3725	1/1	0.93	0.12	25,25,25,25	0
55	MG	2A	3268	1/1	0.93	0.11	32,32,32,32	0
55	MG	2A	3096	1/1	0.93	0.15	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	2A	3793	1/1	0.93	0.14	13,13,13,13	0
55	MG	1a	3034	1/1	0.93	0.30	49,49,49,49	0
55	MG	2A	3617	1/1	0.93	0.14	23,23,23,23	0
55	MG	2A	3103	1/1	0.93	0.91	34,34,34,34	0
55	MG	2A	3025	1/1	0.93	0.29	35,35,35,35	0
55	MG	1A	3907	1/1	0.93	0.54	61,61,61,61	0
55	MG	2A	3355	1/1	0.93	0.23	30,30,30,30	0
55	MG	1A	3073	1/1	0.93	0.27	22,22,22,22	0
55	MG	1X	101	1/1	0.93	0.25	30,30,30,30	0
55	MG	1A	3747	1/1	0.93	0.13	38,38,38,38	0
55	MG	2O	201	1/1	0.93	0.10	31,31,31,31	0
55	MG	2A	3674	1/1	0.93	0.23	36,36,36,36	0
55	MG	1A	3286	1/1	0.93	0.13	41,41,41,41	0
55	MG	1A	3191	1/1	0.93	0.29	44,44,44,44	0
55	MG	1A	3342	1/1	0.93	0.29	46,46,46,46	0
55	MG	2A	3781	1/1	0.93	0.14	43,43,43,43	0
55	MG	2A	3378	1/1	0.93	0.20	44,44,44,44	0
55	MG	2A	3695	1/1	0.93	0.12	44,44,44,44	0
55	MG	2A	3578	1/1	0.93	0.11	22,22,22,22	0
55	MG	2a	1612	1/1	0.93	0.69	39,39,39,39	0
55	MG	1A	3367	1/1	0.93	0.07	27,27,27,27	0
55	MG	2A	3580	1/1	0.93	0.08	40,40,40,40	0
55	MG	1A	3855	1/1	0.93	0.11	36,36,36,36	0
55	MG	2A	3009	1/1	0.93	0.10	27,27,27,27	0
55	MG	1a	3179	1/1	0.93	0.13	47,47,47,47	0
55	MG	28	103	1/1	0.93	0.13	53,53,53,53	0
55	MG	2D	305	1/1	0.93	0.52	41,41,41,41	0
55	MG	2A	3678	1/1	0.93	0.10	43,43,43,43	0
55	MG	2A	3085	1/1	0.93	0.35	27,27,27,27	0
55	MG	1a	3013	1/1	0.93	0.14	56,56,56,56	0
55	MG	1A	3417	1/1	0.93	0.18	30,30,30,30	0
55	MG	1A	3658	1/1	0.93	0.15	32,32,32,32	0
55	MG	1A	3988	1/1	0.93	0.08	36,36,36,36	0
55	MG	2A	3423	1/1	0.93	0.17	31,31,31,31	0
55	MG	2a	1753	1/1	0.93	0.10	33,33,33,33	0
55	MG	1a	3152	1/1	0.93	0.24	40,40,40,40	0
55	MG	2A	3023	1/1	0.93	0.83	41,41,41,41	0
55	MG	2A	3290	1/1	0.93	0.35	30,30,30,30	0
55	MG	2A	3696	1/1	0.93	0.08	50,50,50,50	0
55	MG	1a	3033	1/1	0.93	0.13	40,40,40,40	0
55	MG	2x	103	1/1	0.93	0.17	29,29,29,29	0
55	MG	2G	201	1/1	0.93	0.15	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	1A	3120	1/1	0.93	0.24	30,30,30,30	0
55	MG	1a	3069	1/1	0.93	0.12	23,23,23,23	0
55	MG	1A	3224	1/1	0.93	0.16	48,48,48,48	0
55	MG	2a	1694	1/1	0.93	0.47	46,46,46,46	0
55	MG	1A	3428	1/1	0.93	0.23	21,21,21,21	0
55	MG	1A	3377	1/1	0.93	0.10	38,38,38,38	0
55	MG	1A	3343	1/1	0.93	0.18	25,25,25,25	0
55	MG	1A	3928	1/1	0.93	0.07	33,33,33,33	0
55	MG	1a	3068	1/1	0.93	0.12	30,30,30,30	0
55	MG	2A	3353	1/1	0.93	0.21	36,36,36,36	0
55	MG	2A	3557	1/1	0.93	0.12	15,15,15,15	0
55	MG	2A	3500	1/1	0.93	0.17	33,33,33,33	0
55	MG	2A	3203	1/1	0.93	0.24	44,44,44,44	0
55	MG	1A	3033	1/1	0.93	0.14	35,35,35,35	0
55	MG	1A	3825	1/1	0.93	0.37	52,52,52,52	0
55	MG	1a	3083	1/1	0.93	0.09	40,40,40,40	0
55	MG	2a	1736	1/1	0.93	0.10	54,54,54,54	0
55	MG	1A	4035	1/1	0.93	0.26	15,15,15,15	0
55	MG	2A	3591	1/1	0.93	0.18	41,41,41,41	0
55	MG	2A	3040	1/1	0.93	0.12	28,28,28,28	0
55	MG	2A	3328	1/1	0.93	0.56	64,64,64,64	0
55	MG	1A	3413	1/1	0.93	0.39	21,21,21,21	0
55	MG	2A	3635	1/1	0.93	0.25	31,31,31,31	0
55	MG	1A	3232	1/1	0.93	0.10	26,26,26,26	0
55	MG	1S	203	1/1	0.93	0.09	44,44,44,44	0
55	MG	1A	3764	1/1	0.93	0.12	41,41,41,41	0
55	MG	1A	3098	1/1	0.93	0.56	32,32,32,32	0
55	MG	1a	3113	1/1	0.93	0.11	41,41,41,41	0
55	MG	2A	3231	1/1	0.93	0.14	55,55,55,55	0
55	MG	2A	3661	1/1	0.93	0.17	41,41,41,41	0
55	MG	1A	3585	1/1	0.93	0.11	22,22,22,22	0
55	MG	1A	3827	1/1	0.93	0.38	22,22,22,22	0
55	MG	1A	3774	1/1	0.93	0.24	37,37,37,37	0
55	MG	2a	1652	1/1	0.93	0.21	40,40,40,40	0
55	MG	1A	3718	1/1	0.93	0.24	46,46,46,46	0
55	MG	2A	3283	1/1	0.93	0.11	31,31,31,31	0
55	MG	2a	1669	1/1	0.93	0.08	40,40,40,40	0
55	MG	1A	3140	1/1	0.93	0.38	33,33,33,33	0
55	MG	1a	3168	1/1	0.93	0.16	50,50,50,50	0
55	MG	1N	203	1/1	0.93	0.31	45,45,45,45	0
55	MG	2A	3571	1/1	0.93	0.17	29,29,29,29	0
55	MG	1f	201	1/1	0.93	0.19	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	1A	3510	1/1	0.93	0.15	21,21,21,21	0
55	MG	2A	3441	1/1	0.93	0.12	31,31,31,31	0
55	MG	1A	3716	1/1	0.93	0.11	20,20,20,20	0
55	MG	2a	1615	1/1	0.93	0.17	37,37,37,37	0
55	MG	2A	3179	1/1	0.93	0.27	30,30,30,30	0
55	MG	1A	4023	1/1	0.93	0.15	40,40,40,40	0
55	MG	2A	3254	1/1	0.93	0.33	41,41,41,41	0
55	MG	1A	3331	1/1	0.93	0.13	21,21,21,21	0
55	MG	1A	3155	1/1	0.93	0.19	23,23,23,23	0
55	MG	1a	3154	1/1	0.93	0.08	41,41,41,41	0
55	MG	2a	1636	1/1	0.93	0.12	49,49,49,49	0
55	MG	2A	3053	1/1	0.93	0.17	34,34,34,34	0
55	MG	1T	202	1/1	0.93	0.22	46,46,46,46	0
55	MG	1A	3765	1/1	0.93	0.24	26,26,26,26	0
55	MG	1A	3790	1/1	0.93	0.21	28,28,28,28	0
55	MG	1A	3862	1/1	0.93	0.10	39,39,39,39	0
55	MG	1A	3803	1/1	0.93	0.44	29,29,29,29	0
55	MG	2E	304	1/1	0.93	0.20	30,30,30,30	0
55	MG	1A	3438	1/1	0.93	0.23	33,33,33,33	0
55	MG	2a	1728	1/1	0.93	0.21	41,41,41,41	0
55	MG	2A	3284	1/1	0.93	0.11	33,33,33,33	0
55	MG	2A	3391	1/1	0.93	0.11	30,30,30,30	0
55	MG	2Z	301	1/1	0.93	0.19	68,68,68,68	0
55	MG	1A	3457	1/1	0.93	0.18	38,38,38,38	0
55	MG	15	102	1/1	0.93	0.64	33,33,33,33	0
55	MG	1A	3201	1/1	0.93	0.20	36,36,36,36	0
55	MG	2a	1679	1/1	0.93	0.09	45,45,45,45	0
55	MG	2A	3681	1/1	0.93	0.21	50,50,50,50	0
55	MG	1B	213	1/1	0.93	0.11	48,48,48,48	0
55	MG	2A	3239	1/1	0.93	0.66	34,34,34,34	0
55	MG	2A	3166	1/1	0.93	0.23	38,38,38,38	0
55	MG	1A	3480	1/1	0.93	0.13	20,20,20,20	0
55	MG	1a	3108	1/1	0.93	0.13	63,63,63,63	0
55	MG	2a	1719	1/1	0.93	0.14	43,43,43,43	0
55	MG	2A	3324	1/1	0.93	0.11	26,26,26,26	0
55	MG	1l	202	1/1	0.93	0.08	18,18,18,18	0
55	MG	1A	3230	1/1	0.93	0.21	23,23,23,23	0
55	MG	1A	3564	1/1	0.93	0.18	15,15,15,15	0
55	MG	1a	3145	1/1	0.93	0.14	23,23,23,23	0
55	MG	1A	3007	1/1	0.93	0.12	27,27,27,27	0
55	MG	2Q	201	1/1	0.93	0.10	53,53,53,53	0
55	MG	1a	3117	1/1	0.93	0.16	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	2I	105	1/1	0.93	0.14	49,49,49,49	0
55	MG	1A	3282	1/1	0.93	0.27	24,24,24,24	0
55	MG	1a	3209	1/1	0.93	0.09	38,38,38,38	0
55	MG	1A	3640	1/1	0.93	0.53	47,47,47,47	0
55	MG	1A	3556	1/1	0.93	0.13	26,26,26,26	0
55	MG	2a	1660	1/1	0.93	0.09	46,46,46,46	0
55	MG	1A	3316	1/1	0.93	0.37	14,14,14,14	0
55	MG	2a	1788	1/1	0.93	0.07	54,54,54,54	0
55	MG	2a	1657	1/1	0.93	0.26	45,45,45,45	0
55	MG	2a	1634	1/1	0.93	0.14	51,51,51,51	0
55	MG	1A	3831	1/1	0.93	0.12	26,26,26,26	0
55	MG	2a	1690	1/1	0.93	0.18	39,39,39,39	0
55	MG	2x	104	1/1	0.93	0.22	50,50,50,50	0
55	MG	1A	3630	1/1	0.93	0.13	18,18,18,18	0
55	MG	1A	3509	1/1	0.93	0.17	24,24,24,24	0
55	MG	1S	201	1/1	0.93	0.21	47,47,47,47	0
55	MG	1A	3918	1/1	0.93	0.13	19,19,19,19	0
55	MG	1A	3733	1/1	0.93	0.15	17,17,17,17	0
55	MG	2A	3037	1/1	0.93	0.17	17,17,17,17	0
55	MG	1A	3415	1/1	0.93	0.52	26,26,26,26	0
55	MG	2a	1797	1/1	0.93	0.15	47,47,47,47	0
55	MG	1A	3011	1/1	0.93	0.37	16,16,16,16	0
55	MG	2A	3684	1/1	0.93	0.09	36,36,36,36	0
55	MG	2A	3175	1/1	0.93	0.75	37,37,37,37	0
55	MG	1B	223	1/1	0.93	0.12	28,28,28,28	0
55	MG	2B	206	1/1	0.93	0.14	40,40,40,40	0
55	MG	1A	3981	1/1	0.93	0.15	47,47,47,47	0
55	MG	1F	305	1/1	0.93	0.10	34,34,34,34	0
55	MG	2a	1735	1/1	0.93	0.07	33,33,33,33	0
55	MG	2A	3679	1/1	0.93	0.08	40,40,40,40	0
55	MG	2A	3506	1/1	0.93	0.17	33,33,33,33	0
55	MG	1A	3885	1/1	0.93	0.23	46,46,46,46	0
55	MG	2A	3004	1/1	0.93	0.10	24,24,24,24	0
55	MG	2A	3371	1/1	0.93	0.35	27,27,27,27	0
55	MG	2B	204	1/1	0.93	0.21	47,47,47,47	0
55	MG	2A	3756	1/1	0.93	0.24	25,25,25,25	0
55	MG	2a	1742	1/1	0.93	0.19	44,44,44,44	0
55	MG	2A	3260	1/1	0.93	0.29	23,23,23,23	0
55	MG	1A	3264	1/1	0.93	0.19	42,42,42,42	0
55	MG	1A	3805	1/1	0.93	0.11	41,41,41,41	0
55	MG	1A	3216	1/1	0.93	0.11	30,30,30,30	0
55	MG	1A	3202	1/1	0.93	0.35	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	2A	3173	1/1	0.93	0.10	31,31,31,31	0
55	MG	1a	3124	1/1	0.93	0.09	34,34,34,34	0
55	MG	1A	3223	1/1	0.93	0.16	31,31,31,31	0
55	MG	1A	3247	1/1	0.94	0.20	37,37,37,37	0
55	MG	2A	3125	1/1	0.94	0.17	18,18,18,18	0
55	MG	1A	3812	1/1	0.94	0.11	39,39,39,39	0
55	MG	2A	3438	1/1	0.94	0.91	30,30,30,30	0
55	MG	2A	3596	1/1	0.94	0.17	26,26,26,26	0
55	MG	1A	3464	1/1	0.94	0.59	29,29,29,29	0
55	MG	1A	3338	1/1	0.94	0.12	55,55,55,55	0
55	MG	2A	3447	1/1	0.94	0.65	39,39,39,39	0
55	MG	1A	3886	1/1	0.94	0.22	36,36,36,36	0
55	MG	1A	3108	1/1	0.94	0.11	33,33,33,33	0
55	MG	1E	303	1/1	0.94	0.49	22,22,22,22	0
55	MG	2A	3605	1/1	0.94	0.12	33,33,33,33	0
55	MG	1A	3913	1/1	0.94	0.27	50,50,50,50	0
55	MG	2A	3012	1/1	0.94	0.25	40,40,40,40	0
55	MG	1A	3839	1/1	0.94	0.11	36,36,36,36	0
55	MG	1A	3196	1/1	0.94	0.12	24,24,24,24	0
55	MG	2B	201	1/1	0.94	0.14	40,40,40,40	0
55	MG	2A	3421	1/1	0.94	0.21	22,22,22,22	0
55	MG	2A	3542	1/1	0.94	0.09	29,29,29,29	0
55	MG	1A	3577	1/1	0.94	0.12	15,15,15,15	0
55	MG	1A	3096	1/1	0.94	0.13	23,23,23,23	0
55	MG	1A	3863	1/1	0.94	0.10	49,49,49,49	0
55	MG	2A	3773	1/1	0.94	0.35	36,36,36,36	0
55	MG	1A	3261	1/1	0.94	0.18	23,23,23,23	0
55	MG	1a	3020	1/1	0.94	0.13	34,34,34,34	0
55	MG	1A	3372	1/1	0.94	0.47	22,22,22,22	0
55	MG	1A	3351	1/1	0.94	0.26	28,28,28,28	0
55	MG	1A	3817	1/1	0.94	0.19	40,40,40,40	0
55	MG	1A	3983	1/1	0.94	0.17	25,25,25,25	0
55	MG	1A	3229	1/1	0.94	0.62	29,29,29,29	0
55	MG	2a	1777	1/1	0.94	0.17	38,38,38,38	0
55	MG	2E	301	1/1	0.94	0.12	31,31,31,31	0
55	MG	1Q	201	1/1	0.94	0.17	26,26,26,26	0
55	MG	1a	3026	1/1	0.94	0.11	27,27,27,27	0
55	MG	1A	3748	1/1	0.94	0.12	27,27,27,27	0
55	MG	1W	206	1/1	0.94	0.53	27,27,27,27	0
55	MG	2B	214	1/1	0.94	0.17	49,49,49,49	0
55	MG	2A	3809	1/1	0.94	0.08	40,40,40,40	0
55	MG	2A	3298	1/1	0.94	0.33	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	1A	3301	1/1	0.94	0.95	29,29,29,29	0
55	MG	1A	3165	1/1	0.94	0.74	40,40,40,40	0
55	MG	2A	3496	1/1	0.94	0.19	27,27,27,27	0
55	MG	2A	3036	1/1	0.94	0.18	23,23,23,23	0
55	MG	1A	3771	1/1	0.94	0.11	44,44,44,44	0
55	MG	1A	4025	1/1	0.94	0.15	45,45,45,45	0
55	MG	1a	3114	1/1	0.94	0.07	51,51,51,51	0
55	MG	2a	1720	1/1	0.94	0.11	23,23,23,23	0
55	MG	1a	3118	1/1	0.94	0.15	42,42,42,42	0
55	MG	2P	204	1/1	0.94	0.26	44,44,44,44	0
55	MG	2A	3245	1/1	0.94	0.21	24,24,24,24	0
55	MG	1A	3699	1/1	0.94	0.10	22,22,22,22	0
55	MG	1A	3160	1/1	0.94	0.32	45,45,45,45	0
55	MG	2A	3501	1/1	0.94	0.18	26,26,26,26	0
55	MG	1A	3141	1/1	0.94	0.19	37,37,37,37	0
55	MG	10	107	1/1	0.94	0.11	24,24,24,24	0
55	MG	2A	3603	1/1	0.94	0.09	45,45,45,45	0
55	MG	1N	204	1/1	0.94	0.14	33,33,33,33	0
55	MG	2A	3365	1/1	0.94	0.57	34,34,34,34	0
55	MG	2a	1771	1/1	0.94	0.14	39,39,39,39	0
55	MG	1a	3139	1/1	0.94	0.06	30,30,30,30	0
55	MG	1A	3446	1/1	0.94	0.20	42,42,42,42	0
55	MG	2A	3338	1/1	0.94	0.10	32,32,32,32	0
55	MG	1a	3024	1/1	0.94	0.11	30,30,30,30	0
55	MG	2A	3823	1/1	0.94	0.10	26,26,26,26	0
55	MG	1A	3451	1/1	0.94	0.31	47,47,47,47	0
55	MG	2A	3575	1/1	0.94	0.12	26,26,26,26	0
55	MG	2A	3519	1/1	0.94	0.14	60,60,60,60	0
55	MG	25	101	1/1	0.94	0.13	38,38,38,38	0
55	MG	2A	3034	1/1	0.94	0.44	32,32,32,32	0
55	MG	2a	1623	1/1	0.94	0.43	48,48,48,48	0
55	MG	2A	3847	1/1	0.94	0.14	47,47,47,47	0
55	MG	1A	3514	1/1	0.94	0.96	33,33,33,33	0
55	MG	2A	3776	1/1	0.94	0.32	57,57,57,57	0
55	MG	1A	3060	1/1	0.94	0.14	21,21,21,21	0
55	MG	2d	302	1/1	0.94	0.11	47,47,47,47	0
55	MG	2A	3382	1/1	0.94	0.21	22,22,22,22	0
55	MG	1A	4038	1/1	0.94	0.23	35,35,35,35	0
55	MG	1a	3206	1/1	0.94	0.11	60,60,60,60	0
55	MG	1A	3739	1/1	0.94	0.17	34,34,34,34	0
55	MG	1a	3199	1/1	0.94	0.06	55,55,55,55	0
55	MG	2A	3534	1/1	0.94	0.16	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	2A	3777	1/1	0.94	0.25	46,46,46,46	0
55	MG	1A	3398	1/1	0.94	1.12	29,29,29,29	0
55	MG	1A	3460	1/1	0.94	0.18	41,41,41,41	0
55	MG	1A	3511	1/1	0.94	0.14	21,21,21,21	0
55	MG	2A	3363	1/1	0.94	0.15	49,49,49,49	0
55	MG	2A	3521	1/1	0.94	0.08	33,33,33,33	0
55	MG	1A	3666	1/1	0.94	0.10	23,23,23,23	0
55	MG	1A	3976	1/1	0.94	0.22	26,26,26,26	0
55	MG	2A	3761	1/1	0.94	0.12	55,55,55,55	0
55	MG	2A	3499	1/1	0.94	0.24	45,45,45,45	0
55	MG	1A	3154	1/1	0.94	0.29	17,17,17,17	0
55	MG	2A	3273	1/1	0.94	0.14	24,24,24,24	0
55	MG	2A	3079	1/1	0.94	0.25	50,50,50,50	0
55	MG	1A	3634	1/1	0.94	0.20	32,32,32,32	0
55	MG	1A	3222	1/1	0.94	0.16	19,19,19,19	0
55	MG	2a	1678	1/1	0.94	0.14	40,40,40,40	0
55	MG	1A	3921	1/1	0.94	0.16	54,54,54,54	0
55	MG	1A	3305	1/1	0.94	0.15	23,23,23,23	0
55	MG	2A	3815	1/1	0.94	0.15	44,44,44,44	0
55	MG	1A	3624	1/1	0.94	0.15	43,43,43,43	0
55	MG	2A	3802	1/1	0.94	0.12	17,17,17,17	0
55	MG	2a	1772	1/1	0.94	0.27	28,28,28,28	0
55	MG	2E	303	1/1	0.94	0.29	28,28,28,28	0
55	MG	2A	3653	1/1	0.94	0.10	41,41,41,41	0
55	MG	1A	3383	1/1	0.94	0.56	27,27,27,27	0
55	MG	1A	3051	1/1	0.94	0.11	16,16,16,16	0
55	MG	1A	3652	1/1	0.94	0.26	29,29,29,29	0
55	MG	1x	107	1/1	0.94	0.13	48,48,48,48	0
55	MG	2A	3114	1/1	0.94	0.35	30,30,30,30	0
55	MG	2A	3352	1/1	0.94	0.67	31,31,31,31	0
55	MG	2a	1793	1/1	0.94	0.18	57,57,57,57	0
55	MG	2A	3639	1/1	0.94	0.05	44,44,44,44	0
55	MG	2A	3484	1/1	0.94	0.22	29,29,29,29	0
55	MG	1A	3403	1/1	0.94	0.11	30,30,30,30	0
55	MG	1A	3754	1/1	0.94	0.14	33,33,33,33	0
55	MG	2A	3820	1/1	0.94	0.11	33,33,33,33	0
55	MG	1A	3300	1/1	0.94	0.15	27,27,27,27	0
55	MG	1A	3984	1/1	0.94	0.18	43,43,43,43	0
55	MG	1A	3635	1/1	0.94	0.12	22,22,22,22	0
55	MG	1A	3694	1/1	0.94	0.10	35,35,35,35	0
55	MG	2A	3300	1/1	0.94	0.14	31,31,31,31	0
55	MG	11	102	1/1	0.94	0.12	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	1A	3402	1/1	0.94	0.16	35,35,35,35	0
55	MG	1a	3127	1/1	0.94	0.13	21,21,21,21	0
55	MG	2A	3465	1/1	0.94	0.15	50,50,50,50	0
55	MG	2A	3197	1/1	0.94	0.20	34,34,34,34	0
55	MG	2A	3388	1/1	0.94	0.17	34,34,34,34	0
55	MG	1a	3070	1/1	0.94	0.13	25,25,25,25	0
55	MG	1A	3544	1/1	0.94	0.30	40,40,40,40	0
55	MG	2Z	302	1/1	0.94	0.21	26,26,26,26	0
55	MG	2A	3758	1/1	0.94	0.15	59,59,59,59	0
55	MG	2A	3337	1/1	0.94	0.10	35,35,35,35	0
55	MG	2a	1655	1/1	0.94	0.12	57,57,57,57	0
55	MG	1A	3982	1/1	0.94	0.13	36,36,36,36	0
55	MG	1N	202	1/1	0.94	0.33	41,41,41,41	0
55	MG	1A	3778	1/1	0.94	0.08	55,55,55,55	0
55	MG	2A	3177	1/1	0.94	0.21	33,33,33,33	0
55	MG	1A	3148	1/1	0.94	0.29	26,26,26,26	0
55	MG	2A	3306	1/1	0.94	0.23	19,19,19,19	0
55	MG	2A	3622	1/1	0.94	0.16	37,37,37,37	0
55	MG	2A	3318	1/1	0.94	0.28	44,44,44,44	0
55	MG	1A	3106	1/1	0.94	0.29	33,33,33,33	0
55	MG	1A	3245	1/1	0.94	0.22	48,48,48,48	0
55	MG	1A	3035	1/1	0.94	0.18	18,18,18,18	0
55	MG	2A	3513	1/1	0.94	0.13	56,56,56,56	0
55	MG	2A	3060	1/1	0.94	0.11	41,41,41,41	0
55	MG	1A	3526	1/1	0.94	0.21	31,31,31,31	0
55	MG	1a	3023	1/1	0.94	0.18	44,44,44,44	0
55	MG	2A	3632	1/1	0.94	0.13	37,37,37,37	0
55	MG	2A	3372	1/1	0.94	0.15	42,42,42,42	0
55	MG	2a	1674	1/1	0.94	0.29	67,67,67,67	0
55	MG	2A	3790	1/1	0.94	0.25	42,42,42,42	0
55	MG	1A	3319	1/1	0.94	0.42	16,16,16,16	0
55	MG	2A	3261	1/1	0.94	0.38	43,43,43,43	0
55	MG	1a	3137	1/1	0.94	0.16	34,34,34,34	0
55	MG	1A	4018	1/1	0.94	0.11	40,40,40,40	0
55	MG	1a	3073	1/1	0.94	0.13	50,50,50,50	0
55	MG	2a	1731	1/1	0.94	0.10	33,33,33,33	0
55	MG	2A	3233	1/1	0.94	0.38	50,50,50,50	0
55	MG	1A	3837	1/1	0.94	0.14	51,51,51,51	0
55	MG	1A	3416	1/1	0.94	0.22	44,44,44,44	0
55	MG	2A	3486	1/1	0.94	0.12	29,29,29,29	0
55	MG	2A	3276	1/1	0.94	0.23	59,59,59,59	0
55	MG	1A	3948	1/1	0.94	0.13	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	2a	1812	1/1	0.94	0.14	54,54,54,54	0
55	MG	1A	3758	1/1	0.94	0.87	49,49,49,49	0
55	MG	1D	301	1/1	0.94	0.55	22,22,22,22	0
55	MG	1a	3203	1/1	0.94	0.08	39,39,39,39	0
55	MG	2A	3470	1/1	0.94	0.22	21,21,21,21	0
55	MG	2A	3189	1/1	0.94	0.12	32,32,32,32	0
55	MG	1A	3789	1/1	0.94	0.15	24,24,24,24	0
55	MG	2a	1697	1/1	0.94	0.15	23,23,23,23	0
55	MG	2A	3691	1/1	0.94	0.12	24,24,24,24	0
55	MG	2A	3644	1/1	0.94	0.18	52,52,52,52	0
55	MG	2A	3164	1/1	0.94	0.14	36,36,36,36	0
55	MG	12	101	1/1	0.94	0.33	34,34,34,34	0
55	MG	2A	3146	1/1	0.94	0.14	40,40,40,40	0
55	MG	2A	3081	1/1	0.94	0.16	54,54,54,54	0
55	MG	2A	3686	1/1	0.94	0.16	31,31,31,31	0
55	MG	2i	201	1/1	0.94	0.08	70,70,70,70	0
55	MG	1A	3991	1/1	0.94	0.15	34,34,34,34	0
55	MG	2A	3724	1/1	0.94	0.19	41,41,41,41	0
55	MG	17	107	1/1	0.94	0.35	32,32,32,32	0
55	MG	1A	3392	1/1	0.94	0.72	31,31,31,31	0
55	MG	2A	3072	1/1	0.94	0.38	26,26,26,26	0
55	MG	1B	205	1/1	0.94	0.14	44,44,44,44	0
55	MG	1A	3206	1/1	0.94	0.09	28,28,28,28	0
55	MG	1A	4007	1/1	0.94	0.21	50,50,50,50	0
55	MG	2A	3666	1/1	0.94	0.10	26,26,26,26	0
55	MG	1A	3665	1/1	0.94	0.13	10,10,10,10	0
55	MG	1A	3103	1/1	0.94	0.14	32,32,32,32	0
55	MG	1A	3272	1/1	0.94	0.08	23,23,23,23	0
55	MG	1A	4002	1/1	0.94	0.24	17,17,17,17	0
55	MG	1a	3014	1/1	0.94	0.12	33,33,33,33	0
55	MG	1A	3878	1/1	0.94	0.19	20,20,20,20	0
55	MG	1A	3459	1/1	0.94	0.12	28,28,28,28	0
55	MG	2A	3669	1/1	0.94	0.38	37,37,37,37	0
55	MG	1A	4021	1/1	0.94	0.17	42,42,42,42	0
55	MG	1a	3078	1/1	0.94	0.47	19,19,19,19	0
55	MG	2A	3313	1/1	0.94	0.17	52,52,52,52	0
55	MG	2A	3405	1/1	0.94	0.45	41,41,41,41	0
55	MG	1A	3944	1/1	0.94	0.08	20,20,20,20	0
55	MG	2A	3694	1/1	0.94	0.16	21,21,21,21	0
55	MG	2A	3330	1/1	0.94	0.30	26,26,26,26	0
55	MG	21	106	1/1	0.94	0.26	35,35,35,35	0
55	MG	2B	219	1/1	0.94	0.10	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	1A	3712	1/1	0.94	0.08	36,36,36,36	0
55	MG	2A	3148	1/1	0.94	0.13	31,31,31,31	0
55	MG	2A	3779	1/1	0.94	0.14	34,34,34,34	0
55	MG	1A	3328	1/1	0.94	0.12	22,22,22,22	0
55	MG	2I	202	1/1	0.94	0.11	42,42,42,42	0
55	MG	1A	3467	1/1	0.94	0.28	28,28,28,28	0
55	MG	1A	3522	1/1	0.94	0.16	33,33,33,33	0
55	MG	1R	206	1/1	0.94	0.17	24,24,24,24	0
55	MG	1A	3127	1/1	0.94	0.63	18,18,18,18	0
55	MG	2A	3464	1/1	0.94	0.13	20,20,20,20	0
55	MG	1A	3581	1/1	0.94	0.11	15,15,15,15	0
55	MG	2A	3305	1/1	0.94	0.15	29,29,29,29	0
55	MG	1B	220	1/1	0.94	0.15	25,25,25,25	0
55	MG	1A	3761	1/1	0.94	0.12	51,51,51,51	0
55	MG	1A	3345	1/1	0.94	0.14	21,21,21,21	0
55	MG	1A	3381	1/1	0.94	0.12	22,22,22,22	0
55	MG	1A	3078	1/1	0.94	0.18	23,23,23,23	0
55	MG	1A	3255	1/1	0.94	0.26	32,32,32,32	0
55	MG	1A	3434	1/1	0.94	0.12	43,43,43,43	0
55	MG	10	106	1/1	0.94	0.08	35,35,35,35	0
55	MG	1A	3816	1/1	0.94	0.16	15,15,15,15	0
55	MG	1A	3749	1/1	0.94	0.14	53,53,53,53	0
55	MG	2A	3522	1/1	0.94	0.20	34,34,34,34	0
55	MG	1A	3361	1/1	0.94	0.31	37,37,37,37	0
55	MG	2A	3066	1/1	0.94	0.12	46,46,46,46	0
55	MG	2A	3573	1/1	0.94	0.13	23,23,23,23	0
55	MG	1A	3999	1/1	0.94	0.18	32,32,32,32	0
55	MG	2A	3671	1/1	0.94	0.09	35,35,35,35	0
55	MG	1Z	302	1/1	0.94	0.13	32,32,32,32	0
55	MG	2a	1638	1/1	0.94	0.12	42,42,42,42	0
55	MG	26	101	1/1	0.94	0.17	40,40,40,40	0
55	MG	1A	3558	1/1	0.94	0.16	21,21,21,21	0
55	MG	1a	3052	1/1	0.94	0.17	53,53,53,53	0
55	MG	1A	3334	1/1	0.94	0.80	51,51,51,51	0
55	MG	1A	3961	1/1	0.94	0.13	37,37,37,37	0
55	MG	1A	3017	1/1	0.94	0.18	10,10,10,10	0
55	MG	2A	3253	1/1	0.94	0.09	30,30,30,30	0
55	MG	1A	3555	1/1	0.94	0.53	34,34,34,34	0
55	MG	1A	3071	1/1	0.94	0.53	35,35,35,35	0
55	MG	1A	3105	1/1	0.94	0.39	19,19,19,19	0
55	MG	1a	3109	1/1	0.94	0.10	40,40,40,40	0
55	MG	1A	3490	1/1	0.94	0.17	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	2A	3334	1/1	0.94	0.07	30,30,30,30	0
55	MG	1A	3408	1/1	0.94	0.10	18,18,18,18	0
55	MG	1A	3810	1/1	0.94	0.27	23,23,23,23	0
55	MG	2A	3601	1/1	0.94	0.21	44,44,44,44	0
55	MG	1A	3426	1/1	0.94	0.29	15,15,15,15	0
55	MG	2A	3366	1/1	0.94	0.71	31,31,31,31	0
55	MG	2A	3374	1/1	0.94	0.13	35,35,35,35	0
55	MG	1x	105	1/1	0.94	0.19	54,54,54,54	0
55	MG	1a	3128	1/1	0.94	0.32	30,30,30,30	0
55	MG	2A	3402	1/1	0.94	0.10	34,34,34,34	0
55	MG	2A	3105	1/1	0.94	0.40	45,45,45,45	0
55	MG	1A	3029	1/1	0.94	0.45	23,23,23,23	0
55	MG	2a	1811	1/1	0.94	0.13	42,42,42,42	0
55	MG	2A	3089	1/1	0.94	0.12	32,32,32,32	0
55	MG	2a	1796	1/1	0.94	0.17	50,50,50,50	0
55	MG	1A	3922	1/1	0.94	0.14	68,68,68,68	0
55	MG	1a	3064	1/1	0.94	0.22	59,59,59,59	0
55	MG	1A	3763	1/1	0.94	0.09	37,37,37,37	0
55	MG	2A	3810	1/1	0.94	0.09	29,29,29,29	0
55	MG	2A	3124	1/1	0.94	0.15	29,29,29,29	0
55	MG	1A	3579	1/1	0.94	0.16	15,15,15,15	0
55	MG	2A	3035	1/1	0.94	0.11	30,30,30,30	0
55	MG	1a	3031	1/1	0.94	0.15	29,29,29,29	0
55	MG	1A	3580	1/1	0.94	0.21	42,42,42,42	0
55	MG	1A	4020	1/1	0.94	0.08	35,35,35,35	0
55	MG	2D	302	1/1	0.94	0.23	28,28,28,28	0
55	MG	2a	1773	1/1	0.95	0.23	48,48,48,48	0
55	MG	1a	3211	1/1	0.95	0.32	36,36,36,36	0
55	MG	2E	302	1/1	0.95	0.13	27,27,27,27	0
55	MG	2A	3507	1/1	0.95	0.19	10,10,10,10	0
55	MG	2A	3052	1/1	0.95	0.23	34,34,34,34	0
55	MG	1A	3872	1/1	0.95	0.26	52,52,52,52	0
55	MG	1A	3170	1/1	0.95	0.13	32,32,32,32	0
55	MG	1A	4006	1/1	0.95	0.11	42,42,42,42	0
55	MG	2a	1668	1/1	0.95	0.14	28,28,28,28	0
55	MG	1A	3671	1/1	0.95	0.13	28,28,28,28	0
55	MG	2a	1738	1/1	0.95	0.12	59,59,59,59	0
55	MG	1A	3690	1/1	0.95	0.10	27,27,27,27	0
55	MG	2a	1734	1/1	0.95	0.15	40,40,40,40	0
55	MG	1A	3137	1/1	0.95	0.27	30,30,30,30	0
55	MG	17	101	1/1	0.95	0.55	19,19,19,19	0
55	MG	2a	1783	1/1	0.95	0.08	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	1A	3775	1/1	0.95	0.10	40,40,40,40	0
55	MG	2a	1799	1/1	0.95	0.18	49,49,49,49	0
55	MG	1E	308	1/1	0.95	0.52	34,34,34,34	0
55	MG	2A	3749	1/1	0.95	0.11	35,35,35,35	0
55	MG	1A	3811	1/1	0.95	0.11	39,39,39,39	0
55	MG	2A	3159	1/1	0.95	0.10	31,31,31,31	0
55	MG	1A	3368	1/1	0.95	0.14	29,29,29,29	0
55	MG	2A	3818	1/1	0.95	0.10	30,30,30,30	0
55	MG	2A	3220	1/1	0.95	0.26	38,38,38,38	0
55	MG	2x	101	1/1	0.95	0.14	35,35,35,35	0
55	MG	2a	1804	1/1	0.95	0.12	31,31,31,31	0
55	MG	1A	3488	1/1	0.95	0.11	30,30,30,30	0
55	MG	2a	1693	1/1	0.95	0.10	57,57,57,57	0
55	MG	1A	3786	1/1	0.95	0.22	37,37,37,37	0
55	MG	1A	3797	1/1	0.95	0.13	20,20,20,20	0
55	MG	1B	221	1/1	0.95	0.09	56,56,56,56	0
55	MG	1A	3661	1/1	0.95	0.11	45,45,45,45	0
55	MG	1x	110	1/1	0.95	0.22	29,29,29,29	0
55	MG	1A	3882	1/1	0.95	0.07	24,24,24,24	0
55	MG	1A	3183	1/1	0.95	0.41	29,29,29,29	0
55	MG	2A	3547	1/1	0.95	0.18	29,29,29,29	0
55	MG	1A	3168	1/1	0.95	0.41	31,31,31,31	0
55	MG	1A	3039	1/1	0.95	0.34	38,38,38,38	0
55	MG	1A	3953	1/1	0.95	0.11	46,46,46,46	0
55	MG	2A	3608	1/1	0.95	0.14	31,31,31,31	0
55	MG	1A	3551	1/1	0.95	0.18	19,19,19,19	0
55	MG	1A	3541	1/1	0.95	0.17	32,32,32,32	0
55	MG	1A	3151	1/1	0.95	0.11	25,25,25,25	0
55	MG	2A	3631	1/1	0.95	0.14	19,19,19,19	0
55	MG	1A	3806	1/1	0.95	0.06	30,30,30,30	0
55	MG	1d	301	1/1	0.95	0.14	21,21,21,21	0
55	MG	18	103	1/1	0.95	0.81	40,40,40,40	0
55	MG	1A	3299	1/1	0.95	0.18	34,34,34,34	0
55	MG	1A	3639	1/1	0.95	0.24	15,15,15,15	0
55	MG	1A	3642	1/1	0.95	0.18	21,21,21,21	0
55	MG	15	104	1/1	0.95	0.10	17,17,17,17	0
55	MG	2A	3093	1/1	0.95	0.28	22,22,22,22	0
55	MG	1A	3476	1/1	0.95	0.40	38,38,38,38	0
55	MG	1A	3128	1/1	0.95	0.17	23,23,23,23	0
55	MG	2A	3760	1/1	0.95	0.46	50,50,50,50	0
55	MG	1a	3185	1/1	0.95	0.17	32,32,32,32	0
55	MG	1A	3397	1/1	0.95	0.21	16,16,16,16	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	1a	3161	1/1	0.95	0.11	41,41,41,41	0
55	MG	1A	3292	1/1	0.95	0.14	25,25,25,25	0
55	MG	2A	3357	1/1	0.95	0.13	14,14,14,14	0
55	MG	2A	3343	1/1	0.95	0.11	25,25,25,25	0
55	MG	1A	3550	1/1	0.95	0.13	24,24,24,24	0
55	MG	1A	3870	1/1	0.95	0.08	14,14,14,14	0
55	MG	1A	3044	1/1	0.95	0.10	22,22,22,22	0
55	MG	2a	1708	1/1	0.95	0.09	69,69,69,69	0
55	MG	2F	305	1/1	0.95	0.09	27,27,27,27	0
55	MG	1D	306	1/1	0.95	0.11	35,35,35,35	0
55	MG	1A	3731	1/1	0.95	0.21	25,25,25,25	0
55	MG	1v	105	1/1	0.95	0.13	35,35,35,35	0
55	MG	1a	3196	1/1	0.95	0.08	34,34,34,34	0
55	MG	1A	3016	1/1	0.95	0.11	28,28,28,28	0
55	MG	1A	3531	1/1	0.95	0.13	30,30,30,30	0
55	MG	2A	3210	1/1	0.95	0.12	15,15,15,15	0
55	MG	1A	3394	1/1	0.95	0.36	31,31,31,31	0
55	MG	1A	4032	1/1	0.95	0.14	39,39,39,39	0
55	MG	1A	3032	1/1	0.95	0.40	16,16,16,16	0
55	MG	1W	207	1/1	0.95	0.20	23,23,23,23	0
55	MG	1H	201	1/1	0.95	0.18	32,32,32,32	0
55	MG	2A	3498	1/1	0.95	0.40	32,32,32,32	0
55	MG	2A	3729	1/1	0.95	0.08	24,24,24,24	0
55	MG	1A	3309	1/1	0.95	0.51	25,25,25,25	0
55	MG	2A	3562	1/1	0.95	0.15	29,29,29,29	0
55	MG	1A	3285	1/1	0.95	0.16	42,42,42,42	0
55	MG	1A	3638	1/1	0.95	0.12	10,10,10,10	0
55	MG	2A	3772	1/1	0.95	0.14	31,31,31,31	0
55	MG	1a	3037	1/1	0.95	0.10	39,39,39,39	0
55	MG	1W	201	1/1	0.95	0.30	35,35,35,35	0
55	MG	2a	1758	1/1	0.95	0.09	46,46,46,46	0
55	MG	1A	3395	1/1	0.95	0.22	13,13,13,13	0
55	MG	1A	4030	1/1	0.95	0.49	20,20,20,20	0
55	MG	1A	3964	1/1	0.95	0.14	40,40,40,40	0
55	MG	2a	1801	1/1	0.95	0.15	47,47,47,47	0
55	MG	1A	3942	1/1	0.95	0.24	35,35,35,35	0
55	MG	1A	3539	1/1	0.95	0.14	20,20,20,20	0
55	MG	1B	204	1/1	0.95	0.14	25,25,25,25	0
55	MG	2A	3503	1/1	0.95	0.17	26,26,26,26	0
55	MG	2A	3335	1/1	0.95	0.13	25,25,25,25	0
56	K	2A	3433	1/1	0.95	0.17	43,43,43,43	0
55	MG	1a	3021	1/1	0.95	0.10	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	1A	3860	1/1	0.95	0.24	45,45,45,45	0
55	MG	1A	3985	1/1	0.95	0.22	37,37,37,37	0
55	MG	1A	4041	1/1	0.95	0.53	29,29,29,29	0
55	MG	1B	222	1/1	0.95	0.17	22,22,22,22	0
55	MG	1A	3379	1/1	0.95	0.20	27,27,27,27	0
55	MG	2A	3138	1/1	0.95	0.34	31,31,31,31	0
55	MG	2A	3843	1/1	0.95	0.11	39,39,39,39	0
55	MG	1F	302	1/1	0.95	0.52	16,16,16,16	0
55	MG	1A	3024	1/1	0.95	0.40	38,38,38,38	0
55	MG	1A	3171	1/1	0.95	0.18	34,34,34,34	0
55	MG	1A	3380	1/1	0.95	0.50	24,24,24,24	0
55	MG	1A	3501	1/1	0.95	0.43	36,36,36,36	0
55	MG	10	102	1/1	0.95	0.17	34,34,34,34	0
55	MG	2A	3230	1/1	0.95	0.07	42,42,42,42	0
55	MG	2T	204	1/1	0.95	0.17	39,39,39,39	0
55	MG	1A	3968	1/1	0.95	0.13	42,42,42,42	0
55	MG	1A	3833	1/1	0.95	0.20	28,28,28,28	0
55	MG	1a	3015	1/1	0.95	0.14	31,31,31,31	0
55	MG	1A	3157	1/1	0.95	0.25	29,29,29,29	0
55	MG	13	104	1/1	0.95	0.11	38,38,38,38	0
55	MG	2a	1747	1/1	0.95	0.15	29,29,29,29	0
55	MG	2A	3437	1/1	0.95	0.44	37,37,37,37	0
55	MG	1A	3233	1/1	0.95	0.14	24,24,24,24	0
55	MG	2A	3703	1/1	0.95	0.12	30,30,30,30	0
55	MG	1A	3213	1/1	0.95	0.50	35,35,35,35	0
55	MG	1A	3696	1/1	0.95	0.18	25,25,25,25	0
55	MG	1A	3294	1/1	0.95	0.09	10,10,10,10	0
55	MG	2A	3140	1/1	0.95	0.16	37,37,37,37	0
55	MG	1U	203	1/1	0.95	0.36	32,32,32,32	0
55	MG	2A	3216	1/1	0.95	0.18	28,28,28,28	0
55	MG	2A	3136	1/1	0.95	0.12	39,39,39,39	0
55	MG	1A	3681	1/1	0.95	0.17	22,22,22,22	0
55	MG	1A	3347	1/1	0.95	0.35	34,34,34,34	0
55	MG	2F	303	1/1	0.95	0.09	30,30,30,30	0
55	MG	1A	3989	1/1	0.95	0.11	35,35,35,35	0
55	MG	1F	301	1/1	0.95	0.83	29,29,29,29	0
55	MG	1a	3165	1/1	0.95	0.10	48,48,48,48	0
55	MG	1A	3188	1/1	0.95	0.21	22,22,22,22	0
55	MG	1n	101	1/1	0.95	0.10	34,34,34,34	0
55	MG	1A	3836	1/1	0.95	0.08	45,45,45,45	0
55	MG	1A	3721	1/1	0.95	0.12	26,26,26,26	0
55	MG	2a	1785	1/1	0.95	0.07	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	2A	3797	1/1	0.95	0.15	21,21,21,21	0
55	MG	1A	3008	1/1	0.95	0.15	21,21,21,21	0
55	MG	2A	3119	1/1	0.95	0.26	29,29,29,29	0
55	MG	1A	3876	1/1	0.95	0.35	42,42,42,42	0
55	MG	1a	3095	1/1	0.95	0.50	28,28,28,28	0
55	MG	2A	3610	1/1	0.95	0.77	41,41,41,41	0
55	MG	2B	210	1/1	0.95	0.17	45,45,45,45	0
56	K	1A	3470	1/1	0.95	0.28	51,51,51,51	0
55	MG	1A	3344	1/1	0.95	0.40	19,19,19,19	0
55	MG	2A	3690	1/1	0.95	0.13	43,43,43,43	0
55	MG	2a	1692	1/1	0.95	0.11	46,46,46,46	0
55	MG	1B	210	1/1	0.95	0.13	30,30,30,30	0
55	MG	2a	1807	1/1	0.95	0.18	45,45,45,45	0
55	MG	2A	3564	1/1	0.95	0.10	25,25,25,25	0
55	MG	1A	3791	1/1	0.95	0.12	46,46,46,46	0
55	MG	2A	3011	1/1	0.95	0.53	41,41,41,41	0
55	MG	1A	3374	1/1	0.95	0.41	33,33,33,33	0
55	MG	2A	3808	1/1	0.95	0.08	22,22,22,22	0
55	MG	1A	3235	1/1	0.95	0.15	20,20,20,20	0
55	MG	1N	205	1/1	0.95	0.12	22,22,22,22	0
55	MG	2B	202	1/1	0.95	0.13	40,40,40,40	0
55	MG	1A	3934	1/1	0.95	0.10	49,49,49,49	0
55	MG	1A	3974	1/1	0.95	0.12	30,30,30,30	0
55	MG	1A	3766	1/1	0.95	0.10	26,26,26,26	0
55	MG	1A	3930	1/1	0.95	0.18	17,17,17,17	0
55	MG	1A	3239	1/1	0.95	0.14	43,43,43,43	0
55	MG	1A	3373	1/1	0.95	0.24	28,28,28,28	0
55	MG	2A	3080	1/1	0.95	0.30	26,26,26,26	0
55	MG	2A	3071	1/1	0.95	0.39	45,45,45,45	0
55	MG	2a	1765	1/1	0.95	0.13	42,42,42,42	0
55	MG	1A	3021	1/1	0.95	0.16	21,21,21,21	0
55	MG	2A	3393	1/1	0.95	0.15	31,31,31,31	0
55	MG	1A	3130	1/1	0.95	0.57	18,18,18,18	0
55	MG	2A	3077	1/1	0.95	0.10	23,23,23,23	0
55	MG	1A	3265	1/1	0.95	0.23	19,19,19,19	0
55	MG	1A	3329	1/1	0.95	0.53	25,25,25,25	0
55	MG	2B	209	1/1	0.95	0.08	40,40,40,40	0
55	MG	2A	3786	1/1	0.95	0.13	37,37,37,37	0
55	MG	2A	3688	1/1	0.95	0.20	53,53,53,53	0
55	MG	1F	307	1/1	0.95	0.27	30,30,30,30	0
55	MG	2j	201	1/1	0.95	0.08	64,64,64,64	0
55	MG	2A	3157	1/1	0.95	0.24	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	1A	3826	1/1	0.95	0.12	29,29,29,29	0
55	MG	1a	3080	1/1	0.95	0.09	63,63,63,63	0
55	MG	1A	3058	1/1	0.95	0.18	39,39,39,39	0
55	MG	1a	3057	1/1	0.95	0.08	31,31,31,31	0
55	MG	2A	3552	1/1	0.95	0.22	15,15,15,15	0
55	MG	1A	3517	1/1	0.95	0.15	34,34,34,34	0
55	MG	1A	3097	1/1	0.95	0.57	30,30,30,30	0
55	MG	1A	3175	1/1	0.95	0.28	26,26,26,26	0
55	MG	2A	3204	1/1	0.95	0.19	18,18,18,18	0
55	MG	2A	3842	1/1	0.95	0.15	42,42,42,42	0
55	MG	1a	3040	1/1	0.95	0.10	34,34,34,34	0
55	MG	1A	3466	1/1	0.95	1.04	38,38,38,38	0
55	MG	2A	3831	1/1	0.95	0.23	35,35,35,35	0
55	MG	1A	3990	1/1	0.95	0.10	25,25,25,25	0
55	MG	2A	3699	1/1	0.95	0.10	20,20,20,20	0
55	MG	2A	3568	1/1	0.95	0.14	50,50,50,50	0
55	MG	2A	3827	1/1	0.95	0.18	45,45,45,45	0
55	MG	2A	3139	1/1	0.95	0.20	22,22,22,22	0
55	MG	2A	3211	1/1	0.95	0.67	26,26,26,26	0
55	MG	1A	3491	1/1	0.95	0.27	37,37,37,37	0
55	MG	2A	3485	1/1	0.95	0.10	22,22,22,22	0
55	MG	10	105	1/1	0.95	0.17	29,29,29,29	0
55	MG	1A	3804	1/1	0.95	0.17	35,35,35,35	0
55	MG	1A	3538	1/1	0.95	0.27	29,29,29,29	0
55	MG	1A	4000	1/1	0.95	0.14	32,32,32,32	0
55	MG	1a	3082	1/1	0.95	0.16	28,28,28,28	0
55	MG	1A	3698	1/1	0.95	0.13	12,12,12,12	0
55	MG	1A	3949	1/1	0.95	0.08	31,31,31,31	0
55	MG	1A	3891	1/1	0.95	0.10	42,42,42,42	0
55	MG	1A	3251	1/1	0.95	0.22	26,26,26,26	0
55	MG	1A	3670	1/1	0.95	0.19	57,57,57,57	0
55	MG	2A	3130	1/1	0.95	0.23	28,28,28,28	0
55	MG	2A	3611	1/1	0.95	0.30	43,43,43,43	0
55	MG	2A	3491	1/1	0.95	0.16	27,27,27,27	0
55	MG	2A	3523	1/1	0.95	0.33	27,27,27,27	0
55	MG	1A	3087	1/1	0.95	0.09	30,30,30,30	0
55	MG	2A	3700	1/1	0.95	0.20	31,31,31,31	0
55	MG	2A	3297	1/1	0.95	0.23	17,17,17,17	0
55	MG	1A	3248	1/1	0.95	0.09	16,16,16,16	0
55	MG	2A	3828	1/1	0.95	0.13	24,24,24,24	0
55	MG	2A	3574	1/1	0.95	0.08	31,31,31,31	0
55	MG	2a	1701	1/1	0.95	0.11	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	1A	3659	1/1	0.95	0.12	31,31,31,31	0
55	MG	1A	4033	1/1	0.95	0.11	42,42,42,42	0
55	MG	1A	3866	1/1	0.95	0.15	62,62,62,62	0
55	MG	2A	3097	1/1	0.95	0.27	40,40,40,40	0
55	MG	2A	3750	1/1	0.95	0.10	41,41,41,41	0
55	MG	1a	3025	1/1	0.95	0.16	30,30,30,30	0
55	MG	2a	1763	1/1	0.95	0.08	31,31,31,31	0
55	MG	1A	3005	1/1	0.95	0.34	20,20,20,20	0
55	MG	1a	3043	1/1	0.95	0.12	35,35,35,35	0
55	MG	1A	3909	1/1	0.95	0.28	80,80,80,80	0
55	MG	2A	3144	1/1	0.95	0.17	44,44,44,44	0
55	MG	2A	3459	1/1	0.95	0.12	29,29,29,29	0
55	MG	1A	3880	1/1	0.95	0.08	55,55,55,55	0
55	MG	2A	3322	1/1	0.95	0.11	33,33,33,33	0
55	MG	2A	3354	1/1	0.95	0.07	31,31,31,31	0
55	MG	1Y	202	1/1	0.95	0.07	44,44,44,44	0
55	MG	1A	3350	1/1	0.95	0.16	28,28,28,28	0
55	MG	2A	3782	1/1	0.95	0.23	37,37,37,37	0
55	MG	1A	3955	1/1	0.95	0.11	39,39,39,39	0
55	MG	1A	3992	1/1	0.95	0.39	40,40,40,40	0
55	MG	1A	3455	1/1	0.95	0.12	35,35,35,35	0
55	MG	1A	3621	1/1	0.95	0.24	36,36,36,36	0
55	MG	2A	3757	1/1	0.95	0.09	34,34,34,34	0
55	MG	2a	1648	1/1	0.95	0.46	58,58,58,58	0
55	MG	1A	3519	1/1	0.95	0.18	26,26,26,26	0
55	MG	2B	205	1/1	0.95	0.16	34,34,34,34	0
55	MG	2A	3431	1/1	0.95	0.14	37,37,37,37	0
55	MG	2A	3657	1/1	0.95	0.36	50,50,50,50	0
55	MG	1A	3542	1/1	0.95	0.25	51,51,51,51	0
55	MG	1D	304	1/1	0.95	0.81	30,30,30,30	0
55	MG	2A	3753	1/1	0.95	0.11	31,31,31,31	0
55	MG	2A	3509	1/1	0.95	0.09	26,26,26,26	0
55	MG	1A	3851	1/1	0.95	0.11	43,43,43,43	0
55	MG	1A	3869	1/1	0.95	0.10	61,61,61,61	0
55	MG	1A	3102	1/1	0.95	0.36	17,17,17,17	0
55	MG	2B	215	1/1	0.95	0.17	60,60,60,60	0
55	MG	1A	3905	1/1	0.95	0.15	63,63,63,63	0
55	MG	1A	3619	1/1	0.95	0.10	23,23,23,23	0
55	MG	2D	303	1/1	0.95	0.29	40,40,40,40	0
55	MG	2A	3430	1/1	0.95	0.11	29,29,29,29	0
55	MG	1A	3089	1/1	0.95	0.19	39,39,39,39	0
55	MG	1A	3675	1/1	0.95	0.14	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	2A	3198	1/1	0.95	0.25	26,26,26,26	0
55	MG	1A	3561	1/1	0.95	0.24	52,52,52,52	0
55	MG	1A	3772	1/1	0.95	0.56	47,47,47,47	0
55	MG	10	101	1/1	0.95	0.38	33,33,33,33	0
55	MG	2A	3592	1/1	0.95	0.24	31,31,31,31	0
55	MG	2Y	201	1/1	0.95	0.23	27,27,27,27	0
55	MG	2A	3102	1/1	0.95	0.12	31,31,31,31	0
55	MG	1A	3959	1/1	0.95	0.13	56,56,56,56	0
55	MG	1G	203	1/1	0.95	0.12	40,40,40,40	0
55	MG	2A	3167	1/1	0.95	0.17	51,51,51,51	0
55	MG	2a	1637	1/1	0.95	0.83	39,39,39,39	0
55	MG	2A	3821	1/1	0.95	0.29	33,33,33,33	0
55	MG	1A	3346	1/1	0.95	0.29	15,15,15,15	0
55	MG	1A	3485	1/1	0.96	0.13	39,39,39,39	0
55	MG	28	102	1/1	0.96	0.12	29,29,29,29	0
55	MG	1A	3461	1/1	0.96	0.18	38,38,38,38	0
55	MG	2A	3602	1/1	0.96	0.15	36,36,36,36	0
55	MG	1A	3225	1/1	0.96	0.18	54,54,54,54	0
55	MG	2A	3410	1/1	0.96	0.10	43,43,43,43	0
55	MG	2A	3247	1/1	0.96	0.15	25,25,25,25	0
55	MG	2A	3062	1/1	0.96	0.11	17,17,17,17	0
55	MG	1U	206	1/1	0.96	0.29	19,19,19,19	0
55	MG	1A	3604	1/1	0.96	0.11	20,20,20,20	0
55	MG	1W	205	1/1	0.96	0.61	34,34,34,34	0
55	MG	1F	306	1/1	0.96	0.35	11,11,11,11	0
55	MG	2A	3620	1/1	0.96	0.26	21,21,21,21	0
55	MG	2A	3404	1/1	0.96	0.09	12,12,12,12	0
55	MG	1a	3056	1/1	0.96	0.10	37,37,37,37	0
55	MG	1A	3031	1/1	0.96	0.74	26,26,26,26	0
55	MG	2A	3563	1/1	0.96	0.18	27,27,27,27	0
55	MG	2A	3594	1/1	0.96	0.51	37,37,37,37	0
55	MG	2A	3419	1/1	0.96	0.13	31,31,31,31	0
55	MG	2B	218	1/1	0.96	0.21	37,37,37,37	0
55	MG	2A	3598	1/1	0.96	0.19	32,32,32,32	0
55	MG	2A	3833	1/1	0.96	0.09	47,47,47,47	0
55	MG	2A	3307	1/1	0.96	0.29	38,38,38,38	0
55	MG	1A	3946	1/1	0.96	0.10	30,30,30,30	0
55	MG	1A	3177	1/1	0.96	0.10	26,26,26,26	0
55	MG	2A	3609	1/1	0.96	0.11	27,27,27,27	0
55	MG	1A	3926	1/1	0.96	0.06	34,34,34,34	0
55	MG	2A	3269	1/1	0.96	0.11	30,30,30,30	0
55	MG	1A	3504	1/1	0.96	0.50	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	1A	4022	1/1	0.96	0.13	27,27,27,27	0
55	MG	1A	4017	1/1	0.96	0.11	25,25,25,25	0
55	MG	2a	1781	1/1	0.96	0.06	53,53,53,53	0
55	MG	1A	3092	1/1	0.96	0.29	22,22,22,22	0
55	MG	1A	3682	1/1	0.96	0.11	56,56,56,56	0
55	MG	2A	3640	1/1	0.96	0.35	39,39,39,39	0
55	MG	1A	3091	1/1	0.96	0.21	32,32,32,32	0
55	MG	1a	3055	1/1	0.96	0.10	46,46,46,46	0
55	MG	18	105	1/1	0.96	0.13	35,35,35,35	0
55	MG	1A	3074	1/1	0.96	0.39	19,19,19,19	0
55	MG	15	103	1/1	0.96	0.16	23,23,23,23	0
55	MG	10	103	1/1	0.96	0.18	25,25,25,25	0
55	MG	1A	3212	1/1	0.96	0.08	10,10,10,10	0
55	MG	1A	3242	1/1	0.96	1.00	28,28,28,28	0
55	MG	1B	216	1/1	0.96	0.23	67,67,67,67	0
55	MG	1A	3449	1/1	0.96	0.21	15,15,15,15	0
55	MG	2A	3315	1/1	0.96	0.07	14,14,14,14	0
55	MG	2A	3668	1/1	0.96	0.13	29,29,29,29	0
55	MG	1A	3176	1/1	0.96	0.17	21,21,21,21	0
55	MG	2A	3147	1/1	0.96	0.26	51,51,51,51	0
55	MG	1a	3036	1/1	0.96	0.14	34,34,34,34	0
55	MG	1A	3014	1/1	0.96	0.13	30,30,30,30	0
55	MG	2A	3458	1/1	0.96	0.10	28,28,28,28	0
55	MG	2A	3348	1/1	0.96	0.62	32,32,32,32	0
55	MG	2A	3110	1/1	0.96	0.18	17,17,17,17	0
55	MG	2A	3508	1/1	0.96	0.13	15,15,15,15	0
55	MG	1A	3207	1/1	0.96	0.16	22,22,22,22	0
55	MG	1a	3183	1/1	0.96	0.12	44,44,44,44	0
55	MG	1a	3063	1/1	0.96	0.11	42,42,42,42	0
55	MG	2A	3188	1/1	0.96	0.08	30,30,30,30	0
55	MG	1A	3923	1/1	0.96	0.23	36,36,36,36	0
55	MG	2A	3044	1/1	0.96	1.07	33,33,33,33	0
55	MG	2A	3532	1/1	0.96	0.10	24,24,24,24	0
55	MG	1A	3605	1/1	0.96	0.29	53,53,53,53	0
55	MG	2a	1754	1/1	0.96	0.13	45,45,45,45	0
55	MG	1D	307	1/1	0.96	0.14	10,10,10,10	0
55	MG	1A	3424	1/1	0.96	0.10	21,21,21,21	0
55	MG	1a	3038	1/1	0.96	0.13	54,54,54,54	0
55	MG	1A	3987	1/1	0.96	0.23	34,34,34,34	0
55	MG	1A	4016	1/1	0.96	0.24	54,54,54,54	0
55	MG	23	101	1/1	0.96	0.45	21,21,21,21	0
55	MG	1A	3275	1/1	0.96	0.54	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	1A	3899	1/1	0.96	0.13	22,22,22,22	0
55	MG	23	103	1/1	0.96	0.23	17,17,17,17	0
55	MG	2a	1809	1/1	0.96	0.13	26,26,26,26	0
55	MG	2A	3046	1/1	0.96	0.13	56,56,56,56	0
55	MG	2A	3399	1/1	0.96	0.28	32,32,32,32	0
55	MG	1A	3951	1/1	0.96	0.16	33,33,33,33	0
55	MG	2A	3844	1/1	0.96	0.20	40,40,40,40	0
55	MG	2A	3638	1/1	0.96	0.09	26,26,26,26	0
55	MG	2A	3082	1/1	0.96	0.22	44,44,44,44	0
55	MG	2F	302	1/1	0.96	0.24	32,32,32,32	0
55	MG	1A	3432	1/1	0.96	0.10	20,20,20,20	0
55	MG	1A	3291	1/1	0.96	0.15	18,18,18,18	0
55	MG	1A	3152	1/1	0.96	0.12	29,29,29,29	0
55	MG	2A	3664	1/1	0.96	0.32	34,34,34,34	0
55	MG	1A	3503	1/1	0.96	0.24	40,40,40,40	0
55	MG	1A	3219	1/1	0.96	0.20	36,36,36,36	0
55	MG	2A	3656	1/1	0.96	0.09	35,35,35,35	0
55	MG	2A	3845	1/1	0.96	0.13	38,38,38,38	0
55	MG	1A	3768	1/1	0.96	0.59	24,24,24,24	0
55	MG	2A	3581	1/1	0.96	0.11	33,33,33,33	0
55	MG	2A	3654	1/1	0.96	0.31	41,41,41,41	0
55	MG	1R	204	1/1	0.96	0.26	41,41,41,41	0
55	MG	1A	3685	1/1	0.96	0.24	26,26,26,26	0
55	MG	2a	1713	1/1	0.96	0.10	31,31,31,31	0
55	MG	2a	1620	1/1	0.96	0.25	63,63,63,63	0
55	MG	1A	3651	1/1	0.96	0.14	15,15,15,15	0
55	MG	2A	3303	1/1	0.96	0.24	44,44,44,44	0
55	MG	1a	3091	1/1	0.96	0.17	53,53,53,53	0
55	MG	2a	1752	1/1	0.96	0.17	37,37,37,37	0
55	MG	1B	201	1/1	0.96	0.14	23,23,23,23	0
55	MG	1a	3123	1/1	0.96	0.13	27,27,27,27	0
55	MG	1a	3106	1/1	0.96	0.10	10,10,10,10	0
55	MG	1A	4019	1/1	0.96	0.20	41,41,41,41	0
55	MG	1A	3757	1/1	0.96	0.33	23,23,23,23	0
55	MG	2A	3073	1/1	0.96	0.12	30,30,30,30	0
55	MG	1A	3792	1/1	0.96	0.08	37,37,37,37	0
55	MG	1A	3340	1/1	0.96	0.16	39,39,39,39	0
55	MG	1A	3647	1/1	0.96	0.13	43,43,43,43	0
55	MG	2A	3599	1/1	0.96	0.14	40,40,40,40	0
55	MG	1A	3814	1/1	0.96	0.09	25,25,25,25	0
55	MG	2A	3615	1/1	0.96	0.15	25,25,25,25	0
55	MG	16	101	1/1	0.96	0.12	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	1a	3111	1/1	0.96	0.12	25,25,25,25	0
55	MG	2A	3510	1/1	0.96	0.20	32,32,32,32	0
55	MG	1A	3156	1/1	0.96	0.13	24,24,24,24	0
55	MG	1A	3378	1/1	0.96	0.09	29,29,29,29	0
55	MG	1A	3375	1/1	0.96	0.79	29,29,29,29	0
55	MG	1A	3277	1/1	0.96	0.19	25,25,25,25	0
55	MG	1A	3116	1/1	0.96	0.17	29,29,29,29	0
55	MG	1A	3892	1/1	0.96	0.08	25,25,25,25	0
55	MG	1A	3474	1/1	0.96	0.38	23,23,23,23	0
55	MG	2a	1726	1/1	0.96	0.20	26,26,26,26	0
55	MG	1A	3858	1/1	0.96	0.12	41,41,41,41	0
55	MG	1A	3363	1/1	0.96	0.21	33,33,33,33	0
55	MG	19	102	1/1	0.96	0.12	31,31,31,31	0
55	MG	2A	3397	1/1	0.96	0.11	21,21,21,21	0
55	MG	1a	3150	1/1	0.96	0.09	41,41,41,41	0
55	MG	1A	3034	1/1	0.96	0.23	22,22,22,22	0
55	MG	2A	3050	1/1	0.96	0.12	31,31,31,31	0
55	MG	2r	101	1/1	0.96	0.18	40,40,40,40	0
55	MG	2A	3623	1/1	0.96	0.11	14,14,14,14	0
55	MG	1A	3084	1/1	0.96	0.09	32,32,32,32	0
55	MG	1a	3074	1/1	0.96	0.56	42,42,42,42	0
55	MG	2A	3742	1/1	0.96	0.32	50,50,50,50	0
55	MG	2A	3735	1/1	0.96	0.14	22,22,22,22	0
55	MG	1A	3019	1/1	0.96	0.44	30,30,30,30	0
55	MG	1Z	301	1/1	0.96	0.10	23,23,23,23	0
55	MG	2A	3743	1/1	0.96	0.12	35,35,35,35	0
55	MG	2A	3648	1/1	0.96	0.07	32,32,32,32	0
55	MG	2A	3454	1/1	0.96	0.15	28,28,28,28	0
55	MG	2A	3333	1/1	0.96	0.09	34,34,34,34	0
55	MG	1A	3266	1/1	0.96	0.97	52,52,52,52	0
55	MG	1A	3776	1/1	0.96	0.12	32,32,32,32	0
55	MG	1a	3156	1/1	0.96	0.17	39,39,39,39	0
55	MG	12	102	1/1	0.96	0.37	32,32,32,32	0
55	MG	1A	3136	1/1	0.96	0.54	30,30,30,30	0
55	MG	1a	3159	1/1	0.96	0.07	34,34,34,34	0
55	MG	1a	3019	1/1	0.96	0.14	50,50,50,50	0
55	MG	1A	3138	1/1	0.96	0.65	29,29,29,29	0
55	MG	1A	3107	1/1	0.96	0.08	14,14,14,14	0
55	MG	1A	3628	1/1	0.96	0.10	22,22,22,22	0
55	MG	1A	3534	1/1	0.96	0.64	37,37,37,37	0
55	MG	2a	1695	1/1	0.96	0.12	43,43,43,43	0
55	MG	1P	201	1/1	0.96	0.47	15,15,15,15	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	1A	3041	1/1	0.96	0.20	30,30,30,30	0
55	MG	1A	3134	1/1	0.96	0.99	34,34,34,34	0
55	MG	1A	3486	1/1	0.96	0.13	38,38,38,38	0
55	MG	2A	3106	1/1	0.96	0.12	23,23,23,23	0
55	MG	17	104	1/1	0.96	0.45	28,28,28,28	0
55	MG	1A	3925	1/1	0.96	0.13	20,20,20,20	0
55	MG	1B	232	1/1	0.96	0.16	59,59,59,59	0
55	MG	2A	3259	1/1	0.96	0.63	40,40,40,40	0
55	MG	2A	3476	1/1	0.96	0.23	24,24,24,24	0
55	MG	2A	3389	1/1	0.96	0.12	28,28,28,28	0
55	MG	2A	3473	1/1	0.96	0.19	19,19,19,19	0
55	MG	1a	3110	1/1	0.96	0.12	40,40,40,40	0
55	MG	1A	3552	1/1	0.96	0.07	21,21,21,21	0
55	MG	1A	3896	1/1	0.96	0.13	28,28,28,28	0
55	MG	1F	311	1/1	0.96	0.16	29,29,29,29	0
55	MG	1A	3453	1/1	0.96	0.22	24,24,24,24	0
55	MG	1A	3386	1/1	0.96	0.17	10,10,10,10	0
55	MG	1A	3799	1/1	0.96	0.66	51,51,51,51	0
55	MG	2a	1745	1/1	0.96	0.08	53,53,53,53	0
55	MG	1a	3120	1/1	0.96	0.15	42,42,42,42	0
55	MG	1A	3214	1/1	0.96	0.17	23,23,23,23	0
55	MG	2T	201	1/1	0.96	0.11	36,36,36,36	0
55	MG	2n	101	1/1	0.96	0.11	56,56,56,56	0
55	MG	2A	3813	1/1	0.96	0.13	34,34,34,34	0
55	MG	2A	3748	1/1	0.96	0.12	44,44,44,44	0
55	MG	1A	3283	1/1	0.96	0.11	12,12,12,12	0
55	MG	2A	3270	1/1	0.96	0.17	25,25,25,25	0
55	MG	1a	3143	1/1	0.96	0.10	34,34,34,34	0
55	MG	2A	3013	1/1	0.96	0.47	36,36,36,36	0
55	MG	1A	3742	1/1	0.96	0.10	22,22,22,22	0
55	MG	1A	3770	1/1	0.96	0.13	32,32,32,32	0
55	MG	2a	1737	1/1	0.96	0.17	28,28,28,28	0
55	MG	2x	106	1/1	0.96	0.14	60,60,60,60	0
55	MG	2A	3032	1/1	0.96	0.11	28,28,28,28	0
55	MG	2A	3043	1/1	0.96	0.10	20,20,20,20	0
55	MG	2A	3182	1/1	0.96	0.33	25,25,25,25	0
55	MG	1A	3390	1/1	0.96	0.12	30,30,30,30	0
55	MG	2A	3734	1/1	0.96	0.34	39,39,39,39	0
55	MG	1A	3389	1/1	0.96	0.11	21,21,21,21	0
55	MG	2A	3274	1/1	0.96	0.42	46,46,46,46	0
55	MG	1A	3220	1/1	0.96	0.22	34,34,34,34	0
55	MG	1a	3006	1/1	0.96	0.29	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	2A	3846	1/1	0.96	0.43	43,43,43,43	0
55	MG	1A	3956	1/1	0.96	0.25	39,39,39,39	0
55	MG	1F	304	1/1	0.96	0.08	30,30,30,30	0
55	MG	2a	1627	1/1	0.96	0.17	27,27,27,27	0
55	MG	2D	306	1/1	0.96	0.58	28,28,28,28	0
55	MG	1A	3777	1/1	0.96	0.04	51,51,51,51	0
55	MG	1A	3023	1/1	0.96	0.19	24,24,24,24	0
55	MG	2A	3358	1/1	0.96	0.15	17,17,17,17	0
55	MG	1A	3209	1/1	0.96	0.07	24,24,24,24	0
55	MG	1A	3149	1/1	0.96	0.28	23,23,23,23	0
55	MG	1A	3668	1/1	0.96	0.19	10,10,10,10	0
55	MG	2a	1663	1/1	0.96	0.15	31,31,31,31	0
55	MG	1A	3646	1/1	0.96	0.12	16,16,16,16	0
55	MG	1A	3673	1/1	0.96	0.41	39,39,39,39	0
55	MG	1A	3469	1/1	0.96	0.12	25,25,25,25	0
55	MG	1a	3178	1/1	0.96	0.14	36,36,36,36	0
55	MG	2A	3788	1/1	0.96	0.10	40,40,40,40	0
55	MG	2A	3807	1/1	0.96	0.17	21,21,21,21	0
55	MG	2A	3117	1/1	0.96	0.31	33,33,33,33	0
55	MG	2A	3715	1/1	0.96	0.29	46,46,46,46	0
55	MG	1a	3164	1/1	0.96	0.15	52,52,52,52	0
55	MG	1A	3657	1/1	0.96	0.10	19,19,19,19	0
55	MG	2A	3698	1/1	0.96	0.29	34,34,34,34	0
55	MG	1A	3759	1/1	0.96	0.14	20,20,20,20	0
55	MG	1A	3730	1/1	0.96	0.14	37,37,37,37	0
55	MG	1A	3090	1/1	0.96	0.10	42,42,42,42	0
55	MG	1A	4008	1/1	0.96	0.21	24,24,24,24	0
55	MG	2A	3228	1/1	0.96	0.18	45,45,45,45	0
55	MG	1A	3002	1/1	0.96	0.22	39,39,39,39	0
55	MG	1A	3357	1/1	0.96	0.10	39,39,39,39	0
55	MG	2A	3796	1/1	0.96	0.15	22,22,22,22	0
55	MG	2A	3084	1/1	0.96	0.17	28,28,28,28	0
55	MG	1A	3565	1/1	0.96	0.16	16,16,16,16	0
55	MG	2A	3652	1/1	0.96	0.30	31,31,31,31	0
55	MG	2A	3375	1/1	0.96	0.14	35,35,35,35	0
55	MG	2A	3369	1/1	0.96	0.09	19,19,19,19	0
55	MG	2A	3708	1/1	0.96	0.07	20,20,20,20	0
55	MG	1A	3028	1/1	0.96	0.24	39,39,39,39	0
55	MG	1A	3043	1/1	0.96	0.19	25,25,25,25	0
55	MG	1A	3879	1/1	0.96	0.22	41,41,41,41	0
55	MG	1A	3995	1/1	0.96	0.59	48,48,48,48	0
55	MG	1A	3632	1/1	0.96	0.10	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	2A	3597	1/1	0.96	0.14	26,26,26,26	0
55	MG	2A	3212	1/1	0.96	0.21	26,26,26,26	0
55	MG	2A	3226	1/1	0.96	0.14	32,32,32,32	0
55	MG	1A	3444	1/1	0.96	0.12	18,18,18,18	0
55	MG	1A	3410	1/1	0.96	0.24	34,34,34,34	0
55	MG	2a	1779	1/1	0.96	0.11	19,19,19,19	0
55	MG	1A	3900	1/1	0.96	0.09	22,22,22,22	0
55	MG	2A	3120	1/1	0.96	0.17	30,30,30,30	0
55	MG	1A	3185	1/1	0.96	0.10	23,23,23,23	0
55	MG	2A	3063	1/1	0.96	0.10	26,26,26,26	0
55	MG	2A	3555	1/1	0.96	0.10	32,32,32,32	0
55	MG	1A	3993	1/1	0.96	0.20	10,10,10,10	0
55	MG	1A	3713	1/1	0.96	0.15	40,40,40,40	0
55	MG	1A	4029	1/1	0.96	0.19	36,36,36,36	0
55	MG	1A	3633	1/1	0.96	0.14	26,26,26,26	0
55	MG	2A	3395	1/1	0.96	0.67	38,38,38,38	0
55	MG	1Q	204	1/1	0.96	0.14	35,35,35,35	0
55	MG	2A	3535	1/1	0.96	0.15	24,24,24,24	0
55	MG	2A	3520	1/1	0.96	0.22	48,48,48,48	0
55	MG	2A	3670	1/1	0.96	0.11	43,43,43,43	0
57	ZN	1n	104	1/1	0.96	0.11	68,68,68,68	0
55	MG	1A	3745	1/1	0.96	0.48	32,32,32,32	0
55	MG	2a	1808	1/1	0.96	0.06	56,56,56,56	0
55	MG	1A	3873	1/1	0.96	0.06	50,50,50,50	0
55	MG	1E	304	1/1	0.96	0.08	24,24,24,24	0
55	MG	1x	109	1/1	0.96	0.07	53,53,53,53	0
55	MG	1W	203	1/1	0.96	0.13	13,13,13,13	0
55	MG	2A	3019	1/1	0.96	0.36	47,47,47,47	0
55	MG	2A	3516	1/1	0.96	0.07	36,36,36,36	0
55	MG	1A	3653	1/1	0.96	0.08	21,21,21,21	0
55	MG	1A	3210	1/1	0.96	0.16	25,25,25,25	0
55	MG	1A	3420	1/1	0.96	0.18	29,29,29,29	0
55	MG	1A	3788	1/1	0.96	0.07	35,35,35,35	0
55	MG	1A	3298	1/1	0.96	0.13	38,38,38,38	0
55	MG	2a	1750	1/1	0.96	0.10	32,32,32,32	0
55	MG	2A	3789	1/1	0.96	0.17	34,34,34,34	0
55	MG	1a	3134	1/1	0.96	0.12	28,28,28,28	0
55	MG	1a	3180	1/1	0.96	0.08	55,55,55,55	0
55	MG	1a	3039	1/1	0.96	0.08	20,20,20,20	0
55	MG	1A	3494	1/1	0.96	0.15	10,10,10,10	0
55	MG	1A	3997	1/1	0.96	0.18	37,37,37,37	0
55	MG	2a	1633	1/1	0.96	0.12	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	1A	3260	1/1	0.96	0.14	35,35,35,35	0
55	MG	2A	3837	1/1	0.96	0.18	23,23,23,23	0
55	MG	1A	3489	1/1	0.96	0.11	28,28,28,28	0
55	MG	2A	3439	1/1	0.96	0.12	15,15,15,15	0
55	MG	2A	3099	1/1	0.96	0.13	26,26,26,26	0
55	MG	1R	202	1/1	0.96	0.08	32,32,32,32	0
55	MG	1A	3535	1/1	0.96	0.64	22,22,22,22	0
55	MG	1A	3901	1/1	0.96	0.25	28,28,28,28	0
55	MG	1A	3727	1/1	0.96	0.16	39,39,39,39	0
55	MG	1A	3895	1/1	0.96	0.15	48,48,48,48	0
55	MG	1A	3365	1/1	0.96	0.20	41,41,41,41	0
55	MG	2A	3451	1/1	0.96	0.12	19,19,19,19	0
55	MG	1a	3018	1/1	0.96	0.25	42,42,42,42	0
55	MG	2A	3746	1/1	0.96	0.36	31,31,31,31	0
55	MG	2A	3049	1/1	0.96	0.09	21,21,21,21	0
55	MG	2A	3537	1/1	0.96	0.11	22,22,22,22	0
55	MG	2a	1760	1/1	0.96	0.17	38,38,38,38	0
55	MG	1A	3241	1/1	0.96	0.28	34,34,34,34	0
55	MG	2A	3163	1/1	0.96	0.21	33,33,33,33	0
55	MG	1A	3462	1/1	0.96	0.77	30,30,30,30	0
55	MG	1l	103	1/1	0.96	0.16	47,47,47,47	0
55	MG	1A	3609	1/1	0.97	0.08	17,17,17,17	0
55	MG	2A	3026	1/1	0.97	0.25	27,27,27,27	0
55	MG	1l	203	1/1	0.97	0.08	35,35,35,35	0
55	MG	2A	3692	1/1	0.97	0.18	48,48,48,48	0
55	MG	2A	3479	1/1	0.97	0.15	23,23,23,23	0
55	MG	1A	3482	1/1	0.97	0.34	28,28,28,28	0
55	MG	2A	3726	1/1	0.97	0.08	52,52,52,52	0
55	MG	2A	3463	1/1	0.97	0.19	16,16,16,16	0
55	MG	1a	3201	1/1	0.97	0.09	33,33,33,33	0
55	MG	1A	3276	1/1	0.97	0.14	40,40,40,40	0
55	MG	1a	3136	1/1	0.97	0.06	32,32,32,32	0
55	MG	1a	3167	1/1	0.97	0.28	31,31,31,31	0
55	MG	2A	3448	1/1	0.97	0.10	32,32,32,32	0
55	MG	1A	3769	1/1	0.97	0.10	48,48,48,48	0
55	MG	1a	3192	1/1	0.97	0.10	33,33,33,33	0
55	MG	1A	3088	1/1	0.97	0.20	28,28,28,28	0
55	MG	1A	3845	1/1	0.97	0.12	19,19,19,19	0
55	MG	1A	3082	1/1	0.97	0.17	36,36,36,36	0
55	MG	1A	3263	1/1	0.97	0.14	15,15,15,15	0
55	MG	2A	3481	1/1	0.97	1.08	39,39,39,39	0
55	MG	2A	3745	1/1	0.97	0.18	17,17,17,17	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	1A	3677	1/1	0.97	0.27	36,36,36,36	0
55	MG	1A	3054	1/1	0.97	0.18	21,21,21,21	0
55	MG	1A	3963	1/1	0.97	0.07	42,42,42,42	0
55	MG	1I	201	1/1	0.97	0.07	52,52,52,52	0
55	MG	1A	3664	1/1	0.97	0.14	20,20,20,20	0
55	MG	1a	3086	1/1	0.97	0.48	50,50,50,50	0
55	MG	2a	1644	1/1	0.97	0.19	31,31,31,31	0
55	MG	1A	3832	1/1	0.97	0.16	17,17,17,17	0
55	MG	1A	3117	1/1	0.97	0.09	24,24,24,24	0
55	MG	2A	3432	1/1	0.97	0.19	45,45,45,45	0
55	MG	2A	3712	1/1	0.97	0.11	22,22,22,22	0
55	MG	1A	3382	1/1	0.97	0.46	26,26,26,26	0
55	MG	2A	3413	1/1	0.97	0.08	30,30,30,30	0
55	MG	1a	3010	1/1	0.97	0.16	55,55,55,55	0
55	MG	1A	3547	1/1	0.97	0.22	24,24,24,24	0
55	MG	1A	3607	1/1	0.97	0.12	15,15,15,15	0
55	MG	2A	3474	1/1	0.97	0.20	10,10,10,10	0
55	MG	1A	3110	1/1	0.97	0.81	43,43,43,43	0
55	MG	2A	3561	1/1	0.97	0.15	27,27,27,27	0
55	MG	2A	3565	1/1	0.97	0.15	22,22,22,22	0
55	MG	1A	3966	1/1	0.97	0.16	28,28,28,28	0
55	MG	1A	3708	1/1	0.97	0.07	26,26,26,26	0
55	MG	1A	3254	1/1	0.97	0.23	27,27,27,27	0
55	MG	1A	4028	1/1	0.97	0.13	17,17,17,17	0
55	MG	1S	202	1/1	0.97	0.12	33,33,33,33	0
55	MG	1A	3818	1/1	0.97	0.14	28,28,28,28	0
55	MG	1E	302	1/1	0.97	0.28	32,32,32,32	0
55	MG	1A	3431	1/1	0.97	0.26	14,14,14,14	0
55	MG	1A	3163	1/1	0.97	0.14	19,19,19,19	0
55	MG	1A	3174	1/1	0.97	0.14	23,23,23,23	0
55	MG	1A	3971	1/1	0.97	0.14	20,20,20,20	0
55	MG	2A	3007	1/1	0.97	0.08	38,38,38,38	0
55	MG	1A	3289	1/1	0.97	0.25	10,10,10,10	0
55	MG	2A	3469	1/1	0.97	0.17	21,21,21,21	0
55	MG	1a	3077	1/1	0.97	0.11	46,46,46,46	0
55	MG	2a	1658	1/1	0.97	0.08	20,20,20,20	0
55	MG	2A	3281	1/1	0.97	0.28	40,40,40,40	0
55	MG	1A	3124	1/1	0.97	0.18	27,27,27,27	0
55	MG	1A	3576	1/1	0.97	0.13	10,10,10,10	0
55	MG	1A	3064	1/1	0.97	0.46	13,13,13,13	0
55	MG	2a	1769	1/1	0.97	0.11	64,64,64,64	0
55	MG	1A	3598	1/1	0.97	0.29	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	2A	3650	1/1	0.97	0.27	41,41,41,41	0
55	MG	1a	3099	1/1	0.97	0.13	18,18,18,18	0
55	MG	1a	3045	1/1	0.97	0.07	30,30,30,30	0
55	MG	2A	3031	1/1	0.97	0.38	46,46,46,46	0
55	MG	1x	101	1/1	0.97	0.19	38,38,38,38	0
55	MG	2q	201	1/1	0.97	0.09	30,30,30,30	0
55	MG	2A	3100	1/1	0.97	0.16	22,22,22,22	0
55	MG	1A	3794	1/1	0.97	0.07	35,35,35,35	0
55	MG	1a	3140	1/1	0.97	0.23	42,42,42,42	0
55	MG	1A	3973	1/1	0.97	0.12	38,38,38,38	0
55	MG	2U	201	1/1	0.97	1.21	48,48,48,48	0
55	MG	1A	3575	1/1	0.97	0.08	27,27,27,27	0
55	MG	2A	3047	1/1	0.97	0.08	33,33,33,33	0
55	MG	2A	3834	1/1	0.97	0.11	43,43,43,43	0
55	MG	1a	3195	1/1	0.97	0.06	25,25,25,25	0
55	MG	1A	3954	1/1	0.97	0.10	38,38,38,38	0
55	MG	1A	3445	1/1	0.97	0.08	19,19,19,19	0
55	MG	1A	4026	1/1	0.97	0.12	26,26,26,26	0
55	MG	1a	3147	1/1	0.97	0.10	44,44,44,44	0
55	MG	2A	3637	1/1	0.97	0.09	31,31,31,31	0
55	MG	1A	3560	1/1	0.97	0.17	19,19,19,19	0
55	MG	1A	3256	1/1	0.97	0.27	25,25,25,25	0
55	MG	1A	3571	1/1	0.97	0.08	25,25,25,25	0
55	MG	1a	3207	1/1	0.97	0.29	50,50,50,50	0
57	ZN	29	501	1/1	0.97	0.09	60,60,60,60	0
55	MG	2A	3548	1/1	0.97	0.29	22,22,22,22	0
55	MG	1A	4009	1/1	0.97	0.08	41,41,41,41	0
55	MG	1A	3941	1/1	0.97	0.12	15,15,15,15	0
55	MG	1A	3978	1/1	0.97	0.11	21,21,21,21	0
55	MG	1A	3114	1/1	0.97	0.38	10,10,10,10	0
55	MG	1A	3487	1/1	0.97	0.14	25,25,25,25	0
57	ZN	16	104	1/1	0.97	0.19	36,36,36,36	0
55	MG	1B	209	1/1	0.97	0.12	27,27,27,27	0
55	MG	2A	3401	1/1	0.97	0.17	38,38,38,38	0
55	MG	2A	3287	1/1	0.97	0.44	46,46,46,46	0
55	MG	1A	3126	1/1	0.97	0.12	48,48,48,48	0
55	MG	1A	3513	1/1	0.97	0.18	53,53,53,53	0
55	MG	2A	3238	1/1	0.97	0.60	18,18,18,18	0
55	MG	1A	3554	1/1	0.97	0.15	18,18,18,18	0
55	MG	2U	202	1/1	0.97	0.08	23,23,23,23	0
55	MG	2A	3628	1/1	0.97	0.14	31,31,31,31	0
55	MG	2A	3665	1/1	0.97	0.50	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	1A	3689	1/1	0.97	0.17	54,54,54,54	0
55	MG	1A	3859	1/1	0.97	0.06	51,51,51,51	0
55	MG	1A	3122	1/1	0.97	0.37	22,22,22,22	0
55	MG	1A	3669	1/1	0.97	0.10	26,26,26,26	0
55	MG	2a	1619	1/1	0.97	0.47	27,27,27,27	0
55	MG	1A	3563	1/1	0.97	0.12	19,19,19,19	0
55	MG	1A	3076	1/1	0.97	0.26	42,42,42,42	0
55	MG	1A	3703	1/1	0.97	0.20	25,25,25,25	0
55	MG	13	105	1/1	0.97	0.27	26,26,26,26	0
55	MG	21	103	1/1	0.97	0.16	18,18,18,18	0
55	MG	1Z	303	1/1	0.97	0.15	28,28,28,28	0
55	MG	1A	3049	1/1	0.97	0.24	26,26,26,26	0
55	MG	2A	3739	1/1	0.97	0.11	43,43,43,43	0
55	MG	2A	3579	1/1	0.97	0.20	25,25,25,25	0
55	MG	2A	3830	1/1	0.97	0.11	31,31,31,31	0
55	MG	1A	3548	1/1	0.97	0.15	23,23,23,23	0
55	MG	1F	309	1/1	0.97	0.14	45,45,45,45	0
55	MG	1A	3700	1/1	0.97	0.08	20,20,20,20	0
55	MG	2A	3525	1/1	0.97	0.19	29,29,29,29	0
55	MG	2A	3285	1/1	0.97	0.12	21,21,21,21	0
55	MG	2A	3386	1/1	0.97	0.15	31,31,31,31	0
55	MG	2A	3682	1/1	0.97	0.11	61,61,61,61	0
55	MG	1A	3663	1/1	0.97	0.20	44,44,44,44	0
55	MG	2a	1664	1/1	0.97	0.14	37,37,37,37	0
55	MG	2R	201	1/1	0.97	0.16	17,17,17,17	0
55	MG	2A	3784	1/1	0.97	0.11	43,43,43,43	0
55	MG	2A	3792	1/1	0.97	0.07	30,30,30,30	0
55	MG	2A	3647	1/1	0.97	0.13	41,41,41,41	0
55	MG	1a	3022	1/1	0.97	0.17	16,16,16,16	0
55	MG	2a	1686	1/1	0.97	0.23	37,37,37,37	0
55	MG	1Q	202	1/1	0.97	0.32	30,30,30,30	0
55	MG	18	104	1/1	0.97	0.07	33,33,33,33	0
55	MG	2A	3627	1/1	0.97	0.20	23,23,23,23	0
55	MG	1v	104	1/1	0.97	0.10	35,35,35,35	0
55	MG	1A	3599	1/1	0.97	0.11	27,27,27,27	0
55	MG	1A	3795	1/1	0.97	0.20	27,27,27,27	0
55	MG	1A	3573	1/1	0.97	0.14	24,24,24,24	0
55	MG	1A	3045	1/1	0.97	0.10	15,15,15,15	0
55	MG	1a	3158	1/1	0.97	0.12	19,19,19,19	0
55	MG	1A	3916	1/1	0.97	0.10	21,21,21,21	0
55	MG	2A	3747	1/1	0.97	0.16	49,49,49,49	0
55	MG	2a	1635	1/1	0.97	0.12	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	2A	3221	1/1	0.97	0.12	33,33,33,33	0
55	MG	1A	3782	1/1	0.97	0.09	29,29,29,29	0
55	MG	18	101	1/1	0.97	0.58	27,27,27,27	0
55	MG	1A	3936	1/1	0.97	0.18	39,39,39,39	0
55	MG	1a	3182	1/1	0.97	0.14	39,39,39,39	0
55	MG	1A	3603	1/1	0.97	0.07	36,36,36,36	0
55	MG	1A	3203	1/1	0.97	0.64	14,14,14,14	0
55	MG	2A	3452	1/1	0.97	0.28	37,37,37,37	0
55	MG	1A	3574	1/1	0.97	0.25	46,46,46,46	0
55	MG	1A	3672	1/1	0.97	0.13	32,32,32,32	0
55	MG	1a	3053	1/1	0.97	0.19	38,38,38,38	0
55	MG	1A	3578	1/1	0.97	0.09	26,26,26,26	0
55	MG	1a	3163	1/1	0.97	0.14	42,42,42,42	0
55	MG	1a	3188	1/1	0.97	0.07	41,41,41,41	0
55	MG	2A	3153	1/1	0.97	0.18	50,50,50,50	0
55	MG	2A	3311	1/1	0.97	0.20	33,33,33,33	0
55	MG	2A	3477	1/1	0.97	0.12	16,16,16,16	0
55	MG	1A	3543	1/1	0.97	0.24	30,30,30,30	0
55	MG	2A	3517	1/1	0.97	0.37	44,44,44,44	0
55	MG	2A	3604	1/1	0.97	0.21	34,34,34,34	0
55	MG	1a	3173	1/1	0.97	0.11	51,51,51,51	0
55	MG	1A	3660	1/1	0.97	0.13	10,10,10,10	0
55	MG	2A	3677	1/1	0.97	0.09	37,37,37,37	0
55	MG	1A	3559	1/1	0.97	0.15	42,42,42,42	0
55	MG	2A	3687	1/1	0.97	0.19	49,49,49,49	0
55	MG	2x	105	1/1	0.97	0.22	31,31,31,31	0
55	MG	1A	3318	1/1	0.97	0.32	27,27,27,27	0
55	MG	2A	3806	1/1	0.97	0.16	36,36,36,36	0
55	MG	2A	3229	1/1	0.97	0.12	22,22,22,22	0
55	MG	1A	3970	1/1	0.97	0.10	22,22,22,22	0
55	MG	1X	103	1/1	0.97	0.14	34,34,34,34	0
55	MG	1A	3259	1/1	0.97	0.08	10,10,10,10	0
55	MG	1A	3425	1/1	0.97	0.10	33,33,33,33	0
55	MG	1A	3409	1/1	0.97	0.08	50,50,50,50	0
55	MG	1a	3130	1/1	0.97	0.27	38,38,38,38	0
55	MG	1A	3649	1/1	0.97	0.18	31,31,31,31	0
55	MG	1A	3725	1/1	0.97	0.11	26,26,26,26	0
55	MG	1A	3710	1/1	0.97	0.06	13,13,13,13	0
55	MG	11	101	1/1	0.97	0.52	32,32,32,32	0
55	MG	1A	3221	1/1	0.97	0.62	30,30,30,30	0
55	MG	1A	3617	1/1	0.97	0.11	27,27,27,27	0
55	MG	1A	3906	1/1	0.97	0.18	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	1A	3325	1/1	0.97	0.43	41,41,41,41	0
55	MG	1a	3011	1/1	0.97	0.09	70,70,70,70	0
55	MG	18	102	1/1	0.97	0.56	26,26,26,26	0
55	MG	1A	3515	1/1	0.97	0.19	10,10,10,10	0
55	MG	2A	3816	1/1	0.97	0.19	25,25,25,25	0
55	MG	2A	3723	1/1	0.97	0.12	36,36,36,36	0
55	MG	1A	3667	1/1	0.97	0.15	18,18,18,18	0
55	MG	1A	3038	1/1	0.97	0.28	21,21,21,21	0
55	MG	1A	3838	1/1	0.97	0.14	26,26,26,26	0
55	MG	2A	3710	1/1	0.97	0.30	27,27,27,27	0
55	MG	2A	3394	1/1	0.97	0.14	27,27,27,27	0
55	MG	1A	3829	1/1	0.97	0.17	28,28,28,28	0
55	MG	1A	3267	1/1	0.97	0.36	37,37,37,37	0
55	MG	2Q	204	1/1	0.97	0.28	33,33,33,33	0
55	MG	1v	101	1/1	0.97	0.16	36,36,36,36	0
55	MG	2A	3567	1/1	0.97	0.15	33,33,33,33	0
55	MG	1A	3429	1/1	0.97	0.09	23,23,23,23	0
55	MG	1A	3135	1/1	0.97	0.13	23,23,23,23	0
55	MG	1P	202	1/1	0.97	0.57	15,15,15,15	0
55	MG	1A	3648	1/1	0.97	0.23	34,34,34,34	0
55	MG	1A	3238	1/1	0.97	0.09	27,27,27,27	0
55	MG	2A	3475	1/1	0.97	0.14	17,17,17,17	0
55	MG	1B	212	1/1	0.97	0.15	25,25,25,25	0
55	MG	2A	3667	1/1	0.97	0.09	32,32,32,32	0
55	MG	1A	3902	1/1	0.97	0.09	25,25,25,25	0
55	MG	1A	3396	1/1	0.97	0.19	22,22,22,22	0
55	MG	1A	3592	1/1	0.97	0.09	27,27,27,27	0
55	MG	1B	207	1/1	0.97	0.13	42,42,42,42	0
55	MG	2A	3478	1/1	0.97	0.20	15,15,15,15	0
55	MG	2A	3021	1/1	0.97	0.20	55,55,55,55	0
55	MG	2A	3744	1/1	0.97	0.08	51,51,51,51	0
55	MG	1A	3100	1/1	0.97	0.16	38,38,38,38	0
55	MG	2A	3029	1/1	0.97	0.11	21,21,21,21	0
55	MG	1a	3141	1/1	0.97	0.47	45,45,45,45	0
55	MG	1U	207	1/1	0.97	0.50	31,31,31,31	0
55	MG	1A	3234	1/1	0.97	0.39	28,28,28,28	0
55	MG	1a	3001	1/1	0.97	0.07	47,47,47,47	0
55	MG	1W	209	1/1	0.97	0.21	29,29,29,29	0
55	MG	1A	3187	1/1	0.97	0.80	33,33,33,33	0
55	MG	1n	103	1/1	0.97	0.12	37,37,37,37	0
55	MG	1V	204	1/1	0.97	0.09	51,51,51,51	0
55	MG	2A	3002	1/1	0.97	0.10	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	1A	3931	1/1	0.97	0.20	20,20,20,20	0
55	MG	1A	3456	1/1	0.97	0.33	24,24,24,24	0
55	MG	2e	202	1/1	0.97	0.16	47,47,47,47	0
55	MG	1A	3525	1/1	0.97	0.12	25,25,25,25	0
55	MG	2A	3783	1/1	0.97	0.12	19,19,19,19	0
55	MG	2A	3383	1/1	0.97	0.20	37,37,37,37	0
55	MG	1A	3917	1/1	0.97	0.12	16,16,16,16	0
55	MG	1U	201	1/1	0.97	0.56	24,24,24,24	0
55	MG	1A	3414	1/1	0.97	0.35	26,26,26,26	0
55	MG	2A	3116	1/1	0.97	0.47	38,38,38,38	0
55	MG	2A	3755	1/1	0.97	0.15	42,42,42,42	0
55	MG	2A	3554	1/1	0.97	0.27	28,28,28,28	0
55	MG	2A	3118	1/1	0.97	0.07	51,51,51,51	0
55	MG	1A	3693	1/1	0.97	0.20	46,46,46,46	0
55	MG	1A	3195	1/1	0.97	0.36	31,31,31,31	0
55	MG	2a	1700	1/1	0.97	0.21	43,43,43,43	0
55	MG	2e	201	1/1	0.97	0.13	43,43,43,43	0
55	MG	1A	3533	1/1	0.97	0.12	21,21,21,21	0
55	MG	1A	3821	1/1	0.97	0.14	10,10,10,10	0
55	MG	2A	3553	1/1	0.97	0.24	45,45,45,45	0
55	MG	1A	3947	1/1	0.97	0.15	25,25,25,25	0
55	MG	1A	3819	1/1	0.97	0.13	22,22,22,22	0
55	MG	1A	3732	1/1	0.97	0.13	18,18,18,18	0
55	MG	1R	205	1/1	0.97	0.06	30,30,30,30	0
55	MG	2A	3069	1/1	0.97	0.13	28,28,28,28	0
55	MG	1A	3194	1/1	0.97	0.66	32,32,32,32	0
55	MG	1A	4011	1/1	0.97	0.26	54,54,54,54	0
55	MG	1A	3779	1/1	0.97	0.19	27,27,27,27	0
55	MG	2A	3588	1/1	0.97	0.08	42,42,42,42	0
55	MG	1x	113	1/1	0.97	0.22	50,50,50,50	0
55	MG	2A	3483	1/1	0.97	0.14	29,29,29,29	0
55	MG	1A	3785	1/1	0.97	0.14	14,14,14,14	0
55	MG	1A	3724	1/1	0.97	0.12	20,20,20,20	0
55	MG	1F	303	1/1	0.97	0.31	29,29,29,29	0
55	MG	2A	3527	1/1	0.97	0.12	40,40,40,40	0
55	MG	1A	3349	1/1	0.97	0.14	26,26,26,26	0
55	MG	2A	3342	1/1	0.97	0.08	21,21,21,21	0
55	MG	2A	3450	1/1	0.97	0.15	19,19,19,19	0
55	MG	1A	3042	1/1	0.97	0.09	18,18,18,18	0
55	MG	1a	3103	1/1	0.97	0.11	44,44,44,44	0
55	MG	2x	107	1/1	0.97	0.11	47,47,47,47	0
55	MG	1A	3037	1/1	0.97	0.28	15,15,15,15	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	1x	111	1/1	0.97	0.12	32,32,32,32	0
55	MG	2A	3408	1/1	0.97	0.20	34,34,34,34	0
55	MG	2I	102	1/1	0.97	0.44	40,40,40,40	0
55	MG	1A	3231	1/1	0.97	0.12	22,22,22,22	0
55	MG	2A	3329	1/1	0.97	0.31	23,23,23,23	0
55	MG	1A	3010	1/1	0.97	0.28	33,33,33,33	0
55	MG	1a	3084	1/1	0.97	0.10	10,10,10,10	0
55	MG	1A	3656	1/1	0.97	0.09	36,36,36,36	0
55	MG	1A	3085	1/1	0.97	0.16	14,14,14,14	0
55	MG	1A	3781	1/1	0.97	0.07	41,41,41,41	0
55	MG	1a	3115	1/1	0.97	0.20	38,38,38,38	0
55	MG	1A	3809	1/1	0.97	0.68	32,32,32,32	0
55	MG	1A	3800	1/1	0.97	0.12	24,24,24,24	0
55	MG	1A	3614	1/1	0.97	0.16	14,14,14,14	0
55	MG	2A	3384	1/1	0.97	0.11	24,24,24,24	0
55	MG	2A	3719	1/1	0.97	0.20	47,47,47,47	0
55	MG	1A	3643	1/1	0.97	0.17	35,35,35,35	0
55	MG	2A	3467	1/1	0.97	0.15	34,34,34,34	0
55	MG	1A	3545	1/1	0.97	0.19	22,22,22,22	0
55	MG	2A	3780	1/1	0.97	0.23	51,51,51,51	0
55	MG	1A	3086	1/1	0.97	0.10	37,37,37,37	0
55	MG	1F	312	1/1	0.97	0.09	19,19,19,19	0
55	MG	1O	202	1/1	0.97	0.21	47,47,47,47	0
55	MG	1A	3843	1/1	0.97	0.55	35,35,35,35	0
55	MG	1A	3679	1/1	0.97	0.46	23,23,23,23	0
55	MG	1A	3369	1/1	0.97	0.13	32,32,32,32	0
55	MG	2A	3176	1/1	0.97	0.09	19,19,19,19	0
55	MG	1A	3067	1/1	0.97	0.11	21,21,21,21	0
55	MG	1A	3119	1/1	0.97	0.20	34,34,34,34	0
55	MG	1A	3594	1/1	0.97	0.24	25,25,25,25	0
55	MG	1a	3044	1/1	0.97	0.10	56,56,56,56	0
55	MG	25	103	1/1	0.97	0.16	27,27,27,27	0
55	MG	1A	3484	1/1	0.97	0.46	24,24,24,24	0
55	MG	1A	3756	1/1	0.97	0.11	23,23,23,23	0
55	MG	1A	3711	1/1	0.98	0.09	10,10,10,10	0
55	MG	1a	3138	1/1	0.98	0.12	19,19,19,19	0
55	MG	2a	1711	1/1	0.98	0.12	49,49,49,49	0
55	MG	1A	3856	1/1	0.98	0.46	39,39,39,39	0
55	MG	1a	3008	1/1	0.98	0.12	54,54,54,54	0
55	MG	2a	1683	1/1	0.98	0.11	36,36,36,36	0
55	MG	2A	3427	1/1	0.98	0.65	45,45,45,45	0
55	MG	2A	3490	1/1	0.98	0.20	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	1a	3194	1/1	0.98	0.07	27,27,27,27	0
55	MG	1A	3674	1/1	0.98	0.12	32,32,32,32	0
55	MG	2A	3417	1/1	0.98	0.13	16,16,16,16	0
55	MG	1a	3092	1/1	0.98	0.15	51,51,51,51	0
55	MG	1A	3636	1/1	0.98	0.07	29,29,29,29	0
55	MG	2A	3083	1/1	0.98	0.35	27,27,27,27	0
55	MG	2A	3020	1/1	0.98	0.23	26,26,26,26	0
55	MG	2A	3633	1/1	0.98	0.23	30,30,30,30	0
55	MG	2A	3798	1/1	0.98	0.20	23,23,23,23	0
55	MG	2A	3551	1/1	0.98	0.10	32,32,32,32	0
55	MG	2A	3271	1/1	0.98	0.12	57,57,57,57	0
55	MG	2A	3685	1/1	0.98	0.11	10,10,10,10	0
55	MG	2a	1696	1/1	0.98	0.11	53,53,53,53	0
55	MG	1A	3131	1/1	0.98	0.27	21,21,21,21	0
55	MG	13	101	1/1	0.98	0.37	30,30,30,30	0
55	MG	1A	3823	1/1	0.98	0.10	16,16,16,16	0
55	MG	2A	3524	1/1	0.98	0.14	23,23,23,23	0
55	MG	1A	3890	1/1	0.98	0.28	43,43,43,43	0
55	MG	2A	3771	1/1	0.98	0.13	26,26,26,26	0
55	MG	1A	3101	1/1	0.98	0.33	34,34,34,34	0
55	MG	2A	3070	1/1	0.98	0.11	34,34,34,34	0
55	MG	1A	3129	1/1	0.98	0.64	24,24,24,24	0
55	MG	2A	3488	1/1	0.98	0.19	16,16,16,16	0
55	MG	2A	3010	1/1	0.98	0.07	42,42,42,42	0
55	MG	1A	4015	1/1	0.98	0.33	19,19,19,19	0
55	MG	1A	3093	1/1	0.98	0.12	18,18,18,18	0
55	MG	1A	3939	1/1	0.98	0.11	14,14,14,14	0
55	MG	2A	3586	1/1	0.98	0.12	31,31,31,31	0
55	MG	2A	3344	1/1	0.98	0.14	37,37,37,37	0
55	MG	2A	3721	1/1	0.98	0.13	40,40,40,40	0
55	MG	1A	3150	1/1	0.98	0.09	27,27,27,27	0
55	MG	17	106	1/1	0.98	0.22	17,17,17,17	0
55	MG	1A	3540	1/1	0.98	0.15	14,14,14,14	0
55	MG	1a	3132	1/1	0.98	0.18	31,31,31,31	0
55	MG	2A	3185	1/1	0.98	0.30	54,54,54,54	0
55	MG	1A	3979	1/1	0.98	0.21	36,36,36,36	0
55	MG	2A	3038	1/1	0.98	0.25	51,51,51,51	0
55	MG	1A	3692	1/1	0.98	0.11	44,44,44,44	0
55	MG	1A	3773	1/1	0.98	0.10	21,21,21,21	0
55	MG	1X	104	1/1	0.98	0.10	22,22,22,22	0
55	MG	1A	3980	1/1	0.98	0.08	24,24,24,24	0
55	MG	1A	3920	1/1	0.98	0.13	15,15,15,15	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	2a	1722	1/1	0.98	0.10	26,26,26,26	0
55	MG	1A	3627	1/1	0.98	0.19	10,10,10,10	0
55	MG	1A	3958	1/1	0.98	0.15	27,27,27,27	0
55	MG	1a	3135	1/1	0.98	0.14	26,26,26,26	0
55	MG	1A	3068	1/1	0.98	0.27	34,34,34,34	0
55	MG	17	105	1/1	0.98	0.29	22,22,22,22	0
55	MG	1A	3854	1/1	0.98	0.08	38,38,38,38	0
55	MG	1A	3046	1/1	0.98	0.12	30,30,30,30	0
55	MG	1A	3115	1/1	0.98	0.28	20,20,20,20	0
55	MG	1a	3046	1/1	0.98	0.11	33,33,33,33	0
55	MG	1A	3686	1/1	0.98	0.14	39,39,39,39	0
55	MG	2A	3121	1/1	0.98	0.06	29,29,29,29	0
55	MG	2a	1689	1/1	0.98	0.14	42,42,42,42	0
55	MG	2B	208	1/1	0.98	0.08	22,22,22,22	0
55	MG	2A	3208	1/1	0.98	0.10	37,37,37,37	0
55	MG	1H	202	1/1	0.98	0.12	22,22,22,22	0
55	MG	2A	3129	1/1	0.98	0.22	27,27,27,27	0
55	MG	2a	1677	1/1	0.98	0.06	45,45,45,45	0
55	MG	1A	4013	1/1	0.98	0.13	28,28,28,28	0
55	MG	1A	3937	1/1	0.98	0.08	29,29,29,29	0
55	MG	1A	3654	1/1	0.98	0.11	43,43,43,43	0
55	MG	1E	314	1/1	0.98	0.11	36,36,36,36	0
55	MG	1A	3065	1/1	0.98	0.12	16,16,16,16	0
55	MG	1A	3056	1/1	0.98	0.12	42,42,42,42	0
55	MG	2A	3590	1/1	0.98	0.12	27,27,27,27	0
55	MG	2A	3512	1/1	0.98	0.14	27,27,27,27	0
55	MG	1V	201	1/1	0.98	0.40	27,27,27,27	0
55	MG	2a	1629	1/1	0.98	0.10	30,30,30,30	0
55	MG	2A	3390	1/1	0.98	0.11	37,37,37,37	0
55	MG	1A	3520	1/1	0.98	0.16	11,11,11,11	0
55	MG	2a	1816	1/1	0.98	0.05	35,35,35,35	0
55	MG	2D	308	1/1	0.98	0.24	22,22,22,22	0
55	MG	1A	3047	1/1	0.98	0.17	21,21,21,21	0
55	MG	2D	307	1/1	0.98	0.20	25,25,25,25	0
55	MG	1U	204	1/1	0.98	0.34	17,17,17,17	0
55	MG	2a	1707	1/1	0.98	0.60	43,43,43,43	0
55	MG	1A	3572	1/1	0.98	0.10	36,36,36,36	0
55	MG	1T	201	1/1	0.98	0.32	13,13,13,13	0
55	MG	1B	227	1/1	0.98	0.10	31,31,31,31	0
55	MG	2A	3825	1/1	0.98	0.10	31,31,31,31	0
55	MG	1A	3388	1/1	0.98	0.23	19,19,19,19	0
55	MG	2A	3826	1/1	0.98	0.09	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	1A	3755	1/1	0.98	0.41	26,26,26,26	0
55	MG	1A	3478	1/1	0.98	0.45	27,27,27,27	0
55	MG	1A	3052	1/1	0.98	0.08	19,19,19,19	0
55	MG	2a	1630	1/1	0.98	0.13	48,48,48,48	0
57	ZN	2n	102	1/1	0.98	0.12	52,52,52,52	0
55	MG	18	106	1/1	0.98	0.11	10,10,10,10	0
55	MG	1A	3500	1/1	0.98	0.35	34,34,34,34	0
55	MG	1a	3146	1/1	0.98	0.16	29,29,29,29	0
55	MG	1A	3798	1/1	0.98	0.11	17,17,17,17	0
55	MG	1a	3175	1/1	0.98	0.07	74,74,74,74	0
55	MG	2A	3360	1/1	0.98	0.06	38,38,38,38	0
55	MG	1A	3095	1/1	0.98	0.51	29,29,29,29	0
55	MG	1A	3278	1/1	0.98	0.28	32,32,32,32	0
55	MG	2A	3492	1/1	0.98	0.15	10,10,10,10	0
55	MG	2a	1803	1/1	0.98	0.08	29,29,29,29	0
55	MG	1A	3527	1/1	0.98	0.14	17,17,17,17	0
55	MG	2A	3800	1/1	0.98	0.12	20,20,20,20	0
55	MG	1A	3111	1/1	0.98	0.22	40,40,40,40	0
55	MG	1A	3499	1/1	0.98	0.15	39,39,39,39	0
55	MG	1E	310	1/1	0.98	0.11	20,20,20,20	0
55	MG	15	101	1/1	0.98	0.67	36,36,36,36	0
55	MG	1W	202	1/1	0.98	0.23	20,20,20,20	0
55	MG	2A	3472	1/1	0.98	0.23	15,15,15,15	0
55	MG	2A	3152	1/1	0.98	0.19	50,50,50,50	0
55	MG	2A	3266	1/1	0.98	0.27	32,32,32,32	0
55	MG	1l	201	1/1	0.98	0.19	24,24,24,24	0
55	MG	1A	3729	1/1	0.98	0.15	29,29,29,29	0
55	MG	21	104	1/1	0.98	0.11	27,27,27,27	0
55	MG	1A	3867	1/1	0.98	0.16	18,18,18,18	0
55	MG	2A	3543	1/1	0.98	0.08	23,23,23,23	0
55	MG	1A	3596	1/1	0.98	0.09	34,34,34,34	0
55	MG	1A	3864	1/1	0.98	0.10	31,31,31,31	0
55	MG	1A	3253	1/1	0.98	0.31	21,21,21,21	0
55	MG	1A	3211	1/1	0.98	0.11	37,37,37,37	0
55	MG	2A	3795	1/1	0.98	0.15	30,30,30,30	0
55	MG	1A	3404	1/1	0.98	0.11	21,21,21,21	0
55	MG	1A	3353	1/1	0.98	0.35	34,34,34,34	0
55	MG	1A	3081	1/1	0.98	0.09	15,15,15,15	0
55	MG	1A	3452	1/1	0.98	0.14	21,21,21,21	0
55	MG	1A	4027	1/1	0.98	0.09	11,11,11,11	0
55	MG	1A	3874	1/1	0.98	0.11	30,30,30,30	0
55	MG	2a	1715	1/1	0.98	0.12	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	1A	3977	1/1	0.98	0.11	23,23,23,23	0
55	MG	1A	3743	1/1	0.98	0.11	10,10,10,10	0
55	MG	2A	3468	1/1	0.98	0.30	19,19,19,19	0
55	MG	1A	3153	1/1	0.98	0.13	30,30,30,30	0
55	MG	1A	3302	1/1	0.98	0.17	26,26,26,26	0
55	MG	1A	3003	1/1	0.98	0.10	28,28,28,28	0
55	MG	1A	3407	1/1	0.98	0.16	37,37,37,37	0
55	MG	2A	3033	1/1	0.98	0.10	22,22,22,22	0
55	MG	1A	3717	1/1	0.98	0.11	25,25,25,25	0
55	MG	1A	3077	1/1	0.98	0.12	24,24,24,24	0
55	MG	1A	3940	1/1	0.98	0.20	22,22,22,22	0
55	MG	1a	3119	1/1	0.98	0.12	16,16,16,16	0
55	MG	2A	3702	1/1	0.98	0.07	31,31,31,31	0
55	MG	2A	3293	1/1	0.98	0.38	16,16,16,16	0
55	MG	1A	3178	1/1	0.98	0.09	17,17,17,17	0
55	MG	2A	3529	1/1	0.98	0.12	28,28,28,28	0
55	MG	2A	3018	1/1	0.98	0.14	10,10,10,10	0
55	MG	1A	3246	1/1	0.98	0.22	37,37,37,37	0
55	MG	2A	3804	1/1	0.98	0.09	31,31,31,31	0
55	MG	1a	3186	1/1	0.98	0.18	31,31,31,31	0
55	MG	2A	3636	1/1	0.98	0.12	28,28,28,28	0
55	MG	1A	3142	1/1	0.98	0.41	25,25,25,25	0
55	MG	2A	3803	1/1	0.98	0.18	32,32,32,32	0
55	MG	1A	3728	1/1	0.98	0.09	24,24,24,24	0
55	MG	2A	3022	1/1	0.98	0.22	27,27,27,27	0
55	MG	1x	108	1/1	0.98	0.21	28,28,28,28	0
55	MG	1A	3258	1/1	0.98	0.08	22,22,22,22	0
55	MG	1A	3705	1/1	0.98	0.12	36,36,36,36	0
55	MG	1A	3927	1/1	0.98	0.44	31,31,31,31	0
55	MG	2A	3446	1/1	0.98	0.44	59,59,59,59	0
55	MG	1A	3050	1/1	0.98	0.38	25,25,25,25	0
55	MG	2A	3400	1/1	0.98	0.22	13,13,13,13	0
55	MG	2A	3165	1/1	0.98	0.15	33,33,33,33	0
55	MG	2A	3257	1/1	0.98	0.19	35,35,35,35	0
55	MG	1A	3871	1/1	0.98	0.09	12,12,12,12	0
55	MG	1A	3237	1/1	0.98	0.09	25,25,25,25	0
55	MG	1A	3620	1/1	0.98	0.11	15,15,15,15	0
55	MG	1a	3097	1/1	0.98	0.14	23,23,23,23	0
55	MG	2A	3767	1/1	0.98	0.12	40,40,40,40	0
55	MG	1F	313	1/1	0.98	0.18	49,49,49,49	0
55	MG	2a	1672	1/1	0.98	0.10	21,21,21,21	0
55	MG	1A	3613	1/1	0.98	0.21	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	2A	3368	1/1	0.98	0.40	22,22,22,22	0
55	MG	1A	3181	1/1	0.98	0.09	27,27,27,27	0
55	MG	2A	3706	1/1	0.98	0.09	31,31,31,31	0
55	MG	2A	3295	1/1	0.98	0.42	31,31,31,31	0
55	MG	2A	3533	1/1	0.98	0.12	42,42,42,42	0
55	MG	2Q	203	1/1	0.98	0.41	49,49,49,49	0
55	MG	1A	3629	1/1	0.98	0.16	16,16,16,16	0
55	MG	2A	3626	1/1	0.98	0.07	21,21,21,21	0
55	MG	1B	217	1/1	0.98	0.23	32,32,32,32	0
55	MG	1A	3549	1/1	0.98	0.15	16,16,16,16	0
55	MG	16	102	1/1	0.98	0.12	18,18,18,18	0
55	MG	1A	3352	1/1	0.98	0.15	16,16,16,16	0
55	MG	1A	3676	1/1	0.98	0.11	25,25,25,25	0
55	MG	1a	3204	1/1	0.98	0.19	22,22,22,22	0
55	MG	2A	3192	1/1	0.98	0.11	25,25,25,25	0
55	MG	2A	3791	1/1	0.98	0.09	22,22,22,22	0
55	MG	1A	3020	1/1	0.98	0.17	24,24,24,24	0
55	MG	1A	3536	1/1	0.98	0.17	16,16,16,16	0
55	MG	1A	3645	1/1	0.98	0.16	30,30,30,30	0
55	MG	1A	3688	1/1	0.98	0.11	33,33,33,33	0
55	MG	2A	3370	1/1	0.98	0.13	25,25,25,25	0
55	MG	2A	3065	1/1	0.98	0.10	26,26,26,26	0
55	MG	1A	3321	1/1	0.98	0.22	18,18,18,18	0
55	MG	1A	3244	1/1	0.98	0.20	20,20,20,20	0
55	MG	1a	3125	1/1	0.98	0.20	21,21,21,21	0
55	MG	1A	3641	1/1	0.98	0.20	17,17,17,17	0
55	MG	2a	1764	1/1	0.98	0.36	41,41,41,41	0
55	MG	2A	3642	1/1	0.98	0.13	12,12,12,12	0
55	MG	2A	3127	1/1	0.98	0.19	32,32,32,32	0
55	MG	1R	201	1/1	0.98	0.36	40,40,40,40	0
55	MG	1A	3802	1/1	0.98	0.12	38,38,38,38	0
55	MG	2A	3190	1/1	0.98	0.20	42,42,42,42	0
55	MG	2A	3538	1/1	0.98	0.10	35,35,35,35	0
55	MG	1A	3454	1/1	0.98	0.14	21,21,21,21	0
55	MG	2A	3154	1/1	0.98	0.27	32,32,32,32	0
55	MG	1A	3950	1/1	0.98	0.15	27,27,27,27	0
55	MG	1A	3505	1/1	0.98	0.09	27,27,27,27	0
55	MG	1A	3626	1/1	0.98	0.15	14,14,14,14	0
55	MG	1A	3888	1/1	0.98	0.15	58,58,58,58	0
55	MG	1A	3844	1/1	0.98	0.18	23,23,23,23	0
55	MG	1R	203	1/1	0.98	0.34	30,30,30,30	0
55	MG	1A	3796	1/1	0.98	0.09	10,10,10,10	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	2A	3024	1/1	0.98	0.12	25,25,25,25	0
55	MG	1A	3830	1/1	0.98	0.12	30,30,30,30	0
55	MG	1A	3197	1/1	0.98	0.07	16,16,16,16	0
55	MG	2x	102	1/1	0.98	0.21	41,41,41,41	0
55	MG	1E	307	1/1	0.98	0.21	23,23,23,23	0
55	MG	1A	3701	1/1	0.98	0.21	42,42,42,42	0
55	MG	1A	3537	1/1	0.98	0.07	30,30,30,30	0
55	MG	1F	310	1/1	0.98	0.56	25,25,25,25	0
55	MG	1E	305	1/1	0.98	0.20	34,34,34,34	0
55	MG	1A	3053	1/1	0.98	0.17	31,31,31,31	0
55	MG	1D	302	1/1	0.98	0.20	30,30,30,30	0
55	MG	1A	3441	1/1	0.98	0.34	38,38,38,38	0
55	MG	2A	3339	1/1	0.98	0.09	34,34,34,34	0
55	MG	1A	3631	1/1	0.98	0.08	42,42,42,42	0
55	MG	1A	4004	1/1	0.98	0.23	31,31,31,31	0
55	MG	1A	3824	1/1	0.98	0.18	14,14,14,14	0
55	MG	2A	3570	1/1	0.98	0.10	33,33,33,33	0
55	MG	2A	3559	1/1	0.98	0.12	24,24,24,24	0
55	MG	2A	3003	1/1	0.98	0.21	29,29,29,29	0
55	MG	1D	310	1/1	0.98	0.09	36,36,36,36	0
55	MG	2A	3001	1/1	0.98	0.14	29,29,29,29	0
55	MG	2A	3518	1/1	0.98	0.26	34,34,34,34	0
55	MG	1a	3208	1/1	0.98	0.10	41,41,41,41	0
55	MG	1O	204	1/1	0.98	0.38	38,38,38,38	0
55	MG	2A	3822	1/1	0.98	0.05	28,28,28,28	0
55	MG	1A	3847	1/1	0.98	0.10	21,21,21,21	0
55	MG	1A	3139	1/1	0.98	0.23	35,35,35,35	0
55	MG	2a	1631	1/1	0.98	0.12	42,42,42,42	0
55	MG	1A	3465	1/1	0.98	0.31	22,22,22,22	0
55	MG	2A	3624	1/1	0.98	0.18	27,27,27,27	0
55	MG	2a	1661	1/1	0.98	0.14	46,46,46,46	0
55	MG	1A	3566	1/1	0.98	0.07	18,18,18,18	0
55	MG	2A	3415	1/1	0.98	0.08	36,36,36,36	0
55	MG	1A	3738	1/1	0.98	0.20	42,42,42,42	0
55	MG	2A	3196	1/1	0.98	0.42	29,29,29,29	0
55	MG	1A	3741	1/1	0.98	0.13	16,16,16,16	0
55	MG	2A	3713	1/1	0.98	0.28	39,39,39,39	0
55	MG	1A	3387	1/1	0.98	0.21	24,24,24,24	0
55	MG	1a	3087	1/1	0.98	0.05	36,36,36,36	0
55	MG	2A	3133	1/1	0.98	0.23	33,33,33,33	0
55	MG	1A	3857	1/1	0.98	0.21	23,23,23,23	0
55	MG	2A	3109	1/1	0.98	0.33	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	1A	3850	1/1	0.98	0.29	17,17,17,17	0
55	MG	2A	3373	1/1	0.98	0.18	31,31,31,31	0
55	MG	2a	1684	1/1	0.98	0.09	68,68,68,68	0
55	MG	1A	3279	1/1	0.98	0.10	16,16,16,16	0
55	MG	1A	3483	1/1	0.98	0.19	40,40,40,40	0
55	MG	1a	3131	1/1	0.98	0.15	42,42,42,42	0
55	MG	2A	3829	1/1	0.98	0.19	33,33,33,33	0
55	MG	1a	3153	1/1	0.98	0.11	26,26,26,26	0
55	MG	1A	3341	1/1	0.98	0.09	43,43,43,43	0
55	MG	2a	1732	1/1	0.98	0.10	39,39,39,39	0
55	MG	1A	3257	1/1	0.98	0.16	25,25,25,25	0
55	MG	1A	3846	1/1	0.98	0.28	18,18,18,18	0
55	MG	2a	1729	1/1	0.98	0.12	48,48,48,48	0
55	MG	2A	3799	1/1	0.99	0.13	29,29,29,29	0
55	MG	2a	1800	1/1	0.99	0.13	28,28,28,28	0
55	MG	1A	3144	1/1	0.99	0.14	38,38,38,38	0
55	MG	1A	3960	1/1	0.99	0.14	14,14,14,14	0
55	MG	2A	3299	1/1	0.99	0.12	46,46,46,46	0
55	MG	1A	3975	1/1	0.99	0.10	23,23,23,23	0
55	MG	1A	3061	1/1	0.99	0.06	37,37,37,37	0
55	MG	1a	3133	1/1	0.99	0.09	47,47,47,47	0
55	MG	2a	1682	1/1	0.99	0.07	26,26,26,26	0
55	MG	2A	3556	1/1	0.99	0.11	26,26,26,26	0
55	MG	1A	3945	1/1	0.99	0.21	24,24,24,24	0
57	ZN	19	103	1/1	0.99	0.16	41,41,41,41	0
55	MG	2a	1786	1/1	0.99	0.15	39,39,39,39	0
55	MG	1A	3075	1/1	0.99	0.16	10,10,10,10	0
55	MG	1A	3625	1/1	0.99	0.12	20,20,20,20	0
55	MG	2A	3030	1/1	0.99	0.12	33,33,33,33	0
55	MG	1A	3399	1/1	0.99	0.15	17,17,17,17	0
55	MG	1a	3002	1/1	0.99	0.12	30,30,30,30	0
55	MG	1A	3929	1/1	0.99	0.12	18,18,18,18	0
55	MG	2A	3585	1/1	0.99	0.13	43,43,43,43	0
55	MG	1a	3160	1/1	0.99	0.15	39,39,39,39	0
59	SF4	2d	303	8/8	0.99	0.16	45,64,72,73	0
55	MG	1A	3894	1/1	0.99	0.15	16,16,16,16	0
55	MG	1A	3337	1/1	0.99	0.19	16,16,16,16	0
55	MG	1a	3157	1/1	0.99	0.13	34,34,34,34	0
55	MG	2A	3206	1/1	0.99	0.12	42,42,42,42	0
55	MG	1A	3584	1/1	0.99	0.14	31,31,31,31	0
55	MG	1A	3495	1/1	0.99	0.14	33,33,33,33	0
55	MG	2A	3227	1/1	0.99	0.19	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	1A	3269	1/1	0.99	0.14	25,25,25,25	0
55	MG	2A	3741	1/1	0.99	0.08	25,25,25,25	0
55	MG	1A	3072	1/1	0.99	0.11	27,27,27,27	0
55	MG	2A	3325	1/1	0.99	0.27	22,22,22,22	0
55	MG	1A	3709	1/1	0.99	0.06	28,28,28,28	0
55	MG	1A	3109	1/1	0.99	0.16	21,21,21,21	0
57	ZN	1Y	203	1/1	0.99	0.12	62,62,62,62	0
55	MG	1A	3784	1/1	0.99	0.31	24,24,24,24	0
55	MG	2A	3017	1/1	0.99	0.12	24,24,24,24	0
55	MG	1U	205	1/1	0.99	0.56	27,27,27,27	0
55	MG	1A	3036	1/1	0.99	0.27	30,30,30,30	0
55	MG	1A	3723	1/1	0.99	0.07	36,36,36,36	0
55	MG	2A	3811	1/1	0.99	0.17	10,10,10,10	0
55	MG	2a	1602	1/1	0.99	0.10	51,51,51,51	0
55	MG	1A	3385	1/1	0.99	0.16	26,26,26,26	0
55	MG	2A	3426	1/1	0.99	0.16	55,55,55,55	0
55	MG	1A	3477	1/1	0.99	0.15	25,25,25,25	0
55	MG	1A	3391	1/1	0.99	0.13	37,37,37,37	0
55	MG	1A	3303	1/1	0.99	0.19	37,37,37,37	0
55	MG	1A	3112	1/1	0.99	0.09	16,16,16,16	0
55	MG	2A	3385	1/1	0.99	0.09	21,21,21,21	0
55	MG	1a	3151	1/1	0.99	0.13	28,28,28,28	0
55	MG	1A	3099	1/1	0.99	0.12	23,23,23,23	0
55	MG	2A	3641	1/1	0.99	0.14	41,41,41,41	0
55	MG	2A	3606	1/1	0.99	0.17	34,34,34,34	0
55	MG	2P	202	1/1	0.99	0.21	29,29,29,29	0
55	MG	2A	3056	1/1	0.99	0.20	23,23,23,23	0
55	MG	1A	3834	1/1	0.99	0.26	11,11,11,11	0
55	MG	1A	3450	1/1	0.99	0.07	14,14,14,14	0
55	MG	1A	3783	1/1	0.99	0.26	21,21,21,21	0
55	MG	1A	3243	1/1	0.99	0.35	26,26,26,26	0
55	MG	1A	3422	1/1	0.99	0.11	36,36,36,36	0
55	MG	1a	3129	1/1	0.99	0.11	32,32,32,32	0
55	MG	1A	3616	1/1	0.99	0.08	12,12,12,12	0
55	MG	2a	1784	1/1	0.99	0.27	32,32,32,32	0
55	MG	2A	3801	1/1	0.99	0.05	44,44,44,44	0
55	MG	2Y	202	1/1	0.99	0.20	20,20,20,20	0
55	MG	2A	3445	1/1	0.99	0.36	32,32,32,32	0
55	MG	1A	3637	1/1	0.99	0.19	16,16,16,16	0
55	MG	2A	3123	1/1	0.99	0.14	16,16,16,16	0
55	MG	2A	3704	1/1	0.99	0.06	26,26,26,26	0
55	MG	1A	3118	1/1	0.99	0.24	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	2D	304	1/1	0.99	0.19	22,22,22,22	0
55	MG	1D	308	1/1	0.99	0.13	42,42,42,42	0
55	MG	2A	3462	1/1	0.99	0.24	15,15,15,15	0
55	MG	1A	3442	1/1	0.99	0.18	22,22,22,22	0
55	MG	2A	3104	1/1	0.99	0.33	28,28,28,28	0
55	MG	2A	3515	1/1	0.99	0.14	24,24,24,24	0
55	MG	1a	3190	1/1	0.99	0.32	44,44,44,44	0
55	MG	1A	3384	1/1	0.99	0.09	21,21,21,21	0
55	MG	2A	3583	1/1	0.99	0.09	19,19,19,19	0
55	MG	1A	3335	1/1	0.99	0.10	19,19,19,19	0
55	MG	2A	3219	1/1	0.99	0.15	24,24,24,24	0
57	ZN	26	102	1/1	0.99	0.18	40,40,40,40	0
55	MG	1B	206	1/1	0.99	0.14	45,45,45,45	0
55	MG	2a	1675	1/1	0.99	0.14	44,44,44,44	0
55	MG	1A	3848	1/1	0.99	0.18	22,22,22,22	0
55	MG	2A	3387	1/1	0.99	0.21	25,25,25,25	0
55	MG	1A	3440	1/1	0.99	0.17	19,19,19,19	0
55	MG	1A	3132	1/1	0.99	0.10	35,35,35,35	0
55	MG	1a	3126	1/1	0.99	0.09	30,30,30,30	0
55	MG	2A	3309	1/1	0.99	0.11	48,48,48,48	0
55	MG	1A	3828	1/1	0.99	0.24	28,28,28,28	0
55	MG	1N	201	1/1	0.99	0.24	47,47,47,47	0
55	MG	1A	3593	1/1	0.99	0.14	22,22,22,22	0
55	MG	2A	3505	1/1	0.99	0.13	18,18,18,18	0
55	MG	1A	3801	1/1	0.99	0.14	10,10,10,10	0
55	MG	1A	3123	1/1	0.99	0.13	10,10,10,10	0
55	MG	1A	3186	1/1	0.99	0.17	34,34,34,34	0
55	MG	1a	3098	1/1	0.99	0.10	26,26,26,26	0
59	SF4	1d	302	8/8	0.99	0.16	47,72,75,78	0
55	MG	1A	3327	1/1	0.99	0.19	26,26,26,26	0
55	MG	1B	236	1/1	0.99	0.17	21,21,21,21	0
55	MG	1A	3562	1/1	0.99	0.06	25,25,25,25	0
55	MG	2A	3107	1/1	0.99	0.09	39,39,39,39	0
55	MG	1A	3753	1/1	0.99	0.06	28,28,28,28	0
55	MG	1A	3018	1/1	0.99	0.13	16,16,16,16	0
55	MG	1a	3205	1/1	0.99	0.07	41,41,41,41	0
55	MG	1A	3546	1/1	0.99	0.13	35,35,35,35	0
55	MG	1A	3557	1/1	0.99	0.21	54,54,54,54	0
55	MG	2A	3812	1/1	0.99	0.12	28,28,28,28	0
55	MG	1B	202	1/1	0.99	0.22	48,48,48,48	0
55	MG	1A	3393	1/1	0.99	0.70	21,21,21,21	0
55	MG	2a	1766	1/1	1.00	0.06	39,39,39,39	0

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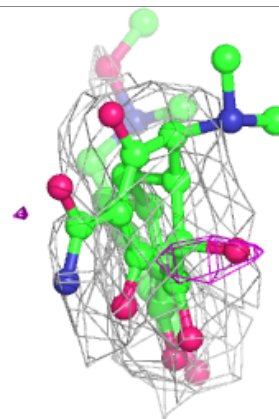
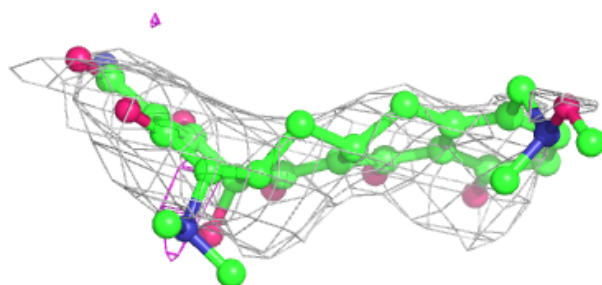
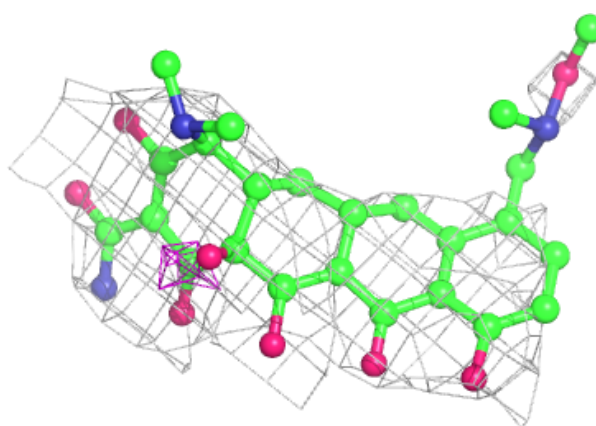
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	1A	3022	1/1	1.00	0.23	29,29,29,29	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

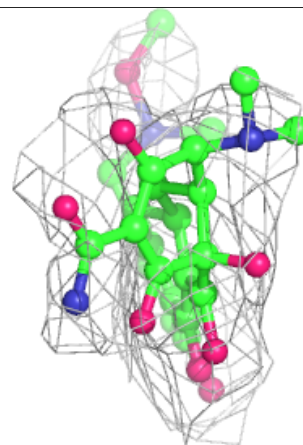
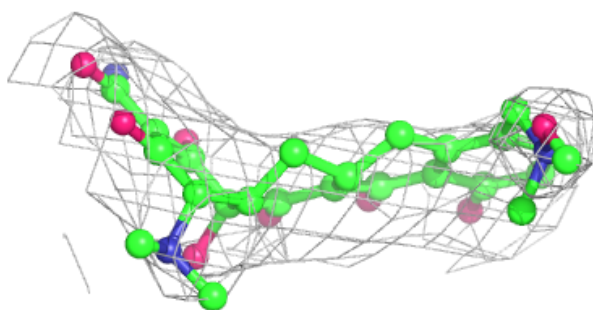
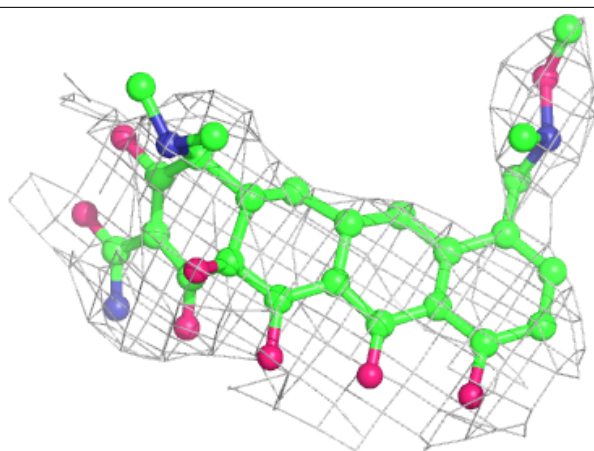
Electron density around V7A 2a 1817:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around V7A 1a 3213:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers ⓘ

There are no such residues in this entry.