Full wwPDB X-ray Structure Validation Report (i)

Feb 25, 2024 – 02:59 PM EST

PDB ID	:	5HCP
Title	:	Crystal structure of antimicrobial peptide Metalnikowin bound to the Thermus thermophilus 70S ribosome
Authors	:	Gagnon, M.G.; Roy, R.N.; Lomakin, I.B.; Florin, T.; Mankin, A.S.; Steitz, T.A.
Deposited on	:	2016-01-04
Resolution	:	2.89 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 (i) symbol.

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

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

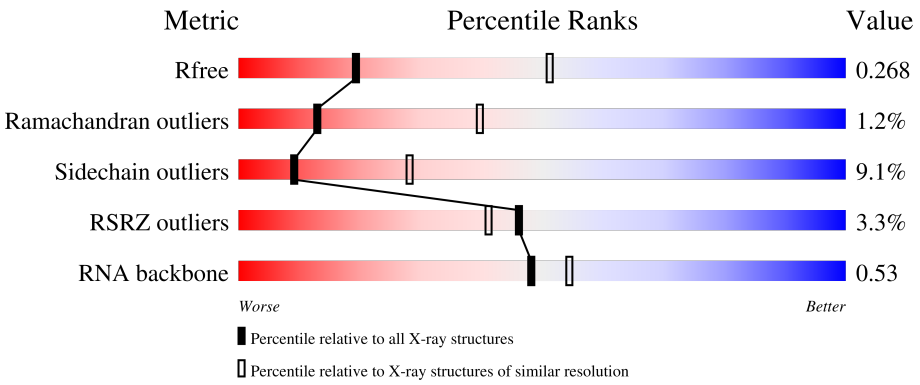
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.89 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	1957 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)
RNA backbone	3102	1007 (3.16-2.64)

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

Mol	Chain	Length	Quality of chain
1	1A	2915	.% 80% 14% • 6%
1	2A	2915	2% 78% 17% • •
2	1B	121	92% 7% •
2	2B	121	2% 80% 18% ••
3	1D	276	93% 7%

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Mol	Chain	Length	Quality of chain
3	2D	276	%, 89%, 10%
4	1E	206	91%, 8%
4	2E	206	91%, 8%
5	1F	210	88%, 9%
5	2F	210	%, 90%, 7%
6	1G	182	3%, 90%, 9%
6	2G	182	8%, 87%, 12%
7	1H	180	%, 89%, 7%
7	2H	180	15%, 89%, 8%
8	1I	148	84%, 14%
8	2I	148	9%, 92%, 7%
9	1N	140	91%, 9%
9	2N	140	91%, 9%
10	1O	122	97%
10	2O	122	96%
11	1P	150	90%, 9%
11	2P	150	7%, 89%, 10%
12	1Q	141	%, 94%, 6%
12	2Q	141	%, 94%, 6%
13	1R	118	87%, 13%
13	2R	118	86%, 14%
14	1S	112	90%, 8%
14	2S	112	10%, 88%, 10%
15	1T	146	85%, 5%, 10%
15	2T	146	88%, 10%

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Mol	Chain	Length	Quality of chain
16	1U	118	93% 5%
16	2U	118	3% 94%
17	1V	101	90% 9%
17	2V	101	% 93% 6%
18	1W	113	94% 5%
18	2W	113	95%
19	1X	96	95%
19	2X	96	3% 96%
20	1Y	110	% 90% 7%
20	2Y	110	10% 94%
21	1Z	206	84% 6% 10%
21	2Z	206	6% 84% 6% 10%
22	10	85	81% 7% 12%
22	20	85	4% 84% 5% 12%
23	11	98	% 95%
23	21	98	% 95%
24	12	72	92% 6%
24	22	72	90% 7%
25	13	60	92% 7%
25	23	60	8% 92% 7%
26	14	71	8% 75% 21%
26	24	71	10% 80% 15%
27	15	60	92% 7%
27	25	60	93% 5%
28	16	54	93% 6%

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Mol	Chain	Length	Quality of chain
28	26	54	93% 6%
29	17	49	2% 88% 10%
29	27	49	6% 92%
30	18	65	92% 6%
30	28	65	2% 92% 6%
31	19	37	97%
31	29	37	5% 97%
32	1a	1521	2% 80% 17%
32	2a	1521	3% 79% 18%
33	1b	256	10% 77% 12% 10%
33	2b	256	11% 79% 10% 10%
34	1c	239	6% 80% 5% 14%
34	2c	239	10% 78% 8% 14%
35	1d	209	2% 89% 10%
35	2d	209	% 89% 10%
36	1e	162	83% 8% 9%
36	2e	162	% 81% 10% 9%
37	1f	101	93% 6%
37	2f	101	2% 95%
38	1g	156	8% 92% 7%
38	2g	156	12% 92% 7%
39	1h	138	% 91% 8%
39	2h	138	4% 89% 10%
40	1i	128	9% 90% 9%
40	2i	128	24% 87% 12%

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Mol	Chain	Length	Quality of chain
41	1j	105	11% 81% 11% 8%
41	2j	105	22% 81% 10% 9%
42	1k	129	% 83% 5% 12%
42	2k	129	4% 83% 5% 12%
43	1l	132	2% 88% 5% 8%
43	2l	132	% 89% 8%
44	1m	126	% 83% 10% 6%
44	2m	126	13% 83% 8% 8%
45	1n	61	8% 89% 10%
45	2n	61	25% 87% 11%
46	1o	89	3% 90% 9%
46	2o	89	3% 89% 10%
47	1p	88	6% 81% 11% 7%
47	2p	88	6% 83% 10% 7%
48	1q	105	89% 6%
48	2q	105	2% 92% 6%
49	1r	88	5% 68% 9% 23%
49	2r	88	11% 69% 8% 23%
50	1s	93	8% 82% 8% 10%
50	2s	93	33% 81% 9% 11%
51	1t	106	% 79% 11% 9%
51	2t	106	2% 83% 7% 9%
52	1u	27	7% 81% 15%
52	2u	27	33% 78% 7% 15%
53	1v	24	17% 79%

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Mol	Chain	Length	Quality of chain
53	2v	24	8% 17% 79%
54	1x	77	66% 32%
54	2x	77	% 66% 32%
55	1z	15	80% 20%
55	2z	15	13% 80% 7% 13%

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
56	MG	12	3001	-	-	-	X
56	MG	1A	3007	-	-	-	X
56	MG	1A	3320	-	-	-	X
56	MG	1A	3333	-	-	-	X
56	MG	1A	3384	-	-	-	X
56	MG	1A	3411	-	-	-	X
56	MG	1A	3901	-	-	-	X
56	MG	1A	3916	-	-	-	X
56	MG	1A	4027	-	-	-	X
56	MG	1A	4054	-	-	-	X
56	MG	1F	304	-	-	-	X
56	MG	1T	206	-	-	-	X
56	MG	1a	1639	-	-	-	X
56	MG	1a	1756	-	-	-	X
56	MG	1a	1757	-	-	-	X
56	MG	2A	3093	-	-	-	X
56	MG	2a	3001	-	-	-	X
56	MG	2a	3039	-	-	-	X
56	MG	2a	3043	-	-	-	X
56	MG	2a	3138	-	-	-	X
56	MG	2a	3254	-	-	-	X

2 Entry composition (i)

There are 59 unique types of molecules in this entry. The entry contains 288976 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
			Total	C	N	O	P			
1	1A	2746	59154	26327	11077	19005	2745	0	0	0
1	2A	2790	60091	26746	11243	19313	2789	0	0	0

- Molecule 2 is a RNA chain called 5S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	1B	120	2572	1146	476	831	119	0	0	0
2	2B	120	2573	1146	476	832	119	0	0	0

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	1D	275	2136	1349	423	361	3	0	0	0
3	2D	275	2142	1352	426	361	3	0	0	0

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	1E	204	1559	985	298	270	6	0	0	0
4	2E	204	1559	985	298	270	6	0	0	0

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	1F	203	1584	1009	298	275	2	0	0	1
5	2F	203	1580	1007	297	274	2	0	0	1

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	1G	181	1425	914	256	251	4	0	0	0
6	2G	181	1424	911	258	251	4	0	0	0

- Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	1H	174	1330	845	248	236	1	0	0	0
7	2H	174	1330	845	248	236	1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	1I	146	1085	693	189	202	1	0	0	0
8	2I	146	1061	680	186	194	1	0	0	0

- Molecule 9 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
9	1N	140	1117	719	207	187	4	0	0	0
9	2N	140	1117	719	207	187	4	0	0	0

- Molecule 10 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	1O	122	933	588	171	170	4	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	2O	122	933	588	171	170	4	0	0	0

- Molecule 11 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	1P	149	1139	709	231	196	3	0	0	0
			Total	C	N	O	S			
11	2P	149	1135	706	230	196	3	0	0	0

- Molecule 12 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	1Q	141	1122	715	212	188	7	0	0	0
			Total	C	N	O	S			
12	2Q	141	1122	715	212	188	7	0	0	0

- Molecule 13 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
13	1R	118	968	604	203	160	1	0	0	0
			Total	C	N	O	S			
13	2R	118	968	604	203	160	1	0	0	0

- Molecule 14 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
14	1S	110	877	553	175	149	0	0	0
			Total	C	N	O			
14	2S	110	870	549	173	148	0	0	0

- Molecule 15 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
15	1T	131	1091	680	225	185	1	0	0	0
			Total	C	N	O	S			
15	2T	131	1083	675	224	183	1	0	0	0

- Molecule 16 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
16	1U	116	959	608	201	149	1	0	0	0
16	2U	116	959	608	201	149	1	0	0	0

- Molecule 17 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
17	1V	101	771	495	140	135	1	0	0	0
17	2V	101	771	495	140	135	1	0	0	0

- Molecule 18 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
18	1W	112	886	557	174	153	2	0	0	0
18	2W	112	886	557	174	153	2	0	0	0

- Molecule 19 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
19	1X	95	750	488	135	126	1	0	0	0
19	2X	95	750	488	135	126	1	0	0	0

- Molecule 20 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
20	1Y	107	806	517	152	131	6	0	0	0
20	2Y	107	806	517	152	131	6	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
21	1Z	186	1470	937	262	269	2	0	0	0
21	2Z	186	1454	929	256	267	2	0	0	0

- Molecule 22 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
22	10	75	598	370	127	100	1	0	0	0
22	20	75	598	370	127	100	1	0	0	0

- Molecule 23 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
23	11	97	755	475	148	131	1	0	0	0
23	21	97	755	475	148	131	1	0	0	0

- Molecule 24 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
24	12	70	588	365	118	103	2	0	0	0
24	22	70	588	365	118	103	2	0	0	0

- Molecule 25 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
25	13	59	469	298	90	81	0	0	0
25	23	59	464	296	90	78	0	0	0

- Molecule 26 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
26	14	69	558	352	102	99	5	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
26	24	69	532	339	97	91	5	0	0	0

- Molecule 27 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
27	15	59	455	285	89	76	5	0	0	0
			Total	C	N	O	S			
27	25	59	455	285	89	76	5	0	0	0

- Molecule 28 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
28	16	53	453	281	91	77	4	0	0	0
			Total	C	N	O	S			
28	26	53	449	279	91	75	4	0	0	0

- Molecule 29 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
29	17	48	418	257	104	55	2	0	0	0
			Total	C	N	O	S			
29	27	48	418	257	104	55	2	0	0	0

- Molecule 30 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
30	18	64	517	331	102	82	2	0	0	0
			Total	C	N	O	S			
30	28	64	517	331	102	82	2	0	0	0

- Molecule 31 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
31	19	37	307	188	68	47	4	0	0	0
			Total	C	N	O	S			
31	29	37	307	188	68	47	4	0	0	0

- Molecule 32 is a RNA chain called 16S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
32	1a	1477	31750	14131	5883	10259	1477	0	0	0
32	2a	1483	31877	14188	5905	10301	1483	0	0	0

- Molecule 33 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
33	1b	231	1786	1136	321	325	4	0	0	0
33	2b	231	1697	1079	292	321	5	0	0	0

- Molecule 34 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
34	1c	206	1480	932	281	266	1	0	0	0
34	2c	206	1412	883	269	259	1	0	0	0

- Molecule 35 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
35	1d	208	1618	1013	312	286	7	0	0	0
35	2d	208	1630	1022	321	280	7	0	0	0

- Molecule 36 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
36	1e	148	1129	714	213	198	4	0	0	0
36	2e	148	1095	695	203	193	4	0	0	0

- Molecule 37 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
37	1f	100	806	511	143	149	3	0	0	0
37	2f	100	817	516	146	152	3	0	0	0

- Molecule 38 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
38	1g	155	1183	732	232	213	6	0	0	0
38	2g	155	1167	728	220	213	6	0	0	0

- Molecule 39 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
39	1h	137	1088	689	206	191	2	0	0	0
39	2h	137	1074	681	202	189	2	0	0	0

- Molecule 40 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
40	1i	127	976	620	189	167	0	0	0
40	2i	127	932	589	177	166	0	0	0

- Molecule 41 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
41	1j	97	682	424	130	128	0	0	0
41	2j	96	678	424	126	128	0	0	0

- Molecule 42 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
42	1k	114	826	513	156	154	3	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
42	2k	114	829	516	155	155	3	0	0	0

- Molecule 43 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
43	1l	122	920	579	181	159	1	0	0	0
			Total	C	N	O	S			
43	2l	122	918	576	182	159	1	0	0	0

- Molecule 44 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
44	1m	118	923	569	191	161	2	0	0	0
			Total	C	N	O	S			
44	2m	116	903	555	187	159	2	0	0	0

- Molecule 45 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
45	1n	60	482	306	100	72	4	0	0	0
			Total	C	N	O	S			
45	2n	60	459	291	93	71	4	0	0	0

- Molecule 46 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
46	1o	88	715	447	140	126	2	0	0	0
			Total	C	N	O	S			
46	2o	88	728	456	144	126	2	0	0	0

- Molecule 47 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
47	1p	82	671	424	133	113	1	0	0	0
			Total	C	N	O	S			
47	2p	82	677	430	133	113	1	0	0	0

- Molecule 48 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
48	1q	99	811	519	148	142	2	0	0	0
48	2q	99	823	528	151	142	2	0	0	0

- Molecule 49 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
49	1r	68	555	355	108	92	0	0	0
49	2r	68	555	355	108	92	0	0	0

- Molecule 50 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
50	1s	84	642	409	119	112	2	0	0	0
50	2s	83	646	412	119	113	2	0	0	0

- Molecule 51 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
51	1t	96	712	435	152	123	2	0	0	0
51	2t	96	731	449	156	124	2	0	0	0

- Molecule 52 is a protein called 30S ribosomal protein Thx.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
52	1u	23	187	116	42	29	0	0	0
52	2u	23	199	122	48	29	0	0	0

- Molecule 53 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
53	1v	5	109	49	22	33	5	0	0	0
53	2v	5	109	49	22	33	5	0	0	0

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

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

- Molecule 55 is a protein called Metalnikowin-1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
55	1z	12	105	66	22	17	0	0	0
55	2z	13	112	71	23	18	0	0	0

- Molecule 56 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
56	1A	1090	1090	1090	0	0
56	1B	30	30	30	0	0
56	1D	13	13	13	0	0
56	1E	12	12	12	0	0
56	1F	8	8	8	0	0
56	1G	3	3	3	0	0
56	1H	4	4	4	0	0
56	1N	7	7	7	0	0
56	1O	3	3	3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
56	1P	6	6	6	0	0
56	1Q	9	9	9	0	0
56	1R	6	6	6	0	0
56	1T	6	6	6	0	0
56	1U	6	6	6	0	0
56	1V	2	2	2	0	0
56	1W	6	6	6	0	0
56	1X	1	1	1	0	0
56	1Y	1	1	1	0	0
56	1Z	2	2	2	0	0
56	10	6	6	6	0	0
56	11	3	3	3	0	0
56	12	1	1	1	0	0
56	13	2	2	2	0	0
56	14	1	1	1	0	0
56	15	3	3	3	0	0
56	16	4	4	4	0	0
56	17	2	2	2	0	0
56	18	3	3	3	0	0
56	19	5	5	5	0	0
56	1a	309	309	309	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
56	1b	1	1	1	0	0
56	1d	2	2	2	0	0
56	1e	3	3	3	0	0
56	1f	1	1	1	0	0
56	1h	2	2	2	0	0
56	1k	1	1	1	0	0
56	1l	2	2	2	0	0
56	1m	1	1	1	0	0
56	1n	1	1	1	0	0
56	1o	3	3	3	0	0
56	1p	2	2	2	0	0
56	1q	3	3	3	0	0
56	1r	3	3	3	0	0
56	1t	1	1	1	0	0
56	1u	1	1	1	0	0
56	1v	1	1	1	0	0
56	1x	10	10	10	0	0
56	1z	1	1	1	0	0
56	2A	561	561	561	0	0
56	2B	10	10	10	0	0
56	2D	5	5	5	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
56	2E	4	4	4	0	0
56	2F	4	4	4	0	0
56	2G	1	1	1	0	0
56	2N	1	1	1	0	0
56	2O	3	3	3	0	0
56	2P	1	1	1	0	0
56	2Q	5	5	5	0	0
56	2R	2	2	2	0	0
56	2T	1	1	1	0	0
56	2U	1	1	1	0	0
56	2X	1	1	1	0	0
56	2Y	1	1	1	0	0
56	2Z	1	1	1	0	0
56	20	1	1	1	0	0
56	23	1	1	1	0	0
56	25	1	1	1	0	0
56	28	3	3	3	0	0
56	2a	255	255	255	0	0
56	2d	2	2	2	0	0
56	2e	2	2	2	0	0
56	2f	1	1	1	0	0

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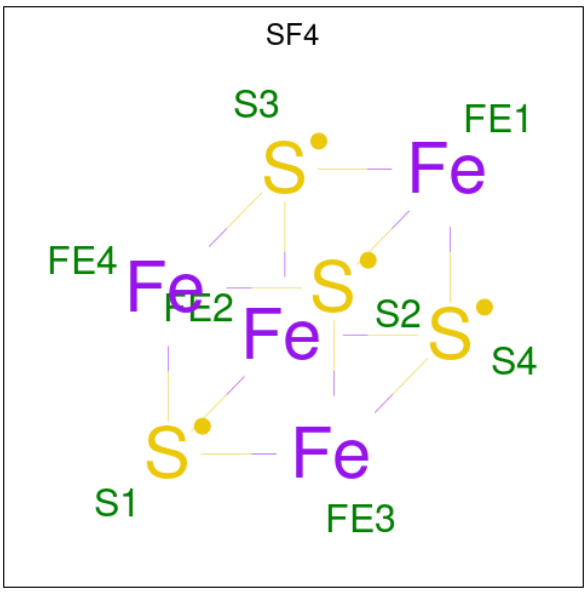
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	2l	5	Total Mg 5 5	0	0
56	2q	3	Total Mg 3 3	0	0
56	2r	1	Total Mg 1 1	0	0
56	2t	1	Total Mg 1 1	0	0
56	2v	1	Total Mg 1 1	0	0
56	2x	7	Total Mg 7 7	0	0
56	2z	1	Total Mg 1 1	0	0

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

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

- Molecule 58 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	1d	1	Total Fe S 8 4 4	0	0
58	2d	1	Total Fe S 8 4 4	0	0

- Molecule 59 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	1A	2412	Total O 2412 2412	0	0
59	1B	46	Total O 46 46	0	0
59	1D	25	Total O 25 25	0	0
59	1E	30	Total O 30 30	0	0
59	1F	21	Total O 21 21	0	0
59	1G	8	Total O 8 8	0	0
59	1H	4	Total O 4 4	0	0
59	1I	3	Total O 3 3	0	0
59	1N	8	Total O 8 8	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	1O	5	Total O 5 5	0	0
59	1P	25	Total O 25 25	0	0
59	1Q	13	Total O 13 13	0	0
59	1R	18	Total O 18 18	0	0
59	1S	2	Total O 2 2	0	0
59	1T	13	Total O 13 13	0	0
59	1U	18	Total O 18 18	0	0
59	1V	5	Total O 5 5	0	0
59	1W	14	Total O 14 14	0	0
59	1X	5	Total O 5 5	0	0
59	1Y	1	Total O 1 1	0	0
59	1Z	6	Total O 6 6	0	0
59	10	8	Total O 8 8	0	0
59	11	7	Total O 7 7	0	0
59	12	2	Total O 2 2	0	0
59	13	3	Total O 3 3	0	0
59	15	7	Total O 7 7	0	0
59	16	11	Total O 11 11	0	0
59	17	9	Total O 9 9	0	0
59	18	16	Total O 16 16	0	0
59	19	3	Total O 3 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	1a	394	Total O 394 394	0	0
59	1b	1	Total O 1 1	0	0
59	1c	1	Total O 1 1	0	0
59	1d	3	Total O 3 3	0	0
59	1e	4	Total O 4 4	0	0
59	1f	1	Total O 1 1	0	0
59	1h	2	Total O 2 2	0	0
59	1j	1	Total O 1 1	0	0
59	1k	2	Total O 2 2	0	0
59	1l	3	Total O 3 3	0	0
59	1m	1	Total O 1 1	0	0
59	1p	1	Total O 1 1	0	0
59	1q	1	Total O 1 1	0	0
59	1s	1	Total O 1 1	0	0
59	1u	1	Total O 1 1	0	0
59	1v	3	Total O 3 3	0	0
59	1x	10	Total O 10 10	0	0
59	1z	5	Total O 5 5	0	0
59	2A	824	Total O 824 824	0	0
59	2B	9	Total O 9 9	0	0
59	2D	18	Total O 18 18	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	2E	11	Total O 11 11	0	0
59	2F	6	Total O 6 6	0	0
59	2N	2	Total O 2 2	0	0
59	2O	1	Total O 1 1	0	0
59	2P	6	Total O 6 6	0	0
59	2R	1	Total O 1 1	0	0
59	2T	1	Total O 1 1	0	0
59	2U	3	Total O 3 3	0	0
59	2W	1	Total O 1 1	0	0
59	2X	3	Total O 3 3	0	0
59	2Y	2	Total O 2 2	0	0
59	2Z	5	Total O 5 5	0	0
59	20	2	Total O 2 2	0	0
59	21	1	Total O 1 1	0	0
59	23	2	Total O 2 2	0	0
59	25	1	Total O 1 1	0	0
59	27	1	Total O 1 1	0	0
59	28	4	Total O 4 4	0	0
59	2a	329	Total O 329 329	0	0
59	2c	1	Total O 1 1	0	0
59	2d	1	Total O 1 1	0	0

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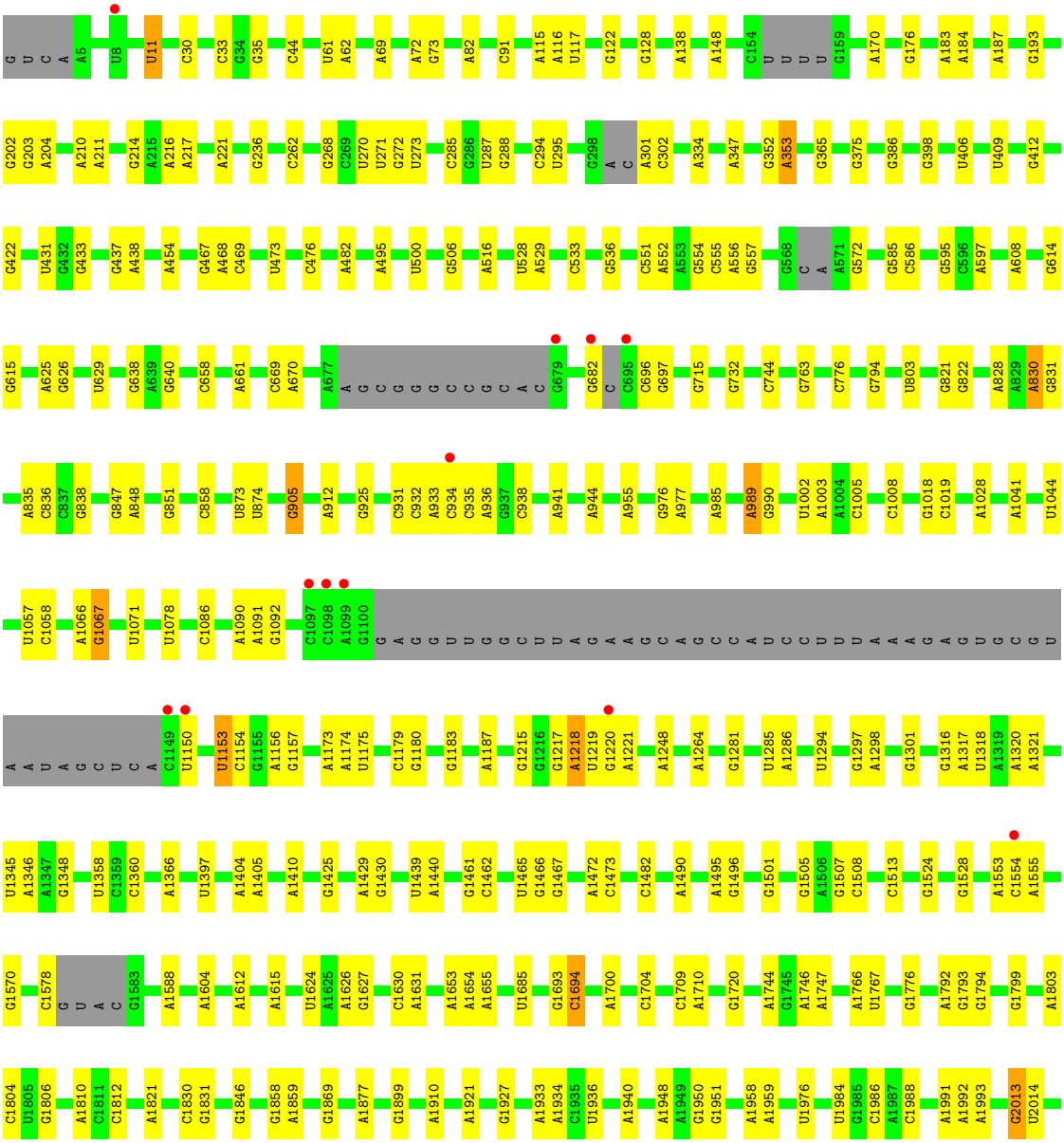
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	2e	4	Total O 4 4	0	0
59	2g	1	Total O 1 1	0	0
59	2i	2	Total O 2 2	0	0
59	2l	2	Total O 2 2	0	0
59	2m	1	Total O 1 1	0	0
59	2o	1	Total O 1 1	0	0
59	2p	2	Total O 2 2	0	0
59	2q	1	Total O 1 1	0	0
59	2t	4	Total O 4 4	0	0
59	2u	1	Total O 1 1	0	0
59	2x	6	Total O 6 6	0	0
59	2z	2	Total O 2 2	0	0

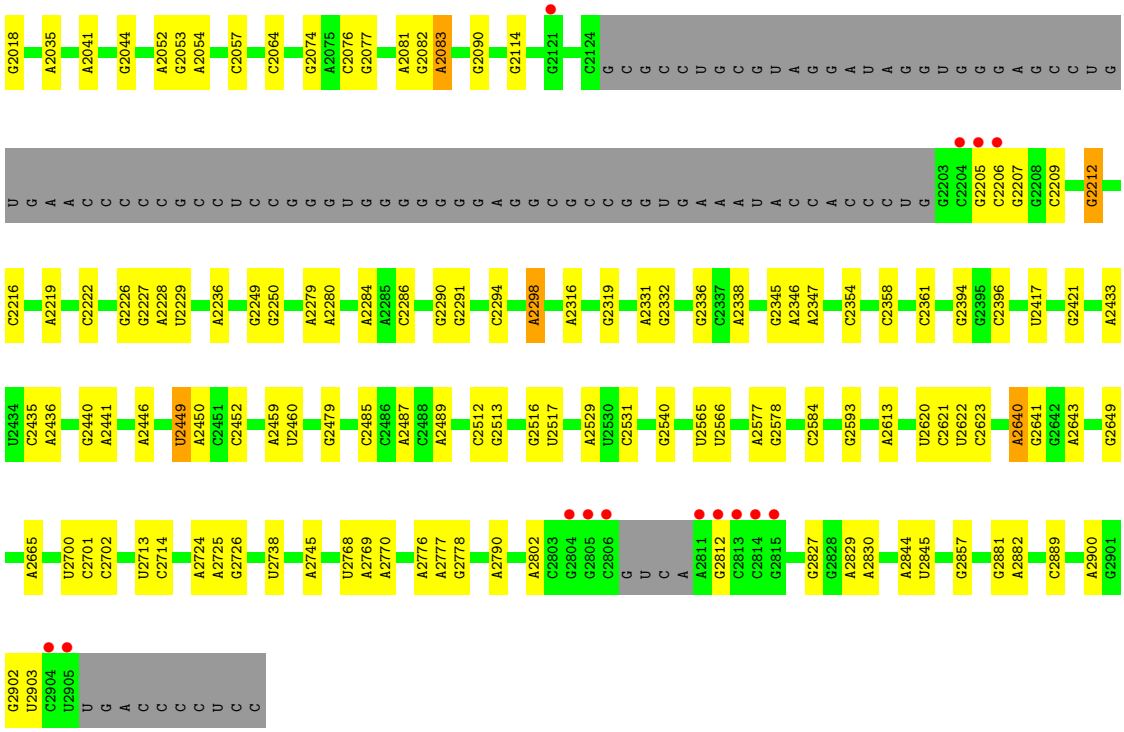
3 Residue-property plots (i)

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

- Molecule 1: 23S Ribosomal RNA

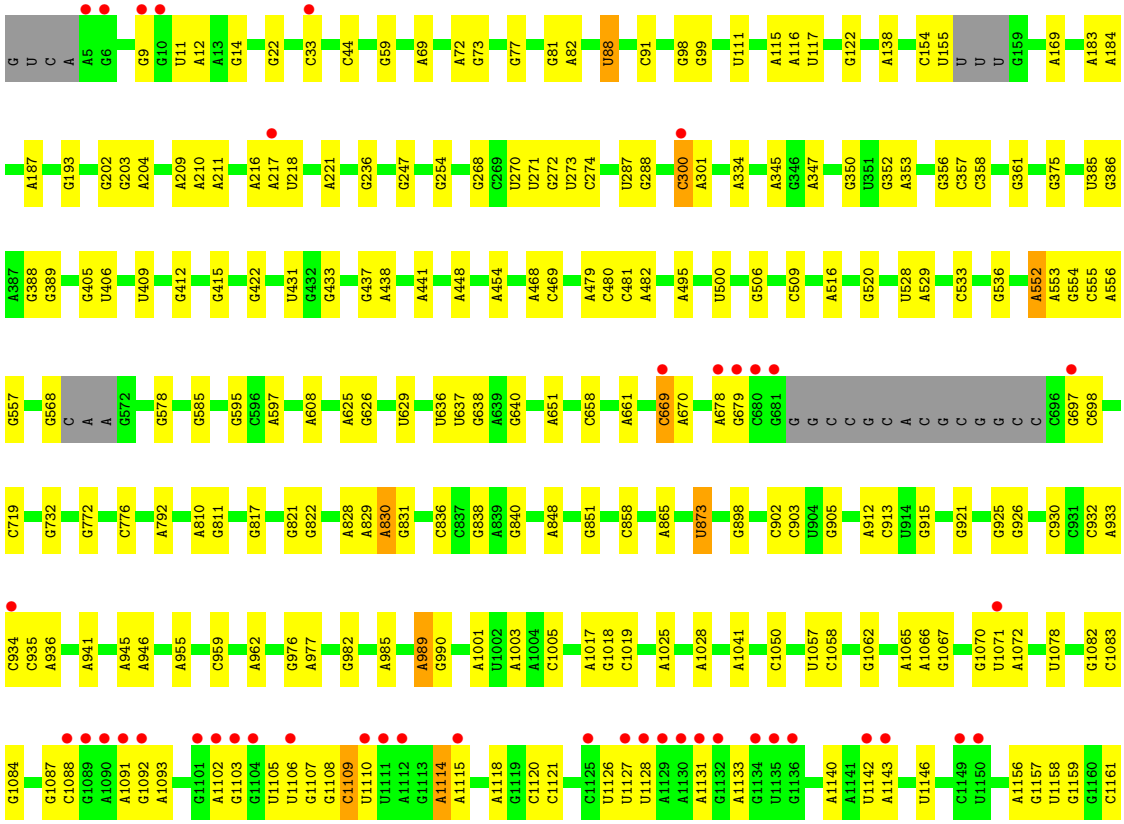
Chain 1A:

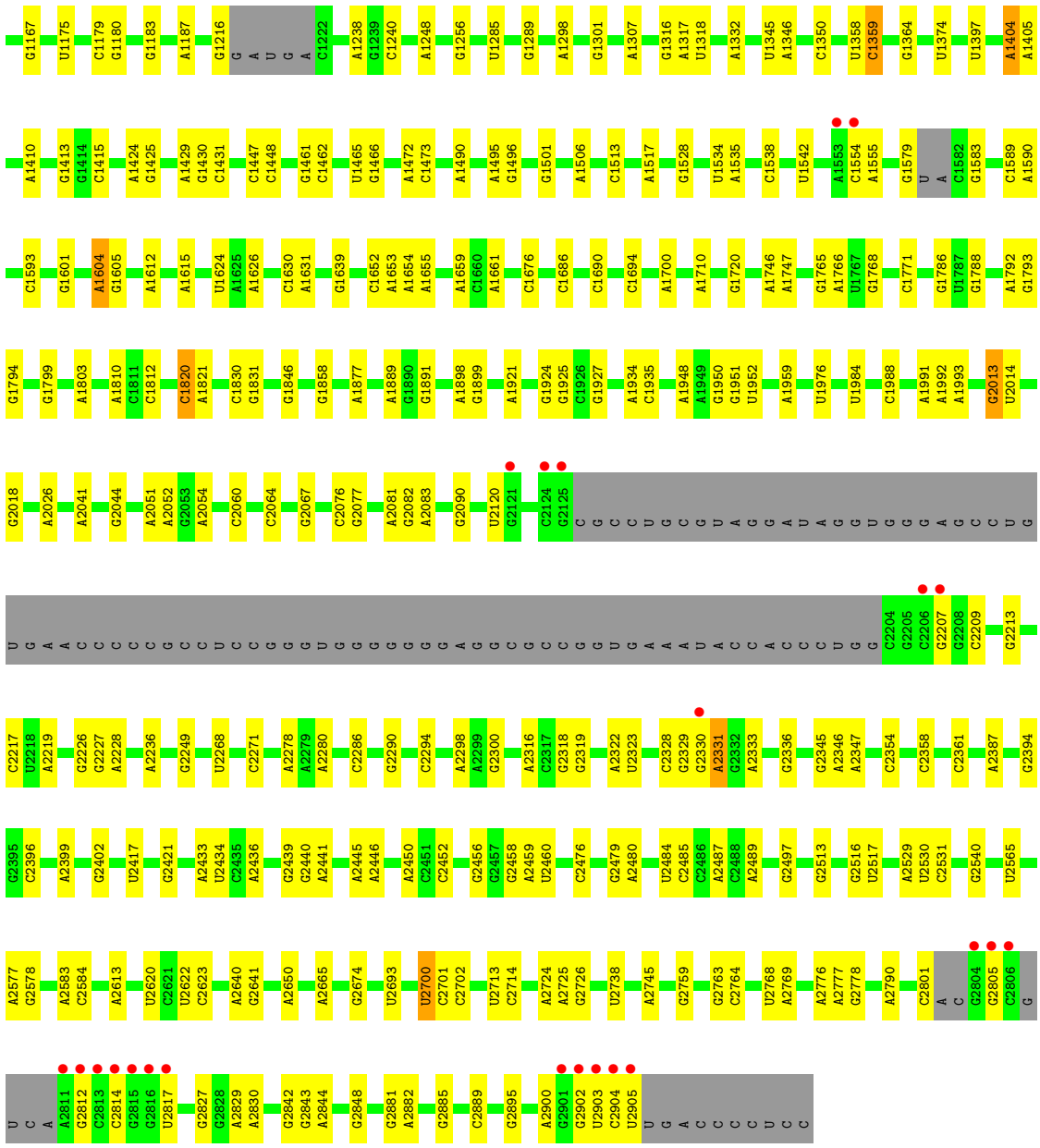




• Molecule 1: 23S Ribosomal RNA

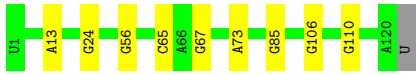
Chain 2A:





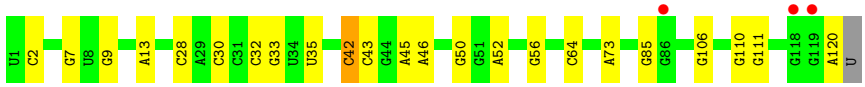
- Molecule 2: 5S Ribosomal RNA

Chain 1B:



- Molecule 2: 5S Ribosomal RNA

Chain 2B:



• Molecule 3: 50S ribosomal protein L2

Chain 1D: 93% 7%

MET A2 R13 R54 L61 R69 W70 D71 L94 D99 R103 L111 V142 L155 V193 L206 R211 R217 V229 R242 L257 R260 K276

• Molecule 3: 50S ribosomal protein L2

Chain 2D: % 89% 10%

MET A2 V3 R14 K38 R54 L61 D71 L94 I106 L111 Q112 V113 I125 R134 V138 V141 V142 L155 R183 T192 V193 R211 R217 V229 R242 L257 R260 K261 R262 I270 R273 R274 K275 K276

• Molecule 4: 50S ribosomal protein L3

Chain 1E: 91% 8%

M1 V7 V21 L52 P53 Q54 V75 R79 R82 R111 V116 R119 R144 E163 V175 L181 V184 L195 A204 ALA LYS

• Molecule 4: 50S ribosomal protein L3

Chain 2E: 91% 8%

M1 V7 T12 V21 T24 L49 L52 V75 R76 I77 R82 V116 R119 R144 E163 V175 L181 V184 K202 K203 A204 ALA LYS

• Molecule 5: 50S ribosomal protein L4

Chain 1F: 88% 9%

MET LYS GLU VAL ALA V6 R18 E19 L20 L33 R38 V57 R74 R106 L110 L125 A130 L162 L170 V183 R191 L192 D195 L196 D197 V201 G208 GLU ALA

• Molecule 5: 50S ribosomal protein L4

Chain 2F: % 90% 7%

MET LYS GLU VAL ALA V6 P14 S15 R18 E19 L20 L24 E27 L33 V57 R74 R106 A130 L162 V183 L192 L196 D197 V201 G208 GLU ALA

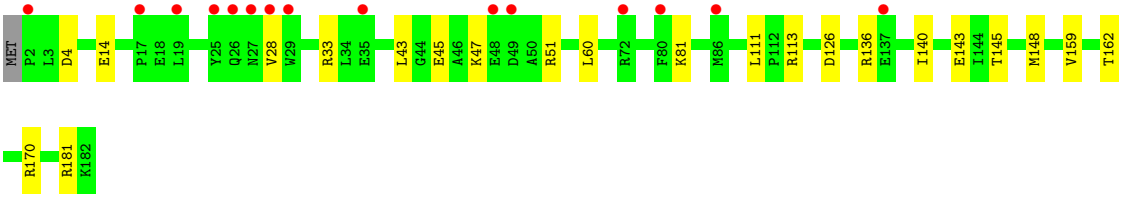
• Molecule 6: 50S ribosomal protein L5

Chain 1G: 3% 90% 9%

MET P2 L3 L7 L43 G44 E45 A46 K47 E48 D49 A50 R51 K75 S78 L82 D126 I140 E143 M148 V159 V160 T161 T162 T165 R170 E174 K182

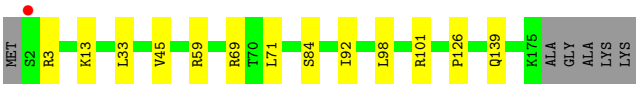
• Molecule 6: 50S ribosomal protein L5

Chain 2G:



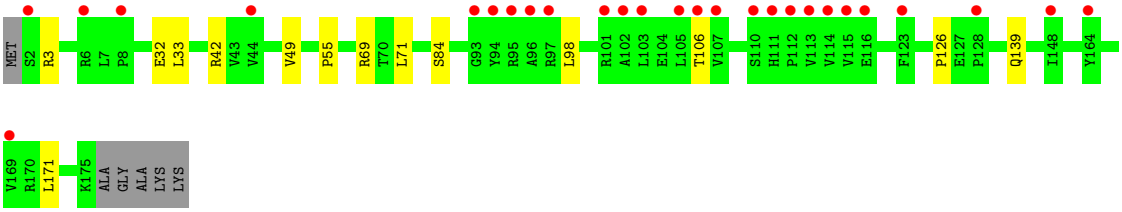
• Molecule 7: 50S ribosomal protein L6

Chain 1H:



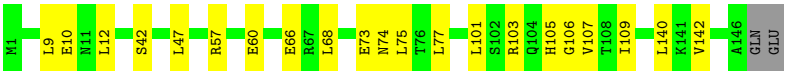
• Molecule 7: 50S ribosomal protein L6

Chain 2H:



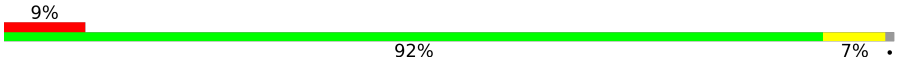
• Molecule 8: 50S ribosomal protein L9

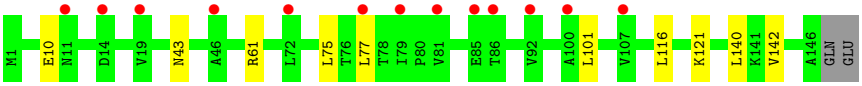
Chain 1I:



• Molecule 8: 50S ribosomal protein L9

Chain 2I:





• Molecule 9: 50S ribosomal protein L13

Chain 1N:

• Molecule 9: 50S ribosomal protein L13

Chain 2N: 91% 9%

M1 K2 V5 L33 L34 V46 A47 M48 V62 T73 L87 L120 K137 L138 E139 V140

• Molecule 10: 50S ribosomal protein L14

Chain 1O: 97%

M1 Q5 K18 V24 E105 L122

• Molecule 10: 50S ribosomal protein L14

Chain 2O: 96%

M1 Q5 L8 V24 I69 R94 L122

• Molecule 11: 50S ribosomal protein L15

Chain 1P: 90% 9%

M1 K2 L3 R55 S56 L59 Q70 K76 E98 L99 L106 L112 P122 V125 E136 L148 E149 ALA

• Molecule 11: 50S ribosomal protein L15

Chain 2P: 7% 89% 10%

M1 K2 L3 K29 L45 R55 S56 L59 R65 L85 L88 A89 R90 F91 E92 V95 T96 L100 V101 R102 L112 G116 E117 G118 K121 P122 L123 K124 V125 L148 E149 ALA

• Molecule 12: 50S ribosomal protein L16

Chain 1Q: % 94% 6%

M1 R6 M7 K8 R16 V35 Q45 R59 R60 Q141

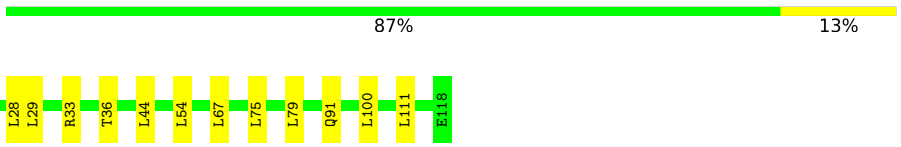
• Molecule 12: 50S ribosomal protein L16

Chain 2Q: % 94% 6%

M1 T21 A28 V35 Q45 R60 V106 V109 T110 Q141

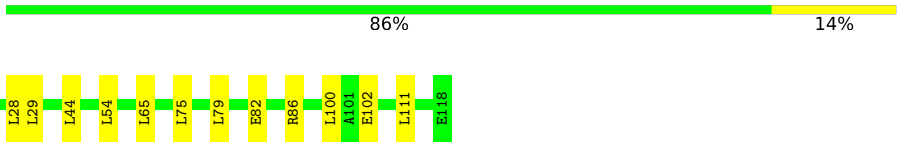
• Molecule 13: 50S ribosomal protein L17

Chain 1R:



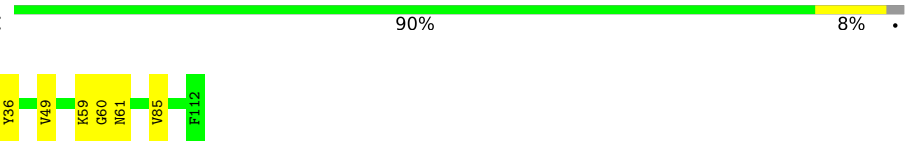
• Molecule 13: 50S ribosomal protein L17

Chain 2R:



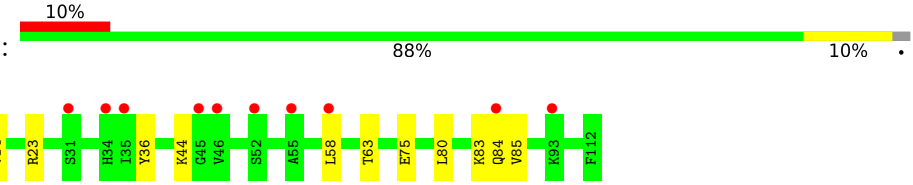
• Molecule 14: 50S ribosomal protein L18

Chain 1S:



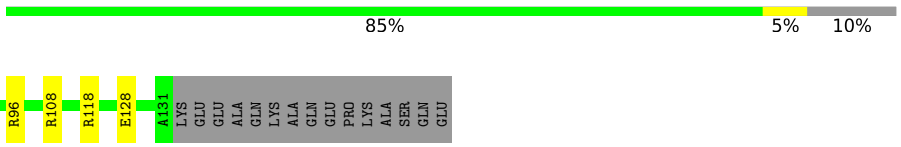
• Molecule 14: 50S ribosomal protein L18

Chain 2S:



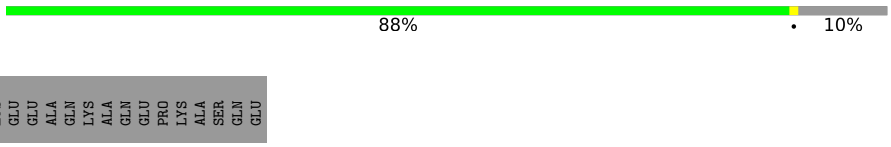
• Molecule 15: 50S ribosomal protein L19

Chain 1T:



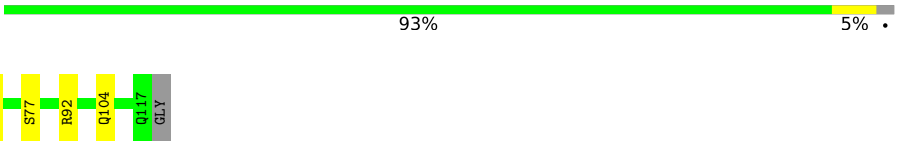
• Molecule 15: 50S ribosomal protein L19

Chain 2T:



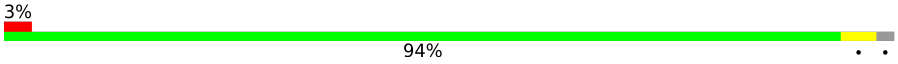
• Molecule 16: 50S ribosomal protein L20

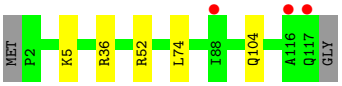
Chain 1U:



• Molecule 16: 50S ribosomal protein L20

Chain 2U:



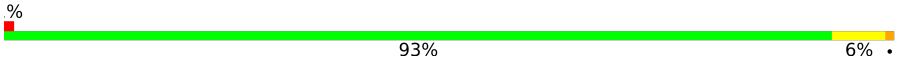


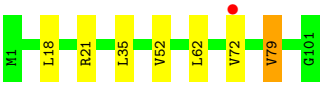
• Molecule 17: 50S ribosomal protein L21

Chain 1V:

• Molecule 17: 50S ribosomal protein L21

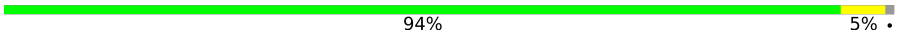
Chain 2V:

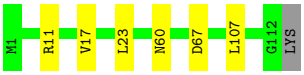




• Molecule 18: 50S ribosomal protein L22

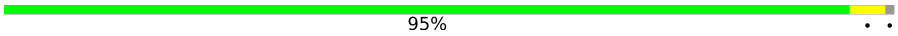
Chain 1W:

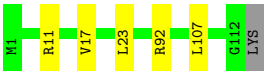




• Molecule 18: 50S ribosomal protein L22

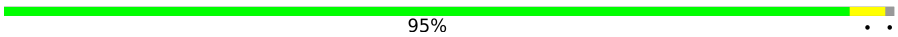
Chain 2W:

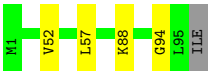




• Molecule 19: 50S ribosomal protein L23

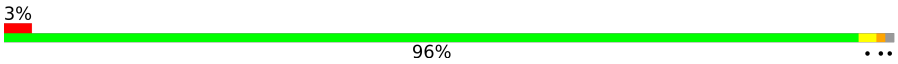
Chain 1X:

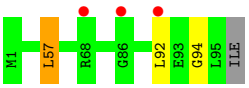




• Molecule 19: 50S ribosomal protein L23

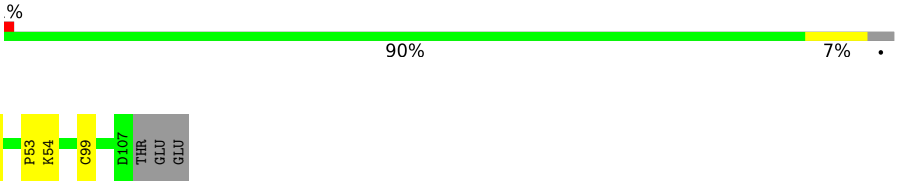
Chain 2X:





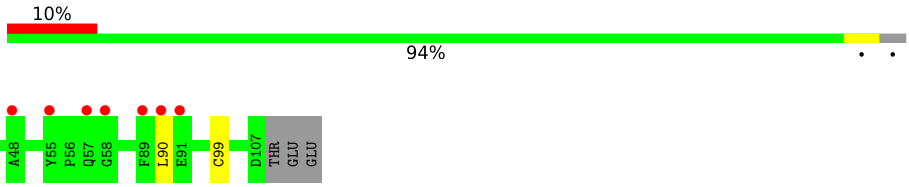
• Molecule 20: 50S ribosomal protein L24

Chain 1Y:



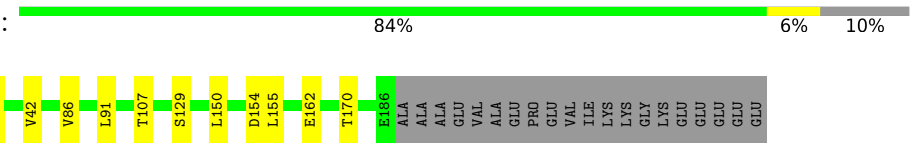
• Molecule 20: 50S ribosomal protein L24

Chain 2Y:



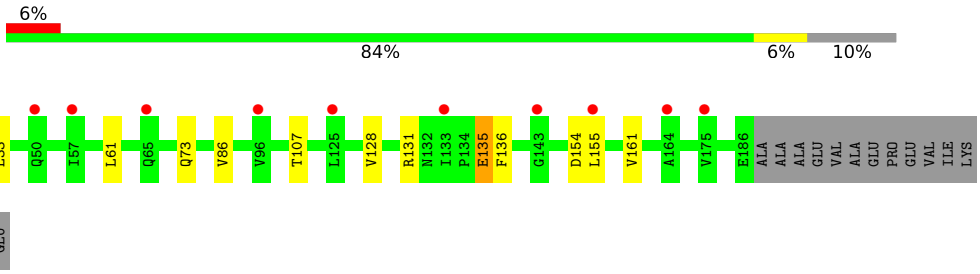
• Molecule 21: 50S ribosomal protein L25

Chain 1Z:



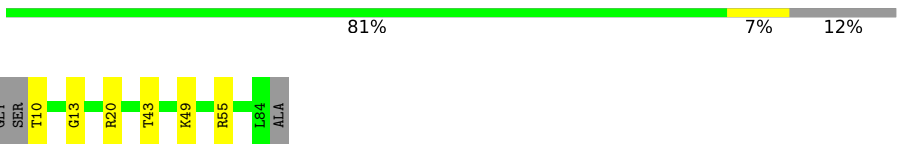
• Molecule 21: 50S ribosomal protein L25

Chain 2Z:



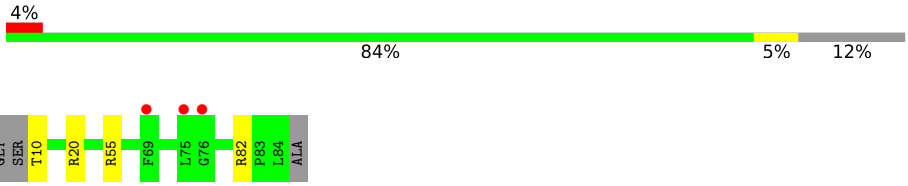
• Molecule 22: 50S ribosomal protein L27

Chain 10:



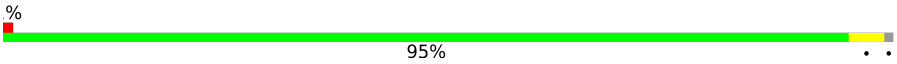
• Molecule 22: 50S ribosomal protein L27

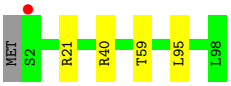
Chain 20:



• Molecule 23: 50S ribosomal protein L28

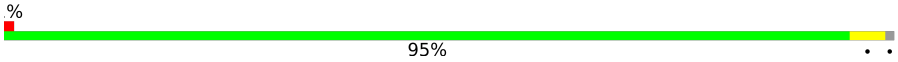
Chain 11:

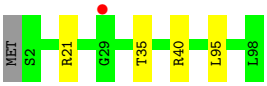




• Molecule 23: 50S ribosomal protein L28

Chain 21:



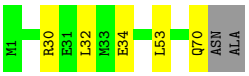


• Molecule 24: 50S ribosomal protein L29

Chain 12:

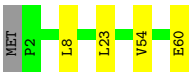
• Molecule 24: 50S ribosomal protein L29

Chain 22:



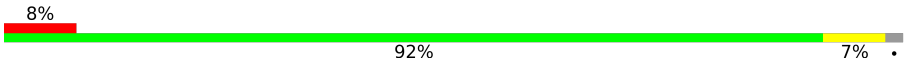
• Molecule 25: 50S ribosomal protein L30

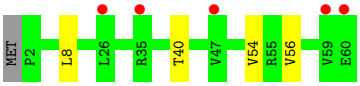
Chain 13:



• Molecule 25: 50S ribosomal protein L30

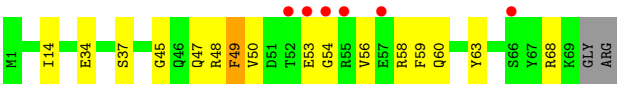
Chain 23:





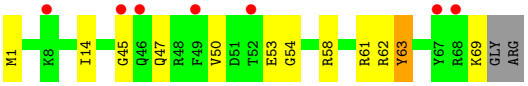
• Molecule 26: 50S ribosomal protein L31

Chain 14:



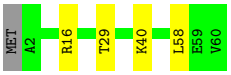
• Molecule 26: 50S ribosomal protein L31

Chain 24:



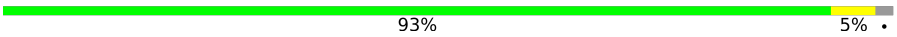
• Molecule 27: 50S ribosomal protein L32

Chain 15:



• Molecule 27: 50S ribosomal protein L32

Chain 25:



• Molecule 28: 50S ribosomal protein L33

Chain 16:

• Molecule 28: 50S ribosomal protein L33

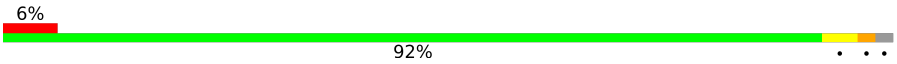
Chain 26:

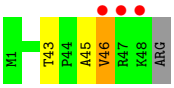
• Molecule 29: 50S ribosomal protein L34

Chain 17:

• Molecule 29: 50S ribosomal protein L34

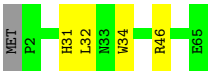
Chain 27:





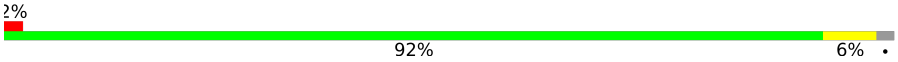
• Molecule 30: 50S ribosomal protein L35

Chain 18:



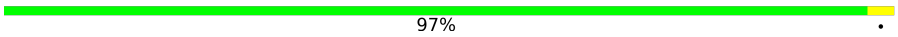
• Molecule 30: 50S ribosomal protein L35

Chain 28:



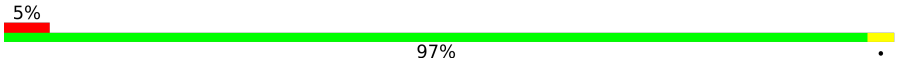
• Molecule 31: 50S ribosomal protein L36

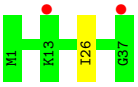
Chain 19:



• Molecule 31: 50S ribosomal protein L36

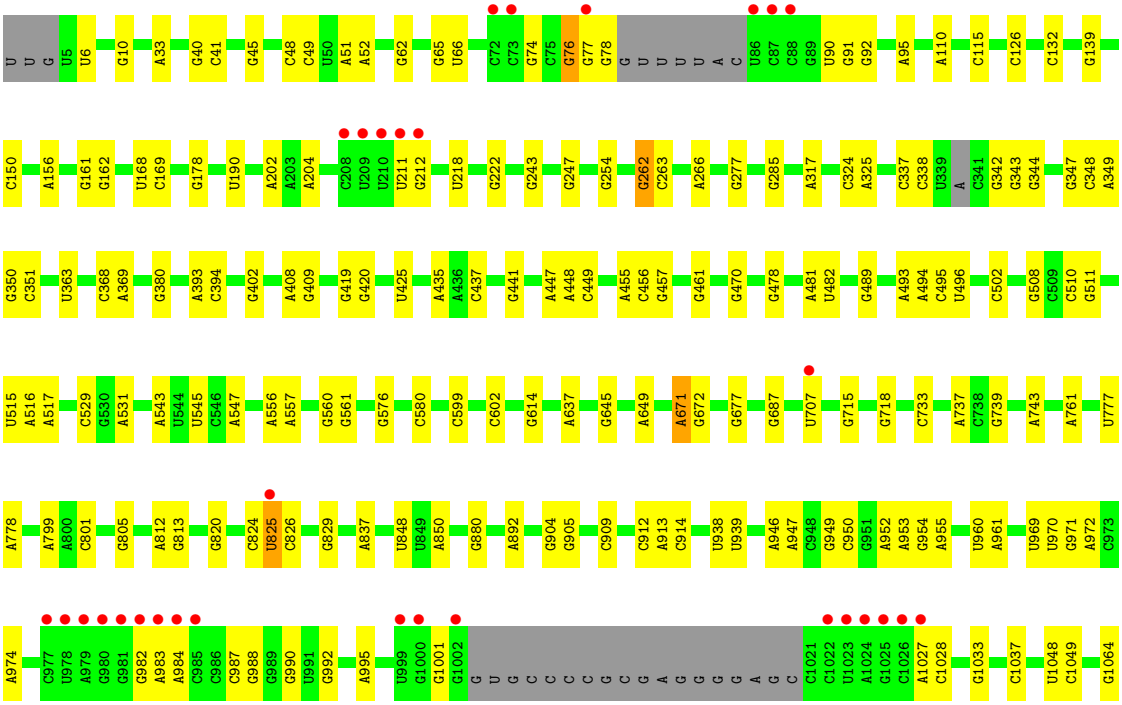
Chain 29:

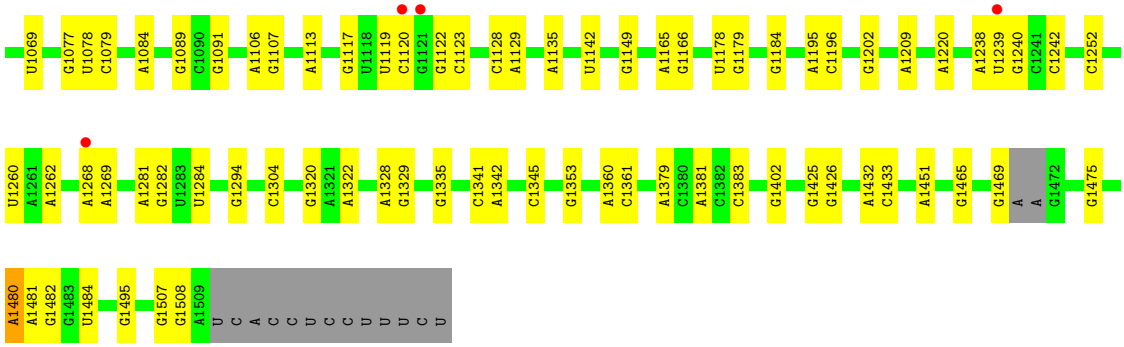




• Molecule 32: 16S Ribosomal RNA

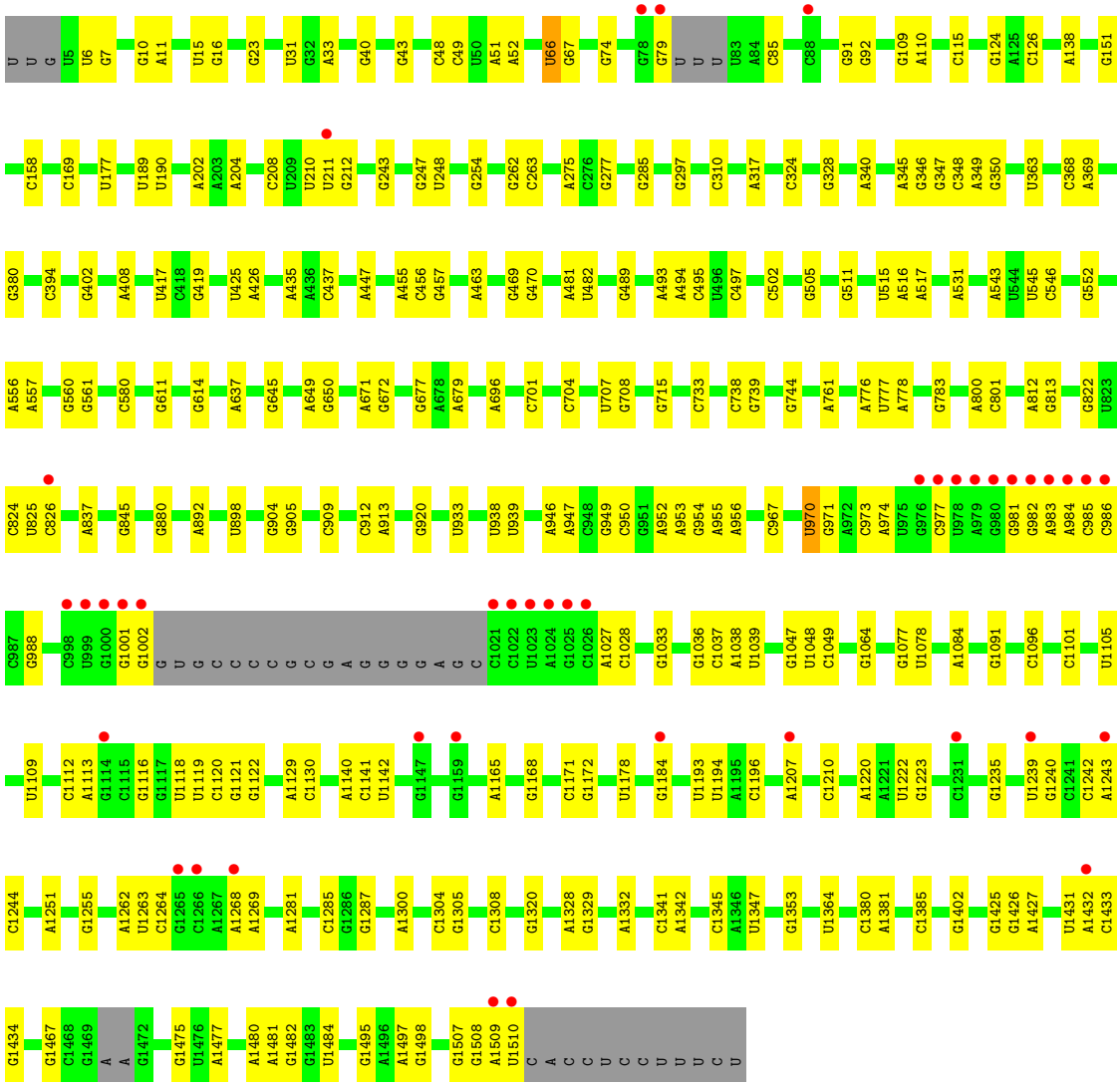
Chain 1a:





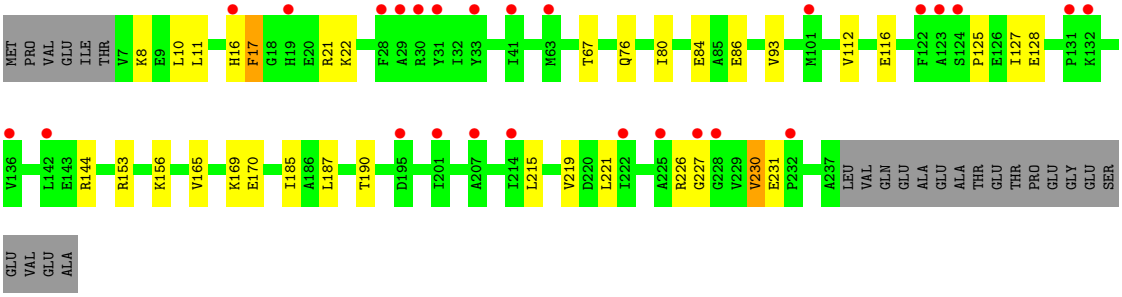
• Molecule 32: 16S Ribosomal RNA

Chain 2a:



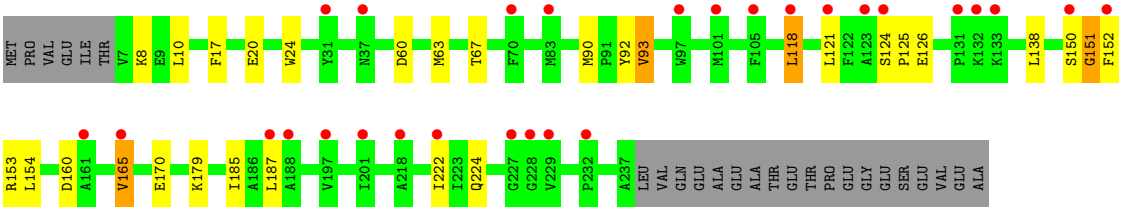
• Molecule 33: 30S ribosomal protein S2

Chain 1b:



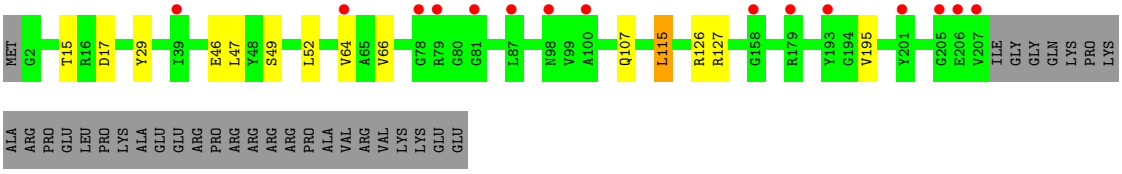
- Molecule 33: 30S ribosomal protein S2

Chain 2b:



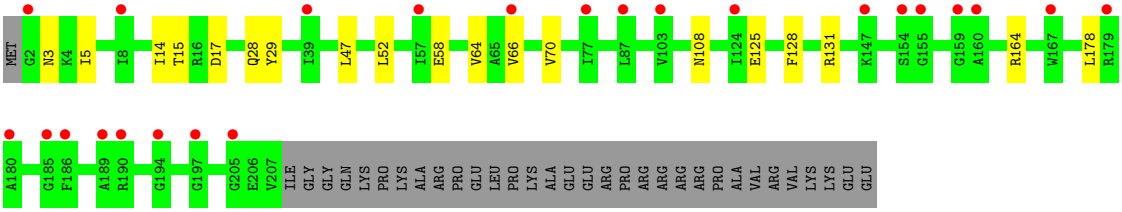
- Molecule 34: 30S ribosomal protein S3

Chain 1c:



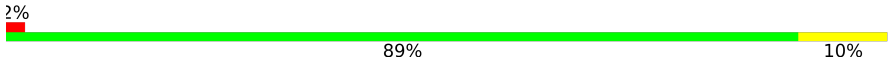
- Molecule 34: 30S ribosomal protein S3

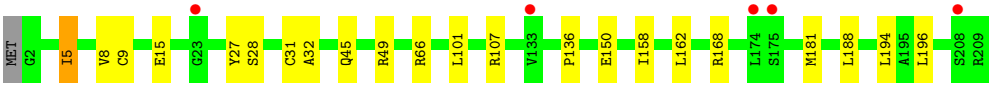
Chain 2c:



- Molecule 35: 30S ribosomal protein S4

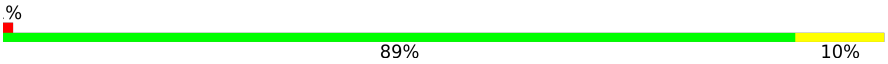
Chain 1d:

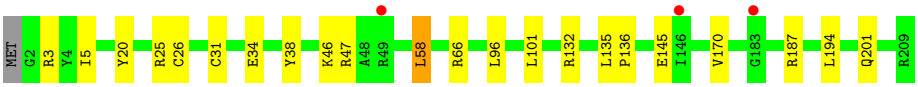




- Molecule 35: 30S ribosomal protein S4

Chain 2d:



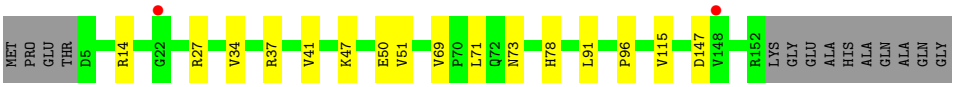


• Molecule 36: 30S ribosomal protein S5

Chain 1e:

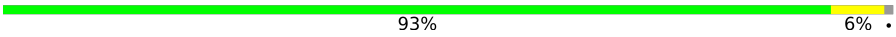
• Molecule 36: 30S ribosomal protein S5

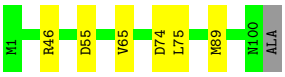
Chain 2e:



• Molecule 37: 30S ribosomal protein S6

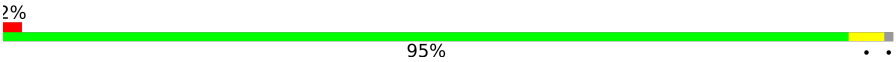
Chain 1f:





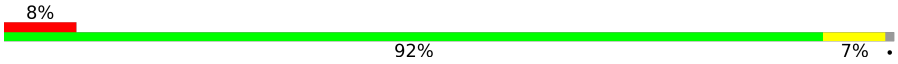
• Molecule 37: 30S ribosomal protein S6

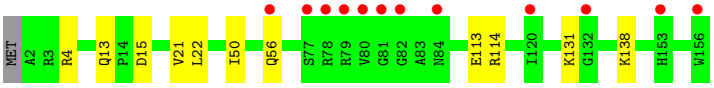
Chain 2f:



• Molecule 38: 30S ribosomal protein S7

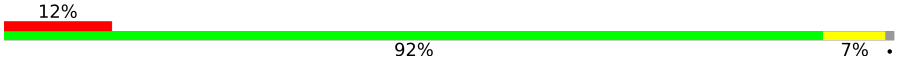
Chain 1g:

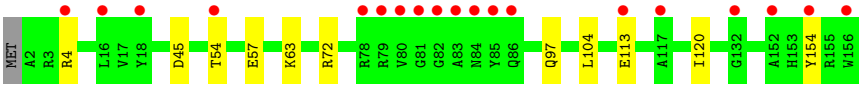




• Molecule 38: 30S ribosomal protein S7

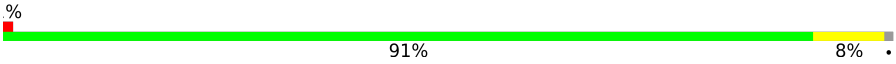
Chain 2g:

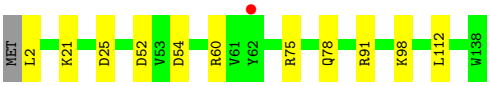




• Molecule 39: 30S ribosomal protein S8

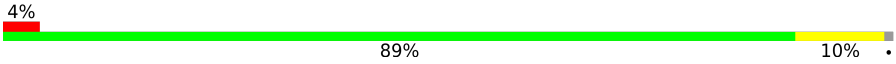
Chain 1h:

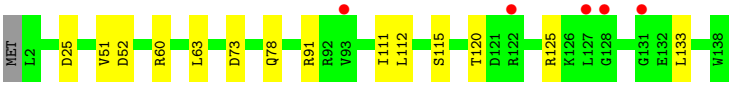




• Molecule 39: 30S ribosomal protein S8

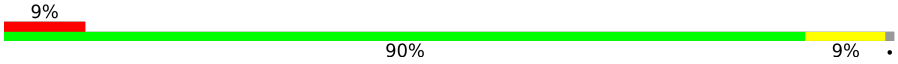
Chain 2h:

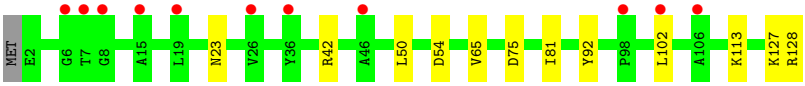




• Molecule 40: 30S ribosomal protein S9

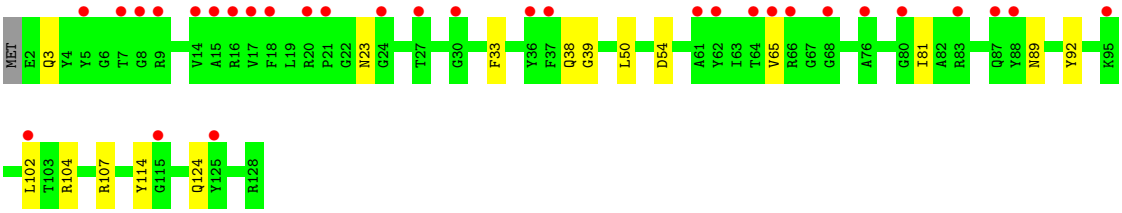
Chain 1i:





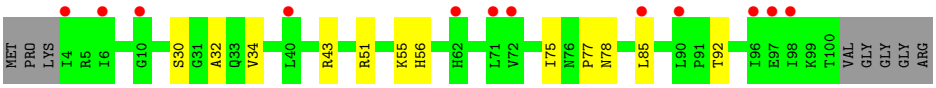
• Molecule 40: 30S ribosomal protein S9

Chain 2i:



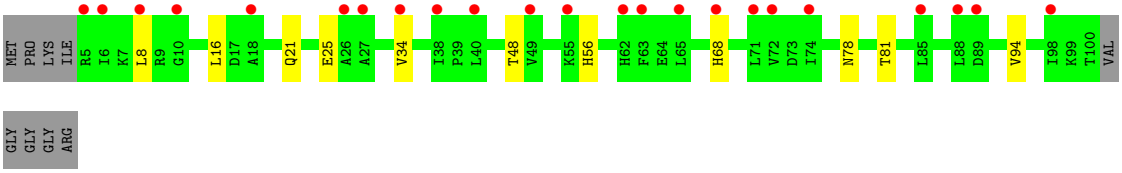
• Molecule 41: 30S ribosomal protein S10

Chain 1j:



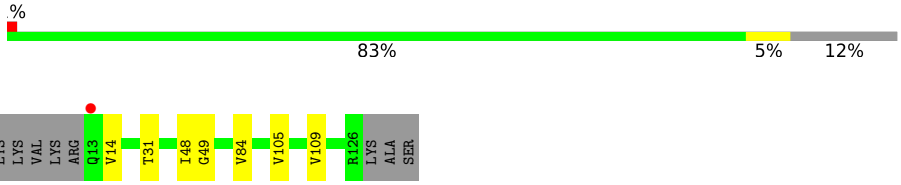
• Molecule 41: 30S ribosomal protein S10

Chain 2j:



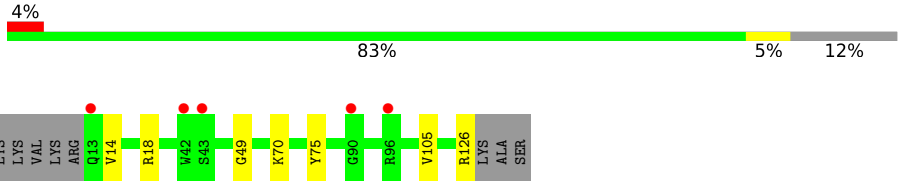
• Molecule 42: 30S ribosomal protein S11

Chain 1k:



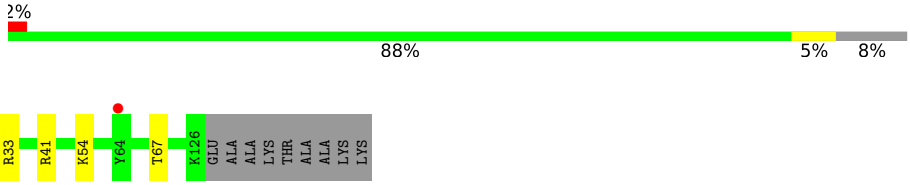
• Molecule 42: 30S ribosomal protein S11

Chain 2k:



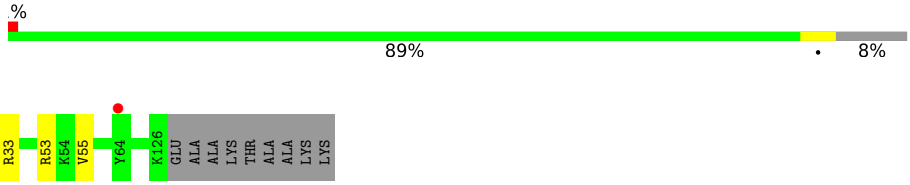
• Molecule 43: 30S ribosomal protein S12

Chain 1l:



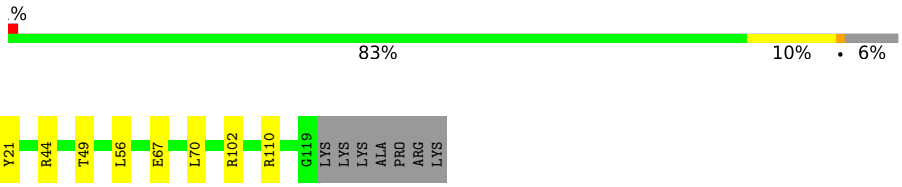
• Molecule 43: 30S ribosomal protein S12

Chain 2l:



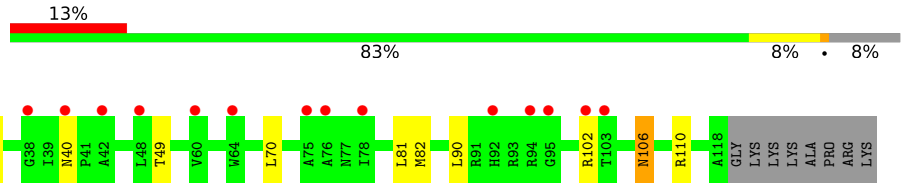
• Molecule 44: 30S ribosomal protein S13

Chain 1m:



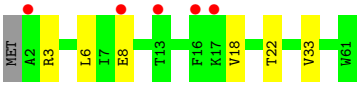
• Molecule 44: 30S ribosomal protein S13

Chain 2m:



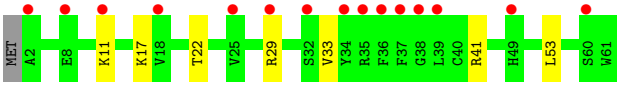
• Molecule 45: 30S ribosomal protein S14 type Z

Chain 1n:



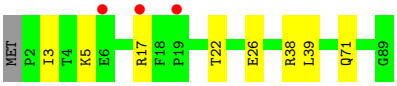
• Molecule 45: 30S ribosomal protein S14 type Z

Chain 2n:



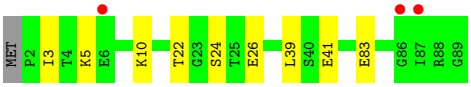
• Molecule 46: 30S ribosomal protein S15

Chain 1o:



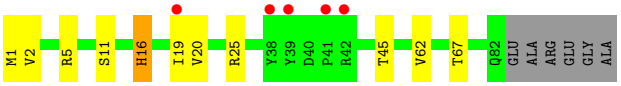
• Molecule 46: 30S ribosomal protein S15

Chain 2o:



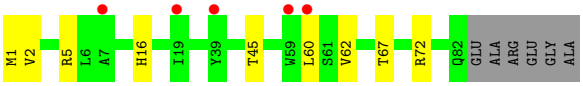
• Molecule 47: 30S ribosomal protein S16

Chain 1p:



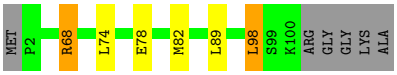
• Molecule 47: 30S ribosomal protein S16

Chain 2p:



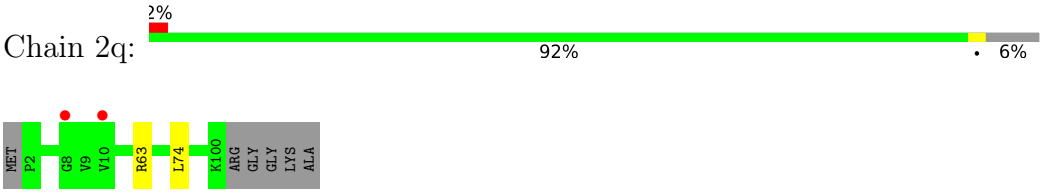
• Molecule 48: 30S ribosomal protein S17

Chain 1q:



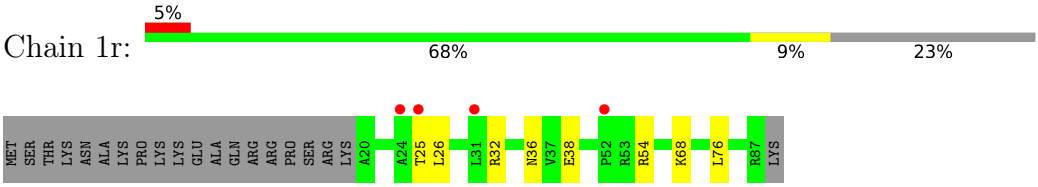
• Molecule 48: 30S ribosomal protein S17

Chain 2q:



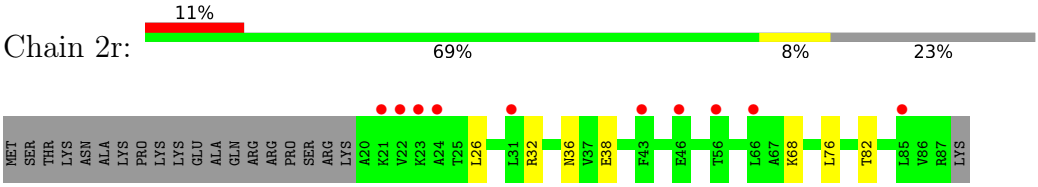
• Molecule 49: 30S ribosomal protein S18

Chain 1r:



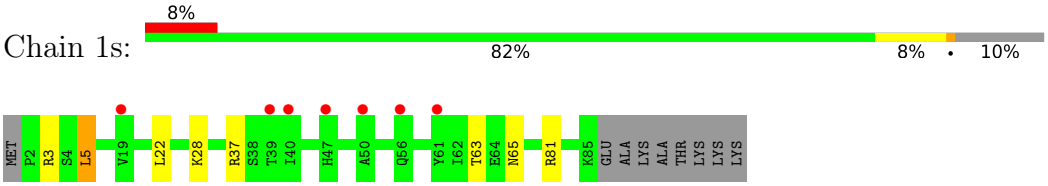
• Molecule 49: 30S ribosomal protein S18

Chain 2r:



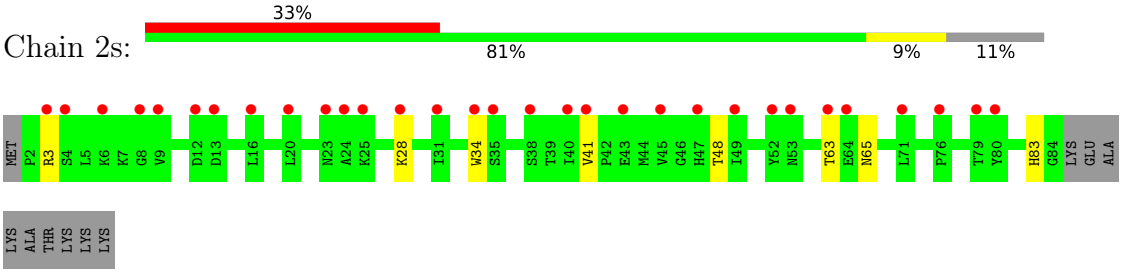
• Molecule 50: 30S ribosomal protein S19

Chain 1s:



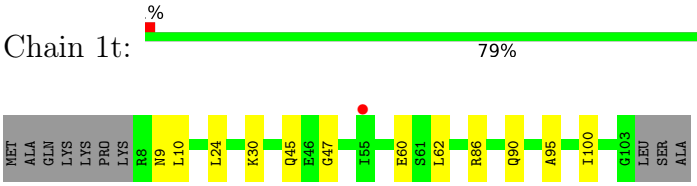
• Molecule 50: 30S ribosomal protein S19

Chain 2s:



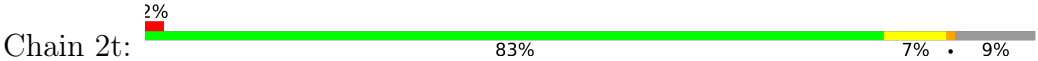
• Molecule 51: 30S ribosomal protein S20

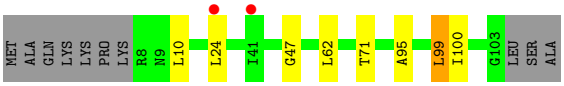
Chain 1t:



• Molecule 51: 30S ribosomal protein S20

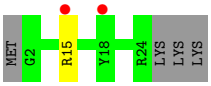
Chain 2t:





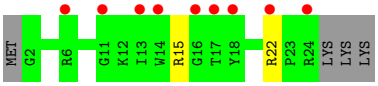
• Molecule 52: 30S ribosomal protein Thx

Chain 1u:



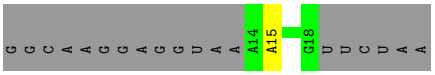
• Molecule 52: 30S ribosomal protein Thx

Chain 2u:



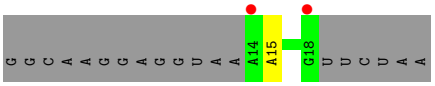
• Molecule 53: mRNA

Chain 1v:



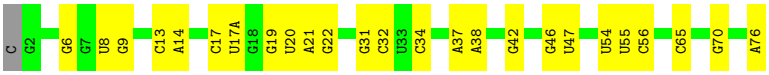
• Molecule 53: mRNA

Chain 2v:



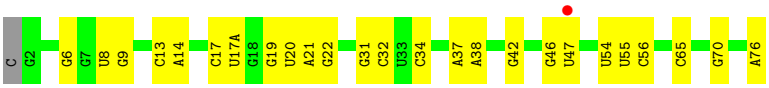
• Molecule 54: P-site tRNA

Chain 1x:



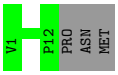
• Molecule 54: P-site tRNA

Chain 2x:



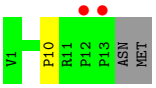
• Molecule 55: Metalnikowin-1

Chain 1z:



• Molecule 55: Metalnikowin-1

Chain 2z:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	209.87Å 450.49Å 623.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.85 – 2.89 49.85 – 2.89	Depositor EDS
% Data completeness (in resolution range)	98.6 (49.85-2.89) 98.6 (49.85-2.89)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.25 (at 2.91Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.212 , 0.268 0.212 , 0.268	Depositor DCC
R_{free} test set	64043 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	56.9	Xtriage
Anisotropy	0.146	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 65.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	288976	wwPDB-VP
Average B, all atoms (Å^2)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.69% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, MG, SF4, ZN, 4SU, PSU, 5MC

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	0.60	4/66249 (0.0%)	0.96	66/103407 (0.1%)
1	2A	0.47	1/67298 (0.0%)	0.95	48/105044 (0.0%)
2	1B	0.45	0/2877	0.86	0/4488
2	2B	0.52	0/2878	0.97	1/4490 (0.0%)
3	1D	0.41	0/2186	0.58	0/2944
3	2D	0.36	0/2192	0.58	0/2951
4	1E	0.44	0/1592	0.58	0/2149
4	2E	0.37	0/1592	0.58	0/2149
5	1F	0.41	0/1619	0.57	0/2193
5	2F	0.35	0/1615	0.57	0/2188
6	1G	0.32	0/1450	0.53	0/1959
6	2G	0.35	0/1449	0.57	0/1958
7	1H	0.35	0/1356	0.54	0/1834
7	2H	0.31	0/1356	0.51	0/1834
8	1I	0.31	0/1100	0.56	0/1501
8	2I	0.31	0/1076	0.56	0/1471
9	1N	0.41	0/1144	0.54	0/1543
9	2N	0.34	0/1144	0.55	0/1543
10	1O	0.42	0/943	0.57	0/1269
10	2O	0.37	0/943	0.59	1/1269 (0.1%)
11	1P	0.38	0/1156	0.60	1/1537 (0.1%)
11	2P	0.36	0/1152	0.58	0/1533
12	1Q	0.41	0/1143	0.53	0/1527
12	2Q	0.36	0/1143	0.59	0/1527
13	1R	0.42	0/982	0.65	0/1312
13	2R	0.32	0/982	0.57	0/1312
14	1S	0.35	0/887	0.60	0/1180
14	2S	0.32	0/880	0.54	0/1172
15	1T	0.39	0/1105	0.59	0/1477
15	2T	0.33	0/1097	0.53	0/1468
16	1U	0.44	0/977	0.56	0/1301
16	2U	0.33	0/977	0.51	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	1V	0.42	0/782	0.58	0/1049
17	2V	0.36	0/782	0.53	0/1049
18	1W	0.45	0/897	0.58	0/1205
18	2W	0.37	0/897	0.57	0/1205
19	1X	0.41	0/764	0.55	0/1025
19	2X	0.37	0/764	0.58	1/1025 (0.1%)
20	1Y	0.40	0/819	0.59	0/1095
20	2Y	0.33	0/819	0.54	0/1095
21	1Z	0.32	0/1502	0.51	0/2041
21	2Z	0.34	0/1486	0.54	0/2022
22	10	0.42	0/606	0.59	0/808
22	20	0.36	0/606	0.55	0/808
23	11	0.41	0/762	0.54	0/1014
23	21	0.35	0/762	0.53	0/1014
24	12	0.35	0/590	0.52	0/781
24	22	0.33	0/590	0.47	0/781
25	13	0.40	0/474	0.56	0/635
25	23	0.33	0/469	0.58	0/630
26	14	0.38	0/571	0.67	0/768
26	24	0.34	0/545	0.65	0/737
27	15	0.41	0/469	0.58	0/635
27	25	0.35	0/469	0.59	0/635
28	16	0.43	0/460	0.53	0/613
28	26	0.37	0/456	0.53	0/608
29	17	0.41	0/426	0.58	0/561
29	27	0.38	0/426	0.54	0/561
30	18	0.42	0/525	0.60	0/691
30	28	0.36	0/525	0.55	0/691
31	19	0.42	0/310	0.54	0/407
31	29	0.36	0/310	0.54	0/407
32	1a	0.40	0/35537	0.89	8/55456 (0.0%)
32	2a	0.38	0/35680	0.88	19/55681 (0.0%)
33	1b	0.31	0/1820	0.56	0/2468
33	2b	2.72	8/1728 (0.5%)	0.70	3/2352 (0.1%)
34	1c	0.28	0/1504	0.49	1/2047 (0.0%)
34	2c	0.33	0/1435	0.55	0/1960
35	1d	0.31	0/1648	0.54	0/2222
35	2d	0.30	0/1659	0.54	1/2230 (0.0%)
36	1e	0.31	0/1145	0.55	0/1543
36	2e	0.30	0/1111	0.58	0/1504
37	1f	0.31	0/819	0.51	0/1111
37	2f	0.31	0/830	0.52	0/1125
38	1g	0.30	0/1198	0.48	0/1613

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
38	2g	0.31	0/1185	0.49	0/1602
39	1h	0.30	0/1108	0.52	0/1494
39	2h	0.29	0/1094	0.51	0/1478
40	1i	0.31	0/995	0.55	0/1339
40	2i	0.33	0/949	0.58	0/1284
41	1j	0.31	0/695	0.56	0/950
41	2j	0.30	0/690	0.55	0/943
42	1k	0.31	0/840	0.52	0/1138
42	2k	0.29	0/844	0.50	0/1145
43	1l	0.32	0/936	0.53	0/1263
43	2l	0.33	0/934	0.59	1/1262 (0.1%)
44	1m	0.29	0/933	0.56	0/1254
44	2m	0.31	0/913	0.52	0/1230
45	1n	0.33	0/491	0.57	0/653
45	2n	0.33	0/467	0.49	0/624
46	1o	0.31	0/726	0.56	0/970
46	2o	0.31	0/739	0.50	0/985
47	1p	0.29	0/686	0.52	0/926
47	2p	0.31	0/693	0.53	0/935
48	1q	0.32	0/824	0.55	1/1105 (0.1%)
48	2q	0.30	0/836	0.48	0/1117
49	1r	0.30	0/560	0.50	0/746
49	2r	0.30	0/560	0.52	0/746
50	1s	0.29	0/657	0.56	1/890 (0.1%)
50	2s	0.32	0/661	0.60	0/893
51	1t	0.28	0/714	0.61	0/948
51	2t	0.29	0/733	0.52	0/969
52	1u	0.24	0/191	0.46	0/252
52	2u	0.30	0/203	0.52	0/266
53	1v	0.64	0/122	1.10	0/188
53	2v	0.53	0/122	0.94	0/188
54	1x	0.57	2/1725 (0.1%)	1.14	18/2689 (0.7%)
54	2x	0.54	1/1725 (0.1%)	1.14	14/2689 (0.5%)
55	1z	0.38	0/109	0.70	0/148
55	2z	0.35	0/117	0.64	0/160
All	All	0.50	16/306294 (0.0%)	0.85	185/458208 (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
5	2F	0	1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	2b	92	TYR	CD1-CE1	59.23	2.28	1.39
33	2b	92	TYR	CD2-CE2	53.18	2.19	1.39
33	2b	92	TYR	CE1-CZ	41.65	1.92	1.38
33	2b	92	TYR	CE2-CZ	41.39	1.92	1.38
33	2b	92	TYR	CG-CD1	33.82	1.83	1.39
33	2b	92	TYR	CG-CD2	32.39	1.81	1.39
33	2b	151	GLY	N-CA	22.82	1.80	1.46
33	2b	150	SER	C-N	10.50	1.51	1.33
1	1A	552	A	N9-C4	-7.88	1.33	1.37
1	1A	1187	A	N9-C4	-7.20	1.33	1.37
1	2A	552	A	N9-C4	-6.75	1.33	1.37
1	1A	1066	A	N9-C4	-6.05	1.34	1.37
54	1x	22	G	N7-C5	5.76	1.42	1.39
54	1x	14	A	C8-N7	-5.24	1.27	1.31
1	1A	2298	A	N9-C4	-5.13	1.34	1.37
54	2x	22	G	N7-C5	5.01	1.42	1.39

All (185) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	2b	150	SER	C-N-CA	16.39	156.71	122.30
1	1A	552	A	C2-N3-C4	-11.05	105.07	110.60
54	1x	46	G	C6-N1-C2	-10.06	119.06	125.10
1	1A	1066	A	C2-N3-C4	-9.89	105.66	110.60
54	2x	46	G	C6-N1-C2	-9.72	119.27	125.10
1	2A	552	A	C2-N3-C4	-8.87	106.16	110.60
1	1A	552	A	N3-C4-C5	8.78	132.94	126.80
33	2b	151	GLY	N-CA-C	8.74	134.95	113.10
1	1A	552	A	N3-C4-N9	-8.51	120.59	127.40
54	1x	14	A	C5-N7-C8	8.50	108.15	103.90
54	2x	14	A	C4-C5-C6	8.45	121.23	117.00
1	1A	1187	A	C2-N3-C4	-8.39	106.41	110.60
1	1A	989	A	C5-N7-C8	-8.31	99.75	103.90
54	2x	14	A	C5-N7-C8	8.19	107.99	103.90
1	1A	847	G	O5'-P-OP2	-7.93	98.57	105.70
32	2a	1141	C	C2-N1-C1'	7.89	127.48	118.80
1	1A	2083	A	O4'-C1'-N9	7.54	114.23	108.20
54	1x	22	G	C5-N7-C8	-7.48	100.56	104.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1A	2083	A	C2-N3-C4	-7.47	106.87	110.60
1	1A	1067	G	N3-C4-N9	-7.41	121.56	126.00
1	1A	214	G	O4'-C1'-N9	7.40	114.12	108.20
1	2A	552	A	N3-C4-C5	7.39	131.97	126.80
54	2x	22	G	C5-N7-C8	-7.35	100.62	104.30
1	1A	1187	A	N3-C4-C5	7.33	131.93	126.80
32	1a	825	U	C5-C6-N1	7.32	126.36	122.70
1	1A	138	A	N7-C8-N9	7.28	117.44	113.80
54	1x	22	G	N3-C4-N9	-7.15	121.71	126.00
54	1x	14	A	C4-C5-C6	7.13	120.56	117.00
1	1A	989	A	N7-C8-N9	7.07	117.34	113.80
19	2X	57	LEU	CA-CB-CG	6.99	131.37	115.30
54	2x	46	G	C5-C6-N1	6.97	114.98	111.50
1	1A	536	G	O4'-C1'-N9	6.93	113.75	108.20
32	2a	738	C	C2-N1-C1'	6.91	126.40	118.80
43	2l	29	GLY	N-CA-C	-6.87	95.92	113.10
54	1x	46	G	C5-C6-N1	6.84	114.92	111.50
54	1x	22	G	N1-C6-O6	-6.77	115.84	119.90
54	2x	22	G	C4-C5-C6	-6.67	114.80	118.80
1	1A	1066	A	N1-C2-N3	6.64	132.62	129.30
54	1x	22	G	C4-C5-C6	-6.63	114.82	118.80
1	1A	138	A	C5-N7-C8	-6.59	100.60	103.90
1	1A	1685	U	O5'-P-OP2	-6.57	99.79	105.70
1	1A	977	A	C5-N7-C8	-6.55	100.62	103.90
1	2A	2583	A	C8-N9-C4	6.52	108.41	105.80
1	1A	1044	U	O5'-P-OP2	-6.47	99.88	105.70
32	2a	738	C	N1-C2-O2	6.40	122.74	118.90
32	2a	1141	C	N1-C2-O2	6.40	122.74	118.90
1	2A	138	A	N7-C8-N9	6.40	117.00	113.80
54	1x	14	A	C5-C6-N1	-6.37	114.52	117.70
1	1A	353	A	C2-N3-C4	-6.36	107.42	110.60
1	1A	2212	G	C5-C6-O6	-6.32	124.81	128.60
1	1A	1694	C	O5'-P-OP1	-6.31	100.02	105.70
1	1A	989	A	C8-N9-C4	-6.31	103.28	105.80
1	1A	1153	U	C2-N1-C1'	6.28	125.23	117.70
54	1x	22	G	C8-N9-C1'	6.26	135.13	127.00
1	2A	830	A	O4'-C1'-N9	6.24	113.19	108.20
1	1A	1294	U	O5'-P-OP1	-6.16	100.16	105.70
1	1A	409	U	C2-N1-C1'	-6.13	110.34	117.70
32	2a	1207	A	C5-C6-N6	6.13	128.60	123.70
1	2A	409	U	O4'-C1'-N1	6.12	113.10	108.20
1	1A	2013	G	P-O3'-C3'	6.11	127.03	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1067	G	N3-C2-N2	-6.10	115.63	119.90
1	2A	138	A	C8-N9-C4	-6.10	103.36	105.80
32	1a	150	C	N1-C2-O2	6.10	122.56	118.90
1	2A	552	A	N3-C4-N9	-6.08	122.54	127.40
1	1A	11	U	C2-N1-C1'	6.07	124.98	117.70
1	1A	1806	G	O5'-P-OP2	-6.05	100.25	105.70
1	2A	2484	U	C2-N1-C1'	6.04	124.94	117.70
32	2a	1207	A	N1-C6-N6	-6.03	114.98	118.60
1	1A	1066	A	C5-N7-C8	-5.95	100.93	103.90
1	1A	2057	C	O5'-P-OP1	-5.89	100.40	105.70
10	2O	8	LEU	CA-CB-CG	5.89	128.84	115.30
1	1A	138	A	C8-N9-C4	-5.89	103.44	105.80
1	1A	551	C	N3-C2-O2	-5.88	117.79	121.90
1	1A	2035	A	C8-N9-C4	5.87	108.15	105.80
32	2a	66	U	P-O3'-C3'	5.87	126.75	119.70
54	2x	46	G	N3-C2-N2	-5.87	115.79	119.90
54	2x	22	G	C8-N9-C1'	5.86	134.62	127.00
54	2x	46	G	C5-C6-O6	-5.85	125.09	128.60
1	2A	300	C	C2-N1-C1'	5.79	125.17	118.80
1	2A	536	G	O4'-C1'-N9	5.78	112.82	108.20
54	1x	14	A	C8-N9-C1'	-5.78	117.30	127.70
1	1A	1187	A	N3-C4-N9	-5.74	122.81	127.40
32	2a	982	G	C8-N9-C4	-5.73	104.11	106.40
32	2a	1141	C	C6-N1-C2	-5.68	118.03	120.30
1	2A	989	A	N1-C6-N6	5.66	122.00	118.60
54	1x	22	G	N7-C8-N9	5.66	115.93	113.10
1	1A	1297	G	O4'-C1'-N9	-5.66	103.68	108.20
1	2A	1248	A	O4'-C1'-N9	5.63	112.70	108.20
1	1A	1744	A	C2-N3-C4	-5.63	107.79	110.60
1	2A	2271	C	C6-N1-C2	-5.62	118.05	120.30
1	1A	1248	A	O4'-C1'-N9	5.62	112.69	108.20
1	2A	1109	C	C2-N1-C1'	5.62	124.98	118.80
54	2x	22	G	N3-C4-N9	-5.61	122.63	126.00
1	2A	989	A	O4'-C1'-N9	5.60	112.68	108.20
35	2d	58	LEU	CA-CB-CG	5.59	128.16	115.30
1	1A	2857	G	O4'-C1'-N9	5.59	112.67	108.20
1	2A	873	U	N3-C2-O2	5.57	126.10	122.20
1	2A	300	C	N1-C2-O2	5.55	122.23	118.90
1	2A	2484	U	N1-C2-O2	5.55	126.69	122.80
1	1A	138	A	O4'-C1'-N9	5.53	112.62	108.20
54	1x	22	G	C6-C5-N7	5.52	133.71	130.40
1	2A	1358	U	C2-N1-C1'	5.52	124.33	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2A	2013	G	P-O3'-C3'	5.51	126.32	119.70
1	2A	1359	C	C2-N1-C1'	5.50	124.85	118.80
1	2A	1820	C	P-O3'-C3'	5.50	126.30	119.70
1	1A	2222	C	N3-C2-O2	-5.50	118.05	121.90
1	2A	1659	A	O5'-P-OP1	-5.49	100.76	105.70
1	2A	829	A	C2-N3-C4	5.48	113.34	110.60
1	1A	1218	A	OP1-P-O3'	5.48	117.25	105.20
54	1x	22	G	N9-C4-C5	5.46	107.58	105.40
54	2x	14	A	C8-N9-C1'	-5.46	117.88	127.70
32	2a	982	G	N3-C4-C5	-5.41	125.89	128.60
1	2A	88	U	C2-N1-C1'	5.40	124.18	117.70
1	1A	30	C	O5'-P-OP1	-5.40	100.84	105.70
32	2a	671	A	P-O3'-C3'	5.38	126.16	119.70
1	2A	2759	G	N1-C6-O6	5.38	123.13	119.90
1	1A	989	A	C2-N3-C4	-5.38	107.91	110.60
1	2A	2268	U	N3-C2-O2	5.36	125.95	122.20
1	2A	1114	A	P-O3'-C3'	5.36	126.13	119.70
1	1A	1358	U	C2-N1-C1'	5.36	124.13	117.70
1	2A	1248	A	N1-C6-N6	5.35	121.81	118.60
1	1A	1693	G	O4'-C1'-N9	-5.35	103.92	108.20
1	2A	1676	C	N3-C2-O2	5.34	125.64	121.90
54	2x	14	A	C4-N9-C1'	5.33	135.90	126.30
11	1P	99	LEU	CA-CB-CG	5.31	127.50	115.30
1	1A	977	A	O4'-C1'-N9	5.30	112.44	108.20
1	2A	1604	A	P-O3'-C3'	5.29	126.05	119.70
1	2A	2700	U	P-O3'-C3'	5.28	126.04	119.70
54	1x	14	A	C4-N9-C1'	5.28	135.81	126.30
1	1A	977	A	C4-C5-N7	5.27	113.33	110.70
54	1x	46	G	C5-C6-O6	-5.27	125.44	128.60
1	2A	2583	A	N7-C8-N9	-5.27	111.17	113.80
32	2a	1141	C	C6-N1-C1'	-5.26	114.49	120.80
32	1a	825	U	C6-N1-C2	-5.26	117.85	121.00
1	1A	1218	A	P-O3'-C3'	5.25	126.00	119.70
1	1A	1066	A	N7-C8-N9	5.24	116.42	113.80
32	2a	738	C	N3-C2-O2	-5.24	118.23	121.90
1	1A	2512	C	C6-N1-C2	5.24	122.40	120.30
54	1x	46	G	N3-C2-N2	-5.23	116.24	119.90
32	2a	1141	C	N3-C2-O2	-5.22	118.24	121.90
1	1A	552	A	C4-N9-C1'	-5.22	116.90	126.30
1	2A	2331	A	C2-N3-C4	5.22	113.21	110.60
1	2A	719	C	N1-C2-O2	-5.21	115.77	118.90
1	2A	202	G	O4'-C1'-N9	5.21	112.37	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2A	1676	C	N1-C2-O2	-5.21	115.78	118.90
2	2B	42	C	P-O3'-C3'	5.20	125.94	119.70
32	2a	933	U	C2-N3-C4	5.20	130.12	127.00
1	2A	792	A	O4'-C1'-N9	5.19	112.36	108.20
1	2A	1404	A	C2-N3-C4	5.18	113.19	110.60
1	2A	2530	U	N3-C2-O2	5.18	125.82	122.20
54	2x	14	A	C5-C6-N1	-5.17	115.11	117.70
1	1A	1439	U	O5'-P-OP1	-5.17	101.05	105.70
1	2A	2458	G	C4-N9-C1'	-5.16	119.79	126.50
1	1A	830	A	P-O3'-C3'	5.14	125.87	119.70
1	1A	2640	A	O4'-C1'-N9	5.14	112.31	108.20
48	1q	98	LEU	CA-CB-CG	5.13	127.11	115.30
54	2x	22	G	C4-N9-C1'	-5.13	119.83	126.50
32	1a	969	U	P-O3'-C3'	5.13	125.86	119.70
32	2a	982	G	C4-N9-C1'	5.12	133.16	126.50
1	2A	669	C	C2-N1-C1'	5.12	124.43	118.80
1	1A	794	G	O4'-C1'-N9	5.11	112.29	108.20
1	1A	202	G	O4'-C1'-N9	5.10	112.28	108.20
1	2A	2814	C	C6-N1-C2	-5.10	118.26	120.30
1	2A	636	U	N3-C2-O2	-5.09	118.64	122.20
32	1a	76	G	N3-C4-N9	5.08	129.05	126.00
1	1A	1153	U	C5-C6-N1	5.08	125.24	122.70
1	1A	2449	U	OP2-P-O3'	5.08	116.38	105.20
1	2A	111	U	C2-N1-C1'	5.07	123.79	117.70
1	2A	830	A	P-O3'-C3'	5.06	125.78	119.70
32	1a	671	A	P-O3'-C3'	5.06	125.77	119.70
50	1s	5	LEU	CA-CB-CG	5.05	126.93	115.30
1	1A	552	A	C8-N9-C1'	5.05	136.80	127.70
33	2b	118	LEU	CA-CB-CG	5.05	126.92	115.30
54	1x	14	A	C4-C5-N7	-5.05	108.18	110.70
1	1A	1281	G	C8-N9-C4	5.04	108.42	106.40
34	1c	115	LEU	CA-CB-CG	5.04	126.90	115.30
32	1a	262	G	P-O3'-C3'	5.04	125.74	119.70
1	2A	1690	C	C2-N1-C1'	5.04	124.34	118.80
32	2a	970	U	P-O3'-C3'	5.03	125.74	119.70
1	1A	586	C	N1-C2-O2	-5.03	115.88	118.90
1	1A	1066	A	N3-C4-N9	-5.03	123.38	127.40
1	1A	905	G	N3-C4-C5	5.01	131.11	128.60
32	2a	1385	C	C6-N1-C2	-5.01	118.30	120.30
32	2a	109	G	P-O3'-C3'	5.01	125.71	119.70
32	1a	1480	A	N7-C8-N9	5.01	116.30	113.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	2F	20	LEU	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%)	253 (93%)	20 (7%)	0	100	100
3	2D	273/276 (99%)	252 (92%)	19 (7%)	2 (1%)	22	54
4	1E	202/206 (98%)	195 (96%)	6 (3%)	1 (0%)	29	61
4	2E	202/206 (98%)	194 (96%)	7 (4%)	1 (0%)	29	61
5	1F	201/210 (96%)	196 (98%)	3 (2%)	2 (1%)	15	45
5	2F	201/210 (96%)	193 (96%)	6 (3%)	2 (1%)	15	45
6	1G	179/182 (98%)	161 (90%)	15 (8%)	3 (2%)	9	31
6	2G	179/182 (98%)	156 (87%)	18 (10%)	5 (3%)	5	19
7	1H	172/180 (96%)	161 (94%)	9 (5%)	2 (1%)	13	40
7	2H	172/180 (96%)	159 (92%)	11 (6%)	2 (1%)	13	40
8	1I	144/148 (97%)	126 (88%)	14 (10%)	4 (3%)	5	19
8	2I	144/148 (97%)	124 (86%)	19 (13%)	1 (1%)	22	54
9	1N	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
9	2N	138/140 (99%)	135 (98%)	2 (1%)	1 (1%)	22	54
10	1O	120/122 (98%)	115 (96%)	4 (3%)	1 (1%)	19	51
10	2O	120/122 (98%)	115 (96%)	4 (3%)	1 (1%)	19	51
11	1P	147/150 (98%)	137 (93%)	9 (6%)	1 (1%)	22	54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	2P	147/150 (98%)	135 (92%)	10 (7%)	2 (1%)	11	36
12	1Q	139/141 (99%)	132 (95%)	7 (5%)	0	100	100
12	2Q	139/141 (99%)	129 (93%)	9 (6%)	1 (1%)	22	54
13	1R	116/118 (98%)	107 (92%)	9 (8%)	0	100	100
13	2R	116/118 (98%)	107 (92%)	9 (8%)	0	100	100
14	1S	108/112 (96%)	98 (91%)	9 (8%)	1 (1%)	17	48
14	2S	108/112 (96%)	98 (91%)	9 (8%)	1 (1%)	17	48
15	1T	129/146 (88%)	123 (95%)	6 (5%)	0	100	100
15	2T	129/146 (88%)	124 (96%)	5 (4%)	0	100	100
16	1U	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
16	2U	114/118 (97%)	112 (98%)	2 (2%)	0	100	100
17	1V	99/101 (98%)	96 (97%)	2 (2%)	1 (1%)	15	45
17	2V	99/101 (98%)	95 (96%)	3 (3%)	1 (1%)	15	45
18	1W	110/113 (97%)	109 (99%)	1 (1%)	0	100	100
18	2W	110/113 (97%)	107 (97%)	3 (3%)	0	100	100
19	1X	93/96 (97%)	92 (99%)	0	1 (1%)	14	42
19	2X	93/96 (97%)	91 (98%)	1 (1%)	1 (1%)	14	42
20	1Y	105/110 (96%)	93 (89%)	10 (10%)	2 (2%)	8	28
20	2Y	105/110 (96%)	94 (90%)	11 (10%)	0	100	100
21	1Z	184/206 (89%)	169 (92%)	15 (8%)	0	100	100
21	2Z	184/206 (89%)	167 (91%)	15 (8%)	2 (1%)	14	42
22	10	73/85 (86%)	70 (96%)	2 (3%)	1 (1%)	11	36
22	20	73/85 (86%)	70 (96%)	3 (4%)	0	100	100
23	11	95/98 (97%)	92 (97%)	3 (3%)	0	100	100
23	21	95/98 (97%)	90 (95%)	5 (5%)	0	100	100
24	12	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
24	22	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
25	13	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
25	23	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
26	14	67/71 (94%)	50 (75%)	8 (12%)	9 (13%)	0	0
26	24	67/71 (94%)	53 (79%)	9 (13%)	5 (8%)	1	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	15	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
27	25	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
28	16	51/54 (94%)	50 (98%)	1 (2%)	0	100	100
28	26	51/54 (94%)	50 (98%)	1 (2%)	0	100	100
29	17	46/49 (94%)	46 (100%)	0	0	100	100
29	27	46/49 (94%)	43 (94%)	1 (2%)	2 (4%)	2	10
30	18	62/65 (95%)	59 (95%)	3 (5%)	0	100	100
30	28	62/65 (95%)	59 (95%)	3 (5%)	0	100	100
31	19	35/37 (95%)	35 (100%)	0	0	100	100
31	29	35/37 (95%)	35 (100%)	0	0	100	100
33	1b	229/256 (90%)	190 (83%)	31 (14%)	8 (4%)	3	14
33	2b	229/256 (90%)	188 (82%)	32 (14%)	9 (4%)	3	12
34	1c	204/239 (85%)	178 (87%)	22 (11%)	4 (2%)	7	27
34	2c	204/239 (85%)	173 (85%)	29 (14%)	2 (1%)	15	45
35	1d	206/209 (99%)	188 (91%)	13 (6%)	5 (2%)	6	22
35	2d	206/209 (99%)	188 (91%)	15 (7%)	3 (2%)	10	34
36	1e	146/162 (90%)	126 (86%)	15 (10%)	5 (3%)	3	15
36	2e	146/162 (90%)	129 (88%)	13 (9%)	4 (3%)	5	19
37	1f	98/101 (97%)	94 (96%)	4 (4%)	0	100	100
37	2f	98/101 (97%)	93 (95%)	5 (5%)	0	100	100
38	1g	153/156 (98%)	132 (86%)	20 (13%)	1 (1%)	22	54
38	2g	153/156 (98%)	132 (86%)	19 (12%)	2 (1%)	12	37
39	1h	135/138 (98%)	128 (95%)	7 (5%)	0	100	100
39	2h	135/138 (98%)	130 (96%)	3 (2%)	2 (2%)	10	34
40	1i	125/128 (98%)	110 (88%)	14 (11%)	1 (1%)	19	51
40	2i	125/128 (98%)	110 (88%)	13 (10%)	2 (2%)	9	32
41	1j	95/105 (90%)	80 (84%)	8 (8%)	7 (7%)	1	2
41	2j	94/105 (90%)	79 (84%)	13 (14%)	2 (2%)	7	26
42	1k	112/129 (87%)	100 (89%)	10 (9%)	2 (2%)	8	29
42	2k	112/129 (87%)	101 (90%)	9 (8%)	2 (2%)	8	29
43	1l	120/132 (91%)	115 (96%)	4 (3%)	1 (1%)	19	51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	2l	120/132 (91%)	113 (94%)	7 (6%)	0	100	100
44	1m	116/126 (92%)	103 (89%)	9 (8%)	4 (3%)	3	15
44	2m	114/126 (90%)	101 (89%)	11 (10%)	2 (2%)	8	29
45	1n	58/61 (95%)	53 (91%)	4 (7%)	1 (2%)	9	31
45	2n	58/61 (95%)	52 (90%)	6 (10%)	0	100	100
46	1o	86/89 (97%)	82 (95%)	4 (5%)	0	100	100
46	2o	86/89 (97%)	82 (95%)	4 (5%)	0	100	100
47	1p	80/88 (91%)	70 (88%)	9 (11%)	1 (1%)	12	37
47	2p	80/88 (91%)	69 (86%)	11 (14%)	0	100	100
48	1q	97/105 (92%)	89 (92%)	7 (7%)	1 (1%)	15	45
48	2q	97/105 (92%)	91 (94%)	6 (6%)	0	100	100
49	1r	66/88 (75%)	59 (89%)	5 (8%)	2 (3%)	4	17
49	2r	66/88 (75%)	60 (91%)	5 (8%)	1 (2%)	10	34
50	1s	82/93 (88%)	72 (88%)	10 (12%)	0	100	100
50	2s	81/93 (87%)	69 (85%)	12 (15%)	0	100	100
51	1t	94/106 (89%)	79 (84%)	12 (13%)	3 (3%)	4	16
51	2t	94/106 (89%)	82 (87%)	8 (8%)	4 (4%)	2	10
52	1u	21/27 (78%)	18 (86%)	3 (14%)	0	100	100
52	2u	21/27 (78%)	18 (86%)	3 (14%)	0	100	100
55	1z	10/15 (67%)	9 (90%)	1 (10%)	0	100	100
55	2z	11/15 (73%)	7 (64%)	3 (27%)	1 (9%)	1	1
All	All	11431/12158 (94%)	10499 (92%)	791 (7%)	141 (1%)	13	40

All (141) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	1F	130	ALA
6	1G	51	ARG
6	1G	126	ASP
7	1H	126	PRO
14	1S	60	GLY
19	1X	94	GLY
26	14	50	VAL
26	14	53	GLU
26	14	59	PHE

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Mol	Chain	Res	Type
26	14	68	ARG
33	1b	17	PHE
33	1b	125	PRO
33	1b	128	GLU
34	1c	107	GLN
35	1d	32	ALA
36	1e	73	ASN
40	1i	54	ASP
41	1j	55	LYS
41	1j	56	HIS
43	1l	29	GLY
44	1m	4	ILE
45	1n	3	ARG
51	1t	95	ALA
3	2D	125	ILE
5	2F	130	ALA
6	2G	14	GLU
6	2G	47	LYS
6	2G	51	ARG
6	2G	81	LYS
7	2H	55	PRO
7	2H	126	PRO
8	2I	10	GLU
12	2Q	28	ALA
17	2V	79	VAL
19	2X	94	GLY
21	2Z	128	VAL
26	24	47	GLN
26	24	50	VAL
26	24	63	TYR
29	27	46	VAL
33	2b	17	PHE
33	2b	121	LEU
33	2b	124	SER
36	2e	37	ARG
36	2e	73	ASN
51	2t	95	ALA
51	2t	99	LEU
55	2z	10	PRO
6	1G	47	LYS
7	1H	92	ILE
8	1I	106	GLY

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Mol	Chain	Res	Type
17	1V	79	VAL
22	10	13	GLY
26	14	45	GLY
26	14	49	PHE
33	1b	165	VAL
34	1c	127	ARG
42	1k	49	GLY
44	1m	5	ALA
51	1t	47	GLY
26	24	45	GLY
26	24	54	GLY
33	2b	20	GLU
33	2b	93	VAL
33	2b	126	GLU
33	2b	165	VAL
34	2c	66	VAL
35	2d	20	TYR
41	2j	78	ASN
4	1E	52	LEU
8	1I	73	GLU
10	1O	5	GLN
11	1P	122	PRO
26	14	48	ARG
33	1b	231	GLU
35	1d	9	CYS
35	1d	136	PRO
38	1g	4	ARG
41	1j	78	ASN
44	1m	21	TYR
6	2G	126	ASP
9	2N	2	LYS
35	2d	136	PRO
40	2i	39	GLY
40	2i	54	ASP
44	2m	106	ASN
49	2r	36	ASN
20	1Y	54	LYS
36	1e	72	GLN
41	1j	32	ALA
48	1q	68	ARG
4	2E	52	LEU
5	2F	18	ARG

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Mol	Chain	Res	Type
10	2O	5	GLN
33	2b	125	PRO
33	2b	151	GLY
35	2d	46	LYS
36	2e	69	VAL
44	2m	21	TYR
20	1Y	53	PRO
34	1c	66	VAL
36	1e	69	VAL
36	1e	98	THR
47	1p	16	HIS
51	1t	100	ILE
3	2D	3	VAL
11	2P	29	LYS
11	2P	122	PRO
14	2S	84	GLN
34	2c	108	ASN
38	2g	4	ARG
38	2g	54	THR
39	2h	73	ASP
39	2h	133	LEU
42	2k	49	GLY
51	2t	47	GLY
5	1F	18	ARG
8	1I	105	HIS
8	1I	107	VAL
26	14	47	GLN
33	1b	22	LYS
34	1c	126	ARG
41	1j	51	ARG
44	1m	67	GLU
49	1r	25	THR
49	1r	36	ASN
21	2Z	135	GLU
29	27	45	ALA
41	2j	56	HIS
26	14	54	GLY
42	1k	105	VAL
33	1b	230	VAL
35	1d	8	VAL
41	1j	77	PRO
42	2k	105	VAL

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Mol	Chain	Res	Type
51	2t	100	ILE
36	1e	85	GLY
33	1b	227	GLY
35	1d	5	ILE
41	1j	75	ILE
36	2e	96	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	1D	215/218 (99%)	196 (91%)	19 (9%)	10 30
3	2D	216/218 (99%)	190 (88%)	26 (12%)	5 15
4	1E	164/166 (99%)	149 (91%)	15 (9%)	9 28
4	2E	164/166 (99%)	147 (90%)	17 (10%)	7 21
5	1F	160/166 (96%)	144 (90%)	16 (10%)	7 23
5	2F	159/166 (96%)	146 (92%)	13 (8%)	11 32
6	1G	143/156 (92%)	129 (90%)	14 (10%)	8 24
6	2G	142/156 (91%)	125 (88%)	17 (12%)	5 15
7	1H	144/148 (97%)	133 (92%)	11 (8%)	13 36
7	2H	144/148 (97%)	132 (92%)	12 (8%)	11 32
8	1I	110/124 (89%)	93 (84%)	17 (16%)	2 8
8	2I	104/124 (84%)	95 (91%)	9 (9%)	10 30
9	1N	118/119 (99%)	106 (90%)	12 (10%)	7 22
9	2N	118/119 (99%)	107 (91%)	11 (9%)	9 27
10	1O	100/100 (100%)	97 (97%)	3 (3%)	41 75
10	2O	100/100 (100%)	97 (97%)	3 (3%)	41 75
11	1P	116/116 (100%)	103 (89%)	13 (11%)	6 18
11	2P	115/116 (99%)	102 (89%)	13 (11%)	6 18
12	1Q	111/111 (100%)	103 (93%)	8 (7%)	14 39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	2Q	111/111 (100%)	104 (94%)	7 (6%)	18	46
13	1R	101/101 (100%)	86 (85%)	15 (15%)	3	9
13	2R	101/101 (100%)	85 (84%)	16 (16%)	2	8
14	1S	87/88 (99%)	79 (91%)	8 (9%)	9	27
14	2S	85/88 (97%)	75 (88%)	10 (12%)	5	16
15	1T	115/127 (91%)	108 (94%)	7 (6%)	18	48
15	2T	113/127 (89%)	111 (98%)	2 (2%)	59	85
16	1U	93/94 (99%)	87 (94%)	6 (6%)	17	45
16	2U	93/94 (99%)	88 (95%)	5 (5%)	22	54
17	1V	80/82 (98%)	70 (88%)	10 (12%)	4	14
17	2V	80/82 (98%)	73 (91%)	7 (9%)	10	30
18	1W	90/92 (98%)	84 (93%)	6 (7%)	16	43
18	2W	90/92 (98%)	85 (94%)	5 (6%)	21	52
19	1X	77/78 (99%)	74 (96%)	3 (4%)	32	66
19	2X	77/78 (99%)	75 (97%)	2 (3%)	46	77
20	1Y	85/91 (93%)	79 (93%)	6 (7%)	14	40
20	2Y	85/91 (93%)	81 (95%)	4 (5%)	26	59
21	1Z	159/179 (89%)	146 (92%)	13 (8%)	11	32
21	2Z	156/179 (87%)	144 (92%)	12 (8%)	13	35
22	10	60/67 (90%)	55 (92%)	5 (8%)	11	32
22	20	60/67 (90%)	56 (93%)	4 (7%)	16	43
23	11	80/83 (96%)	76 (95%)	4 (5%)	24	57
23	21	80/83 (96%)	76 (95%)	4 (5%)	24	57
24	12	65/67 (97%)	61 (94%)	4 (6%)	18	47
24	22	65/67 (97%)	60 (92%)	5 (8%)	13	35
25	13	51/52 (98%)	47 (92%)	4 (8%)	12	34
25	23	50/52 (96%)	46 (92%)	4 (8%)	12	33
26	14	60/63 (95%)	52 (87%)	8 (13%)	4	11
26	24	53/63 (84%)	45 (85%)	8 (15%)	3	9
27	15	50/52 (96%)	46 (92%)	4 (8%)	12	33
27	25	50/52 (96%)	47 (94%)	3 (6%)	19	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	16	51/52 (98%)	48 (94%)	3 (6%)	19	49
28	26	50/52 (96%)	47 (94%)	3 (6%)	19	49
29	17	41/42 (98%)	36 (88%)	5 (12%)	5	15
29	27	41/42 (98%)	39 (95%)	2 (5%)	25	57
30	18	54/55 (98%)	50 (93%)	4 (7%)	13	38
30	28	54/55 (98%)	50 (93%)	4 (7%)	13	38
31	19	34/34 (100%)	33 (97%)	1 (3%)	42	76
31	29	34/34 (100%)	33 (97%)	1 (3%)	42	76
33	1b	177/220 (80%)	149 (84%)	28 (16%)	2	8
33	2b	158/220 (72%)	137 (87%)	21 (13%)	4	11
34	1c	127/188 (68%)	117 (92%)	10 (8%)	12	34
34	2c	108/188 (57%)	91 (84%)	17 (16%)	2	8
35	1d	161/181 (89%)	144 (89%)	17 (11%)	6	20
35	2d	164/181 (91%)	145 (88%)	19 (12%)	5	16
36	1e	113/123 (92%)	103 (91%)	10 (9%)	10	30
36	2e	106/123 (86%)	94 (89%)	12 (11%)	6	18
37	1f	83/90 (92%)	77 (93%)	6 (7%)	14	39
37	2f	86/90 (96%)	83 (96%)	3 (4%)	36	70
38	1g	111/127 (87%)	101 (91%)	10 (9%)	9	29
38	2g	107/127 (84%)	98 (92%)	9 (8%)	11	31
39	1h	114/119 (96%)	103 (90%)	11 (10%)	8	25
39	2h	111/119 (93%)	99 (89%)	12 (11%)	6	20
40	1i	89/99 (90%)	78 (88%)	11 (12%)	4	14
40	2i	80/99 (81%)	66 (82%)	14 (18%)	2	6
41	1j	60/92 (65%)	55 (92%)	5 (8%)	11	32
41	2j	62/92 (67%)	53 (86%)	9 (14%)	3	9
42	1k	82/99 (83%)	77 (94%)	5 (6%)	18	48
42	2k	82/99 (83%)	77 (94%)	5 (6%)	18	48
43	1l	95/109 (87%)	90 (95%)	5 (5%)	22	54
43	2l	94/109 (86%)	90 (96%)	4 (4%)	29	62
44	1m	90/101 (89%)	80 (89%)	10 (11%)	6	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
44	2m	87/101 (86%)	77 (88%)	10 (12%)	5	17
45	1n	47/50 (94%)	42 (89%)	5 (11%)	6	20
45	2n	43/50 (86%)	36 (84%)	7 (16%)	2	7
46	1o	75/80 (94%)	67 (89%)	8 (11%)	6	20
46	2o	78/80 (98%)	69 (88%)	9 (12%)	5	17
47	1p	67/74 (90%)	56 (84%)	11 (16%)	2	7
47	2p	68/74 (92%)	59 (87%)	9 (13%)	4	12
48	1q	91/97 (94%)	85 (93%)	6 (7%)	16	44
48	2q	94/97 (97%)	92 (98%)	2 (2%)	53	81
49	1r	59/77 (77%)	53 (90%)	6 (10%)	7	22
49	2r	59/77 (77%)	53 (90%)	6 (10%)	7	22
50	1s	65/80 (81%)	57 (88%)	8 (12%)	4	14
50	2s	67/80 (84%)	59 (88%)	8 (12%)	5	15
51	1t	66/82 (80%)	57 (86%)	9 (14%)	3	11
51	2t	71/82 (87%)	66 (93%)	5 (7%)	15	41
52	1u	16/22 (73%)	15 (94%)	1 (6%)	18	46
52	2u	18/22 (82%)	16 (89%)	2 (11%)	6	19
55	1z	12/15 (80%)	12 (100%)	0	100	100
55	2z	13/15 (87%)	13 (100%)	0	100	100
All	All	9160/10096 (91%)	8322 (91%)	838 (9%)	9	28

All (838) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	1D	13	ARG
3	1D	54	ARG
3	1D	61	LEU
3	1D	69	ARG
3	1D	71	ASP
3	1D	94	LEU
3	1D	99	ASP
3	1D	103	ARG
3	1D	111	LEU
3	1D	142	VAL
3	1D	155	LEU

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Mol	Chain	Res	Type
3	1D	193	VAL
3	1D	206	LEU
3	1D	211	ARG
3	1D	217	ARG
3	1D	229	VAL
3	1D	242	ARG
3	1D	257	LEU
3	1D	260	ARG
4	1E	7	VAL
4	1E	21	VAL
4	1E	54	GLN
4	1E	75	VAL
4	1E	79	ARG
4	1E	82	ARG
4	1E	111	ARG
4	1E	116	VAL
4	1E	119	ARG
4	1E	144	ARG
4	1E	163	GLU
4	1E	175	VAL
4	1E	181	LEU
4	1E	184	VAL
4	1E	195	LEU
5	1F	20	LEU
5	1F	33	LEU
5	1F	38	ARG
5	1F	57	VAL
5	1F	74	ARG
5	1F	106	ARG
5	1F	110	LEU
5	1F	125	LEU
5	1F	162	LEU
5	1F	170	LEU
5	1F	183	VAL
5	1F	191	ARG
5	1F	192	LEU
5	1F	195	ASP
5	1F	197	ASP
5	1F	201	VAL
6	1G	3	LEU
6	1G	7	LEU
6	1G	43	LEU

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Mol	Chain	Res	Type
6	1G	45	GLU
6	1G	82	LEU
6	1G	140	ILE
6	1G	143	GLU
6	1G	148	MET
6	1G	159	VAL
6	1G	161	THR
6	1G	162	THR
6	1G	165	THR
6	1G	170	ARG
6	1G	174	GLU
7	1H	3	ARG
7	1H	13	LYS
7	1H	33	LEU
7	1H	45	VAL
7	1H	59	ARG
7	1H	69	ARG
7	1H	71	LEU
7	1H	84	SER
7	1H	98	LEU
7	1H	101	ARG
7	1H	139	GLN
8	1I	9	LEU
8	1I	10	GLU
8	1I	12	LEU
8	1I	42	SER
8	1I	47	LEU
8	1I	57	ARG
8	1I	60	GLU
8	1I	66	GLU
8	1I	68	LEU
8	1I	74	ASN
8	1I	75	LEU
8	1I	77	LEU
8	1I	101	LEU
8	1I	103	ARG
8	1I	109	ILE
8	1I	140	LEU
8	1I	142	VAL
9	1N	8	GLN
9	1N	28	THR
9	1N	33	LEU

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Mol	Chain	Res	Type
9	1N	34	LEU
9	1N	46	VAL
9	1N	48	MET
9	1N	61	ARG
9	1N	67	LEU
9	1N	73	THR
9	1N	87	LEU
9	1N	120	LEU
9	1N	137	LYS
10	1O	18	LYS
10	1O	24	VAL
10	1O	105	GLU
11	1P	3	LEU
11	1P	55	ARG
11	1P	56	SER
11	1P	59	LEU
11	1P	70	GLN
11	1P	76	LYS
11	1P	98	GLU
11	1P	99	LEU
11	1P	106	LEU
11	1P	112	LEU
11	1P	125	VAL
11	1P	136	GLU
11	1P	148	LEU
12	1Q	1	MET
12	1Q	6	ARG
12	1Q	8	LYS
12	1Q	16	ARG
12	1Q	35	VAL
12	1Q	45	GLN
12	1Q	59	ARG
12	1Q	60	ARG
13	1R	6	SER
13	1R	18	LEU
13	1R	24	GLN
13	1R	28	LEU
13	1R	29	LEU
13	1R	33	ARG
13	1R	36	THR
13	1R	44	LEU
13	1R	54	LEU

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Mol	Chain	Res	Type
13	1R	67	LEU
13	1R	75	LEU
13	1R	79	LEU
13	1R	91	GLN
13	1R	100	LEU
13	1R	111	LEU
14	1S	3	ARG
14	1S	4	LEU
14	1S	20	ARG
14	1S	36	TYR
14	1S	49	VAL
14	1S	59	LYS
14	1S	61	ASN
14	1S	85	VAL
15	1T	49	VAL
15	1T	89	VAL
15	1T	93	ARG
15	1T	96	ARG
15	1T	108	ARG
15	1T	118	ARG
15	1T	128	GLU
16	1U	8	VAL
16	1U	36	ARG
16	1U	74	LEU
16	1U	77	SER
16	1U	92	ARG
16	1U	104	GLN
17	1V	18	LEU
17	1V	35	LEU
17	1V	43	GLU
17	1V	46	VAL
17	1V	51	VAL
17	1V	52	VAL
17	1V	61	VAL
17	1V	62	LEU
17	1V	72	VAL
17	1V	79	VAL
18	1W	11	ARG
18	1W	17	VAL
18	1W	23	LEU
18	1W	60	ASN
18	1W	67	ASP

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Mol	Chain	Res	Type
18	1W	107	LEU
19	1X	52	VAL
19	1X	57	LEU
19	1X	88	LYS
20	1Y	1	MET
20	1Y	2	ARG
20	1Y	23	ARG
20	1Y	26	LYS
20	1Y	43	ASN
20	1Y	99	CYS
21	1Z	6	LYS
21	1Z	11	GLU
21	1Z	33	LEU
21	1Z	42	VAL
21	1Z	86	VAL
21	1Z	91	LEU
21	1Z	107	THR
21	1Z	129	SER
21	1Z	150	LEU
21	1Z	154	ASP
21	1Z	155	LEU
21	1Z	162	GLU
21	1Z	170	THR
22	10	10	THR
22	10	20	ARG
22	10	43	THR
22	10	49	LYS
22	10	55	ARG
23	11	21	ARG
23	11	40	ARG
23	11	59	THR
23	11	95	LEU
24	12	32	LEU
24	12	34	GLU
24	12	53	LEU
24	12	70	GLN
25	13	8	LEU
25	13	23	LEU
25	13	54	VAL
25	13	60	GLU
26	14	14	ILE
26	14	34	GLU

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Mol	Chain	Res	Type
26	14	37	SER
26	14	49	PHE
26	14	56	VAL
26	14	58	ARG
26	14	60	GLN
26	14	63	TYR
27	15	16	ARG
27	15	29	THR
27	15	40	LYS
27	15	58	LEU
28	16	6	ARG
28	16	14	THR
28	16	48	VAL
29	17	1	MET
29	17	9	ARG
29	17	24	THR
29	17	43	THR
29	17	46	VAL
30	18	31	HIS
30	18	32	LEU
30	18	34	TRP
30	18	46	ARG
31	19	26	ILE
33	1b	8	LYS
33	1b	10	LEU
33	1b	11	LEU
33	1b	16	HIS
33	1b	17	PHE
33	1b	21	ARG
33	1b	67	THR
33	1b	76	GLN
33	1b	80	ILE
33	1b	84	GLU
33	1b	86	GLU
33	1b	93	VAL
33	1b	112	VAL
33	1b	116	GLU
33	1b	127	ILE
33	1b	144	ARG
33	1b	153	ARG
33	1b	156	LYS
33	1b	169	LYS

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Mol	Chain	Res	Type
33	1b	170	GLU
33	1b	185	ILE
33	1b	187	LEU
33	1b	190	THR
33	1b	215	LEU
33	1b	219	VAL
33	1b	221	LEU
33	1b	226	ARG
33	1b	230	VAL
34	1c	15	THR
34	1c	17	ASP
34	1c	29	TYR
34	1c	46	GLU
34	1c	47	LEU
34	1c	49	SER
34	1c	52	LEU
34	1c	64	VAL
34	1c	115	LEU
34	1c	195	VAL
35	1d	5	ILE
35	1d	15	GLU
35	1d	28	SER
35	1d	31	CYS
35	1d	45	GLN
35	1d	49	ARG
35	1d	66	ARG
35	1d	101	LEU
35	1d	107	ARG
35	1d	150	GLU
35	1d	158	ILE
35	1d	162	LEU
35	1d	168	ARG
35	1d	181	MET
35	1d	188	LEU
35	1d	194	LEU
35	1d	196	LEU
36	1e	31	LEU
36	1e	40	ARG
36	1e	41	VAL
36	1e	47	LYS
36	1e	51	VAL
36	1e	73	ASN

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Mol	Chain	Res	Type
36	1e	78	HIS
36	1e	79	GLU
36	1e	91	LEU
36	1e	147	ASP
37	1f	46	ARG
37	1f	55	ASP
37	1f	65	VAL
37	1f	74	ASP
37	1f	75	LEU
37	1f	89	MET
38	1g	13	GLN
38	1g	15	ASP
38	1g	21	VAL
38	1g	22	LEU
38	1g	50	ILE
38	1g	56	GLN
38	1g	113	GLU
38	1g	114	ARG
38	1g	131	LYS
38	1g	138	LYS
39	1h	2	LEU
39	1h	21	LYS
39	1h	25	ASP
39	1h	52	ASP
39	1h	54	ASP
39	1h	60	ARG
39	1h	75	ARG
39	1h	78	GLN
39	1h	91	ARG
39	1h	98	LYS
39	1h	112	LEU
40	1i	23	ASN
40	1i	42	ARG
40	1i	50	LEU
40	1i	65	VAL
40	1i	75	ASP
40	1i	81	ILE
40	1i	92	TYR
40	1i	102	LEU
40	1i	113	LYS
40	1i	127	LYS
40	1i	128	ARG

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Mol	Chain	Res	Type
41	1j	30	SER
41	1j	34	VAL
41	1j	43	ARG
41	1j	85	LEU
41	1j	92	THR
42	1k	14	VAL
42	1k	31	THR
42	1k	48	ILE
42	1k	84	VAL
42	1k	109	VAL
43	1l	27	LEU
43	1l	33	ARG
43	1l	41	ARG
43	1l	54	LYS
43	1l	67	THR
44	1m	3	ARG
44	1m	4	ILE
44	1m	19	LEU
44	1m	20	THR
44	1m	44	ARG
44	1m	49	THR
44	1m	56	LEU
44	1m	70	LEU
44	1m	102	ARG
44	1m	110	ARG
45	1n	6	LEU
45	1n	8	GLU
45	1n	18	VAL
45	1n	22	THR
45	1n	33	VAL
46	1o	3	ILE
46	1o	5	LYS
46	1o	17	ARG
46	1o	22	THR
46	1o	26	GLU
46	1o	38	ARG
46	1o	39	LEU
46	1o	71	GLN
47	1p	1	MET
47	1p	2	VAL
47	1p	5	ARG
47	1p	11	SER

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Mol	Chain	Res	Type
47	1p	16	HIS
47	1p	19	ILE
47	1p	20	VAL
47	1p	25	ARG
47	1p	45	THR
47	1p	62	VAL
47	1p	67	THR
48	1q	68	ARG
48	1q	74	LEU
48	1q	78	GLU
48	1q	82	MET
48	1q	89	LEU
48	1q	98	LEU
49	1r	26	LEU
49	1r	32	ARG
49	1r	38	GLU
49	1r	54	ARG
49	1r	68	LYS
49	1r	76	LEU
50	1s	3	ARG
50	1s	5	LEU
50	1s	22	LEU
50	1s	28	LYS
50	1s	37	ARG
50	1s	63	THR
50	1s	65	ASN
50	1s	81	ARG
51	1t	9	ASN
51	1t	10	LEU
51	1t	24	LEU
51	1t	30	LYS
51	1t	45	GLN
51	1t	60	GLU
51	1t	62	LEU
51	1t	86	ARG
51	1t	90	GLN
52	1u	15	ARG
3	2D	14	ARG
3	2D	38	LYS
3	2D	54	ARG
3	2D	61	LEU
3	2D	71	ASP

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Mol	Chain	Res	Type
3	2D	94	LEU
3	2D	106	ILE
3	2D	111	LEU
3	2D	113	VAL
3	2D	134	ARG
3	2D	138	VAL
3	2D	141	VAL
3	2D	142	VAL
3	2D	155	LEU
3	2D	183	ARG
3	2D	192	THR
3	2D	193	VAL
3	2D	211	ARG
3	2D	217	ARG
3	2D	229	VAL
3	2D	242	ARG
3	2D	257	LEU
3	2D	260	ARG
3	2D	262	ARG
3	2D	274	ARG
3	2D	276	LYS
4	2E	7	VAL
4	2E	12	THR
4	2E	21	VAL
4	2E	24	THR
4	2E	49	LEU
4	2E	52	LEU
4	2E	75	VAL
4	2E	77	ILE
4	2E	82	ARG
4	2E	116	VAL
4	2E	119	ARG
4	2E	144	ARG
4	2E	163	GLU
4	2E	175	VAL
4	2E	181	LEU
4	2E	184	VAL
4	2E	202	LYS
5	2F	20	LEU
5	2F	24	LEU
5	2F	27	GLU
5	2F	33	LEU

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Mol	Chain	Res	Type
5	2F	57	VAL
5	2F	74	ARG
5	2F	106	ARG
5	2F	162	LEU
5	2F	183	VAL
5	2F	192	LEU
5	2F	196	LEU
5	2F	197	ASP
5	2F	201	VAL
6	2G	4	ASP
6	2G	28	VAL
6	2G	33	ARG
6	2G	43	LEU
6	2G	45	GLU
6	2G	60	LEU
6	2G	111	LEU
6	2G	113	ARG
6	2G	136	ARG
6	2G	140	ILE
6	2G	143	GLU
6	2G	145	THR
6	2G	148	MET
6	2G	159	VAL
6	2G	162	THR
6	2G	170	ARG
6	2G	181	ARG
7	2H	3	ARG
7	2H	32	GLU
7	2H	33	LEU
7	2H	42	ARG
7	2H	49	VAL
7	2H	69	ARG
7	2H	71	LEU
7	2H	84	SER
7	2H	98	LEU
7	2H	106	THR
7	2H	139	GLN
7	2H	171	LEU
8	2I	43	ASN
8	2I	61	ARG
8	2I	75	LEU
8	2I	77	LEU

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Mol	Chain	Res	Type
8	2I	101	LEU
8	2I	116	LEU
8	2I	121	LYS
8	2I	140	LEU
8	2I	142	VAL
9	2N	5	VAL
9	2N	33	LEU
9	2N	34	LEU
9	2N	46	VAL
9	2N	48	MET
9	2N	62	VAL
9	2N	73	THR
9	2N	87	LEU
9	2N	120	LEU
9	2N	137	LYS
9	2N	138	LEU
10	2O	24	VAL
10	2O	69	ILE
10	2O	94	ARG
11	2P	3	LEU
11	2P	45	LEU
11	2P	55	ARG
11	2P	56	SER
11	2P	59	LEU
11	2P	65	ARG
11	2P	95	VAL
11	2P	96	THR
11	2P	102	ARG
11	2P	112	LEU
11	2P	121	LYS
11	2P	125	VAL
11	2P	148	LEU
12	2Q	1	MET
12	2Q	21	THR
12	2Q	35	VAL
12	2Q	45	GLN
12	2Q	106	VAL
12	2Q	109	VAL
12	2Q	110	THR
13	2R	1	MET
13	2R	6	SER
13	2R	18	LEU

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Mol	Chain	Res	Type
13	2R	24	GLN
13	2R	28	LEU
13	2R	29	LEU
13	2R	44	LEU
13	2R	54	LEU
13	2R	65	LEU
13	2R	75	LEU
13	2R	79	LEU
13	2R	82	GLU
13	2R	86	ARG
13	2R	100	LEU
13	2R	102	GLU
13	2R	111	LEU
14	2S	14	VAL
14	2S	23	ARG
14	2S	36	TYR
14	2S	44	LYS
14	2S	58	LEU
14	2S	63	THR
14	2S	75	GLU
14	2S	80	LEU
14	2S	83	LYS
14	2S	85	VAL
15	2T	89	VAL
15	2T	96	ARG
16	2U	5	LYS
16	2U	36	ARG
16	2U	52	ARG
16	2U	74	LEU
16	2U	104	GLN
17	2V	18	LEU
17	2V	21	ARG
17	2V	35	LEU
17	2V	52	VAL
17	2V	62	LEU
17	2V	72	VAL
17	2V	79	VAL
18	2W	11	ARG
18	2W	17	VAL
18	2W	23	LEU
18	2W	92	ARG
18	2W	107	LEU

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Mol	Chain	Res	Type
19	2X	57	LEU
19	2X	92	LEU
20	2Y	43	ASN
20	2Y	44	ILE
20	2Y	90	LEU
20	2Y	99	CYS
21	2Z	18	LEU
21	2Z	33	LEU
21	2Z	61	LEU
21	2Z	73	GLN
21	2Z	86	VAL
21	2Z	107	THR
21	2Z	131	ARG
21	2Z	135	GLU
21	2Z	136	PHE
21	2Z	154	ASP
21	2Z	155	LEU
21	2Z	161	VAL
22	20	10	THR
22	20	20	ARG
22	20	55	ARG
22	20	82	ARG
23	21	21	ARG
23	21	35	THR
23	21	40	ARG
23	21	95	LEU
24	22	30	ARG
24	22	32	LEU
24	22	34	GLU
24	22	53	LEU
24	22	70	GLN
25	23	8	LEU
25	23	40	THR
25	23	54	VAL
25	23	56	VAL
26	24	1	MET
26	24	14	ILE
26	24	53	GLU
26	24	58	ARG
26	24	61	ARG
26	24	62	ARG
26	24	63	TYR

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Mol	Chain	Res	Type
26	24	69	LYS
27	25	16	ARG
27	25	29	THR
27	25	40	LYS
28	26	6	ARG
28	26	14	THR
28	26	48	VAL
29	27	43	THR
29	27	46	VAL
30	28	30	ARG
30	28	31	HIS
30	28	34	TRP
30	28	37	SER
31	29	26	ILE
33	2b	8	LYS
33	2b	10	LEU
33	2b	24	TRP
33	2b	60	ASP
33	2b	63	MET
33	2b	67	THR
33	2b	90	MET
33	2b	93	VAL
33	2b	118	LEU
33	2b	138	LEU
33	2b	152	PHE
33	2b	153	ARG
33	2b	154	LEU
33	2b	160	ASP
33	2b	165	VAL
33	2b	170	GLU
33	2b	179	LYS
33	2b	185	ILE
33	2b	187	LEU
33	2b	222	ILE
33	2b	224	GLN
34	2c	3	ASN
34	2c	5	ILE
34	2c	14	ILE
34	2c	15	THR
34	2c	17	ASP
34	2c	28	GLN
34	2c	29	TYR

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Mol	Chain	Res	Type
34	2c	47	LEU
34	2c	52	LEU
34	2c	58	GLU
34	2c	64	VAL
34	2c	70	VAL
34	2c	125	GLU
34	2c	128	PHE
34	2c	131	ARG
34	2c	164	ARG
34	2c	178	LEU
35	2d	3	ARG
35	2d	5	ILE
35	2d	25	ARG
35	2d	26	CYS
35	2d	31	CYS
35	2d	34	GLU
35	2d	38	TYR
35	2d	47	ARG
35	2d	58	LEU
35	2d	66	ARG
35	2d	96	LEU
35	2d	101	LEU
35	2d	132	ARG
35	2d	135	LEU
35	2d	145	GLU
35	2d	170	VAL
35	2d	187	ARG
35	2d	194	LEU
35	2d	201	GLN
36	2e	14	ARG
36	2e	27	ARG
36	2e	34	VAL
36	2e	41	VAL
36	2e	47	LYS
36	2e	50	GLU
36	2e	51	VAL
36	2e	71	LEU
36	2e	78	HIS
36	2e	91	LEU
36	2e	115	VAL
36	2e	147	ASP
37	2f	28	ARG

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Mol	Chain	Res	Type
37	2f	65	VAL
37	2f	75	LEU
38	2g	45	ASP
38	2g	57	GLU
38	2g	63	LYS
38	2g	72	ARG
38	2g	97	GLN
38	2g	104	LEU
38	2g	113	GLU
38	2g	120	ILE
38	2g	154	TYR
39	2h	25	ASP
39	2h	51	VAL
39	2h	52	ASP
39	2h	60	ARG
39	2h	63	LEU
39	2h	78	GLN
39	2h	91	ARG
39	2h	111	ILE
39	2h	112	LEU
39	2h	115	SER
39	2h	120	THR
39	2h	125	ARG
40	2i	3	GLN
40	2i	23	ASN
40	2i	33	PHE
40	2i	38	GLN
40	2i	50	LEU
40	2i	65	VAL
40	2i	81	ILE
40	2i	89	ASN
40	2i	92	TYR
40	2i	102	LEU
40	2i	104	ARG
40	2i	107	ARG
40	2i	114	TYR
40	2i	124	GLN
41	2j	8	LEU
41	2j	16	LEU
41	2j	21	GLN
41	2j	25	GLU
41	2j	34	VAL

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Mol	Chain	Res	Type
41	2j	48	THR
41	2j	68	HIS
41	2j	81	THR
41	2j	94	VAL
42	2k	14	VAL
42	2k	18	ARG
42	2k	70	LYS
42	2k	75	TYR
42	2k	126	ARG
43	2l	23	LYS
43	2l	33	ARG
43	2l	53	ARG
43	2l	55	VAL
44	2m	3	ARG
44	2m	40	ASN
44	2m	49	THR
44	2m	70	LEU
44	2m	81	LEU
44	2m	82	MET
44	2m	90	LEU
44	2m	102	ARG
44	2m	106	ASN
44	2m	110	ARG
45	2n	11	LYS
45	2n	17	LYS
45	2n	22	THR
45	2n	29	ARG
45	2n	33	VAL
45	2n	41	ARG
45	2n	53	LEU
46	2o	3	ILE
46	2o	5	LYS
46	2o	10	LYS
46	2o	22	THR
46	2o	24	SER
46	2o	26	GLU
46	2o	39	LEU
46	2o	41	GLU
46	2o	83	GLU
47	2p	1	MET
47	2p	2	VAL
47	2p	5	ARG

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Mol	Chain	Res	Type
47	2p	16	HIS
47	2p	45	THR
47	2p	60	LEU
47	2p	62	VAL
47	2p	67	THR
47	2p	72	ARG
48	2q	63	ARG
48	2q	74	LEU
49	2r	26	LEU
49	2r	32	ARG
49	2r	38	GLU
49	2r	68	LYS
49	2r	76	LEU
49	2r	82	THR
50	2s	3	ARG
50	2s	28	LYS
50	2s	34	TRP
50	2s	41	VAL
50	2s	48	THR
50	2s	63	THR
50	2s	65	ASN
50	2s	83	HIS
51	2t	10	LEU
51	2t	24	LEU
51	2t	62	LEU
51	2t	71	THR
51	2t	99	LEU
52	2u	15	ARG
52	2u	22	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (143) such sidechains are listed below:

Mol	Chain	Res	Type
3	1D	87	ASN
3	1D	164	GLN
3	1D	253	GLN
4	1E	54	GLN
5	1F	8	GLN
5	1F	69	HIS
5	1F	169	ASN
5	1F	203	GLN
5	1F	204	ASN

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Mol	Chain	Res	Type
6	1G	40	ASN
8	1I	43	ASN
8	1I	105	HIS
8	1I	139	GLN
9	1N	8	GLN
9	1N	133	GLN
11	1P	38	GLN
11	1P	70	GLN
12	1Q	45	GLN
13	1R	24	GLN
13	1R	71	GLN
13	1R	91	GLN
14	1S	95	HIS
15	1T	123	GLN
16	1U	81	HIS
16	1U	94	ASN
16	1U	104	GLN
19	1X	31	HIS
20	1Y	6	HIS
20	1Y	43	ASN
20	1Y	92	ASN
21	1Z	73	GLN
21	1Z	151	HIS
24	12	70	GLN
26	14	46	GLN
26	14	60	GLN
30	18	35	GLN
31	19	36	GLN
34	1c	170	GLN
35	1d	43	HIS
35	1d	123	HIS
35	1d	201	GLN
36	1e	141	GLN
37	1f	100	ASN
38	1g	11	GLN
38	1g	56	GLN
38	1g	86	GLN
40	1i	23	ASN
40	1i	73	GLN
40	1i	89	ASN
40	1i	117	HIS
40	1i	124	GLN

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Mol	Chain	Res	Type
41	1j	56	HIS
42	1k	93	GLN
43	1l	78	GLN
43	1l	99	HIS
44	1m	92	HIS
46	1o	28	GLN
46	1o	62	GLN
47	1p	13	HIS
48	1q	16	GLN
48	1q	26	GLN
50	1s	47	HIS
50	1s	56	GLN
50	1s	65	ASN
50	1s	69	HIS
51	1t	9	ASN
51	1t	45	GLN
3	2D	126	GLN
3	2D	129	ASN
3	2D	164	GLN
3	2D	253	GLN
5	2F	69	HIS
5	2F	169	ASN
5	2F	203	GLN
6	2G	40	ASN
6	2G	130	ASN
6	2G	132	ASN
8	2I	43	ASN
8	2I	105	HIS
11	2P	38	GLN
12	2Q	45	GLN
12	2Q	57	HIS
13	2R	24	GLN
13	2R	71	GLN
14	2S	68	GLN
14	2S	95	HIS
15	2T	123	GLN
16	2U	44	ASN
17	2V	64	HIS
19	2X	31	HIS
19	2X	82	GLN
20	2Y	6	HIS
20	2Y	43	ASN

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Mol	Chain	Res	Type
21	2Z	55	HIS
21	2Z	73	GLN
22	20	50	ASN
25	23	32	GLN
25	23	33	GLN
28	26	32	ASN
31	29	36	GLN
33	2b	16	HIS
33	2b	19	HIS
33	2b	45	GLN
33	2b	78	GLN
33	2b	110	GLN
33	2b	224	GLN
34	2c	6	HIS
34	2c	28	GLN
34	2c	37	GLN
34	2c	102	ASN
34	2c	176	HIS
34	2c	181	ASN
35	2d	123	HIS
35	2d	160	GLN
36	2e	78	HIS
36	2e	141	GLN
37	2f	73	ASN
38	2g	28	ASN
38	2g	86	GLN
38	2g	97	GLN
38	2g	110	GLN
38	2g	148	ASN
39	2h	15	ASN
40	2i	3	GLN
40	2i	58	HIS
40	2i	73	GLN
40	2i	89	ASN
41	2j	13	HIS
41	2j	33	GLN
41	2j	56	HIS
41	2j	62	HIS
42	2k	93	GLN
42	2k	104	GLN
43	2l	75	HIS
43	2l	78	GLN

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Mol	Chain	Res	Type
43	2l	99	HIS
44	2m	77	ASN
44	2m	92	HIS
46	2o	28	GLN
47	2p	16	HIS
50	2s	56	GLN
50	2s	69	HIS
50	2s	83	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2737/2915 (93%)	384 (14%)	19 (0%)
1	2A	2781/2915 (95%)	475 (17%)	25 (0%)
2	1B	119/121 (98%)	9 (7%)	0
2	2B	119/121 (98%)	22 (18%)	2 (1%)
32	1a	1472/1521 (96%)	256 (17%)	0
32	2a	1479/1521 (97%)	268 (18%)	0
53	1v	4/24 (16%)	1 (25%)	0
53	2v	4/24 (16%)	1 (25%)	0
54	1x	75/77 (97%)	18 (24%)	0
54	2x	75/77 (97%)	18 (24%)	0
All	All	8865/9316 (95%)	1452 (16%)	46 (0%)

All (1452) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	11	U
1	1A	33	C
1	1A	35	G
1	1A	44	C
1	1A	61	U
1	1A	62	A
1	1A	69	A
1	1A	72	A
1	1A	73	G
1	1A	82	A
1	1A	91	C
1	1A	115	A
1	1A	116	A
1	1A	117	U

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Mol	Chain	Res	Type
1	1A	122	G
1	1A	128	G
1	1A	148	A
1	1A	170	A
1	1A	176	G
1	1A	184	A
1	1A	187	A
1	1A	193	G
1	1A	203	G
1	1A	204	A
1	1A	210	A
1	1A	211	A
1	1A	216	A
1	1A	217	A
1	1A	221	A
1	1A	236	G
1	1A	262	C
1	1A	268	G
1	1A	270	U
1	1A	271	U
1	1A	272	G
1	1A	273	U
1	1A	285	C
1	1A	287	U
1	1A	288	G
1	1A	294	C
1	1A	295	U
1	1A	302	C
1	1A	334	A
1	1A	347	A
1	1A	352	G
1	1A	353	A
1	1A	365	G
1	1A	375	G
1	1A	386	G
1	1A	398	G
1	1A	406	U
1	1A	412	G
1	1A	422	G
1	1A	431	U
1	1A	433	G
1	1A	437	G

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Mol	Chain	Res	Type
1	1A	438	A
1	1A	454	A
1	1A	467	G
1	1A	468	A
1	1A	469	C
1	1A	473	U
1	1A	476	C
1	1A	482	A
1	1A	495	A
1	1A	500	U
1	1A	506	G
1	1A	528	U
1	1A	529	A
1	1A	533	C
1	1A	554	G
1	1A	555	C
1	1A	556	A
1	1A	557	G
1	1A	572	G
1	1A	585	G
1	1A	595	G
1	1A	597	A
1	1A	608	A
1	1A	614	G
1	1A	615	G
1	1A	625	A
1	1A	626	G
1	1A	629	U
1	1A	638	G
1	1A	640	G
1	1A	658	C
1	1A	661	A
1	1A	669	C
1	1A	670	A
1	1A	682	G
1	1A	696	C
1	1A	697	G
1	1A	715	G
1	1A	732	G
1	1A	744	C
1	1A	763	G
1	1A	776	C

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Mol	Chain	Res	Type
1	1A	803	U
1	1A	821	G
1	1A	822	G
1	1A	828	A
1	1A	830	A
1	1A	831	G
1	1A	835	A
1	1A	836	C
1	1A	838	G
1	1A	848	A
1	1A	851	G
1	1A	858	C
1	1A	873	U
1	1A	874	U
1	1A	905	G
1	1A	912	A
1	1A	925	G
1	1A	931	C
1	1A	932	C
1	1A	933	A
1	1A	934	C
1	1A	935	C
1	1A	936	A
1	1A	938	C
1	1A	941	A
1	1A	944	A
1	1A	955	A
1	1A	976	G
1	1A	985	A
1	1A	989	A
1	1A	990	G
1	1A	1002	U
1	1A	1003	A
1	1A	1005	C
1	1A	1008	C
1	1A	1018	G
1	1A	1019	C
1	1A	1028	A
1	1A	1041	A
1	1A	1057	U
1	1A	1058	C
1	1A	1067	G

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Mol	Chain	Res	Type
1	1A	1071	U
1	1A	1078	U
1	1A	1086	C
1	1A	1090	A
1	1A	1091	A
1	1A	1092	G
1	1A	1150	U
1	1A	1153	U
1	1A	1154	C
1	1A	1156	A
1	1A	1157	G
1	1A	1173	A
1	1A	1174	A
1	1A	1175	U
1	1A	1179	C
1	1A	1180	G
1	1A	1183	G
1	1A	1215	G
1	1A	1217	G
1	1A	1218	A
1	1A	1219	U
1	1A	1220	G
1	1A	1221	A
1	1A	1264	A
1	1A	1286	A
1	1A	1298	A
1	1A	1301	G
1	1A	1316	G
1	1A	1317	A
1	1A	1318	U
1	1A	1321	A
1	1A	1345	U
1	1A	1346	A
1	1A	1348	G
1	1A	1360	C
1	1A	1366	A
1	1A	1397	U
1	1A	1404	A
1	1A	1405	A
1	1A	1410	A
1	1A	1429	A
1	1A	1430	G

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Mol	Chain	Res	Type
1	1A	1440	A
1	1A	1461	G
1	1A	1462	C
1	1A	1465	U
1	1A	1466	G
1	1A	1467	G
1	1A	1472	A
1	1A	1473	C
1	1A	1482	C
1	1A	1490	A
1	1A	1495	A
1	1A	1496	G
1	1A	1501	G
1	1A	1505	G
1	1A	1507	G
1	1A	1508	C
1	1A	1513	C
1	1A	1524	G
1	1A	1528	G
1	1A	1553	A
1	1A	1554	C
1	1A	1555	A
1	1A	1570	G
1	1A	1578	C
1	1A	1588	A
1	1A	1604	A
1	1A	1612	A
1	1A	1615	A
1	1A	1624	U
1	1A	1626	A
1	1A	1627	G
1	1A	1630	C
1	1A	1631	A
1	1A	1653	A
1	1A	1654	A
1	1A	1655	A
1	1A	1694	C
1	1A	1700	A
1	1A	1704	C
1	1A	1710	A
1	1A	1720	G
1	1A	1746	A

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Mol	Chain	Res	Type
1	1A	1747	A
1	1A	1766	A
1	1A	1767	U
1	1A	1776	G
1	1A	1793	G
1	1A	1794	G
1	1A	1799	G
1	1A	1803	A
1	1A	1804	C
1	1A	1810	A
1	1A	1812	C
1	1A	1821	A
1	1A	1830	C
1	1A	1831	G
1	1A	1846	G
1	1A	1858	G
1	1A	1859	A
1	1A	1869	G
1	1A	1877	A
1	1A	1899	G
1	1A	1910	A
1	1A	1921	A
1	1A	1927	G
1	1A	1933	A
1	1A	1934	A
1	1A	1936	U
1	1A	1940	A
1	1A	1948	A
1	1A	1950	G
1	1A	1951	G
1	1A	1958	A
1	1A	1959	A
1	1A	1976	U
1	1A	1984	U
1	1A	1986	C
1	1A	1988	C
1	1A	1991	A
1	1A	1992	A
1	1A	1993	A
1	1A	2013	G
1	1A	2014	U
1	1A	2018	G

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Mol	Chain	Res	Type
1	1A	2041	A
1	1A	2044	G
1	1A	2052	A
1	1A	2053	G
1	1A	2054	A
1	1A	2064	C
1	1A	2074	G
1	1A	2076	C
1	1A	2077	G
1	1A	2081	A
1	1A	2082	G
1	1A	2083	A
1	1A	2090	G
1	1A	2114	G
1	1A	2205	G
1	1A	2206	C
1	1A	2207	G
1	1A	2209	C
1	1A	2212	G
1	1A	2216	C
1	1A	2219	A
1	1A	2226	G
1	1A	2227	G
1	1A	2228	A
1	1A	2229	U
1	1A	2236	A
1	1A	2249	G
1	1A	2250	G
1	1A	2279	A
1	1A	2280	A
1	1A	2284	A
1	1A	2286	C
1	1A	2290	G
1	1A	2291	G
1	1A	2294	C
1	1A	2298	A
1	1A	2316	A
1	1A	2319	G
1	1A	2331	A
1	1A	2332	G
1	1A	2336	G
1	1A	2338	A

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Mol	Chain	Res	Type
1	1A	2345	G
1	1A	2346	A
1	1A	2347	A
1	1A	2354	C
1	1A	2358	C
1	1A	2361	C
1	1A	2394	G
1	1A	2396	C
1	1A	2417	U
1	1A	2421	G
1	1A	2433	A
1	1A	2435	C
1	1A	2436	A
1	1A	2440	G
1	1A	2441	A
1	1A	2446	A
1	1A	2449	U
1	1A	2450	A
1	1A	2452	C
1	1A	2459	A
1	1A	2460	U
1	1A	2479	G
1	1A	2485	C
1	1A	2487	A
1	1A	2489	A
1	1A	2513	G
1	1A	2516	G
1	1A	2517	U
1	1A	2529	A
1	1A	2531	C
1	1A	2540	G
1	1A	2565	U
1	1A	2566	U
1	1A	2577	A
1	1A	2578	G
1	1A	2584	C
1	1A	2593	G
1	1A	2613	A
1	1A	2620	U
1	1A	2621	C
1	1A	2622	U
1	1A	2623	C

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Mol	Chain	Res	Type
1	1A	2640	A
1	1A	2641	G
1	1A	2643	A
1	1A	2649	G
1	1A	2665	A
1	1A	2700	U
1	1A	2701	C
1	1A	2702	C
1	1A	2713	U
1	1A	2714	C
1	1A	2724	A
1	1A	2725	A
1	1A	2726	G
1	1A	2738	U
1	1A	2745	A
1	1A	2769	A
1	1A	2770	A
1	1A	2776	A
1	1A	2777	A
1	1A	2778	G
1	1A	2790	A
1	1A	2802	A
1	1A	2812	G
1	1A	2827	G
1	1A	2829	A
1	1A	2830	A
1	1A	2844	A
1	1A	2845	U
1	1A	2881	G
1	1A	2882	A
1	1A	2889	C
1	1A	2900	A
1	1A	2902	G
1	1A	2903	U
2	1B	13	A
2	1B	24	G
2	1B	56	G
2	1B	65	C
2	1B	67	G
2	1B	73	A
2	1B	85	G
2	1B	106	G

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Mol	Chain	Res	Type
2	1B	110	G
32	1a	6	U
32	1a	10	G
32	1a	33	A
32	1a	40	G
32	1a	41	C
32	1a	45	G
32	1a	48	C
32	1a	49	C
32	1a	51	A
32	1a	52	A
32	1a	62	G
32	1a	65	G
32	1a	66	U
32	1a	74	G
32	1a	76	G
32	1a	77	G
32	1a	78	G
32	1a	90	U
32	1a	91	G
32	1a	92	G
32	1a	95	A
32	1a	110	A
32	1a	115	C
32	1a	126	C
32	1a	132	C
32	1a	139	G
32	1a	156	A
32	1a	161	G
32	1a	162	G
32	1a	168	U
32	1a	169	C
32	1a	178	G
32	1a	190	U
32	1a	202	A
32	1a	204	A
32	1a	211	U
32	1a	212	G
32	1a	218	U
32	1a	222	G
32	1a	243	G
32	1a	247	G

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Mol	Chain	Res	Type
32	1a	254	G
32	1a	262	G
32	1a	263	C
32	1a	266	A
32	1a	277	G
32	1a	285	G
32	1a	317	A
32	1a	324	C
32	1a	325	A
32	1a	337	C
32	1a	338	C
32	1a	342	G
32	1a	343	G
32	1a	344	G
32	1a	347	G
32	1a	348	C
32	1a	349	A
32	1a	350	G
32	1a	351	C
32	1a	363	U
32	1a	368	C
32	1a	369	A
32	1a	380	G
32	1a	393	A
32	1a	394	C
32	1a	402	G
32	1a	408	A
32	1a	409	G
32	1a	419	G
32	1a	420	G
32	1a	425	U
32	1a	435	A
32	1a	437	C
32	1a	441	G
32	1a	447	A
32	1a	448	A
32	1a	449	C
32	1a	455	A
32	1a	456	C
32	1a	457	G
32	1a	461	G
32	1a	470	G

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Mol	Chain	Res	Type
32	1a	478	G
32	1a	481	A
32	1a	482	U
32	1a	489	G
32	1a	493	A
32	1a	494	A
32	1a	495	C
32	1a	496	U
32	1a	502	C
32	1a	508	G
32	1a	510	C
32	1a	511	G
32	1a	515	U
32	1a	516	A
32	1a	517	A
32	1a	529	C
32	1a	531	A
32	1a	543	A
32	1a	545	U
32	1a	547	A
32	1a	556	A
32	1a	557	A
32	1a	560	G
32	1a	561	G
32	1a	576	G
32	1a	580	C
32	1a	599	C
32	1a	602	C
32	1a	614	G
32	1a	637	A
32	1a	645	G
32	1a	649	A
32	1a	671	A
32	1a	672	G
32	1a	677	G
32	1a	687	G
32	1a	707	U
32	1a	715	G
32	1a	718	G
32	1a	733	C
32	1a	737	A
32	1a	739	G

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Mol	Chain	Res	Type
32	1a	743	A
32	1a	761	A
32	1a	777	U
32	1a	778	A
32	1a	799	A
32	1a	801	C
32	1a	805	G
32	1a	812	A
32	1a	813	G
32	1a	820	G
32	1a	824	C
32	1a	825	U
32	1a	826	C
32	1a	829	G
32	1a	837	A
32	1a	848	U
32	1a	850	A
32	1a	880	G
32	1a	892	A
32	1a	904	G
32	1a	905	G
32	1a	909	C
32	1a	912	C
32	1a	913	A
32	1a	914	C
32	1a	938	U
32	1a	939	U
32	1a	946	A
32	1a	947	A
32	1a	949	G
32	1a	950	C
32	1a	952	A
32	1a	953	A
32	1a	954	G
32	1a	955	A
32	1a	960	U
32	1a	961	A
32	1a	970	U
32	1a	971	G
32	1a	972	A
32	1a	974	A
32	1a	982	G

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Mol	Chain	Res	Type
32	1a	983	A
32	1a	984	A
32	1a	987	C
32	1a	988	G
32	1a	990	G
32	1a	992	G
32	1a	995	A
32	1a	1001	G
32	1a	1027	A
32	1a	1028	C
32	1a	1033	G
32	1a	1037	C
32	1a	1048	U
32	1a	1049	C
32	1a	1064	G
32	1a	1069	U
32	1a	1077	G
32	1a	1078	U
32	1a	1079	C
32	1a	1084	A
32	1a	1089	G
32	1a	1091	G
32	1a	1106	A
32	1a	1107	G
32	1a	1113	A
32	1a	1117	G
32	1a	1119	U
32	1a	1120	C
32	1a	1122	G
32	1a	1123	C
32	1a	1128	C
32	1a	1129	A
32	1a	1135	A
32	1a	1142	U
32	1a	1149	G
32	1a	1165	A
32	1a	1166	G
32	1a	1178	U
32	1a	1179	G
32	1a	1184	G
32	1a	1195	A
32	1a	1196	C

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Mol	Chain	Res	Type
32	1a	1202	G
32	1a	1209	A
32	1a	1220	A
32	1a	1238	A
32	1a	1239	U
32	1a	1240	G
32	1a	1242	C
32	1a	1252	C
32	1a	1260	U
32	1a	1262	A
32	1a	1268	A
32	1a	1269	A
32	1a	1281	A
32	1a	1282	G
32	1a	1284	U
32	1a	1294	G
32	1a	1304	C
32	1a	1320	G
32	1a	1322	A
32	1a	1328	A
32	1a	1329	G
32	1a	1335	G
32	1a	1341	C
32	1a	1342	A
32	1a	1345	C
32	1a	1353	G
32	1a	1360	A
32	1a	1361	C
32	1a	1379	A
32	1a	1381	A
32	1a	1383	C
32	1a	1402	G
32	1a	1425	G
32	1a	1426	G
32	1a	1432	A
32	1a	1433	C
32	1a	1451	A
32	1a	1465	G
32	1a	1469	G
32	1a	1475	G
32	1a	1480	A
32	1a	1481	A

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Mol	Chain	Res	Type
32	1a	1482	G
32	1a	1484	U
32	1a	1495	G
32	1a	1507	G
32	1a	1508	G
53	1v	15	A
54	1x	6	G
54	1x	9	G
54	1x	13	C
54	1x	17	C
54	1x	17(A)	U
54	1x	19	G
54	1x	20	U
54	1x	21	A
54	1x	31	G
54	1x	34	C
54	1x	37	A
54	1x	38	A
54	1x	42	G
54	1x	47	U
54	1x	56	C
54	1x	65	C
54	1x	70	G
54	1x	76	A
1	2A	9	G
1	2A	11	U
1	2A	12	A
1	2A	14	G
1	2A	22	G
1	2A	33	C
1	2A	44	C
1	2A	59	G
1	2A	69	A
1	2A	72	A
1	2A	73	G
1	2A	77	G
1	2A	81	G
1	2A	82	A
1	2A	88	U
1	2A	91	C
1	2A	98	G
1	2A	99	G

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Mol	Chain	Res	Type
1	2A	115	A
1	2A	116	A
1	2A	117	U
1	2A	122	G
1	2A	154	C
1	2A	155	U
1	2A	169	A
1	2A	184	A
1	2A	187	A
1	2A	193	G
1	2A	203	G
1	2A	204	A
1	2A	209	A
1	2A	210	A
1	2A	211	A
1	2A	216	A
1	2A	217	A
1	2A	218	U
1	2A	221	A
1	2A	236	G
1	2A	254	G
1	2A	268	G
1	2A	270	U
1	2A	271	U
1	2A	272	G
1	2A	273	U
1	2A	274	C
1	2A	287	U
1	2A	288	G
1	2A	300	C
1	2A	301	A
1	2A	334	A
1	2A	345	A
1	2A	347	A
1	2A	350	G
1	2A	352	G
1	2A	353	A
1	2A	356	G
1	2A	357	C
1	2A	358	C
1	2A	361	G
1	2A	375	G

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Mol	Chain	Res	Type
1	2A	385	U
1	2A	386	G
1	2A	388	G
1	2A	389	G
1	2A	405	G
1	2A	406	U
1	2A	412	G
1	2A	415	G
1	2A	422	G
1	2A	431	U
1	2A	433	G
1	2A	437	G
1	2A	438	A
1	2A	441	A
1	2A	448	A
1	2A	454	A
1	2A	468	A
1	2A	469	C
1	2A	479	A
1	2A	480	C
1	2A	481	C
1	2A	482	A
1	2A	495	A
1	2A	500	U
1	2A	506	G
1	2A	509	C
1	2A	516	A
1	2A	520	G
1	2A	528	U
1	2A	529	A
1	2A	533	C
1	2A	552	A
1	2A	553	A
1	2A	554	G
1	2A	555	C
1	2A	556	A
1	2A	557	G
1	2A	568	G
1	2A	578	G
1	2A	585	G
1	2A	595	G
1	2A	597	A

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Mol	Chain	Res	Type
1	2A	608	A
1	2A	625	A
1	2A	626	G
1	2A	629	U
1	2A	637	U
1	2A	638	G
1	2A	640	G
1	2A	651	A
1	2A	658	C
1	2A	661	A
1	2A	669	C
1	2A	670	A
1	2A	678	A
1	2A	679	G
1	2A	697	G
1	2A	698	C
1	2A	732	G
1	2A	772	G
1	2A	776	C
1	2A	811	G
1	2A	817	G
1	2A	821	G
1	2A	822	G
1	2A	828	A
1	2A	830	A
1	2A	831	G
1	2A	836	C
1	2A	838	G
1	2A	840	G
1	2A	848	A
1	2A	851	G
1	2A	858	C
1	2A	865	A
1	2A	873	U
1	2A	898	G
1	2A	903	C
1	2A	905	G
1	2A	912	A
1	2A	913	C
1	2A	915	G
1	2A	921	G
1	2A	925	G

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Mol	Chain	Res	Type
1	2A	926	G
1	2A	930	C
1	2A	932	C
1	2A	933	A
1	2A	934	C
1	2A	935	C
1	2A	936	A
1	2A	941	A
1	2A	945	A
1	2A	946	A
1	2A	955	A
1	2A	959	C
1	2A	962	A
1	2A	976	G
1	2A	977	A
1	2A	982	G
1	2A	985	A
1	2A	989	A
1	2A	990	G
1	2A	1001	A
1	2A	1003	A
1	2A	1005	C
1	2A	1017	A
1	2A	1018	G
1	2A	1019	C
1	2A	1025	A
1	2A	1028	A
1	2A	1041	A
1	2A	1050	C
1	2A	1057	U
1	2A	1058	C
1	2A	1062	G
1	2A	1065	A
1	2A	1066	A
1	2A	1067	G
1	2A	1070	G
1	2A	1072	A
1	2A	1078	U
1	2A	1082	G
1	2A	1083	C
1	2A	1084	G
1	2A	1087	G

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Mol	Chain	Res	Type
1	2A	1088	C
1	2A	1091	A
1	2A	1092	G
1	2A	1093	A
1	2A	1103	G
1	2A	1105	U
1	2A	1106	U
1	2A	1107	G
1	2A	1108	G
1	2A	1109	C
1	2A	1110	U
1	2A	1115	A
1	2A	1118	A
1	2A	1120	C
1	2A	1121	C
1	2A	1126	U
1	2A	1127	U
1	2A	1128	U
1	2A	1131	A
1	2A	1133	A
1	2A	1140	A
1	2A	1142	U
1	2A	1143	A
1	2A	1146	U
1	2A	1156	A
1	2A	1157	G
1	2A	1158	U
1	2A	1159	G
1	2A	1161	C
1	2A	1167	G
1	2A	1175	U
1	2A	1179	C
1	2A	1180	G
1	2A	1183	G
1	2A	1187	A
1	2A	1216	G
1	2A	1240	C
1	2A	1256	G
1	2A	1285	U
1	2A	1289	G
1	2A	1298	A
1	2A	1301	G

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Mol	Chain	Res	Type
1	2A	1307	A
1	2A	1316	G
1	2A	1317	A
1	2A	1318	U
1	2A	1332	A
1	2A	1345	U
1	2A	1346	A
1	2A	1350	C
1	2A	1359	C
1	2A	1364	G
1	2A	1374	U
1	2A	1397	U
1	2A	1404	A
1	2A	1405	A
1	2A	1410	A
1	2A	1413	G
1	2A	1415	C
1	2A	1425	G
1	2A	1429	A
1	2A	1430	G
1	2A	1431	C
1	2A	1447	C
1	2A	1448	C
1	2A	1461	G
1	2A	1462	C
1	2A	1465	U
1	2A	1466	G
1	2A	1472	A
1	2A	1473	C
1	2A	1490	A
1	2A	1495	A
1	2A	1496	G
1	2A	1501	G
1	2A	1506	A
1	2A	1513	C
1	2A	1517	A
1	2A	1528	G
1	2A	1534	U
1	2A	1535	A
1	2A	1538	C
1	2A	1542	U
1	2A	1554	C

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Mol	Chain	Res	Type
1	2A	1555	A
1	2A	1579	G
1	2A	1583	G
1	2A	1589	C
1	2A	1590	A
1	2A	1593	C
1	2A	1601	G
1	2A	1604	A
1	2A	1605	G
1	2A	1612	A
1	2A	1615	A
1	2A	1624	U
1	2A	1626	A
1	2A	1630	C
1	2A	1631	A
1	2A	1639	G
1	2A	1652	C
1	2A	1653	A
1	2A	1654	A
1	2A	1655	A
1	2A	1661	A
1	2A	1686	C
1	2A	1694	C
1	2A	1700	A
1	2A	1710	A
1	2A	1720	G
1	2A	1746	A
1	2A	1747	A
1	2A	1765	G
1	2A	1766	A
1	2A	1768	G
1	2A	1771	C
1	2A	1786	G
1	2A	1788	G
1	2A	1792	A
1	2A	1793	G
1	2A	1794	G
1	2A	1799	G
1	2A	1803	A
1	2A	1810	A
1	2A	1812	C
1	2A	1821	A

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Mol	Chain	Res	Type
1	2A	1830	C
1	2A	1831	G
1	2A	1846	G
1	2A	1858	G
1	2A	1877	A
1	2A	1889	A
1	2A	1891	G
1	2A	1898	A
1	2A	1899	G
1	2A	1921	A
1	2A	1924	G
1	2A	1925	G
1	2A	1927	G
1	2A	1934	A
1	2A	1935	C
1	2A	1948	A
1	2A	1950	G
1	2A	1951	G
1	2A	1952	U
1	2A	1959	A
1	2A	1976	U
1	2A	1984	U
1	2A	1988	C
1	2A	1991	A
1	2A	1992	A
1	2A	1993	A
1	2A	2014	U
1	2A	2018	G
1	2A	2026	A
1	2A	2041	A
1	2A	2044	G
1	2A	2051	A
1	2A	2052	A
1	2A	2054	A
1	2A	2060	C
1	2A	2064	C
1	2A	2067	G
1	2A	2076	C
1	2A	2077	G
1	2A	2081	A
1	2A	2082	G
1	2A	2083	A

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Mol	Chain	Res	Type
1	2A	2090	G
1	2A	2120	U
1	2A	2207	G
1	2A	2209	C
1	2A	2213	G
1	2A	2217	C
1	2A	2219	A
1	2A	2226	G
1	2A	2227	G
1	2A	2228	A
1	2A	2236	A
1	2A	2249	G
1	2A	2278	A
1	2A	2280	A
1	2A	2286	C
1	2A	2290	G
1	2A	2294	C
1	2A	2298	A
1	2A	2300	G
1	2A	2316	A
1	2A	2318	G
1	2A	2319	G
1	2A	2322	A
1	2A	2323	U
1	2A	2328	C
1	2A	2329	G
1	2A	2330	G
1	2A	2331	A
1	2A	2333	A
1	2A	2336	G
1	2A	2345	G
1	2A	2346	A
1	2A	2347	A
1	2A	2354	C
1	2A	2358	C
1	2A	2361	C
1	2A	2387	A
1	2A	2394	G
1	2A	2396	C
1	2A	2399	A
1	2A	2402	G
1	2A	2417	U

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Mol	Chain	Res	Type
1	2A	2421	G
1	2A	2433	A
1	2A	2434	U
1	2A	2436	A
1	2A	2439	G
1	2A	2440	G
1	2A	2441	A
1	2A	2445	A
1	2A	2446	A
1	2A	2450	A
1	2A	2452	C
1	2A	2456	G
1	2A	2459	A
1	2A	2460	U
1	2A	2476	C
1	2A	2479	G
1	2A	2480	A
1	2A	2485	C
1	2A	2487	A
1	2A	2489	A
1	2A	2497	G
1	2A	2513	G
1	2A	2516	G
1	2A	2517	U
1	2A	2529	A
1	2A	2531	C
1	2A	2540	G
1	2A	2565	U
1	2A	2577	A
1	2A	2578	G
1	2A	2584	C
1	2A	2613	A
1	2A	2620	U
1	2A	2622	U
1	2A	2623	C
1	2A	2640	A
1	2A	2641	G
1	2A	2650	A
1	2A	2665	A
1	2A	2674	G
1	2A	2693	U
1	2A	2700	U

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Mol	Chain	Res	Type
1	2A	2701	C
1	2A	2702	C
1	2A	2713	U
1	2A	2714	C
1	2A	2724	A
1	2A	2725	A
1	2A	2726	G
1	2A	2738	U
1	2A	2745	A
1	2A	2763	G
1	2A	2764	C
1	2A	2769	A
1	2A	2776	A
1	2A	2777	A
1	2A	2778	G
1	2A	2790	A
1	2A	2801	C
1	2A	2805	G
1	2A	2812	G
1	2A	2817	U
1	2A	2827	G
1	2A	2829	A
1	2A	2830	A
1	2A	2842	G
1	2A	2843	G
1	2A	2844	A
1	2A	2848	G
1	2A	2881	G
1	2A	2882	A
1	2A	2885	G
1	2A	2889	C
1	2A	2895	G
1	2A	2900	A
1	2A	2902	G
1	2A	2903	U
1	2A	2904	C
1	2A	2905	U
2	2B	2	C
2	2B	7	G
2	2B	9	G
2	2B	13	A
2	2B	28	C

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Mol	Chain	Res	Type
2	2B	30	C
2	2B	32	C
2	2B	33	G
2	2B	35	U
2	2B	43	C
2	2B	45	A
2	2B	46	A
2	2B	50	G
2	2B	52	A
2	2B	56	G
2	2B	64	C
2	2B	73	A
2	2B	85	G
2	2B	106	G
2	2B	110	G
2	2B	111	G
2	2B	120	A
32	2a	6	U
32	2a	7	G
32	2a	10	G
32	2a	11	A
32	2a	15	U
32	2a	16	G
32	2a	23	G
32	2a	31	U
32	2a	33	A
32	2a	40	G
32	2a	43	G
32	2a	48	C
32	2a	49	C
32	2a	51	A
32	2a	52	A
32	2a	66	U
32	2a	67	G
32	2a	74	G
32	2a	79	G
32	2a	85	C
32	2a	91	G
32	2a	92	G
32	2a	110	A
32	2a	115	C
32	2a	124	G

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Mol	Chain	Res	Type
32	2a	126	C
32	2a	138	A
32	2a	151	G
32	2a	158	C
32	2a	169	C
32	2a	177	U
32	2a	189	U
32	2a	190	U
32	2a	202	A
32	2a	204	A
32	2a	208	C
32	2a	210	U
32	2a	211	U
32	2a	212	G
32	2a	243	G
32	2a	247	G
32	2a	248	U
32	2a	254	G
32	2a	262	G
32	2a	263	C
32	2a	275	A
32	2a	277	G
32	2a	285	G
32	2a	297	G
32	2a	310	C
32	2a	317	A
32	2a	324	C
32	2a	328	G
32	2a	340	A
32	2a	345	A
32	2a	346	G
32	2a	347	G
32	2a	348	C
32	2a	349	A
32	2a	350	G
32	2a	363	U
32	2a	368	C
32	2a	369	A
32	2a	380	G
32	2a	394	C
32	2a	402	G
32	2a	408	A

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Mol	Chain	Res	Type
32	2a	417	U
32	2a	419	G
32	2a	425	U
32	2a	426	A
32	2a	435	A
32	2a	437	C
32	2a	447	A
32	2a	455	A
32	2a	456	C
32	2a	457	G
32	2a	463	A
32	2a	469	G
32	2a	470	G
32	2a	481	A
32	2a	482	U
32	2a	489	G
32	2a	493	A
32	2a	494	A
32	2a	495	C
32	2a	497	C
32	2a	502	C
32	2a	505	G
32	2a	511	G
32	2a	515	U
32	2a	516	A
32	2a	517	A
32	2a	531	A
32	2a	543	A
32	2a	545	U
32	2a	546	C
32	2a	552	G
32	2a	556	A
32	2a	557	A
32	2a	560	G
32	2a	561	G
32	2a	580	C
32	2a	611	G
32	2a	614	G
32	2a	637	A
32	2a	645	G
32	2a	649	A
32	2a	650	G

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Mol	Chain	Res	Type
32	2a	672	G
32	2a	677	G
32	2a	679	A
32	2a	696	A
32	2a	701	C
32	2a	704	C
32	2a	707	U
32	2a	708	G
32	2a	715	G
32	2a	733	C
32	2a	739	G
32	2a	744	G
32	2a	761	A
32	2a	776	A
32	2a	777	U
32	2a	778	A
32	2a	783	G
32	2a	800	A
32	2a	801	C
32	2a	812	A
32	2a	813	G
32	2a	822	G
32	2a	824	C
32	2a	825	U
32	2a	826	C
32	2a	837	A
32	2a	845	G
32	2a	880	G
32	2a	892	A
32	2a	898	U
32	2a	904	G
32	2a	905	G
32	2a	909	C
32	2a	912	C
32	2a	913	A
32	2a	920	G
32	2a	938	U
32	2a	939	U
32	2a	946	A
32	2a	947	A
32	2a	949	G
32	2a	950	C

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Mol	Chain	Res	Type
32	2a	952	A
32	2a	953	A
32	2a	954	G
32	2a	955	A
32	2a	956	A
32	2a	967	C
32	2a	970	U
32	2a	971	G
32	2a	973	C
32	2a	974	A
32	2a	977	C
32	2a	981	G
32	2a	983	A
32	2a	984	A
32	2a	985	C
32	2a	986	C
32	2a	988	G
32	2a	1001	G
32	2a	1002	G
32	2a	1027	A
32	2a	1028	C
32	2a	1033	G
32	2a	1036	G
32	2a	1037	C
32	2a	1038	A
32	2a	1039	U
32	2a	1047	G
32	2a	1048	U
32	2a	1049	C
32	2a	1064	G
32	2a	1077	G
32	2a	1078	U
32	2a	1084	A
32	2a	1091	G
32	2a	1096	C
32	2a	1101	C
32	2a	1105	U
32	2a	1109	U
32	2a	1112	C
32	2a	1113	A
32	2a	1116	G
32	2a	1118	U

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Mol	Chain	Res	Type
32	2a	1119	U
32	2a	1120	C
32	2a	1121	G
32	2a	1122	G
32	2a	1129	A
32	2a	1130	C
32	2a	1140	A
32	2a	1142	U
32	2a	1165	A
32	2a	1168	G
32	2a	1171	C
32	2a	1172	G
32	2a	1178	U
32	2a	1184	G
32	2a	1193	U
32	2a	1194	U
32	2a	1196	C
32	2a	1210	C
32	2a	1220	A
32	2a	1222	U
32	2a	1223	G
32	2a	1235	G
32	2a	1239	U
32	2a	1240	G
32	2a	1242	C
32	2a	1243	A
32	2a	1244	C
32	2a	1251	A
32	2a	1255	G
32	2a	1262	A
32	2a	1263	U
32	2a	1264	C
32	2a	1268	A
32	2a	1269	A
32	2a	1281	A
32	2a	1285	C
32	2a	1287	G
32	2a	1300	A
32	2a	1304	C
32	2a	1305	G
32	2a	1308	C
32	2a	1320	G

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Mol	Chain	Res	Type
32	2a	1328	A
32	2a	1329	G
32	2a	1332	A
32	2a	1341	C
32	2a	1342	A
32	2a	1345	C
32	2a	1347	U
32	2a	1353	G
32	2a	1364	U
32	2a	1380	C
32	2a	1381	A
32	2a	1402	G
32	2a	1425	G
32	2a	1426	G
32	2a	1427	A
32	2a	1431	U
32	2a	1432	A
32	2a	1433	C
32	2a	1434	G
32	2a	1467	G
32	2a	1475	G
32	2a	1477	A
32	2a	1480	A
32	2a	1481	A
32	2a	1482	G
32	2a	1484	U
32	2a	1495	G
32	2a	1497	A
32	2a	1498	G
32	2a	1507	G
32	2a	1508	G
32	2a	1509	A
32	2a	1510	U
53	2v	15	A
54	2x	6	G
54	2x	9	G
54	2x	13	C
54	2x	17	C
54	2x	17(A)	U
54	2x	19	G
54	2x	20	U
54	2x	21	A

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Mol	Chain	Res	Type
54	2x	31	G
54	2x	34	C
54	2x	37	A
54	2x	38	A
54	2x	42	G
54	2x	47	U
54	2x	56	C
54	2x	65	C
54	2x	70	G
54	2x	76	A

All (46) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	183	A
1	1A	184	A
1	1A	301	A
1	1A	516	A
1	1A	873	U
1	1A	1153	U
1	1A	1218	A
1	1A	1220	G
1	1A	1285	U
1	1A	1320	A
1	1A	1425	G
1	1A	1465	U
1	1A	1653	A
1	1A	1709	C
1	1A	1792	A
1	1A	2013	G
1	1A	2417	U
1	1A	2700	U
1	1A	2768	U
1	2A	183	A
1	2A	184	A
1	2A	247	G
1	2A	357	C
1	2A	516	A
1	2A	810	A
1	2A	873	U
1	2A	902	C
1	2A	945	A

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Mol	Chain	Res	Type
1	2A	1071	U
1	2A	1087	G
1	2A	1102	A
1	2A	1114	A
1	2A	1238	A
1	2A	1424	A
1	2A	1425	G
1	2A	1465	U
1	2A	1604	A
1	2A	1820	C
1	2A	1934	A
1	2A	2013	G
1	2A	2328	C
1	2A	2417	U
1	2A	2700	U
1	2A	2768	U
2	2B	42	C
2	2B	45	A

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

8 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	1x	8	54	18,21,22	2.04	5 (27%)	26,30,33	1.33	5 (19%)
54	5MU	1x	54	54	19,22,23	1.54	5 (26%)	28,32,35	1.88	5 (17%)
54	5MC	2x	32	54	18,22,23	1.04	1 (5%)	26,32,35	1.27	3 (11%)
54	PSU	2x	55	54	18,21,22	1.34	2 (11%)	22,30,33	1.80	3 (13%)
54	5MC	1x	32	54	18,22,23	1.03	2 (11%)	26,32,35	1.15	2 (7%)
54	PSU	1x	55	54	18,21,22	1.31	2 (11%)	22,30,33	1.74	3 (13%)
54	5MU	2x	54	54	19,22,23	1.43	5 (26%)	28,32,35	1.95	6 (21%)
54	4SU	2x	8	54	18,21,22	1.91	5 (27%)	26,30,33	1.22	3 (11%)

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	1x	8	54	-	0/7/25/26	0/2/2/2
54	5MU	1x	54	54	-	0/7/25/26	0/2/2/2
54	5MC	2x	32	54	-	1/7/25/26	0/2/2/2
54	PSU	2x	55	54	-	2/7/25/26	0/2/2/2
54	5MC	1x	32	54	-	0/7/25/26	0/2/2/2
54	PSU	1x	55	54	-	2/7/25/26	0/2/2/2
54	5MU	2x	54	54	-	1/7/25/26	0/2/2/2
54	4SU	2x	8	54	-	0/7/25/26	0/2/2/2

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	1x	8	4SU	C4-N3	-4.76	1.32	1.37
54	2x	8	4SU	C4-N3	-4.57	1.32	1.37
54	1x	8	4SU	C2-N3	-4.08	1.30	1.38
54	1x	8	4SU	C4-S4	-3.98	1.60	1.68
54	2x	8	4SU	C4-S4	-3.82	1.61	1.68
54	2x	55	PSU	C6-C5	3.44	1.39	1.35
54	1x	54	5MU	C6-C5	3.36	1.40	1.34
54	2x	32	5MC	C6-C5	3.09	1.39	1.34
54	1x	32	5MC	C6-C5	3.08	1.39	1.34
54	1x	54	5MU	C4-N3	-2.95	1.33	1.38
54	1x	55	PSU	C6-C5	2.95	1.38	1.35
54	2x	8	4SU	C2-N3	-2.94	1.32	1.38
54	2x	54	5MU	C6-C5	2.90	1.39	1.34
54	2x	8	4SU	C5-C4	-2.84	1.38	1.42
54	1x	8	4SU	C5-C4	-2.80	1.39	1.42
54	1x	54	5MU	C2-N1	2.59	1.42	1.38
54	1x	54	5MU	C4-C5	2.56	1.49	1.44
54	2x	54	5MU	C4-C5	2.55	1.49	1.44
54	1x	55	PSU	C4-N3	-2.45	1.34	1.38
54	2x	54	5MU	C4-N3	-2.43	1.34	1.38
54	2x	55	PSU	C4-N3	-2.41	1.34	1.38
54	2x	54	5MU	C2-N1	2.34	1.42	1.38
54	1x	32	5MC	C6-N1	-2.24	1.34	1.38
54	2x	8	4SU	C6-C5	2.10	1.39	1.35
54	2x	54	5MU	C6-N1	-2.08	1.34	1.38
54	1x	8	4SU	C6-C5	2.01	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	1x	54	5MU	C2-N3	-2.00	1.34	1.38

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	2x	55	PSU	N1-C2-N3	5.69	121.57	115.13
54	1x	55	PSU	N1-C2-N3	5.17	120.99	115.13
54	1x	54	5MU	N3-C2-N1	5.15	121.72	114.89
54	2x	54	5MU	C4-N3-C2	-4.85	121.07	127.35
54	2x	54	5MU	N3-C2-N1	4.73	121.16	114.89
54	1x	54	5MU	C4-N3-C2	-4.51	121.51	127.35
54	2x	54	5MU	C5-C4-N3	4.05	118.77	115.31
54	1x	54	5MU	C5-C4-N3	3.79	118.55	115.31
54	2x	55	PSU	C4-N3-C2	-3.72	120.97	126.34
54	2x	54	5MU	C5-C6-N1	-3.52	119.72	123.34
54	1x	55	PSU	C4-N3-C2	-3.50	121.29	126.34
54	2x	54	5MU	O4-C4-C5	-3.47	120.88	124.90
54	1x	32	5MC	C5-C6-N1	-3.42	119.82	123.34
54	1x	54	5MU	C5-C6-N1	-3.38	119.86	123.34
54	1x	55	PSU	O2-C2-N1	-3.37	119.08	122.79
54	2x	32	5MC	O2-C2-N3	-3.25	117.04	122.33
54	2x	32	5MC	C5-C6-N1	-3.13	120.12	123.34
54	1x	8	4SU	C6-C5-C4	-3.10	117.27	119.95
54	1x	8	4SU	O2-C2-N1	3.00	126.78	122.79
54	1x	8	4SU	C5-C4-N3	2.99	117.46	114.69
54	2x	55	PSU	O2-C2-N1	-2.89	119.61	122.79
54	2x	32	5MC	C5-C4-N3	-2.82	118.63	121.67
54	2x	8	4SU	C6-C5-C4	-2.82	117.51	119.95
54	1x	32	5MC	C5-C4-N3	-2.78	118.68	121.67
54	2x	8	4SU	C1'-N1-C2	2.69	122.43	117.57
54	2x	8	4SU	C5-C4-N3	2.63	117.13	114.69
54	1x	54	5MU	O4-C4-C5	-2.51	122.00	124.90
54	2x	54	5MU	O2-C2-N1	-2.38	119.62	122.79
54	1x	8	4SU	O2-C2-N3	-2.21	117.39	121.50
54	1x	8	4SU	S4-C4-N3	-2.04	118.20	120.21

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
54	1x	55	PSU	O4'-C4'-C5'-O5'
54	2x	55	PSU	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
54	1x	55	PSU	C3'-C4'-C5'-O5'
54	2x	54	5MU	C3'-C4'-C5'-O5'
54	2x	55	PSU	C3'-C4'-C5'-O5'
54	2x	32	5MC	C2'-C1'-N1-C2

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 2494 ligands modelled in this entry, 2492 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
58	SF4	1d	501	35	0,12,12	-	-	-		
58	SF4	2d	501	35	0,12,12	-	-	-		

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

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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	2746/2915 (94%)	0.04	26 (0%)	84	84	22, 41, 87, 114	0
1	2A	2790/2915 (95%)	-0.21	66 (2%)	59	56	25, 46, 93, 111	0
2	1B	120/121 (99%)	-0.07	0	100	100	36, 65, 80, 91	0
2	2B	120/121 (99%)	0.18	3 (2%)	57	55	41, 70, 83, 92	0
3	1D	275/276 (99%)	-0.28	0	100	100	23, 40, 57, 77	0
3	2D	275/276 (99%)	-0.30	3 (1%)	80	80	24, 43, 59, 78	0
4	1E	204/206 (99%)	-0.14	0	100	100	21, 43, 66, 81	0
4	2E	204/206 (99%)	-0.18	1 (0%)	91	91	23, 45, 67, 82	0
5	1F	203/210 (96%)	-0.09	0	100	100	22, 50, 75, 90	0
5	2F	203/210 (96%)	-0.21	2 (0%)	82	82	24, 54, 76, 93	0
6	1G	181/182 (99%)	-0.09	5 (2%)	53	49	50, 70, 83, 98	0
6	2G	181/182 (99%)	0.59	15 (8%)	11	8	54, 73, 85, 100	0
7	1H	174/180 (96%)	-0.05	1 (0%)	89	89	48, 64, 77, 82	0
7	2H	174/180 (96%)	0.98	27 (15%)	2	1	56, 69, 81, 83	0
8	1I	146/148 (98%)	0.19	0	100	100	45, 75, 84, 89	0
8	2I	146/148 (98%)	0.59	13 (8%)	9	7	47, 76, 85, 92	0
9	1N	140/140 (100%)	-0.13	0	100	100	27, 46, 66, 79	0
9	2N	140/140 (100%)	0.01	0	100	100	30, 50, 70, 81	0
10	1O	122/122 (100%)	-0.18	0	100	100	33, 45, 63, 70	0
10	2O	122/122 (100%)	-0.28	0	100	100	34, 47, 63, 73	0
11	1P	149/150 (99%)	-0.02	0	100	100	22, 52, 75, 86	0
11	2P	149/150 (99%)	0.37	11 (7%)	14	11	25, 56, 78, 89	0
12	1Q	141/141 (100%)	0.00	1 (0%)	87	87	31, 49, 63, 87	0
12	2Q	141/141 (100%)	-0.24	1 (0%)	87	87	35, 52, 66, 85	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
13	1R	118/118 (100%)	-0.38	0	100	100	19, 30, 47, 57	0
13	2R	118/118 (100%)	-0.14	0	100	100	35, 51, 65, 76	0
14	1S	110/112 (98%)	-0.24	0	100	100	33, 49, 65, 68	0
14	2S	110/112 (98%)	0.79	11 (10%)	7	5	65, 79, 88, 93	0
15	1T	131/146 (89%)	-0.29	0	100	100	29, 41, 70, 90	0
15	2T	131/146 (89%)	-0.22	0	100	100	47, 58, 78, 90	0
16	1U	116/118 (98%)	-0.49	0	100	100	19, 27, 44, 64	0
16	2U	116/118 (98%)	0.02	3 (2%)	56	52	37, 59, 77, 88	0
17	1V	101/101 (100%)	-0.17	0	100	100	27, 49, 65, 74	0
17	2V	101/101 (100%)	0.13	1 (0%)	82	82	30, 54, 71, 78	0
18	1W	112/113 (99%)	-0.25	0	100	100	23, 35, 55, 84	0
18	2W	112/113 (99%)	-0.27	0	100	100	26, 37, 56, 87	0
19	1X	95/96 (98%)	-0.09	0	100	100	31, 46, 66, 78	0
19	2X	95/96 (98%)	-0.02	3 (3%)	47	43	34, 49, 69, 78	0
20	1Y	107/110 (97%)	-0.09	1 (0%)	84	84	29, 47, 68, 85	0
20	2Y	107/110 (97%)	0.67	11 (10%)	6	5	55, 72, 83, 98	0
21	1Z	186/206 (90%)	-0.22	0	100	100	51, 68, 82, 92	0
21	2Z	186/206 (90%)	0.57	12 (6%)	18	14	55, 71, 84, 93	0
22	10	75/85 (88%)	-0.15	0	100	100	33, 45, 59, 66	0
22	20	75/85 (88%)	0.27	3 (4%)	38	33	37, 50, 64, 68	0
23	11	97/98 (98%)	-0.04	1 (1%)	82	82	28, 47, 71, 78	0
23	21	97/98 (98%)	-0.04	1 (1%)	82	82	30, 49, 73, 78	0
24	12	70/72 (97%)	-0.02	0	100	100	42, 58, 72, 80	0
24	22	70/72 (97%)	0.10	0	100	100	45, 61, 74, 79	0
25	13	59/60 (98%)	-0.09	0	100	100	32, 45, 65, 78	0
25	23	59/60 (98%)	0.47	5 (8%)	10	8	35, 50, 69, 80	0
26	14	69/71 (97%)	0.28	6 (8%)	10	7	52, 75, 99, 102	0
26	24	69/71 (97%)	0.93	7 (10%)	7	5	78, 93, 98, 103	0
27	15	59/60 (98%)	-0.41	0	100	100	15, 30, 45, 72	0
27	25	59/60 (98%)	-0.22	0	100	100	33, 50, 67, 72	0
28	16	53/54 (98%)	-0.26	0	100	100	38, 48, 59, 70	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
28	26	53/54 (98%)	-0.21	0	100	100	42, 51, 62, 72	0
29	17	48/49 (97%)	-0.07	1 (2%)	63	61	24, 31, 64, 81	0
29	27	48/49 (97%)	-0.01	3 (6%)	20	16	26, 34, 64, 82	0
30	18	64/65 (98%)	-0.09	0	100	100	30, 41, 49, 63	0
30	28	64/65 (98%)	-0.07	1 (1%)	72	71	33, 43, 52, 64	0
31	19	37/37 (100%)	0.25	0	100	100	38, 48, 70, 74	0
31	29	37/37 (100%)	0.24	2 (5%)	25	22	43, 53, 71, 77	0
32	1a	1477/1521 (97%)	0.05	35 (2%)	59	56	34, 72, 98, 114	0
32	2a	1483/1521 (97%)	0.12	41 (2%)	53	49	43, 78, 101, 115	0
33	1b	231/256 (90%)	0.62	26 (11%)	5	4	67, 86, 96, 115	0
33	2b	231/256 (90%)	0.77	28 (12%)	4	3	71, 88, 97, 106	0
34	1c	206/239 (86%)	0.49	15 (7%)	15	11	70, 84, 93, 99	0
34	2c	206/239 (86%)	0.83	24 (11%)	4	3	73, 85, 94, 96	0
35	1d	208/209 (99%)	0.21	5 (2%)	59	56	56, 77, 88, 100	0
35	2d	208/209 (99%)	0.15	3 (1%)	75	75	56, 73, 84, 92	0
36	1e	148/162 (91%)	-0.06	0	100	100	47, 67, 79, 87	0
36	2e	148/162 (91%)	-0.01	2 (1%)	75	75	56, 74, 84, 90	0
37	1f	100/101 (99%)	-0.19	0	100	100	55, 73, 84, 90	0
37	2f	100/101 (99%)	-0.11	2 (2%)	65	63	56, 74, 83, 87	0
38	1g	155/156 (99%)	0.48	12 (7%)	13	10	66, 79, 91, 98	0
38	2g	155/156 (99%)	0.87	19 (12%)	4	3	67, 81, 91, 97	0
39	1h	137/138 (99%)	0.05	1 (0%)	87	87	53, 69, 77, 82	0
39	2h	137/138 (99%)	0.35	5 (3%)	42	37	62, 75, 84, 91	0
40	1i	127/128 (99%)	0.77	11 (8%)	10	7	61, 87, 95, 97	0
40	2i	127/128 (99%)	1.43	31 (24%)	0	0	67, 88, 95, 102	0
41	1j	97/105 (92%)	0.93	12 (12%)	4	3	57, 87, 95, 98	0
41	2j	96/105 (91%)	1.35	23 (23%)	0	0	76, 91, 101, 102	0
42	1k	114/129 (88%)	0.03	1 (0%)	84	84	38, 67, 80, 94	0
42	2k	114/129 (88%)	0.36	5 (4%)	34	30	52, 76, 86, 92	0
43	1l	122/132 (92%)	-0.02	2 (1%)	72	71	49, 63, 76, 89	0
43	2l	122/132 (92%)	0.10	1 (0%)	86	86	56, 67, 76, 82	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
44	1m	118/126 (93%)	0.16	1 (0%)	86	86	58, 80, 87, 92	0
44	2m	116/126 (92%)	0.60	16 (13%)	2	2	70, 83, 89, 96	0
45	1n	60/61 (98%)	0.55	5 (8%)	11	8	60, 77, 86, 92	0
45	2n	60/61 (98%)	1.36	15 (25%)	0	0	77, 88, 94, 96	0
46	1o	88/89 (98%)	0.16	3 (3%)	45	40	50, 65, 82, 86	0
46	2o	88/89 (98%)	0.29	3 (3%)	45	40	60, 74, 87, 92	0
47	1p	82/88 (93%)	0.57	5 (6%)	21	17	62, 77, 88, 93	0
47	2p	82/88 (93%)	0.43	5 (6%)	21	17	59, 70, 79, 91	0
48	1q	99/105 (94%)	0.20	0	100	100	47, 68, 80, 83	0
48	2q	99/105 (94%)	0.25	2 (2%)	65	63	58, 72, 81, 85	0
49	1r	68/88 (77%)	0.48	4 (5%)	22	18	58, 68, 83, 87	0
49	2r	68/88 (77%)	0.84	10 (14%)	2	1	63, 74, 84, 88	0
50	1s	84/93 (90%)	0.69	7 (8%)	11	8	67, 81, 92, 98	0
50	2s	83/93 (89%)	1.65	31 (37%)	0	0	76, 91, 102, 105	0
51	1t	96/106 (90%)	0.42	1 (1%)	82	82	57, 75, 84, 90	0
51	2t	96/106 (90%)	0.30	2 (2%)	63	61	56, 73, 84, 87	0
52	1u	23/27 (85%)	0.74	2 (8%)	10	7	68, 77, 82, 85	0
52	2u	23/27 (85%)	1.80	9 (39%)	0	0	68, 80, 85, 88	0
53	1v	5/24 (20%)	0.36	0	100	100	50, 55, 86, 88	0
53	2v	5/24 (20%)	1.44	2 (40%)	0	0	73, 74, 89, 103	0
54	1x	72/77 (93%)	0.11	0	100	100	34, 68, 85, 99	0
54	2x	72/77 (93%)	0.35	1 (1%)	75	75	36, 71, 87, 101	0
55	1z	12/15 (80%)	0.12	0	100	100	29, 36, 72, 81	0
55	2z	13/15 (86%)	0.48	2 (15%)	2	1	31, 37, 84, 91	0
All	All	20521/21474 (95%)	0.10	677 (3%)	46	41	15, 62, 92, 115	0

All (677) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
38	1g	79	ARG	7.5
32	1a	980	G	7.5
32	2a	980	G	7.1
32	1a	981	G	6.9
33	1b	227	GLY	6.9

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Mol	Chain	Res	Type	RSRZ
38	1g	156	TRP	6.8
34	2c	155	GLY	6.6
32	2a	981	G	6.3
32	1a	979	A	6.0
38	2g	156	TRP	6.0
33	1b	228	GLY	5.9
1	2A	2812	G	5.9
32	2a	979	A	5.7
38	1g	78	ARG	5.5
41	1j	98	ILE	5.4
7	2H	111	HIS	5.4
40	2i	15	ALA	5.4
38	1g	80	VAL	5.3
52	2u	14	TRP	5.3
45	2n	25	VAL	5.3
7	2H	112	PRO	5.1
1	1A	1554	C	5.0
41	2j	85	LEU	5.0
20	2Y	1	MET	5.0
38	2g	78	ARG	4.9
34	2c	189	ALA	4.9
32	1a	982	G	4.8
1	1A	2815	G	4.8
12	1Q	59	ARG	4.7
40	2i	21	PRO	4.7
38	1g	81	GLY	4.6
41	2j	63	PHE	4.6
55	2z	13	PRO	4.5
26	24	68	ARG	4.5
32	2a	1509	A	4.5
40	2i	36	TYR	4.5
20	2Y	5	MET	4.5
38	2g	82	GLY	4.5
1	2A	2815	G	4.5
1	2A	2811	A	4.4
52	2u	13	ILE	4.4
50	2s	71	LEU	4.4
40	2i	5	TYR	4.3
7	2H	106	THR	4.3
49	2r	43	PHE	4.3
38	2g	154	TYR	4.3
38	2g	80	VAL	4.3

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Mol	Chain	Res	Type	RSRZ
40	2i	62	TYR	4.2
41	2j	5	ARG	4.2
32	1a	211	U	4.2
7	2H	115	VAL	4.2
1	2A	2805	G	4.2
32	1a	1023	U	4.2
33	2b	187	LEU	4.1
45	2n	49	HIS	4.1
50	2s	6	LYS	4.1
45	1n	2	ALA	4.0
32	1a	978	U	4.0
16	2U	88	ILE	4.0
29	17	48	LYS	4.0
6	2G	48	GLU	4.0
38	1g	77	SER	3.9
34	2c	8	ILE	3.9
40	2i	30	GLY	3.9
32	2a	1000	G	3.9
40	2i	7	THR	3.9
7	2H	103	LEU	3.9
32	2a	982	G	3.9
1	2A	217	A	3.9
38	2g	83	ALA	3.9
1	2A	2813	C	3.8
33	2b	118	LEU	3.8
20	1Y	1	MET	3.8
33	2b	101	MET	3.8
50	2s	8	GLY	3.8
41	1j	97	GLU	3.8
49	2r	66	LEU	3.8
40	2i	20	ARG	3.8
26	14	53	GLU	3.8
34	2c	2	GLY	3.8
50	2s	80	TYR	3.7
34	2c	180	ALA	3.7
19	2X	92	LEU	3.7
8	2I	11	ASN	3.7
6	2G	86	MET	3.7
40	2i	66	ARG	3.7
33	1b	232	PRO	3.7
1	2A	1149	C	3.7
35	2d	49	ARG	3.7

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Mol	Chain	Res	Type	RSRZ
33	2b	132	LYS	3.6
40	2i	68	GLY	3.6
33	2b	31	TYR	3.6
34	2c	186	PHE	3.6
32	2a	1510	U	3.6
50	2s	12	ASP	3.6
1	2A	1134	G	3.6
22	20	75	LEU	3.6
34	2c	66	VAL	3.6
41	1j	72	VAL	3.6
1	2A	1554	C	3.6
22	20	76	GLY	3.6
7	2H	95	ARG	3.6
50	2s	24	ALA	3.5
1	2A	1091	A	3.5
26	24	45	GLY	3.5
44	2m	94	ARG	3.5
8	2I	81	VAL	3.5
33	2b	131	PRO	3.5
53	2v	14	A	3.5
7	2H	2	SER	3.5
40	2i	9	ARG	3.5
1	1A	1098	C	3.5
7	2H	107	VAL	3.5
1	1A	2904	C	3.5
6	2G	27	ASN	3.4
19	2X	68	ARG	3.4
26	14	55	ARG	3.4
44	2m	95	GLY	3.4
32	2a	1239	U	3.4
40	2i	61	ALA	3.4
50	2s	34	TRP	3.4
41	1j	4	ILE	3.4
6	1G	51	ARG	3.4
8	2I	107	VAL	3.4
1	1A	2905	U	3.4
8	2I	46	ALA	3.4
8	2I	85	GLU	3.4
14	2S	58	LEU	3.4
40	1i	19	LEU	3.4
33	1b	29	ALA	3.4
32	2a	1024	A	3.4

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Mol	Chain	Res	Type	RSRZ
32	1a	1120	C	3.4
1	1A	2814	C	3.4
6	2G	28	VAL	3.4
1	2A	2816	G	3.3
33	2b	37	ASN	3.3
6	2G	26	GLN	3.3
32	1a	209	U	3.3
33	2b	228	GLY	3.3
52	2u	6	ARG	3.3
1	2A	2904	C	3.3
50	2s	38	SER	3.3
32	2a	1025	G	3.3
34	1c	81	GLY	3.3
34	2c	179	ARG	3.3
1	2A	1132	G	3.3
26	24	49	PHE	3.2
7	2H	6	ARG	3.2
40	2i	115	GLY	3.2
41	2j	89	ASP	3.2
33	1b	122	PHE	3.2
47	1p	39	TYR	3.2
21	2Z	96	VAL	3.2
33	2b	188	ALA	3.2
41	2j	71	LEU	3.2
44	2m	102	ARG	3.2
1	2A	1130	A	3.2
34	1c	78	GLY	3.2
34	2c	190	ARG	3.2
52	2u	16	GLY	3.2
1	2A	2905	U	3.2
41	2j	40	LEU	3.2
49	2r	85	LEU	3.2
1	2A	2902	G	3.2
11	2P	118	GLY	3.2
32	2a	1026	C	3.2
32	1a	1024	A	3.2
6	2G	19	LEU	3.2
52	2u	17	THR	3.1
49	2r	31	LEU	3.1
50	2s	52	TYR	3.1
7	2H	101	ARG	3.1
33	1b	63	MET	3.1

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Mol	Chain	Res	Type	RSRZ
39	2h	122	ARG	3.1
26	14	66	SER	3.1
41	2j	6	ILE	3.1
33	2b	165	VAL	3.1
50	2s	41	VAL	3.1
40	2i	16	ARG	3.1
34	2c	154	SER	3.1
41	2j	27	ALA	3.1
1	2A	678	A	3.1
1	1A	2205	G	3.1
47	1p	41	PRO	3.1
7	2H	114	VAL	3.1
17	2V	72	VAL	3.1
34	1c	206	GLU	3.1
41	1j	85	LEU	3.1
41	1j	90	LEU	3.0
1	1A	1220	G	3.0
1	2A	1089	G	3.0
32	1a	1002	G	3.0
41	2j	65	LEU	3.0
1	1A	2811	A	3.0
34	2c	57	ILE	3.0
52	2u	22	ARG	3.0
41	2j	74	ILE	3.0
50	2s	40	ILE	3.0
32	2a	1268	A	3.0
33	1b	33	TYR	3.0
1	2A	2806	C	3.0
32	2a	986	C	3.0
34	2c	124	ILE	3.0
40	2i	14	VAL	3.0
44	2m	7	VAL	3.0
1	2A	1128	U	3.0
31	29	37	GLY	3.0
38	2g	16	LEU	3.0
41	2j	8	LEU	3.0
34	2c	159	GLY	3.0
41	2j	10	GLY	3.0
50	2s	64	GLU	3.0
32	1a	825	U	3.0
1	2A	2804	G	3.0
41	1j	10	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
44	2m	103	THR	3.0
21	2Z	125	LEU	2.9
11	2P	116	GLY	2.9
38	2g	79	ARG	2.9
1	1A	1149	C	2.9
45	2n	32	SER	2.9
32	2a	983	A	2.9
33	1b	16	HIS	2.9
32	2a	999	U	2.9
1	2A	2814	C	2.9
32	1a	72	C	2.9
34	1c	207	VAL	2.9
32	2a	1265	G	2.9
40	2i	76	ALA	2.9
1	1A	2813	C	2.9
26	14	52	THR	2.9
34	2c	167	TRP	2.9
34	1c	100	ALA	2.9
40	1i	15	ALA	2.9
38	1g	153	HIS	2.9
26	24	52	THR	2.9
38	2g	81	GLY	2.9
6	2G	17	PRO	2.9
32	1a	707	U	2.9
50	1s	56	GLN	2.9
50	2s	3	ARG	2.9
6	1G	49	ASP	2.9
33	2b	232	PRO	2.9
1	2A	1129	A	2.9
47	1p	19	ILE	2.9
7	2H	123	PHE	2.9
34	2c	77	ILE	2.9
50	2s	49	ILE	2.9
40	1i	8	GLY	2.9
5	2F	15	SER	2.8
47	2p	59	TRP	2.8
34	1c	64	VAL	2.8
1	1A	2804	G	2.8
32	1a	1000	G	2.8
32	2a	1002	G	2.8
42	2k	13	GLN	2.8
32	2a	1022	C	2.8

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Mol	Chain	Res	Type	RSRZ
32	1a	1268	A	2.8
1	2A	2901	G	2.8
21	2Z	5	LEU	2.8
35	2d	183	GLY	2.8
1	2A	10	G	2.8
41	2j	26	ALA	2.8
49	2r	23	LYS	2.8
32	1a	1027	A	2.8
26	24	67	TYR	2.8
52	1u	18	TYR	2.8
1	2A	697	G	2.8
7	2H	97	ARG	2.8
16	2U	116	ALA	2.8
44	1m	2	ALA	2.8
41	1j	62	HIS	2.8
32	1a	977	C	2.8
44	2m	64	TRP	2.8
1	2A	1101	G	2.8
44	2m	78	ILE	2.8
52	2u	11	GLY	2.8
50	2s	79	THR	2.8
7	2H	102	ALA	2.8
32	1a	88	C	2.8
5	2F	14	PRO	2.8
7	2H	148	ILE	2.8
7	2H	44	VAL	2.8
6	2G	29	TRP	2.7
50	2s	43	GLU	2.7
34	2c	87	LEU	2.7
45	2n	2	ALA	2.7
54	2x	47	U	2.7
40	1i	102	LEU	2.7
26	14	57	GLU	2.7
20	2Y	55	TYR	2.7
39	2h	131	GLY	2.7
32	2a	978	U	2.7
40	2i	17	VAL	2.7
33	1b	123	ALA	2.7
33	1b	124	SER	2.7
14	2S	35	ILE	2.7
33	2b	197	VAL	2.7
11	2P	91	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
32	2a	211	U	2.7
1	2A	669	C	2.7
32	2a	1184	G	2.7
33	1b	131	PRO	2.7
33	2b	123	ALA	2.7
1	2A	1106	U	2.7
1	1A	695	C	2.7
50	2s	20	LEU	2.7
32	2a	976	G	2.7
14	2S	34	HIS	2.7
33	2b	70	PHE	2.7
40	2i	88	TYR	2.7
8	2I	86	THR	2.7
7	2H	113	VAL	2.7
1	1A	2806	C	2.7
29	27	48	LYS	2.7
34	2c	147	LYS	2.7
19	2X	86	GLY	2.7
32	1a	77	G	2.7
45	2n	36	PHE	2.6
32	1a	983	A	2.6
7	2H	169	VAL	2.6
36	2e	22	GLY	2.6
44	2m	75	ALA	2.6
37	2f	97	PHE	2.6
45	2n	34	TYR	2.6
33	1b	132	LYS	2.6
45	1n	16	PHE	2.6
32	1a	1025	G	2.6
21	2Z	143	GLY	2.6
38	2g	132	GLY	2.6
50	2s	9	VAL	2.6
50	2s	53	ASN	2.6
33	1b	225	ALA	2.6
44	2m	42	ALA	2.6
1	1A	934	C	2.6
1	1A	2206	C	2.6
1	2A	934	C	2.6
33	1b	28	PHE	2.6
32	1a	1239	U	2.6
33	1b	31	TYR	2.6
34	1c	87	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
2	2B	119	G	2.6
32	1a	984	A	2.6
38	2g	84	ASN	2.6
34	1c	39	ILE	2.6
40	2i	87	GLN	2.6
41	1j	71	LEU	2.6
45	2n	39	LEU	2.6
41	2j	49	VAL	2.6
50	1s	50	ALA	2.6
1	2A	1090	A	2.6
32	2a	984	A	2.6
32	2a	1023	U	2.6
26	14	54	GLY	2.6
43	2l	64	TYR	2.6
7	2H	93	GLY	2.6
34	1c	205	GLY	2.6
40	2i	8	GLY	2.6
40	2i	102	LEU	2.6
1	2A	2206	C	2.6
32	1a	1026	C	2.6
33	2b	218	ALA	2.6
11	2P	122	PRO	2.6
38	2g	54	THR	2.5
1	2A	9	G	2.5
7	2H	96	ALA	2.5
16	2U	117	GLN	2.5
47	2p	60	LEU	2.5
40	2i	95	LYS	2.5
41	2j	68	HIS	2.5
1	2A	1553	A	2.5
1	1A	2805	G	2.5
38	1g	84	ASN	2.5
46	1o	19	PRO	2.5
21	2Z	133	ILE	2.5
8	2I	77	LEU	2.5
21	2Z	175	VAL	2.5
14	2S	45	GLY	2.5
20	2Y	90	LEU	2.5
49	1r	31	LEU	2.5
32	1a	210	U	2.5
33	2b	152	PHE	2.5
7	1H	2	SER	2.5

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Mol	Chain	Res	Type	RSRZ
26	24	46	GLN	2.5
33	2b	201	ILE	2.5
41	2j	38	ILE	2.5
1	1A	2812	G	2.5
50	1s	61	TYR	2.5
25	23	59	VAL	2.5
33	2b	97	TRP	2.5
20	2Y	57	GLN	2.5
34	1c	193	TYR	2.5
38	2g	86	GLN	2.5
40	1i	36	TYR	2.5
32	2a	977	C	2.5
35	1d	175	SER	2.5
31	29	13	LYS	2.5
8	2I	14	ASP	2.5
47	1p	42	ARG	2.5
40	2i	27	THR	2.5
51	2t	41	ILE	2.5
33	2b	150	SER	2.5
40	1i	98	PRO	2.5
40	1i	6	GLY	2.5
1	2A	2125	G	2.5
11	2P	123	LEU	2.5
50	2s	35	SER	2.4
50	2s	76	PRO	2.4
32	2a	88	C	2.4
32	1a	999	U	2.4
49	2r	22	VAL	2.4
21	2Z	164	ALA	2.4
6	2G	137	GLU	2.4
1	2A	1104	G	2.4
7	2H	110	SER	2.4
40	2i	80	GLY	2.4
44	2m	92	HIS	2.4
1	2A	1150	U	2.4
14	2S	52	SER	2.4
22	20	69	PHE	2.4
35	1d	133	VAL	2.4
1	2A	1092	G	2.4
34	2c	160	ALA	2.4
25	23	60	GLU	2.4
50	2s	47	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
11	2P	85	LEU	2.4
55	2z	12	PRO	2.4
36	2e	148	VAL	2.4
7	2H	116	GLU	2.4
1	2A	5	A	2.4
1	2A	2817	U	2.4
33	2b	124	SER	2.4
52	1u	15	ARG	2.4
44	2m	40	ASN	2.4
50	2s	23	ASN	2.4
1	2A	1088	C	2.4
32	1a	208	C	2.4
32	1a	1022	C	2.4
32	1a	212	G	2.4
32	2a	1159	G	2.4
6	2G	25	TYR	2.4
50	1s	39	THR	2.4
4	2E	1	MET	2.4
1	2A	680	C	2.4
3	2D	270	ILE	2.4
11	2P	100	LEU	2.4
41	1j	6	ILE	2.4
46	2o	87	ILE	2.4
38	2g	113	GLU	2.4
6	1G	50	ALA	2.4
40	1i	46	ALA	2.4
32	2a	998	C	2.4
33	1b	136	VAL	2.4
1	2A	2330	G	2.4
14	2S	55	ALA	2.4
20	2Y	91	GLU	2.3
39	2h	128	GLY	2.3
45	2n	38	GLY	2.3
6	2G	49	ASP	2.3
33	1b	101	MET	2.3
1	1A	679	G	2.3
11	2P	88	LEU	2.3
32	2a	1207	A	2.3
35	1d	174	LEU	2.3
35	2d	146	ILE	2.3
38	1g	120	ILE	2.3
50	2s	16	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
45	1n	8	GLU	2.3
40	2i	37	PHE	2.3
21	2Z	50	GLN	2.3
34	1c	201	TYR	2.3
6	1G	78	SER	2.3
41	2j	98	ILE	2.3
47	2p	19	ILE	2.3
32	1a	985	C	2.3
52	2u	18	TYR	2.3
37	2f	89	MET	2.3
1	2A	1102	A	2.3
1	2A	1136	G	2.3
2	2B	118	G	2.3
6	1G	75	LYS	2.3
23	21	29	GLY	2.3
32	1a	1121	G	2.3
46	1o	17	ARG	2.3
6	2G	2	PRO	2.3
43	1l	64	TYR	2.3
21	2Z	2	GLU	2.3
45	2n	8	GLU	2.3
34	2c	39	ILE	2.3
34	1c	158	GLY	2.3
50	1s	19	VAL	2.3
1	1A	682	G	2.3
32	2a	1001	G	2.3
32	2a	1021	C	2.3
45	2n	35	ARG	2.3
48	2q	10	VAL	2.3
32	2a	1114	G	2.3
32	2a	1147	G	2.3
33	2b	222	ILE	2.3
39	2h	127	LEU	2.3
47	2p	7	ALA	2.3
45	2n	29	ARG	2.3
50	1s	47	HIS	2.3
12	2Q	60	ARG	2.3
33	2b	83	MET	2.3
14	2S	46	VAL	2.3
7	2H	8	PRO	2.3
11	2P	1	MET	2.3
32	1a	73	C	2.3

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Mol	Chain	Res	Type	RSRZ
45	2n	37	PHE	2.3
1	2A	679	G	2.3
45	2n	18	VAL	2.2
50	2s	45	VAL	2.2
33	1b	222	ILE	2.2
34	2c	185	GLY	2.2
34	2c	194	GLY	2.2
42	2k	42	TRP	2.2
43	1l	28	LYS	2.2
39	1h	62	TYR	2.2
51	1t	55	ILE	2.2
11	2P	92	GLU	2.2
38	1g	56	GLN	2.2
49	2r	56	THR	2.2
33	1b	142	LEU	2.2
42	2k	90	GLY	2.2
40	2i	125	TYR	2.2
23	1l	2	SER	2.2
7	2H	128	PRO	2.2
21	2Z	155	LEU	2.2
34	2c	205	GLY	2.2
41	1j	96	ILE	2.2
49	2r	24	ALA	2.2
38	2g	18	TYR	2.2
1	1A	1097	C	2.2
1	2A	1125	C	2.2
14	2S	93	LYS	2.2
1	2A	1112	A	2.2
1	2A	1142	U	2.2
35	1d	23	GLY	2.2
40	2i	64	THR	2.2
20	2Y	48	ALA	2.2
1	2A	2121	G	2.2
7	2H	164	TYR	2.2
34	2c	197	GLY	2.2
50	2s	13	ASP	2.2
11	2P	90	ARG	2.2
30	28	21	LYS	2.2
33	1b	214	ILE	2.2
40	1i	106	ALA	2.2
40	2i	83	ARG	2.2
50	1s	40	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
7	2H	94	TYR	2.2
33	2b	227	GLY	2.2
42	2k	96	ARG	2.2
50	2s	25	LYS	2.2
8	2I	19	VAL	2.2
34	2c	103	VAL	2.2
6	2G	72	ARG	2.2
1	1A	1150	U	2.2
1	2A	1071	U	2.2
1	2A	1127	U	2.2
8	2I	79	ILE	2.2
8	2I	100	ALA	2.2
38	2g	152	ALA	2.2
41	2j	18	ALA	2.2
14	2S	31	SER	2.2
45	2n	60	SER	2.2
49	1r	25	THR	2.2
39	2h	93	VAL	2.2
47	2p	39	TYR	2.2
20	2Y	2	ARG	2.2
33	1b	30	ARG	2.2
1	2A	33	C	2.2
1	2A	1135	U	2.2
32	2a	1266	C	2.2
33	2b	133	LYS	2.2
38	1g	82	GLY	2.1
38	2g	117	ALA	2.1
1	2A	6	G	2.1
45	1n	17	LYS	2.1
52	2u	24	ARG	2.1
38	1g	132	GLY	2.1
33	2b	121	LEU	2.1
41	2j	88	LEU	2.1
1	2A	1111	U	2.1
49	1r	24	ALA	2.1
41	1j	40	LEU	2.1
1	2A	1143	A	2.1
21	2Z	57	ILE	2.1
46	1o	6	GLU	2.1
41	2j	72	VAL	2.1
48	2q	8	GLY	2.1
41	2j	55	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
47	1p	38	TYR	2.1
32	2a	826	C	2.1
49	1r	52	PRO	2.1
44	2m	60	VAL	2.1
49	2r	21	LYS	2.1
14	2S	5	THR	2.1
44	2m	48	LEU	2.1
49	2r	46	GLU	2.1
33	1b	207	ALA	2.1
32	2a	1231	C	2.1
40	2i	65	VAL	2.1
38	2g	4	ARG	2.1
8	2I	72	LEU	2.1
20	2Y	89	PHE	2.1
45	1n	13	THR	2.1
51	2t	24	LEU	2.1
33	1b	195	ASP	2.1
2	2B	86	G	2.1
1	2A	1115	A	2.1
8	2I	92	VAL	2.1
32	2a	1432	A	2.1
21	2Z	65	GLN	2.1
1	1A	8	U	2.1
33	2b	161	ALA	2.1
20	2Y	58	GLY	2.1
25	23	47	VAL	2.1
32	2a	79	G	2.1
34	1c	98	ASN	2.1
6	2G	35	GLU	2.1
1	2A	300	C	2.1
1	2A	1110	U	2.1
1	2A	2903	U	2.1
29	27	47	ARG	2.1
29	27	46	VAL	2.1
33	2b	229	VAL	2.1
1	1A	2121	G	2.1
1	2A	1103	G	2.1
1	2A	2207	G	2.1
53	2v	18	G	2.1
1	2A	1131	A	2.0
14	2S	84	GLN	2.0
32	2a	985	C	2.0

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Mol	Chain	Res	Type	RSRZ
50	2s	4	SER	2.0
3	2D	273	ARG	2.0
32	1a	86	U	2.0
46	2o	86	GLY	2.0
50	2s	63	THR	2.0
6	2G	80	PHE	2.0
42	1k	13	GLN	2.0
1	2A	681	G	2.0
32	2a	1243	A	2.0
33	1b	41	ILE	2.0
3	2D	275	LYS	2.0
33	2b	105	PHE	2.0
33	1b	201	ILE	2.0
42	2k	43	SER	2.0
45	2n	11	LYS	2.0
1	2A	2124	C	2.0
40	2i	24	GLY	2.0
44	2m	6	GLY	2.0
44	2m	76	ALA	2.0
1	1A	1099	A	2.0
40	1i	7	THR	2.0
34	1c	79	ARG	2.0
40	2i	18	PHE	2.0
7	2H	105	LEU	2.0
50	2s	28	LYS	2.0
33	1b	19	HIS	2.0
41	2j	62	HIS	2.0
44	2m	38	GLY	2.0
46	2o	6	GLU	2.0
50	2s	31	ILE	2.0
35	1d	208	SER	2.0
1	1A	2204	C	2.0
32	1a	87	C	2.0
38	2g	85	TYR	2.0
32	2a	78	G	2.0
25	23	35	ARG	2.0
34	1c	179	ARG	2.0
40	1i	26	VAL	2.0
41	2j	34	VAL	2.0
25	23	26	LEU	2.0
26	24	8	LYS	2.0
20	2Y	43	ASN	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
54	PSU	2x	55	20/21	0.88	0.17	62,68,78,88	0
54	5MC	2x	32	21/22	0.91	0.25	68,80,88,91	0
54	5MU	2x	54	21/22	0.93	0.20	72,76,86,101	0
54	5MC	1x	32	21/22	0.94	0.20	51,62,76,86	0
54	PSU	1x	55	20/21	0.94	0.18	57,65,79,80	0
54	5MU	1x	54	21/22	0.94	0.17	50,67,76,78	0
54	4SU	2x	8	20/21	0.95	0.14	57,78,89,92	0
54	4SU	1x	8	20/21	0.96	0.17	47,65,79,80	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3298	1/1	0.35	0.29	81,81,81,81	0
56	MG	1A	3517	1/1	0.35	0.31	69,69,69,69	0
56	MG	1A	3901	1/1	0.36	0.59	86,86,86,86	0
56	MG	1F	304	1/1	0.41	0.57	73,73,73,73	0
56	MG	2A	3074	1/1	0.52	0.21	54,54,54,54	0
56	MG	2a	3006	1/1	0.54	0.14	77,77,77,77	0
56	MG	2A	3093	1/1	0.55	0.55	57,57,57,57	0
56	MG	2G	3001	1/1	0.55	0.22	56,56,56,56	0
56	MG	1a	1639	1/1	0.55	0.55	77,77,77,77	0
56	MG	1A	3411	1/1	0.58	0.41	51,51,51,51	0
56	MG	1a	1756	1/1	0.58	0.49	58,58,58,58	0
56	MG	1a	1645	1/1	0.59	0.40	78,78,78,78	0
56	MG	14	502	1/1	0.61	0.25	64,64,64,64	0
56	MG	1A	4041	1/1	0.61	0.15	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3548	1/1	0.62	0.17	72,72,72,72	0
56	MG	2A	3230	1/1	0.62	0.30	47,47,47,47	0
56	MG	2a	3031	1/1	0.62	0.23	88,88,88,88	0
56	MG	1a	1802	1/1	0.63	0.27	68,68,68,68	0
56	MG	1A	3146	1/1	0.64	0.24	62,62,62,62	0
56	MG	1a	1757	1/1	0.64	0.42	69,69,69,69	0
56	MG	1A	4076	1/1	0.64	0.30	72,72,72,72	0
56	MG	2a	3122	1/1	0.65	0.39	71,71,71,71	0
56	MG	2a	3153	1/1	0.65	0.17	92,92,92,92	0
56	MG	1A	3369	1/1	0.66	0.39	67,67,67,67	0
56	MG	1A	3544	1/1	0.66	0.39	61,61,61,61	0
56	MG	1A	3320	1/1	0.66	0.53	70,70,70,70	0
56	MG	2A	3124	1/1	0.67	0.35	65,65,65,65	0
56	MG	2a	3138	1/1	0.67	0.45	81,81,81,81	0
56	MG	2a	3088	1/1	0.67	0.07	76,76,76,76	0
57	ZN	24	501	1/1	0.67	0.07	133,133,133,133	0
56	MG	2A	3197	1/1	0.68	0.15	63,63,63,63	0
56	MG	1A	3897	1/1	0.68	0.28	60,60,60,60	0
56	MG	2a	3053	1/1	0.68	0.16	99,99,99,99	0
56	MG	2a	3206	1/1	0.68	0.17	56,56,56,56	0
56	MG	2A	3194	1/1	0.68	0.25	56,56,56,56	0
56	MG	1A	3333	1/1	0.69	0.53	57,57,57,57	0
56	MG	2A	3243	1/1	0.69	0.13	69,69,69,69	0
56	MG	1A	3935	1/1	0.69	0.20	52,52,52,52	0
56	MG	2A	3171	1/1	0.69	0.32	49,49,49,49	0
56	MG	1a	1851	1/1	0.69	0.12	56,56,56,56	0
56	MG	1A	3511	1/1	0.69	0.38	55,55,55,55	0
56	MG	1A	3699	1/1	0.70	0.28	58,58,58,58	0
56	MG	2A	3065	1/1	0.70	0.17	55,55,55,55	0
56	MG	2A	3432	1/1	0.71	0.21	55,55,55,55	0
56	MG	2A	3081	1/1	0.71	0.24	54,54,54,54	0
56	MG	2a	3150	1/1	0.71	0.28	76,76,76,76	0
56	MG	2A	3224	1/1	0.72	0.34	73,73,73,73	0
56	MG	1A	3138	1/1	0.72	0.29	48,48,48,48	0
56	MG	1A	3502	1/1	0.72	0.15	70,70,70,70	0
56	MG	1a	1823	1/1	0.72	0.26	71,71,71,71	0
56	MG	1a	1619	1/1	0.72	0.15	75,75,75,75	0
56	MG	1a	1796	1/1	0.73	0.08	85,85,85,85	0
56	MG	1Z	301	1/1	0.73	0.12	94,94,94,94	0
56	MG	2a	3043	1/1	0.73	0.43	78,78,78,78	0
56	MG	1A	3016	1/1	0.73	0.16	56,56,56,56	0
56	MG	1A	3384	1/1	0.73	0.50	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3116	1/1	0.73	0.23	52,52,52,52	0
56	MG	1A	3326	1/1	0.73	0.17	62,62,62,62	0
56	MG	2a	3149	1/1	0.73	0.18	63,63,63,63	0
56	MG	1A	3237	1/1	0.73	0.15	58,58,58,58	0
56	MG	1T	206	1/1	0.73	0.43	76,76,76,76	0
56	MG	2A	3104	1/1	0.73	0.17	59,59,59,59	0
56	MG	2l	3002	1/1	0.73	0.27	68,68,68,68	0
56	MG	2a	3001	1/1	0.73	0.48	62,62,62,62	0
56	MG	1a	1750	1/1	0.74	0.34	69,69,69,69	0
56	MG	2Q	3005	1/1	0.74	0.31	54,54,54,54	0
56	MG	1A	3218	1/1	0.74	0.30	58,58,58,58	0
56	MG	1H	3002	1/1	0.74	0.25	62,62,62,62	0
56	MG	11	102	1/1	0.74	0.24	65,65,65,65	0
56	MG	12	3001	1/1	0.74	0.44	57,57,57,57	0
56	MG	2A	3483	1/1	0.74	0.12	72,72,72,72	0
56	MG	2B	202	1/1	0.74	0.15	55,55,55,55	0
56	MG	1A	3012	1/1	0.75	0.23	66,66,66,66	0
56	MG	2A	3380	1/1	0.75	0.12	59,59,59,59	0
56	MG	1A	4058	1/1	0.75	0.33	48,48,48,48	0
56	MG	1A	4027	1/1	0.75	0.55	62,62,62,62	0
56	MG	2a	3039	1/1	0.75	0.54	67,67,67,67	0
56	MG	2A	3184	1/1	0.75	0.28	45,45,45,45	0
56	MG	2a	3049	1/1	0.75	0.24	79,79,79,79	0
56	MG	2A	3233	1/1	0.75	0.11	52,52,52,52	0
56	MG	2a	3068	1/1	0.75	0.37	56,56,56,56	0
56	MG	1a	1615	1/1	0.76	0.32	66,66,66,66	0
56	MG	2A	3071	1/1	0.76	0.26	46,46,46,46	0
56	MG	1a	1699	1/1	0.76	0.20	58,58,58,58	0
56	MG	1A	3319	1/1	0.76	0.10	75,75,75,75	0
56	MG	1a	1752	1/1	0.76	0.17	61,61,61,61	0
56	MG	2a	3254	1/1	0.76	0.49	76,76,76,76	0
56	MG	2a	3022	1/1	0.76	0.16	77,77,77,77	0
56	MG	1A	3478	1/1	0.76	0.31	49,49,49,49	0
56	MG	1A	3941	1/1	0.77	0.19	60,60,60,60	0
56	MG	1A	3318	1/1	0.77	0.17	65,65,65,65	0
56	MG	2a	3133	1/1	0.77	0.14	63,63,63,63	0
56	MG	1T	202	1/1	0.77	0.27	51,51,51,51	0
56	MG	1A	3593	1/1	0.77	0.26	62,62,62,62	0
56	MG	1a	1628	1/1	0.77	0.29	57,57,57,57	0
56	MG	2a	3151	1/1	0.77	0.11	97,97,97,97	0
56	MG	2a	3044	1/1	0.77	0.12	71,71,71,71	0
56	MG	1a	1786	1/1	0.77	0.19	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3916	1/1	0.77	0.69	45,45,45,45	0
56	MG	2a	3054	1/1	0.77	0.08	96,96,96,96	0
56	MG	1A	3324	1/1	0.77	0.18	57,57,57,57	0
56	MG	1A	4054	1/1	0.78	0.43	69,69,69,69	0
56	MG	2a	3101	1/1	0.78	0.38	77,77,77,77	0
56	MG	1A	3087	1/1	0.78	0.21	45,45,45,45	0
56	MG	2a	3130	1/1	0.78	0.26	50,50,50,50	0
56	MG	1A	3601	1/1	0.78	0.20	36,36,36,36	0
56	MG	1B	205	1/1	0.78	0.16	56,56,56,56	0
56	MG	1a	1816	1/1	0.78	0.24	76,76,76,76	0
56	MG	2A	3261	1/1	0.78	0.13	43,43,43,43	0
56	MG	2A	3114	1/1	0.78	0.26	50,50,50,50	0
56	MG	1a	1820	1/1	0.78	0.09	79,79,79,79	0
56	MG	2a	3164	1/1	0.78	0.10	80,80,80,80	0
56	MG	2a	3191	1/1	0.78	0.35	88,88,88,88	0
56	MG	1A	3007	1/1	0.78	0.63	73,73,73,73	0
56	MG	2A	3488	1/1	0.78	0.10	69,69,69,69	0
56	MG	1A	3086	1/1	0.78	0.40	52,52,52,52	0
56	MG	2x	104	1/1	0.78	0.12	84,84,84,84	0
56	MG	1A	3261	1/1	0.78	0.27	68,68,68,68	0
56	MG	1A	3804	1/1	0.79	0.11	66,66,66,66	0
56	MG	1A	4016	1/1	0.79	0.21	77,77,77,77	0
56	MG	1A	3856	1/1	0.79	0.28	55,55,55,55	0
56	MG	2A	3206	1/1	0.79	0.26	50,50,50,50	0
56	MG	1A	3433	1/1	0.79	0.21	51,51,51,51	0
56	MG	2a	3047	1/1	0.79	0.14	79,79,79,79	0
56	MG	2D	302	1/1	0.79	0.25	57,57,57,57	0
56	MG	2a	3051	1/1	0.79	0.20	91,91,91,91	0
56	MG	1X	3001	1/1	0.79	0.38	56,56,56,56	0
56	MG	2A	3035	1/1	0.79	0.13	54,54,54,54	0
56	MG	2X	8001	1/1	0.79	0.16	45,45,45,45	0
56	MG	2A	3040	1/1	0.79	0.12	57,57,57,57	0
56	MG	1a	1716	1/1	0.79	0.29	54,54,54,54	0
56	MG	2a	3014	1/1	0.79	0.30	64,64,64,64	0
56	MG	1A	3335	1/1	0.80	0.75	58,58,58,58	0
56	MG	2a	3072	1/1	0.80	0.21	65,65,65,65	0
56	MG	1A	3493	1/1	0.80	0.24	64,64,64,64	0
56	MG	2A	3204	1/1	0.80	0.30	53,53,53,53	0
56	MG	1A	3632	1/1	0.80	0.17	67,67,67,67	0
56	MG	2a	3005	1/1	0.80	0.36	72,72,72,72	0
56	MG	1a	1751	1/1	0.80	0.15	64,64,64,64	0
56	MG	1A	3289	1/1	0.80	0.18	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2a	3017	1/1	0.80	0.26	61,61,61,61	0
56	MG	1A	3242	1/1	0.80	0.42	67,67,67,67	0
56	MG	1A	3248	1/1	0.80	0.13	47,47,47,47	0
56	MG	2A	3252	1/1	0.80	0.15	43,43,43,43	0
56	MG	1A	3094	1/1	0.80	0.34	54,54,54,54	0
56	MG	1A	3471	1/1	0.80	0.23	55,55,55,55	0
56	MG	1a	1798	1/1	0.80	0.29	71,71,71,71	0
56	MG	1a	1800	1/1	0.80	0.14	79,79,79,79	0
56	MG	1a	1668	1/1	0.80	0.21	63,63,63,63	0
56	MG	2q	201	1/1	0.80	0.13	58,58,58,58	0
56	MG	2t	201	1/1	0.80	0.26	58,58,58,58	0
56	MG	1a	1671	1/1	0.80	0.21	77,77,77,77	0
56	MG	1a	1686	1/1	0.80	0.12	62,62,62,62	0
56	MG	1A	3494	1/1	0.81	0.57	68,68,68,68	0
56	MG	2A	3116	1/1	0.81	0.16	54,54,54,54	0
56	MG	1A	3828	1/1	0.81	0.12	49,49,49,49	0
56	MG	1H	3003	1/1	0.81	0.30	65,65,65,65	0
56	MG	1A	3847	1/1	0.81	0.16	55,55,55,55	0
56	MG	1A	3011	1/1	0.81	0.23	47,47,47,47	0
56	MG	1a	1763	1/1	0.81	0.39	55,55,55,55	0
56	MG	1A	3019	1/1	0.81	0.45	46,46,46,46	0
56	MG	1A	3512	1/1	0.81	0.33	50,50,50,50	0
56	MG	10	106	1/1	0.81	0.19	54,54,54,54	0
56	MG	1A	3355	1/1	0.81	0.09	64,64,64,64	0
56	MG	1A	3524	1/1	0.81	0.15	68,68,68,68	0
56	MG	1A	3525	1/1	0.81	0.18	74,74,74,74	0
56	MG	1A	3456	1/1	0.81	0.17	71,71,71,71	0
56	MG	2A	3256	1/1	0.81	0.14	43,43,43,43	0
56	MG	1A	3366	1/1	0.81	0.16	42,42,42,42	0
56	MG	2A	3288	1/1	0.81	0.13	41,41,41,41	0
56	MG	1a	1825	1/1	0.81	0.31	73,73,73,73	0
56	MG	1A	3027	1/1	0.81	0.37	47,47,47,47	0
56	MG	1m	201	1/1	0.81	0.37	95,95,95,95	0
56	MG	1n	102	1/1	0.81	0.17	53,53,53,53	0
56	MG	1A	3484	1/1	0.81	0.11	45,45,45,45	0
56	MG	1A	3491	1/1	0.81	0.15	54,54,54,54	0
56	MG	1A	3644	1/1	0.81	0.15	45,45,45,45	0
56	MG	1A	4088	1/1	0.81	0.53	45,45,45,45	0
56	MG	2a	3230	1/1	0.81	0.11	67,67,67,67	0
56	MG	1A	3383	1/1	0.81	0.17	67,67,67,67	0
56	MG	2e	3001	1/1	0.81	0.46	74,74,74,74	0
56	MG	1B	210	1/1	0.81	0.24	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3087	1/1	0.81	0.20	53,53,53,53	0
56	MG	1a	1700	1/1	0.81	0.28	60,60,60,60	0
56	MG	2A	3102	1/1	0.81	0.15	51,51,51,51	0
56	MG	2x	106	1/1	0.81	0.20	82,82,82,82	0
56	MG	1E	304	1/1	0.81	0.29	65,65,65,65	0
56	MG	1a	1653	1/1	0.82	0.18	56,56,56,56	0
56	MG	1a	1784	1/1	0.82	0.29	80,80,80,80	0
56	MG	2a	3114	1/1	0.82	0.27	77,77,77,77	0
56	MG	1A	3404	1/1	0.82	0.34	54,54,54,54	0
56	MG	1A	3759	1/1	0.82	0.10	68,68,68,68	0
56	MG	1A	3123	1/1	0.82	0.25	49,49,49,49	0
56	MG	2a	3137	1/1	0.82	0.17	62,62,62,62	0
56	MG	1a	1602	1/1	0.82	0.24	61,61,61,61	0
56	MG	1A	3417	1/1	0.82	0.18	76,76,76,76	0
56	MG	1A	3174	1/1	0.82	0.13	47,47,47,47	0
56	MG	1a	1738	1/1	0.82	0.24	73,73,73,73	0
56	MG	1A	3448	1/1	0.82	0.19	56,56,56,56	0
56	MG	1a	1629	1/1	0.82	0.11	63,63,63,63	0
56	MG	2a	3173	1/1	0.82	0.13	43,43,43,43	0
56	MG	2a	3175	1/1	0.82	0.15	66,66,66,66	0
56	MG	1a	1636	1/1	0.82	0.72	53,53,53,53	0
56	MG	2A	3340	1/1	0.82	0.29	52,52,52,52	0
56	MG	2a	3217	1/1	0.82	0.46	68,68,68,68	0
56	MG	2a	3226	1/1	0.82	0.08	77,77,77,77	0
56	MG	1B	212	1/1	0.82	0.38	59,59,59,59	0
56	MG	2A	3131	1/1	0.82	0.11	56,56,56,56	0
56	MG	2A	3451	1/1	0.82	0.07	59,59,59,59	0
56	MG	2A	3467	1/1	0.82	0.22	47,47,47,47	0
56	MG	1A	3119	1/1	0.82	0.28	59,59,59,59	0
56	MG	1q	202	1/1	0.82	0.25	53,53,53,53	0
56	MG	2a	3058	1/1	0.82	0.29	66,66,66,66	0
56	MG	2A	3498	1/1	0.82	0.37	69,69,69,69	0
56	MG	2A	3186	1/1	0.82	0.22	59,59,59,59	0
57	ZN	2n	501	1/1	0.82	0.07	110,110,110,110	0
56	MG	1A	3969	1/1	0.83	0.18	77,77,77,77	0
56	MG	1A	3974	1/1	0.83	0.46	59,59,59,59	0
56	MG	2A	3246	1/1	0.83	0.14	55,55,55,55	0
56	MG	1x	108	1/1	0.83	0.23	49,49,49,49	0
56	MG	2A	3007	1/1	0.83	0.49	77,77,77,77	0
56	MG	2a	3055	1/1	0.83	0.21	81,81,81,81	0
56	MG	2A	3028	1/1	0.83	0.20	53,53,53,53	0
56	MG	1A	3376	1/1	0.83	0.25	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1a	1742	1/1	0.83	0.21	68,68,68,68	0
56	MG	1A	3020	1/1	0.83	0.24	40,40,40,40	0
56	MG	2A	3392	1/1	0.83	0.17	55,55,55,55	0
56	MG	1A	3499	1/1	0.83	0.24	64,64,64,64	0
56	MG	2A	3435	1/1	0.83	0.15	46,46,46,46	0
56	MG	2A	3436	1/1	0.83	0.15	44,44,44,44	0
56	MG	1A	3435	1/1	0.83	0.13	66,66,66,66	0
56	MG	1A	3510	1/1	0.83	0.21	46,46,46,46	0
56	MG	2A	3476	1/1	0.83	0.33	66,66,66,66	0
56	MG	1A	3074	1/1	0.83	0.34	63,63,63,63	0
56	MG	1A	4083	1/1	0.83	0.24	65,65,65,65	0
56	MG	1a	1773	1/1	0.83	0.54	77,77,77,77	0
56	MG	2A	3505	1/1	0.83	0.18	50,50,50,50	0
56	MG	1A	3451	1/1	0.83	0.45	66,66,66,66	0
56	MG	1A	3814	1/1	0.83	0.16	49,49,49,49	0
56	MG	1A	3513	1/1	0.83	0.30	59,59,59,59	0
56	MG	1A	3387	1/1	0.83	0.18	54,54,54,54	0
56	MG	2a	3202	1/1	0.83	0.15	52,52,52,52	0
56	MG	1a	1640	1/1	0.83	0.22	78,78,78,78	0
56	MG	1A	3390	1/1	0.83	0.13	52,52,52,52	0
56	MG	1a	1806	1/1	0.83	0.20	51,51,51,51	0
56	MG	2a	3229	1/1	0.83	0.21	57,57,57,57	0
56	MG	1a	1649	1/1	0.83	0.21	59,59,59,59	0
56	MG	1A	3402	1/1	0.83	0.44	60,60,60,60	0
56	MG	1A	3540	1/1	0.83	0.47	48,48,48,48	0
56	MG	1A	3084	1/1	0.83	0.28	53,53,53,53	0
56	MG	2A	3205	1/1	0.83	0.20	43,43,43,43	0
56	MG	2a	3033	1/1	0.83	0.52	64,64,64,64	0
56	MG	2a	3038	1/1	0.83	0.33	58,58,58,58	0
56	MG	1A	3546	1/1	0.83	0.10	66,66,66,66	0
56	MG	1a	1852	1/1	0.83	0.21	82,82,82,82	0
56	MG	1A	3125	1/1	0.83	0.21	52,52,52,52	0
56	MG	1A	3093	1/1	0.84	0.19	48,48,48,48	0
56	MG	1A	3031	1/1	0.84	0.24	60,60,60,60	0
56	MG	1a	1908	1/1	0.84	0.07	53,53,53,53	0
56	MG	1e	201	1/1	0.84	0.19	66,66,66,66	0
56	MG	1A	3426	1/1	0.84	0.14	54,54,54,54	0
56	MG	1A	3103	1/1	0.84	0.44	32,32,32,32	0
56	MG	1A	3042	1/1	0.84	0.25	42,42,42,42	0
56	MG	1r	3002	1/1	0.84	0.13	70,70,70,70	0
56	MG	1P	204	1/1	0.84	0.16	61,61,61,61	0
56	MG	1A	3436	1/1	0.84	0.26	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	4044	1/1	0.84	0.36	44,44,44,44	0
56	MG	1A	3439	1/1	0.84	0.17	50,50,50,50	0
56	MG	1a	1791	1/1	0.84	0.17	82,82,82,82	0
56	MG	2A	3062	1/1	0.84	0.25	46,46,46,46	0
56	MG	1a	1792	1/1	0.84	0.17	92,92,92,92	0
56	MG	1A	3896	1/1	0.84	0.09	72,72,72,72	0
56	MG	2A	3262	1/1	0.84	0.11	53,53,53,53	0
56	MG	2A	3274	1/1	0.84	0.22	37,37,37,37	0
56	MG	1A	4072	1/1	0.84	0.18	48,48,48,48	0
56	MG	1A	3162	1/1	0.84	0.40	38,38,38,38	0
56	MG	1A	3024	1/1	0.84	0.38	56,56,56,56	0
56	MG	1A	3914	1/1	0.84	0.21	41,41,41,41	0
56	MG	1a	1809	1/1	0.84	0.25	54,54,54,54	0
56	MG	18	3001	1/1	0.84	0.38	50,50,50,50	0
56	MG	1A	3193	1/1	0.84	0.14	53,53,53,53	0
56	MG	2A	3443	1/1	0.84	0.15	63,63,63,63	0
56	MG	2q	203	1/1	0.84	0.24	53,53,53,53	0
56	MG	2A	3445	1/1	0.84	0.26	74,74,74,74	0
56	MG	1A	3194	1/1	0.84	0.19	39,39,39,39	0
56	MG	1a	1748	1/1	0.84	0.41	55,55,55,55	0
56	MG	1a	1827	1/1	0.84	0.28	68,68,68,68	0
56	MG	2a	3076	1/1	0.84	0.47	65,65,65,65	0
56	MG	1A	3056	1/1	0.85	0.15	59,59,59,59	0
56	MG	23	101	1/1	0.85	0.26	50,50,50,50	0
56	MG	1a	1605	1/1	0.85	0.13	68,68,68,68	0
56	MG	2A	3120	1/1	0.85	0.36	58,58,58,58	0
56	MG	1A	3770	1/1	0.85	0.10	50,50,50,50	0
56	MG	1A	4047	1/1	0.85	0.23	47,47,47,47	0
56	MG	1A	3014	1/1	0.85	0.10	55,55,55,55	0
56	MG	2a	3019	1/1	0.85	0.31	72,72,72,72	0
56	MG	2a	3020	1/1	0.85	0.47	44,44,44,44	0
56	MG	1A	3322	1/1	0.85	0.32	53,53,53,53	0
56	MG	1A	3827	1/1	0.85	0.20	30,30,30,30	0
56	MG	1A	3446	1/1	0.85	0.18	58,58,58,58	0
56	MG	2A	3196	1/1	0.85	0.17	47,47,47,47	0
56	MG	1A	3101	1/1	0.85	0.18	50,50,50,50	0
56	MG	1a	1818	1/1	0.85	0.17	81,81,81,81	0
56	MG	1A	3287	1/1	0.85	0.30	38,38,38,38	0
56	MG	1A	3873	1/1	0.85	0.20	41,41,41,41	0
56	MG	1B	208	1/1	0.85	0.27	63,63,63,63	0
56	MG	1a	1655	1/1	0.85	0.15	60,60,60,60	0
56	MG	1A	3393	1/1	0.85	0.16	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3395	1/1	0.85	0.16	46,46,46,46	0
56	MG	1a	1874	1/1	0.85	0.14	48,48,48,48	0
56	MG	1a	1899	1/1	0.85	0.47	64,64,64,64	0
56	MG	1a	1903	1/1	0.85	0.24	56,56,56,56	0
56	MG	2a	3070	1/1	0.85	0.22	66,66,66,66	0
56	MG	1B	227	1/1	0.85	0.30	69,69,69,69	0
56	MG	1a	1693	1/1	0.85	0.10	53,53,53,53	0
56	MG	1a	1696	1/1	0.85	0.12	48,48,48,48	0
56	MG	2a	3094	1/1	0.85	0.32	55,55,55,55	0
56	MG	1A	3128	1/1	0.85	0.22	50,50,50,50	0
56	MG	2A	3298	1/1	0.85	0.17	52,52,52,52	0
56	MG	2a	3121	1/1	0.85	0.11	88,88,88,88	0
56	MG	2A	3308	1/1	0.85	0.29	53,53,53,53	0
56	MG	2a	3124	1/1	0.85	0.11	62,62,62,62	0
56	MG	2A	3311	1/1	0.85	0.17	41,41,41,41	0
56	MG	2A	3314	1/1	0.85	0.11	43,43,43,43	0
56	MG	1A	3907	1/1	0.85	0.36	50,50,50,50	0
56	MG	1A	3083	1/1	0.85	0.13	45,45,45,45	0
56	MG	2a	3145	1/1	0.85	0.12	95,95,95,95	0
56	MG	2a	3147	1/1	0.85	0.25	68,68,68,68	0
56	MG	1x	102	1/1	0.85	0.46	67,67,67,67	0
56	MG	1A	3408	1/1	0.85	0.35	58,58,58,58	0
56	MG	2A	3433	1/1	0.85	0.26	43,43,43,43	0
56	MG	1H	3004	1/1	0.85	0.24	66,66,66,66	0
56	MG	2a	3162	1/1	0.85	0.15	79,79,79,79	0
56	MG	1A	3554	1/1	0.85	0.18	65,65,65,65	0
56	MG	2a	3167	1/1	0.85	0.36	59,59,59,59	0
56	MG	2A	3437	1/1	0.85	0.13	69,69,69,69	0
56	MG	1A	3348	1/1	0.85	0.30	52,52,52,52	0
56	MG	1A	3948	1/1	0.85	0.53	41,41,41,41	0
56	MG	2a	3193	1/1	0.85	0.16	65,65,65,65	0
56	MG	1A	3306	1/1	0.85	0.66	69,69,69,69	0
56	MG	1a	1755	1/1	0.85	0.22	57,57,57,57	0
56	MG	2a	3212	1/1	0.85	0.18	46,46,46,46	0
56	MG	1A	3317	1/1	0.85	0.21	63,63,63,63	0
56	MG	1A	3090	1/1	0.85	0.23	47,47,47,47	0
56	MG	2A	3076	1/1	0.85	0.22	56,56,56,56	0
56	MG	1A	3509	1/1	0.85	0.29	68,68,68,68	0
56	MG	2a	3242	1/1	0.85	0.09	73,73,73,73	0
56	MG	2a	3253	1/1	0.85	0.28	54,54,54,54	0
56	MG	1a	1764	1/1	0.85	0.16	59,59,59,59	0
56	MG	2A	3554	1/1	0.85	0.18	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3557	1/1	0.85	0.16	54,54,54,54	0
56	MG	1A	4034	1/1	0.85	0.12	72,72,72,72	0
56	MG	2B	204	1/1	0.85	0.37	65,65,65,65	0
56	MG	2B	210	1/1	0.85	0.34	65,65,65,65	0
56	MG	2A	3097	1/1	0.85	0.15	51,51,51,51	0
56	MG	2D	303	1/1	0.85	0.34	45,45,45,45	0
56	MG	1A	4036	1/1	0.85	0.19	54,54,54,54	0
56	MG	1A	4038	1/1	0.85	0.13	54,54,54,54	0
56	MG	2A	3038	1/1	0.86	0.20	45,45,45,45	0
56	MG	1A	3316	1/1	0.86	0.29	51,51,51,51	0
56	MG	2A	3044	1/1	0.86	0.22	51,51,51,51	0
56	MG	2A	3054	1/1	0.86	0.13	58,58,58,58	0
56	MG	1A	3023	1/1	0.86	0.34	55,55,55,55	0
56	MG	2A	3353	1/1	0.86	0.27	41,41,41,41	0
56	MG	2A	3363	1/1	0.86	0.12	49,49,49,49	0
56	MG	2a	3064	1/1	0.86	0.27	79,79,79,79	0
56	MG	2A	3364	1/1	0.86	0.17	44,44,44,44	0
56	MG	1B	230	1/1	0.86	0.23	67,67,67,67	0
56	MG	1E	302	1/1	0.86	0.41	41,41,41,41	0
56	MG	1A	3356	1/1	0.86	0.16	63,63,63,63	0
56	MG	1A	3357	1/1	0.86	0.13	54,54,54,54	0
56	MG	1A	4020	1/1	0.86	0.14	26,26,26,26	0
56	MG	1A	3238	1/1	0.86	0.38	52,52,52,52	0
56	MG	2a	3111	1/1	0.86	0.37	60,60,60,60	0
56	MG	1A	3327	1/1	0.86	0.15	44,44,44,44	0
56	MG	1A	4035	1/1	0.86	0.18	46,46,46,46	0
56	MG	1a	1685	1/1	0.86	0.72	55,55,55,55	0
56	MG	1A	3467	1/1	0.86	0.22	54,54,54,54	0
56	MG	2a	3128	1/1	0.86	0.28	62,62,62,62	0
56	MG	1a	1687	1/1	0.86	0.12	42,42,42,42	0
56	MG	1A	3329	1/1	0.86	0.16	53,53,53,53	0
56	MG	2A	3481	1/1	0.86	0.19	46,46,46,46	0
56	MG	1A	3300	1/1	0.86	0.57	41,41,41,41	0
56	MG	1A	3527	1/1	0.86	0.34	69,69,69,69	0
56	MG	10	105	1/1	0.86	0.35	52,52,52,52	0
56	MG	2A	3146	1/1	0.86	0.17	35,35,35,35	0
56	MG	2A	3151	1/1	0.86	0.40	54,54,54,54	0
56	MG	1A	3026	1/1	0.86	0.27	47,47,47,47	0
56	MG	2A	3172	1/1	0.86	0.29	63,63,63,63	0
56	MG	1a	1869	1/1	0.86	0.23	68,68,68,68	0
56	MG	1a	1720	1/1	0.86	0.29	45,45,45,45	0
56	MG	1A	3485	1/1	0.86	0.40	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3488	1/1	0.86	0.18	43,43,43,43	0
56	MG	1a	1746	1/1	0.86	0.30	59,59,59,59	0
56	MG	2a	3187	1/1	0.86	0.24	77,77,77,77	0
56	MG	1A	3428	1/1	0.86	0.16	43,43,43,43	0
56	MG	1A	3430	1/1	0.86	0.36	41,41,41,41	0
56	MG	1a	1601	1/1	0.86	0.37	63,63,63,63	0
56	MG	2A	3223	1/1	0.86	0.12	70,70,70,70	0
56	MG	2a	3003	1/1	0.86	0.64	55,55,55,55	0
56	MG	2a	3004	1/1	0.86	0.45	61,61,61,61	0
56	MG	1A	3336	1/1	0.86	0.18	58,58,58,58	0
56	MG	1A	3497	1/1	0.86	0.33	55,55,55,55	0
56	MG	1a	1610	1/1	0.86	0.17	69,69,69,69	0
56	MG	1x	107	1/1	0.86	0.09	48,48,48,48	0
56	MG	1A	3605	1/1	0.86	0.19	31,31,31,31	0
56	MG	1x	109	1/1	0.86	0.11	66,66,66,66	0
56	MG	2d	502	1/1	0.86	0.49	61,61,61,61	0
56	MG	2A	3255	1/1	0.86	0.32	43,43,43,43	0
56	MG	1a	1616	1/1	0.86	0.22	55,55,55,55	0
56	MG	2A	3012	1/1	0.86	0.08	71,71,71,71	0
56	MG	2a	3036	1/1	0.86	0.16	59,59,59,59	0
56	MG	2A	3015	1/1	0.86	0.12	57,57,57,57	0
56	MG	1A	3940	1/1	0.86	0.21	65,65,65,65	0
56	MG	2a	3042	1/1	0.86	0.20	72,72,72,72	0
57	ZN	14	501	1/1	0.86	0.08	103,103,103,103	0
56	MG	2A	3275	1/1	0.86	0.15	51,51,51,51	0
56	MG	1A	3388	1/1	0.86	0.18	55,55,55,55	0
56	MG	2A	3218	1/1	0.87	0.40	54,54,54,54	0
56	MG	2A	3220	1/1	0.87	0.17	72,72,72,72	0
56	MG	2a	3092	1/1	0.87	0.21	62,62,62,62	0
56	MG	1a	1761	1/1	0.87	0.20	65,65,65,65	0
56	MG	2A	3504	1/1	0.87	0.20	42,42,42,42	0
56	MG	2A	3063	1/1	0.87	0.36	48,48,48,48	0
56	MG	2A	3543	1/1	0.87	0.30	49,49,49,49	0
56	MG	2a	3117	1/1	0.87	0.38	66,66,66,66	0
56	MG	1a	1866	1/1	0.87	0.28	73,73,73,73	0
56	MG	1A	3447	1/1	0.87	0.11	54,54,54,54	0
56	MG	2A	3559	1/1	0.87	0.36	56,56,56,56	0
56	MG	2A	3561	1/1	0.87	0.26	55,55,55,55	0
56	MG	1A	3567	1/1	0.87	0.11	40,40,40,40	0
56	MG	2A	3244	1/1	0.87	0.29	85,85,85,85	0
56	MG	1a	1765	1/1	0.87	0.25	58,58,58,58	0
56	MG	1A	3184	1/1	0.87	0.44	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3083	1/1	0.87	0.24	39,39,39,39	0
56	MG	1a	1781	1/1	0.87	0.12	75,75,75,75	0
56	MG	1a	1783	1/1	0.87	0.31	73,73,73,73	0
56	MG	2A	3094	1/1	0.87	0.22	43,43,43,43	0
56	MG	1f	3001	1/1	0.87	0.17	57,57,57,57	0
56	MG	1A	3255	1/1	0.87	0.21	45,45,45,45	0
56	MG	2a	3159	1/1	0.87	0.22	58,58,58,58	0
56	MG	1a	1697	1/1	0.87	0.11	56,56,56,56	0
56	MG	2A	3110	1/1	0.87	0.32	53,53,53,53	0
56	MG	1o	101	1/1	0.87	0.31	81,81,81,81	0
56	MG	1a	1622	1/1	0.87	0.20	49,49,49,49	0
56	MG	1A	3186	1/1	0.87	0.30	24,24,24,24	0
56	MG	1A	3876	1/1	0.87	0.17	33,33,33,33	0
56	MG	2A	3342	1/1	0.87	0.23	61,61,61,61	0
56	MG	2A	3348	1/1	0.87	0.17	60,60,60,60	0
56	MG	2a	3197	1/1	0.87	0.13	78,78,78,78	0
56	MG	2a	3198	1/1	0.87	0.18	65,65,65,65	0
56	MG	1a	1719	1/1	0.87	0.60	68,68,68,68	0
56	MG	2a	3030	1/1	0.87	0.24	51,51,51,51	0
56	MG	1A	3403	1/1	0.87	0.34	50,50,50,50	0
56	MG	1A	3331	1/1	0.87	0.35	62,62,62,62	0
56	MG	2A	3365	1/1	0.87	0.08	41,41,41,41	0
56	MG	2A	3370	1/1	0.87	0.27	65,65,65,65	0
56	MG	1A	3500	1/1	0.87	0.24	53,53,53,53	0
56	MG	2A	3011	1/1	0.87	0.16	48,48,48,48	0
56	MG	2A	3419	1/1	0.87	0.26	61,61,61,61	0
56	MG	2A	3182	1/1	0.87	0.21	36,36,36,36	0
56	MG	1a	1641	1/1	0.87	0.25	47,47,47,47	0
56	MG	1A	3501	1/1	0.87	0.15	51,51,51,51	0
56	MG	2A	3190	1/1	0.87	0.09	48,48,48,48	0
56	MG	2A	3192	1/1	0.87	0.40	43,43,43,43	0
56	MG	2q	202	1/1	0.87	0.15	59,59,59,59	0
56	MG	2A	3439	1/1	0.87	0.17	60,60,60,60	0
56	MG	1A	3100	1/1	0.87	0.19	51,51,51,51	0
56	MG	1A	3802	1/1	0.87	0.10	65,65,65,65	0
56	MG	1A	3360	1/1	0.87	0.40	57,57,57,57	0
56	MG	1A	3005	1/1	0.87	0.18	57,57,57,57	0
56	MG	1a	1603	1/1	0.87	0.30	69,69,69,69	0
56	MG	1A	3826	1/1	0.87	0.16	17,17,17,17	0
56	MG	1a	1692	1/1	0.88	0.21	64,64,64,64	0
56	MG	2A	3208	1/1	0.88	0.22	48,48,48,48	0
56	MG	2A	3214	1/1	0.88	0.61	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1G	3001	1/1	0.88	0.10	50,50,50,50	0
56	MG	1A	3180	1/1	0.88	0.08	34,34,34,34	0
56	MG	1A	3351	1/1	0.88	0.14	46,46,46,46	0
56	MG	1A	3666	1/1	0.88	0.20	25,25,25,25	0
56	MG	1N	3005	1/1	0.88	0.21	45,45,45,45	0
56	MG	1A	3683	1/1	0.88	0.08	42,42,42,42	0
56	MG	2A	3238	1/1	0.88	0.20	30,30,30,30	0
56	MG	1A	3970	1/1	0.88	0.35	64,64,64,64	0
56	MG	1A	3397	1/1	0.88	0.19	36,36,36,36	0
56	MG	1a	1726	1/1	0.88	0.08	68,68,68,68	0
56	MG	1a	1736	1/1	0.88	0.27	51,51,51,51	0
56	MG	1A	3983	1/1	0.88	0.27	31,31,31,31	0
56	MG	1A	3993	1/1	0.88	0.10	34,34,34,34	0
56	MG	2A	3009	1/1	0.88	0.25	50,50,50,50	0
56	MG	1Z	302	1/1	0.88	0.21	65,65,65,65	0
56	MG	1A	3723	1/1	0.88	0.11	29,29,29,29	0
56	MG	1A	3728	1/1	0.88	0.32	62,62,62,62	0
56	MG	1A	4026	1/1	0.88	0.43	63,63,63,63	0
56	MG	1A	3025	1/1	0.88	0.26	55,55,55,55	0
56	MG	2A	3306	1/1	0.88	0.15	32,32,32,32	0
56	MG	1a	1754	1/1	0.88	0.38	51,51,51,51	0
56	MG	1A	3453	1/1	0.88	0.29	72,72,72,72	0
56	MG	17	102	1/1	0.88	0.21	60,60,60,60	0
56	MG	2A	3318	1/1	0.88	0.13	43,43,43,43	0
56	MG	2a	3087	1/1	0.88	0.21	57,57,57,57	0
56	MG	1A	3092	1/1	0.88	0.38	44,44,44,44	0
56	MG	2A	3055	1/1	0.88	0.29	35,35,35,35	0
56	MG	1A	3458	1/1	0.88	0.07	48,48,48,48	0
56	MG	1A	3276	1/1	0.88	0.15	51,51,51,51	0
56	MG	1A	3824	1/1	0.88	0.16	49,49,49,49	0
56	MG	1A	3278	1/1	0.88	0.44	50,50,50,50	0
56	MG	1a	1606	1/1	0.88	0.15	71,71,71,71	0
56	MG	1a	1608	1/1	0.88	0.21	70,70,70,70	0
56	MG	1A	3129	1/1	0.88	0.22	42,42,42,42	0
56	MG	1a	1611	1/1	0.88	0.22	46,46,46,46	0
56	MG	2A	3408	1/1	0.88	0.11	62,62,62,62	0
56	MG	1A	3479	1/1	0.88	0.23	59,59,59,59	0
56	MG	2A	3421	1/1	0.88	0.29	41,41,41,41	0
56	MG	1A	3838	1/1	0.88	0.25	64,64,64,64	0
56	MG	1A	4064	1/1	0.88	0.13	57,57,57,57	0
56	MG	1A	3104	1/1	0.88	0.25	52,52,52,52	0
56	MG	2A	3100	1/1	0.88	0.33	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1a	1623	1/1	0.88	0.15	67,67,67,67	0
56	MG	1A	3529	1/1	0.88	0.19	61,61,61,61	0
56	MG	2A	3442	1/1	0.88	0.10	66,66,66,66	0
56	MG	2A	3107	1/1	0.88	0.23	49,49,49,49	0
56	MG	1A	3373	1/1	0.88	0.18	44,44,44,44	0
56	MG	2A	3112	1/1	0.88	0.16	59,59,59,59	0
56	MG	2a	3163	1/1	0.88	0.46	94,94,94,94	0
56	MG	1A	3486	1/1	0.88	0.15	57,57,57,57	0
56	MG	2A	3470	1/1	0.88	0.08	64,64,64,64	0
56	MG	1A	3297	1/1	0.88	0.20	49,49,49,49	0
56	MG	1a	1814	1/1	0.88	0.10	67,67,67,67	0
56	MG	2A	3121	1/1	0.88	0.17	38,38,38,38	0
56	MG	1A	3063	1/1	0.88	0.14	57,57,57,57	0
56	MG	2A	3128	1/1	0.88	0.10	56,56,56,56	0
56	MG	1A	3150	1/1	0.88	0.45	44,44,44,44	0
56	MG	2A	3142	1/1	0.88	0.21	56,56,56,56	0
56	MG	1A	3029	1/1	0.88	0.34	71,71,71,71	0
56	MG	1B	214	1/1	0.88	0.23	56,56,56,56	0
56	MG	2A	3161	1/1	0.88	0.08	38,38,38,38	0
56	MG	2a	3214	1/1	0.88	0.12	73,73,73,73	0
56	MG	1A	3495	1/1	0.88	0.19	41,41,41,41	0
56	MG	1A	3314	1/1	0.88	0.18	51,51,51,51	0
56	MG	2A	3177	1/1	0.88	0.07	54,54,54,54	0
56	MG	2A	3181	1/1	0.88	0.09	48,48,48,48	0
56	MG	2B	205	1/1	0.88	0.32	59,59,59,59	0
56	MG	2a	3252	1/1	0.88	0.12	67,67,67,67	0
56	MG	1a	1829	1/1	0.88	0.22	45,45,45,45	0
56	MG	2A	3183	1/1	0.88	0.22	46,46,46,46	0
56	MG	1a	1834	1/1	0.88	0.16	57,57,57,57	0
56	MG	2d	503	1/1	0.88	0.13	62,62,62,62	0
56	MG	1a	1661	1/1	0.88	0.22	59,59,59,59	0
56	MG	1D	302	1/1	0.88	0.32	52,52,52,52	0
56	MG	1a	1669	1/1	0.88	0.19	37,37,37,37	0
56	MG	2Z	301	1/1	0.88	0.08	70,70,70,70	0
56	MG	20	8001	1/1	0.88	0.15	62,62,62,62	0
56	MG	1A	3923	1/1	0.88	0.18	40,40,40,40	0
56	MG	2x	101	1/1	0.88	0.08	72,72,72,72	0
56	MG	28	103	1/1	0.88	0.22	56,56,56,56	0
56	MG	1A	3930	1/1	0.88	0.21	55,55,55,55	0
56	MG	1A	3076	1/1	0.88	0.17	51,51,51,51	0
56	MG	1F	306	1/1	0.88	0.37	59,59,59,59	0
56	MG	1a	1905	1/1	0.88	0.24	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1a	1683	1/1	0.89	0.15	58,58,58,58	0
56	MG	1A	3558	1/1	0.89	0.37	43,43,43,43	0
56	MG	1k	201	1/1	0.89	0.19	49,49,49,49	0
56	MG	1A	3563	1/1	0.89	0.13	54,54,54,54	0
56	MG	1A	3091	1/1	0.89	0.80	54,54,54,54	0
56	MG	1D	306	1/1	0.89	0.22	49,49,49,49	0
56	MG	1q	201	1/1	0.89	0.23	58,58,58,58	0
56	MG	2a	3018	1/1	0.89	0.20	62,62,62,62	0
56	MG	1A	3584	1/1	0.89	0.11	39,39,39,39	0
56	MG	1r	3001	1/1	0.89	0.23	61,61,61,61	0
56	MG	2A	3239	1/1	0.89	0.30	59,59,59,59	0
56	MG	2a	3028	1/1	0.89	0.16	38,38,38,38	0
56	MG	1A	3908	1/1	0.89	0.16	51,51,51,51	0
56	MG	1r	3003	1/1	0.89	0.16	49,49,49,49	0
56	MG	1A	3121	1/1	0.89	0.23	72,72,72,72	0
56	MG	2A	3251	1/1	0.89	0.20	49,49,49,49	0
56	MG	1A	3143	1/1	0.89	0.20	34,34,34,34	0
56	MG	2A	3253	1/1	0.89	0.23	59,59,59,59	0
56	MG	1A	3337	1/1	0.89	0.20	44,44,44,44	0
56	MG	1A	3257	1/1	0.89	0.17	39,39,39,39	0
56	MG	1A	3643	1/1	0.89	0.21	49,49,49,49	0
56	MG	1A	3350	1/1	0.89	0.38	60,60,60,60	0
56	MG	2A	3270	1/1	0.89	0.09	59,59,59,59	0
56	MG	1A	3649	1/1	0.89	0.21	26,26,26,26	0
56	MG	1A	3942	1/1	0.89	0.33	91,91,91,91	0
56	MG	1Q	206	1/1	0.89	0.22	53,53,53,53	0
56	MG	2A	3021	1/1	0.89	0.48	58,58,58,58	0
56	MG	1R	204	1/1	0.89	0.21	70,70,70,70	0
56	MG	1A	3504	1/1	0.89	0.20	62,62,62,62	0
56	MG	1A	3678	1/1	0.89	0.12	39,39,39,39	0
56	MG	1W	3006	1/1	0.89	0.38	40,40,40,40	0
56	MG	1A	3508	1/1	0.89	0.24	68,68,68,68	0
56	MG	1A	3690	1/1	0.89	0.14	21,21,21,21	0
56	MG	1A	3979	1/1	0.89	0.20	55,55,55,55	0
56	MG	1A	3396	1/1	0.89	0.10	55,55,55,55	0
56	MG	1A	3989	1/1	0.89	0.53	31,31,31,31	0
56	MG	2A	3359	1/1	0.89	0.15	57,57,57,57	0
56	MG	1A	3711	1/1	0.89	0.14	61,61,61,61	0
56	MG	11	103	1/1	0.89	0.15	42,42,42,42	0
56	MG	2A	3073	1/1	0.89	0.10	38,38,38,38	0
56	MG	2a	3115	1/1	0.89	0.20	50,50,50,50	0
56	MG	1A	4006	1/1	0.89	0.32	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3719	1/1	0.89	0.12	56,56,56,56	0
56	MG	16	104	1/1	0.89	0.21	53,53,53,53	0
56	MG	2A	3401	1/1	0.89	0.29	70,70,70,70	0
56	MG	2A	3082	1/1	0.89	0.13	57,57,57,57	0
56	MG	1a	1767	1/1	0.89	0.13	71,71,71,71	0
56	MG	1A	3017	1/1	0.89	0.31	53,53,53,53	0
56	MG	2A	3090	1/1	0.89	0.21	58,58,58,58	0
56	MG	1A	4025	1/1	0.89	0.31	80,80,80,80	0
56	MG	2a	3141	1/1	0.89	0.08	70,70,70,70	0
56	MG	18	3002	1/1	0.89	0.21	58,58,58,58	0
56	MG	1A	3263	1/1	0.89	0.22	42,42,42,42	0
56	MG	1A	3749	1/1	0.89	0.26	43,43,43,43	0
56	MG	2A	3438	1/1	0.89	0.24	53,53,53,53	0
56	MG	1a	1787	1/1	0.89	0.32	52,52,52,52	0
56	MG	1A	4028	1/1	0.89	0.12	63,63,63,63	0
56	MG	2a	3157	1/1	0.89	0.34	108,108,108,108	0
56	MG	1A	4029	1/1	0.89	0.14	42,42,42,42	0
56	MG	1A	3265	1/1	0.89	0.24	27,27,27,27	0
56	MG	2A	3449	1/1	0.89	0.22	57,57,57,57	0
56	MG	1A	3764	1/1	0.89	0.17	68,68,68,68	0
56	MG	2a	3165	1/1	0.89	0.49	74,74,74,74	0
56	MG	2A	3462	1/1	0.89	0.19	46,46,46,46	0
56	MG	1A	3272	1/1	0.89	0.14	58,58,58,58	0
56	MG	1A	3188	1/1	0.89	0.08	53,53,53,53	0
56	MG	2a	3180	1/1	0.89	0.18	46,46,46,46	0
56	MG	2a	3182	1/1	0.89	0.16	78,78,78,78	0
56	MG	1A	3147	1/1	0.89	0.23	28,28,28,28	0
56	MG	2A	3478	1/1	0.89	0.19	50,50,50,50	0
56	MG	1A	3367	1/1	0.89	0.12	48,48,48,48	0
56	MG	1a	1811	1/1	0.89	0.14	66,66,66,66	0
56	MG	1a	1812	1/1	0.89	0.09	53,53,53,53	0
56	MG	2A	3494	1/1	0.89	0.24	38,38,38,38	0
56	MG	1A	3425	1/1	0.89	0.13	50,50,50,50	0
56	MG	2A	3499	1/1	0.89	0.19	49,49,49,49	0
56	MG	1A	4053	1/1	0.89	0.49	52,52,52,52	0
56	MG	1A	3115	1/1	0.89	0.13	56,56,56,56	0
56	MG	2A	3522	1/1	0.89	0.36	43,43,43,43	0
56	MG	2A	3524	1/1	0.89	0.20	50,50,50,50	0
56	MG	1A	3532	1/1	0.89	0.19	62,62,62,62	0
56	MG	2a	3234	1/1	0.89	0.29	82,82,82,82	0
56	MG	2a	3235	1/1	0.89	0.18	73,73,73,73	0
56	MG	2A	3550	1/1	0.89	0.12	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	4063	1/1	0.89	0.18	47,47,47,47	0
56	MG	1A	3152	1/1	0.89	0.18	30,30,30,30	0
56	MG	1A	3835	1/1	0.89	0.13	47,47,47,47	0
56	MG	1A	3490	1/1	0.89	0.09	57,57,57,57	0
56	MG	1A	4077	1/1	0.89	0.20	47,47,47,47	0
56	MG	1a	1644	1/1	0.89	0.20	75,75,75,75	0
56	MG	1A	3841	1/1	0.89	0.08	44,44,44,44	0
56	MG	1a	1855	1/1	0.89	0.27	48,48,48,48	0
56	MG	1A	3032	1/1	0.89	0.37	44,44,44,44	0
56	MG	1A	3380	1/1	0.89	0.14	49,49,49,49	0
56	MG	1A	3857	1/1	0.89	0.25	51,51,51,51	0
56	MG	1a	1878	1/1	0.89	0.42	67,67,67,67	0
56	MG	1a	1880	1/1	0.89	0.20	69,69,69,69	0
56	MG	1A	3173	1/1	0.89	0.19	40,40,40,40	0
56	MG	1A	3557	1/1	0.89	0.43	71,71,71,71	0
56	MG	1A	3888	1/1	0.89	0.14	43,43,43,43	0
56	MG	1B	225	1/1	0.89	0.11	63,63,63,63	0
56	MG	1A	3004	1/1	0.90	0.27	54,54,54,54	0
56	MG	1A	3137	1/1	0.90	0.20	36,36,36,36	0
56	MG	1A	3095	1/1	0.90	0.22	46,46,46,46	0
56	MG	1A	3955	1/1	0.90	0.12	21,21,21,21	0
56	MG	1A	3774	1/1	0.90	0.12	43,43,43,43	0
56	MG	2a	3059	1/1	0.90	0.14	69,69,69,69	0
56	MG	1A	3775	1/1	0.90	0.18	31,31,31,31	0
56	MG	1A	3358	1/1	0.90	0.20	61,61,61,61	0
56	MG	1A	3301	1/1	0.90	0.20	64,64,64,64	0
56	MG	1A	3398	1/1	0.90	0.19	46,46,46,46	0
56	MG	1A	3399	1/1	0.90	0.37	45,45,45,45	0
56	MG	2a	3086	1/1	0.90	0.14	50,50,50,50	0
56	MG	1a	1621	1/1	0.90	0.28	57,57,57,57	0
56	MG	1D	308	1/1	0.90	0.37	54,54,54,54	0
56	MG	1D	311	1/1	0.90	0.28	51,51,51,51	0
56	MG	1a	1627	1/1	0.90	0.09	70,70,70,70	0
56	MG	2a	3095	1/1	0.90	0.09	41,41,41,41	0
56	MG	2A	3195	1/1	0.90	0.19	47,47,47,47	0
56	MG	2a	3104	1/1	0.90	0.30	54,54,54,54	0
56	MG	1A	3825	1/1	0.90	0.32	45,45,45,45	0
56	MG	2a	3113	1/1	0.90	0.31	50,50,50,50	0
56	MG	2A	3010	1/1	0.90	0.18	68,68,68,68	0
56	MG	1A	3449	1/1	0.90	0.23	67,67,67,67	0
56	MG	2A	3477	1/1	0.90	0.16	47,47,47,47	0
56	MG	2a	3119	1/1	0.90	0.10	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3575	1/1	0.90	0.33	57,57,57,57	0
56	MG	2A	3013	1/1	0.90	0.13	60,60,60,60	0
56	MG	1A	3450	1/1	0.90	0.39	52,52,52,52	0
56	MG	1A	3585	1/1	0.90	0.20	14,14,14,14	0
56	MG	1G	3003	1/1	0.90	0.05	43,43,43,43	0
56	MG	2A	3219	1/1	0.90	0.22	56,56,56,56	0
56	MG	1A	3400	1/1	0.90	0.22	37,37,37,37	0
56	MG	1A	3096	1/1	0.90	0.27	40,40,40,40	0
56	MG	1A	3311	1/1	0.90	0.22	44,44,44,44	0
56	MG	2a	3142	1/1	0.90	0.47	80,80,80,80	0
56	MG	1N	3003	1/1	0.90	0.21	38,38,38,38	0
56	MG	1A	3313	1/1	0.90	0.12	42,42,42,42	0
56	MG	1O	3001	1/1	0.90	0.25	39,39,39,39	0
56	MG	2A	3549	1/1	0.90	0.17	49,49,49,49	0
56	MG	2A	3056	1/1	0.90	0.31	52,52,52,52	0
56	MG	2A	3057	1/1	0.90	0.20	52,52,52,52	0
56	MG	1A	3464	1/1	0.90	0.16	57,57,57,57	0
56	MG	1A	3868	1/1	0.90	0.19	84,84,84,84	0
56	MG	1A	3465	1/1	0.90	0.11	59,59,59,59	0
56	MG	1a	1673	1/1	0.90	0.42	46,46,46,46	0
56	MG	1A	3647	1/1	0.90	0.18	19,19,19,19	0
56	MG	1T	203	1/1	0.90	0.13	75,75,75,75	0
56	MG	2B	206	1/1	0.90	0.21	37,37,37,37	0
56	MG	1A	3406	1/1	0.90	0.23	49,49,49,49	0
56	MG	1A	3047	1/1	0.90	0.29	54,54,54,54	0
56	MG	2a	3178	1/1	0.90	0.21	55,55,55,55	0
56	MG	1A	3670	1/1	0.90	0.26	37,37,37,37	0
56	MG	2A	3263	1/1	0.90	0.09	42,42,42,42	0
56	MG	2A	3265	1/1	0.90	0.16	47,47,47,47	0
56	MG	1A	4049	1/1	0.90	0.25	49,49,49,49	0
56	MG	1A	3899	1/1	0.90	0.19	77,77,77,77	0
56	MG	1A	3477	1/1	0.90	0.37	40,40,40,40	0
56	MG	1a	1837	1/1	0.90	0.15	48,48,48,48	0
56	MG	1A	4057	1/1	0.90	0.41	50,50,50,50	0
56	MG	1A	3030	1/1	0.90	0.09	46,46,46,46	0
56	MG	2A	3099	1/1	0.90	0.08	61,61,61,61	0
56	MG	1a	1703	1/1	0.90	0.19	52,52,52,52	0
56	MG	2A	3312	1/1	0.90	0.17	38,38,38,38	0
56	MG	2a	3223	1/1	0.90	0.17	77,77,77,77	0
56	MG	1a	1713	1/1	0.90	0.20	66,66,66,66	0
56	MG	2a	3009	1/1	0.90	0.07	84,84,84,84	0
56	MG	1A	3281	1/1	0.90	0.07	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3328	1/1	0.90	0.20	70,70,70,70	0
56	MG	1A	3526	1/1	0.90	0.22	47,47,47,47	0
56	MG	1A	3345	1/1	0.90	0.22	63,63,63,63	0
56	MG	2a	3246	1/1	0.90	0.18	60,60,60,60	0
56	MG	1A	3038	1/1	0.90	0.50	55,55,55,55	0
56	MG	1a	1891	1/1	0.90	0.19	51,51,51,51	0
56	MG	2a	3023	1/1	0.90	0.21	66,66,66,66	0
56	MG	1a	1730	1/1	0.90	0.27	44,44,44,44	0
56	MG	2A	3361	1/1	0.90	0.17	34,34,34,34	0
56	MG	1A	3072	1/1	0.90	0.24	46,46,46,46	0
56	MG	1A	3535	1/1	0.90	0.31	59,59,59,59	0
56	MG	2A	3123	1/1	0.90	0.25	57,57,57,57	0
56	MG	2A	3368	1/1	0.90	0.36	48,48,48,48	0
56	MG	1A	4086	1/1	0.90	0.16	63,63,63,63	0
56	MG	2a	3040	1/1	0.90	0.06	58,58,58,58	0
56	MG	2a	3041	1/1	0.90	0.12	50,50,50,50	0
56	MG	2x	102	1/1	0.90	0.18	68,68,68,68	0
56	MG	1b	3001	1/1	0.90	0.20	70,70,70,70	0
56	MG	1a	1744	1/1	0.90	0.63	58,58,58,58	0
56	MG	2A	3393	1/1	0.90	0.21	56,56,56,56	0
56	MG	2A	3136	1/1	0.90	0.22	61,61,61,61	0
56	MG	1A	3296	1/1	0.90	0.22	49,49,49,49	0
56	MG	2A	3164	1/1	0.91	0.45	51,51,51,51	0
56	MG	1B	223	1/1	0.91	0.14	65,65,65,65	0
56	MG	1a	1836	1/1	0.91	0.14	51,51,51,51	0
56	MG	1A	3252	1/1	0.91	0.18	56,56,56,56	0
56	MG	2A	3178	1/1	0.91	0.15	54,54,54,54	0
56	MG	1A	3382	1/1	0.91	0.08	53,53,53,53	0
56	MG	1a	1647	1/1	0.91	0.28	53,53,53,53	0
56	MG	1A	3920	1/1	0.91	0.18	65,65,65,65	0
56	MG	2O	202	1/1	0.91	0.12	37,37,37,37	0
56	MG	1A	3657	1/1	0.91	0.13	34,34,34,34	0
56	MG	1A	3925	1/1	0.91	0.25	56,56,56,56	0
56	MG	1a	1871	1/1	0.91	0.33	69,69,69,69	0
56	MG	1a	1659	1/1	0.91	0.26	52,52,52,52	0
56	MG	1a	1877	1/1	0.91	0.25	52,52,52,52	0
56	MG	25	502	1/1	0.91	0.53	54,54,54,54	0
56	MG	1A	3659	1/1	0.91	0.16	17,17,17,17	0
56	MG	1D	309	1/1	0.91	0.16	56,56,56,56	0
56	MG	1a	1888	1/1	0.91	0.20	60,60,60,60	0
56	MG	2A	3198	1/1	0.91	0.13	56,56,56,56	0
56	MG	1A	3663	1/1	0.91	0.12	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3052	1/1	0.91	0.22	51,51,51,51	0
56	MG	1A	3120	1/1	0.91	0.28	59,59,59,59	0
56	MG	2a	3010	1/1	0.91	0.20	44,44,44,44	0
56	MG	2a	3011	1/1	0.91	0.18	58,58,58,58	0
56	MG	2A	3207	1/1	0.91	0.35	49,49,49,49	0
56	MG	2a	3016	1/1	0.91	0.43	65,65,65,65	0
56	MG	1E	307	1/1	0.91	0.33	57,57,57,57	0
56	MG	1A	3161	1/1	0.91	0.36	47,47,47,47	0
56	MG	1A	3041	1/1	0.91	0.22	51,51,51,51	0
56	MG	1A	3949	1/1	0.91	0.23	35,35,35,35	0
56	MG	1A	3689	1/1	0.91	0.08	65,65,65,65	0
56	MG	1A	3085	1/1	0.91	0.14	48,48,48,48	0
56	MG	2a	3025	1/1	0.91	0.26	60,60,60,60	0
56	MG	1a	1694	1/1	0.91	0.09	51,51,51,51	0
56	MG	1A	3514	1/1	0.91	0.29	59,59,59,59	0
56	MG	1A	3973	1/1	0.91	0.22	50,50,50,50	0
56	MG	1A	3124	1/1	0.91	0.26	36,36,36,36	0
56	MG	1A	3522	1/1	0.91	0.07	50,50,50,50	0
56	MG	2A	3240	1/1	0.91	0.18	34,34,34,34	0
56	MG	1q	203	1/1	0.91	0.19	53,53,53,53	0
56	MG	1A	3057	1/1	0.91	0.06	47,47,47,47	0
56	MG	1A	3008	1/1	0.91	0.22	51,51,51,51	0
56	MG	1a	1715	1/1	0.91	0.13	50,50,50,50	0
56	MG	1u	8001	1/1	0.91	0.16	53,53,53,53	0
56	MG	1x	101	1/1	0.91	0.22	64,64,64,64	0
56	MG	1A	3741	1/1	0.91	0.10	63,63,63,63	0
56	MG	1a	1718	1/1	0.91	0.13	75,75,75,75	0
56	MG	2A	3257	1/1	0.91	0.34	67,67,67,67	0
56	MG	2a	3052	1/1	0.91	0.09	81,81,81,81	0
56	MG	1A	4000	1/1	0.91	0.11	69,69,69,69	0
56	MG	1R	205	1/1	0.91	0.24	28,28,28,28	0
56	MG	2A	3005	1/1	0.91	0.14	59,59,59,59	0
56	MG	1A	3279	1/1	0.91	0.25	41,41,41,41	0
56	MG	2A	3269	1/1	0.91	0.30	38,38,38,38	0
56	MG	1A	3015	1/1	0.91	0.29	51,51,51,51	0
56	MG	1A	3187	1/1	0.91	0.14	52,52,52,52	0
56	MG	1U	202	1/1	0.91	0.53	51,51,51,51	0
56	MG	2A	3276	1/1	0.91	0.09	60,60,60,60	0
56	MG	2A	3281	1/1	0.91	0.12	45,45,45,45	0
56	MG	2A	3284	1/1	0.91	0.18	34,34,34,34	0
56	MG	1a	1741	1/1	0.91	0.13	48,48,48,48	0
56	MG	2A	3295	1/1	0.91	0.17	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1V	202	1/1	0.91	0.18	28,28,28,28	0
56	MG	2a	3093	1/1	0.91	0.33	66,66,66,66	0
56	MG	2A	3301	1/1	0.91	0.08	42,42,42,42	0
56	MG	2A	3305	1/1	0.91	0.14	50,50,50,50	0
56	MG	2a	3098	1/1	0.91	0.35	55,55,55,55	0
56	MG	2A	3014	1/1	0.91	0.18	52,52,52,52	0
56	MG	1a	1743	1/1	0.91	0.18	44,44,44,44	0
56	MG	1A	3133	1/1	0.91	0.38	48,48,48,48	0
56	MG	2A	3025	1/1	0.91	0.37	55,55,55,55	0
56	MG	1A	3533	1/1	0.91	0.09	56,56,56,56	0
56	MG	2A	3030	1/1	0.91	0.37	64,64,64,64	0
56	MG	1a	1747	1/1	0.91	0.24	64,64,64,64	0
56	MG	2a	3118	1/1	0.91	0.23	60,60,60,60	0
56	MG	1A	3475	1/1	0.91	0.08	66,66,66,66	0
56	MG	1A	3290	1/1	0.91	0.18	30,30,30,30	0
56	MG	2A	3346	1/1	0.91	0.06	69,69,69,69	0
56	MG	10	103	1/1	0.91	0.23	62,62,62,62	0
56	MG	2A	3045	1/1	0.91	0.35	48,48,48,48	0
56	MG	2A	3050	1/1	0.91	0.41	55,55,55,55	0
56	MG	2A	3052	1/1	0.91	0.13	37,37,37,37	0
56	MG	1A	3048	1/1	0.91	0.20	51,51,51,51	0
56	MG	1A	3107	1/1	0.91	0.58	53,53,53,53	0
56	MG	1A	3481	1/1	0.91	0.37	46,46,46,46	0
56	MG	1A	3550	1/1	0.91	0.20	68,68,68,68	0
56	MG	1A	3552	1/1	0.91	0.22	51,51,51,51	0
56	MG	1a	1760	1/1	0.91	0.31	79,79,79,79	0
56	MG	2A	3391	1/1	0.91	0.28	52,52,52,52	0
56	MG	1A	3405	1/1	0.91	0.54	41,41,41,41	0
56	MG	1a	1762	1/1	0.91	0.25	71,71,71,71	0
56	MG	2A	3072	1/1	0.91	0.24	29,29,29,29	0
56	MG	2a	3155	1/1	0.91	0.17	87,87,87,87	0
56	MG	1A	3198	1/1	0.91	0.18	50,50,50,50	0
56	MG	2A	3410	1/1	0.91	0.13	52,52,52,52	0
56	MG	2A	3413	1/1	0.91	0.20	55,55,55,55	0
56	MG	2A	3418	1/1	0.91	0.25	52,52,52,52	0
56	MG	1A	3832	1/1	0.91	0.16	34,34,34,34	0
56	MG	1A	3140	1/1	0.91	0.22	36,36,36,36	0
56	MG	2A	3422	1/1	0.91	0.13	73,73,73,73	0
56	MG	2A	3077	1/1	0.91	0.13	43,43,43,43	0
56	MG	1A	3219	1/1	0.91	0.21	56,56,56,56	0
56	MG	1A	3220	1/1	0.91	0.50	41,41,41,41	0
56	MG	2a	3179	1/1	0.91	0.07	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1a	1777	1/1	0.91	0.18	54,54,54,54	0
56	MG	2A	3085	1/1	0.91	0.16	38,38,38,38	0
56	MG	1a	1780	1/1	0.91	0.08	56,56,56,56	0
56	MG	1A	3424	1/1	0.91	0.25	37,37,37,37	0
56	MG	1A	3850	1/1	0.91	0.13	47,47,47,47	0
56	MG	2a	3194	1/1	0.91	0.38	44,44,44,44	0
56	MG	1a	1604	1/1	0.91	0.27	60,60,60,60	0
56	MG	1A	3228	1/1	0.91	0.21	48,48,48,48	0
56	MG	1A	3236	1/1	0.91	0.12	58,58,58,58	0
56	MG	1A	3860	1/1	0.91	0.20	38,38,38,38	0
56	MG	2a	3210	1/1	0.91	0.20	78,78,78,78	0
56	MG	2a	3211	1/1	0.91	0.35	55,55,55,55	0
56	MG	2A	3461	1/1	0.91	0.36	53,53,53,53	0
56	MG	1A	4075	1/1	0.91	0.30	61,61,61,61	0
56	MG	2A	3465	1/1	0.91	0.14	45,45,45,45	0
56	MG	1A	3427	1/1	0.91	0.17	51,51,51,51	0
56	MG	2a	3224	1/1	0.91	0.12	60,60,60,60	0
56	MG	2a	3225	1/1	0.91	0.19	59,59,59,59	0
56	MG	2A	3106	1/1	0.91	0.17	47,47,47,47	0
56	MG	1A	3075	1/1	0.91	0.17	46,46,46,46	0
56	MG	1A	4078	1/1	0.91	0.40	65,65,65,65	0
56	MG	2a	3233	1/1	0.91	0.16	58,58,58,58	0
56	MG	1a	1617	1/1	0.91	0.19	55,55,55,55	0
56	MG	1A	4079	1/1	0.91	0.22	33,33,33,33	0
56	MG	2a	3241	1/1	0.91	0.23	73,73,73,73	0
56	MG	1A	3368	1/1	0.91	0.28	65,65,65,65	0
56	MG	2a	3245	1/1	0.91	0.21	64,64,64,64	0
56	MG	2A	3485	1/1	0.91	0.11	56,56,56,56	0
56	MG	1A	3608	1/1	0.91	0.25	26,26,26,26	0
56	MG	1A	3614	1/1	0.91	0.28	57,57,57,57	0
56	MG	1A	3145	1/1	0.91	0.40	38,38,38,38	0
56	MG	2a	3255	1/1	0.91	0.09	57,57,57,57	0
56	MG	1A	3639	1/1	0.91	0.28	47,47,47,47	0
56	MG	2A	3127	1/1	0.91	0.22	43,43,43,43	0
56	MG	1A	3641	1/1	0.91	0.12	52,52,52,52	0
56	MG	2A	3512	1/1	0.91	0.23	38,38,38,38	0
56	MG	1a	1819	1/1	0.91	0.26	73,73,73,73	0
56	MG	2A	3135	1/1	0.91	0.10	43,43,43,43	0
56	MG	2A	3531	1/1	0.91	0.28	52,52,52,52	0
56	MG	2A	3541	1/1	0.91	0.22	38,38,38,38	0
56	MG	1a	1630	1/1	0.91	0.14	42,42,42,42	0
56	MG	1a	1632	1/1	0.91	0.20	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3051	1/1	0.91	0.60	47,47,47,47	0
56	MG	1A	3117	1/1	0.91	0.10	62,62,62,62	0
56	MG	2x	107	1/1	0.91	0.11	78,78,78,78	0
56	MG	2A	3157	1/1	0.91	0.18	31,31,31,31	0
56	MG	2A	3160	1/1	0.91	0.13	49,49,49,49	0
56	MG	1B	216	1/1	0.91	0.12	70,70,70,70	0
56	MG	2B	208	1/1	0.92	0.10	58,58,58,58	0
56	MG	1A	3999	1/1	0.92	0.15	51,51,51,51	0
56	MG	1A	3604	1/1	0.92	0.10	36,36,36,36	0
56	MG	1A	3034	1/1	0.92	0.14	49,49,49,49	0
56	MG	2E	304	1/1	0.92	0.09	56,56,56,56	0
56	MG	2F	302	1/1	0.92	0.24	48,48,48,48	0
56	MG	1a	1904	1/1	0.92	0.20	76,76,76,76	0
56	MG	2N	8001	1/1	0.92	0.14	63,63,63,63	0
56	MG	1A	4010	1/1	0.92	0.26	37,37,37,37	0
56	MG	2P	201	1/1	0.92	0.22	33,33,33,33	0
56	MG	2Q	3001	1/1	0.92	0.41	45,45,45,45	0
56	MG	2Q	3002	1/1	0.92	0.18	55,55,55,55	0
56	MG	1O	3003	1/1	0.92	0.12	60,60,60,60	0
56	MG	1a	1909	1/1	0.92	0.11	71,71,71,71	0
56	MG	1a	1698	1/1	0.92	0.12	63,63,63,63	0
56	MG	1d	502	1/1	0.92	0.16	82,82,82,82	0
56	MG	1P	201	1/1	0.92	0.16	49,49,49,49	0
56	MG	1e	202	1/1	0.92	0.09	65,65,65,65	0
56	MG	1P	202	1/1	0.92	0.26	59,59,59,59	0
56	MG	2A	3210	1/1	0.92	0.35	31,31,31,31	0
56	MG	2A	3213	1/1	0.92	0.20	42,42,42,42	0
56	MG	1A	3386	1/1	0.92	0.24	68,68,68,68	0
56	MG	1l	202	1/1	0.92	0.09	58,58,58,58	0
56	MG	1a	1709	1/1	0.92	0.25	61,61,61,61	0
56	MG	1A	4019	1/1	0.92	0.22	39,39,39,39	0
56	MG	1A	3022	1/1	0.92	0.17	49,49,49,49	0
56	MG	1o	103	1/1	0.92	0.26	47,47,47,47	0
56	MG	2a	3012	1/1	0.92	0.12	58,58,58,58	0
56	MG	2a	3013	1/1	0.92	0.07	50,50,50,50	0
56	MG	1p	3001	1/1	0.92	0.26	52,52,52,52	0
56	MG	1p	3002	1/1	0.92	0.14	77,77,77,77	0
56	MG	2A	3235	1/1	0.92	0.21	57,57,57,57	0
56	MG	1A	3616	1/1	0.92	0.25	29,29,29,29	0
56	MG	1a	1717	1/1	0.92	0.18	47,47,47,47	0
56	MG	1A	3624	1/1	0.92	0.18	40,40,40,40	0
56	MG	1A	3523	1/1	0.92	0.18	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1T	205	1/1	0.92	0.16	56,56,56,56	0
56	MG	1A	3636	1/1	0.92	0.16	49,49,49,49	0
56	MG	2a	3026	1/1	0.92	0.13	54,54,54,54	0
56	MG	2A	3247	1/1	0.92	0.12	59,59,59,59	0
56	MG	1t	3001	1/1	0.92	0.43	53,53,53,53	0
56	MG	1a	1727	1/1	0.92	0.17	56,56,56,56	0
56	MG	1A	3151	1/1	0.92	0.15	45,45,45,45	0
56	MG	1a	1733	1/1	0.92	0.58	52,52,52,52	0
56	MG	1x	104	1/1	0.92	0.07	56,56,56,56	0
56	MG	1U	205	1/1	0.92	0.48	41,41,41,41	0
56	MG	1A	3354	1/1	0.92	0.07	84,84,84,84	0
56	MG	1a	1739	1/1	0.92	0.06	70,70,70,70	0
56	MG	1A	3061	1/1	0.92	0.17	51,51,51,51	0
56	MG	1A	3848	1/1	0.92	0.18	45,45,45,45	0
56	MG	1A	3286	1/1	0.92	0.12	40,40,40,40	0
56	MG	2a	3045	1/1	0.92	0.38	68,68,68,68	0
56	MG	2a	3046	1/1	0.92	0.12	70,70,70,70	0
56	MG	1A	3158	1/1	0.92	0.20	32,32,32,32	0
56	MG	1A	4042	1/1	0.92	0.33	44,44,44,44	0
56	MG	1A	3648	1/1	0.92	0.18	26,26,26,26	0
56	MG	1A	3122	1/1	0.92	0.28	56,56,56,56	0
56	MG	2A	3279	1/1	0.92	0.13	51,51,51,51	0
56	MG	1a	1749	1/1	0.92	0.15	64,64,64,64	0
56	MG	1A	3656	1/1	0.92	0.18	20,20,20,20	0
56	MG	2a	3056	1/1	0.92	0.17	58,58,58,58	0
56	MG	2A	3018	1/1	0.92	0.22	47,47,47,47	0
56	MG	2A	3289	1/1	0.92	0.18	37,37,37,37	0
56	MG	2a	3061	1/1	0.92	0.22	71,71,71,71	0
56	MG	2A	3019	1/1	0.92	0.16	48,48,48,48	0
56	MG	2a	3065	1/1	0.92	0.21	93,93,93,93	0
56	MG	1A	3872	1/1	0.92	0.13	39,39,39,39	0
56	MG	2a	3069	1/1	0.92	0.18	65,65,65,65	0
56	MG	1A	3081	1/1	0.92	0.15	40,40,40,40	0
56	MG	1A	3534	1/1	0.92	0.21	55,55,55,55	0
56	MG	2A	3029	1/1	0.92	0.15	57,57,57,57	0
56	MG	15	104	1/1	0.92	0.25	53,53,53,53	0
56	MG	2A	3034	1/1	0.92	0.17	44,44,44,44	0
56	MG	1A	3200	1/1	0.92	0.18	39,39,39,39	0
56	MG	1A	4061	1/1	0.92	0.23	61,61,61,61	0
56	MG	2A	3316	1/1	0.92	0.10	55,55,55,55	0
56	MG	1a	1758	1/1	0.92	0.17	67,67,67,67	0
56	MG	2A	3041	1/1	0.92	0.15	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3334	1/1	0.92	0.17	53,53,53,53	0
56	MG	2A	3339	1/1	0.92	0.32	63,63,63,63	0
56	MG	1A	4062	1/1	0.92	0.27	49,49,49,49	0
56	MG	2A	3341	1/1	0.92	0.14	51,51,51,51	0
56	MG	1A	3890	1/1	0.92	0.18	31,31,31,31	0
56	MG	2A	3343	1/1	0.92	0.08	55,55,55,55	0
56	MG	2A	3046	1/1	0.92	0.43	60,60,60,60	0
56	MG	19	102	1/1	0.92	0.23	50,50,50,50	0
56	MG	1A	3892	1/1	0.92	0.11	46,46,46,46	0
56	MG	1A	4066	1/1	0.92	0.30	35,35,35,35	0
56	MG	1A	3205	1/1	0.92	0.30	33,33,33,33	0
56	MG	1A	3209	1/1	0.92	0.38	39,39,39,39	0
56	MG	1A	3040	1/1	0.92	0.24	36,36,36,36	0
56	MG	1A	3053	1/1	0.92	0.25	36,36,36,36	0
56	MG	1A	3684	1/1	0.92	0.17	50,50,50,50	0
56	MG	2A	3064	1/1	0.92	0.45	56,56,56,56	0
56	MG	2A	3372	1/1	0.92	0.11	33,33,33,33	0
56	MG	1A	3304	1/1	0.92	0.23	45,45,45,45	0
56	MG	2A	3386	1/1	0.92	0.25	37,37,37,37	0
56	MG	2A	3389	1/1	0.92	0.21	39,39,39,39	0
56	MG	1A	3452	1/1	0.92	0.16	50,50,50,50	0
56	MG	1A	3269	1/1	0.92	0.19	53,53,53,53	0
56	MG	1A	3701	1/1	0.92	0.15	29,29,29,29	0
56	MG	1B	201	1/1	0.92	0.15	40,40,40,40	0
56	MG	1a	1789	1/1	0.92	0.29	60,60,60,60	0
56	MG	2A	3409	1/1	0.92	0.10	64,64,64,64	0
56	MG	1A	3455	1/1	0.92	0.11	58,58,58,58	0
56	MG	1A	3381	1/1	0.92	0.28	54,54,54,54	0
56	MG	1a	1793	1/1	0.92	0.16	83,83,83,83	0
56	MG	1a	1795	1/1	0.92	0.28	64,64,64,64	0
56	MG	2A	3420	1/1	0.92	0.23	72,72,72,72	0
56	MG	1B	209	1/1	0.92	0.15	56,56,56,56	0
56	MG	1a	1797	1/1	0.92	0.21	73,73,73,73	0
56	MG	2A	3431	1/1	0.92	0.16	50,50,50,50	0
56	MG	2a	3168	1/1	0.92	0.34	67,67,67,67	0
56	MG	2A	3088	1/1	0.92	0.12	44,44,44,44	0
56	MG	1A	3559	1/1	0.92	0.16	55,55,55,55	0
56	MG	1A	3562	1/1	0.92	0.18	54,54,54,54	0
56	MG	1B	213	1/1	0.92	0.09	50,50,50,50	0
56	MG	1a	1803	1/1	0.92	0.21	66,66,66,66	0
56	MG	1A	3937	1/1	0.92	0.18	52,52,52,52	0
56	MG	1A	3938	1/1	0.92	0.11	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3505	1/1	0.92	0.18	49,49,49,49	0
56	MG	1A	3118	1/1	0.92	0.18	47,47,47,47	0
56	MG	1A	3414	1/1	0.92	0.21	50,50,50,50	0
56	MG	1a	1815	1/1	0.92	0.17	73,73,73,73	0
56	MG	1A	3762	1/1	0.92	0.06	39,39,39,39	0
56	MG	2a	3201	1/1	0.92	0.12	66,66,66,66	0
56	MG	2A	3456	1/1	0.92	0.26	64,64,64,64	0
56	MG	2a	3203	1/1	0.92	0.13	58,58,58,58	0
56	MG	1a	1817	1/1	0.92	0.15	54,54,54,54	0
56	MG	2a	3209	1/1	0.92	0.13	53,53,53,53	0
56	MG	1A	3579	1/1	0.92	0.29	41,41,41,41	0
56	MG	1A	3954	1/1	0.92	0.21	16,16,16,16	0
56	MG	1A	3765	1/1	0.92	0.13	45,45,45,45	0
56	MG	1A	3582	1/1	0.92	0.20	25,25,25,25	0
56	MG	2a	3215	1/1	0.92	0.12	53,53,53,53	0
56	MG	1A	3772	1/1	0.92	0.28	43,43,43,43	0
56	MG	2a	3219	1/1	0.92	0.13	62,62,62,62	0
56	MG	1a	1650	1/1	0.92	0.22	49,49,49,49	0
56	MG	1D	312	1/1	0.92	0.18	45,45,45,45	0
56	MG	1E	301	1/1	0.92	0.50	40,40,40,40	0
56	MG	1a	1656	1/1	0.92	0.24	84,84,84,84	0
56	MG	1A	3273	1/1	0.92	0.20	37,37,37,37	0
56	MG	1A	3418	1/1	0.92	0.21	48,48,48,48	0
56	MG	2A	3492	1/1	0.92	0.13	67,67,67,67	0
56	MG	1a	1667	1/1	0.92	0.19	64,64,64,64	0
56	MG	2A	3495	1/1	0.92	0.30	60,60,60,60	0
56	MG	2A	3496	1/1	0.92	0.12	35,35,35,35	0
56	MG	2A	3144	1/1	0.92	0.34	41,41,41,41	0
56	MG	1a	1853	1/1	0.92	0.12	70,70,70,70	0
56	MG	1A	3788	1/1	0.92	0.23	30,30,30,30	0
56	MG	1a	1858	1/1	0.92	0.05	56,56,56,56	0
56	MG	2A	3510	1/1	0.92	0.28	61,61,61,61	0
56	MG	1E	310	1/1	0.92	0.35	49,49,49,49	0
56	MG	1a	1867	1/1	0.92	0.13	64,64,64,64	0
56	MG	1A	3793	1/1	0.92	0.19	55,55,55,55	0
56	MG	2A	3166	1/1	0.92	0.12	32,32,32,32	0
56	MG	2A	3169	1/1	0.92	0.14	37,37,37,37	0
56	MG	2l	3001	1/1	0.92	0.44	65,65,65,65	0
56	MG	1A	3422	1/1	0.92	0.14	40,40,40,40	0
56	MG	2A	3547	1/1	0.92	0.24	52,52,52,52	0
56	MG	1A	3990	1/1	0.92	0.18	17,17,17,17	0
56	MG	2A	3176	1/1	0.92	0.14	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3553	1/1	0.92	0.23	41,41,41,41	0
56	MG	1a	1684	1/1	0.92	0.11	57,57,57,57	0
56	MG	1A	3473	1/1	0.92	0.11	55,55,55,55	0
56	MG	1A	3996	1/1	0.92	0.07	37,37,37,37	0
56	MG	1a	1884	1/1	0.92	0.15	46,46,46,46	0
56	MG	1a	1885	1/1	0.92	0.21	54,54,54,54	0
56	MG	1a	1886	1/1	0.92	0.09	56,56,56,56	0
56	MG	1A	3998	1/1	0.92	0.22	59,59,59,59	0
56	MG	2A	3188	1/1	0.92	0.33	41,41,41,41	0
56	MG	1A	3686	1/1	0.93	0.17	28,28,28,28	0
56	MG	1A	3687	1/1	0.93	0.19	17,17,17,17	0
56	MG	2F	303	1/1	0.93	0.10	52,52,52,52	0
56	MG	1h	8002	1/1	0.93	0.45	80,80,80,80	0
56	MG	1A	3216	1/1	0.93	0.28	39,39,39,39	0
56	MG	1A	3549	1/1	0.93	0.28	73,73,73,73	0
56	MG	1A	3697	1/1	0.93	0.11	41,41,41,41	0
56	MG	1A	3489	1/1	0.93	0.23	41,41,41,41	0
56	MG	1F	302	1/1	0.93	0.12	39,39,39,39	0
56	MG	1o	102	1/1	0.93	0.16	72,72,72,72	0
56	MG	1F	303	1/1	0.93	0.45	32,32,32,32	0
56	MG	1A	3067	1/1	0.93	0.25	56,56,56,56	0
56	MG	1A	3707	1/1	0.93	0.18	32,32,32,32	0
56	MG	1F	307	1/1	0.93	0.66	59,59,59,59	0
56	MG	1A	3178	1/1	0.93	0.12	37,37,37,37	0
56	MG	1A	3713	1/1	0.93	0.09	61,61,61,61	0
56	MG	2A	3241	1/1	0.93	0.15	56,56,56,56	0
56	MG	1A	3716	1/1	0.93	0.14	38,38,38,38	0
56	MG	1A	3555	1/1	0.93	0.14	61,61,61,61	0
56	MG	1A	3556	1/1	0.93	0.27	58,58,58,58	0
56	MG	1N	3001	1/1	0.93	0.21	44,44,44,44	0
56	MG	1N	3002	1/1	0.93	0.29	48,48,48,48	0
56	MG	1A	3726	1/1	0.93	0.18	46,46,46,46	0
56	MG	1A	3963	1/1	0.93	0.13	27,27,27,27	0
56	MG	1N	3007	1/1	0.93	0.22	54,54,54,54	0
56	MG	1A	3492	1/1	0.93	0.55	47,47,47,47	0
56	MG	1A	3045	1/1	0.93	0.18	39,39,39,39	0
56	MG	1A	3282	1/1	0.93	0.22	54,54,54,54	0
56	MG	1x	110	1/1	0.93	0.28	73,73,73,73	0
56	MG	2A	3002	1/1	0.93	0.14	40,40,40,40	0
56	MG	2A	3003	1/1	0.93	0.13	43,43,43,43	0
56	MG	2A	3266	1/1	0.93	0.20	41,41,41,41	0
56	MG	1A	3750	1/1	0.93	0.17	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3754	1/1	0.93	0.34	39,39,39,39	0
56	MG	2A	3271	1/1	0.93	0.14	50,50,50,50	0
56	MG	2A	3272	1/1	0.93	0.22	67,67,67,67	0
56	MG	1Q	204	1/1	0.93	0.21	45,45,45,45	0
56	MG	1A	3127	1/1	0.93	0.23	40,40,40,40	0
56	MG	1Q	209	1/1	0.93	0.21	59,59,59,59	0
56	MG	2A	3277	1/1	0.93	0.14	44,44,44,44	0
56	MG	1R	202	1/1	0.93	0.51	55,55,55,55	0
56	MG	1A	3330	1/1	0.93	0.27	39,39,39,39	0
56	MG	2A	3282	1/1	0.93	0.16	35,35,35,35	0
56	MG	1A	3437	1/1	0.93	0.22	46,46,46,46	0
56	MG	1A	3992	1/1	0.93	0.09	36,36,36,36	0
56	MG	1A	3568	1/1	0.93	0.14	45,45,45,45	0
56	MG	1a	1753	1/1	0.93	0.22	48,48,48,48	0
56	MG	2A	3020	1/1	0.93	0.18	39,39,39,39	0
56	MG	1A	3768	1/1	0.93	0.18	8,8,8,8	0
56	MG	1A	3769	1/1	0.93	0.29	55,55,55,55	0
56	MG	1A	3438	1/1	0.93	0.08	49,49,49,49	0
56	MG	1U	203	1/1	0.93	0.16	29,29,29,29	0
56	MG	1A	3771	1/1	0.93	0.17	55,55,55,55	0
56	MG	2A	3031	1/1	0.93	0.18	47,47,47,47	0
56	MG	1a	1759	1/1	0.93	0.61	66,66,66,66	0
56	MG	1A	3578	1/1	0.93	0.14	48,48,48,48	0
56	MG	2A	3317	1/1	0.93	0.26	36,36,36,36	0
56	MG	1A	3229	1/1	0.93	0.14	50,50,50,50	0
56	MG	1A	3235	1/1	0.93	0.10	53,53,53,53	0
56	MG	1A	4018	1/1	0.93	0.17	45,45,45,45	0
56	MG	2a	3060	1/1	0.93	0.16	81,81,81,81	0
56	MG	2A	3335	1/1	0.93	0.20	35,35,35,35	0
56	MG	2A	3338	1/1	0.93	0.13	46,46,46,46	0
56	MG	1A	3779	1/1	0.93	0.13	35,35,35,35	0
56	MG	1A	3780	1/1	0.93	0.19	26,26,26,26	0
56	MG	1O	104	1/1	0.93	0.10	47,47,47,47	0
56	MG	1a	1769	1/1	0.93	0.11	63,63,63,63	0
56	MG	1A	3334	1/1	0.93	0.19	73,73,73,73	0
56	MG	2a	3075	1/1	0.93	0.11	59,59,59,59	0
56	MG	1A	3035	1/1	0.93	0.32	44,44,44,44	0
56	MG	2a	3079	1/1	0.93	0.09	52,52,52,52	0
56	MG	2a	3082	1/1	0.93	0.22	54,54,54,54	0
56	MG	2a	3083	1/1	0.93	0.10	49,49,49,49	0
56	MG	1a	1778	1/1	0.93	0.09	48,48,48,48	0
56	MG	2A	3352	1/1	0.93	0.19	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3588	1/1	0.93	0.19	60,60,60,60	0
56	MG	2A	3356	1/1	0.93	0.14	38,38,38,38	0
56	MG	1A	3037	1/1	0.93	0.24	40,40,40,40	0
56	MG	1a	1782	1/1	0.93	0.09	73,73,73,73	0
56	MG	1A	3807	1/1	0.93	0.12	46,46,46,46	0
56	MG	1A	4030	1/1	0.93	0.16	43,43,43,43	0
56	MG	2a	3100	1/1	0.93	0.33	80,80,80,80	0
56	MG	1A	4033	1/1	0.93	0.17	62,62,62,62	0
56	MG	2A	3366	1/1	0.93	0.22	50,50,50,50	0
56	MG	2a	3106	1/1	0.93	0.21	52,52,52,52	0
56	MG	1A	3595	1/1	0.93	0.12	66,66,66,66	0
56	MG	1A	3394	1/1	0.93	0.15	42,42,42,42	0
56	MG	1A	3049	1/1	0.93	0.10	37,37,37,37	0
56	MG	2A	3374	1/1	0.93	0.10	58,58,58,58	0
56	MG	1A	4037	1/1	0.93	0.18	75,75,75,75	0
56	MG	19	101	1/1	0.93	0.21	51,51,51,51	0
56	MG	1a	1794	1/1	0.93	0.12	56,56,56,56	0
56	MG	2a	3120	1/1	0.93	0.19	62,62,62,62	0
56	MG	1A	3136	1/1	0.93	0.09	35,35,35,35	0
56	MG	1A	3060	1/1	0.93	0.17	46,46,46,46	0
56	MG	1A	3349	1/1	0.93	0.19	35,35,35,35	0
56	MG	2A	3084	1/1	0.93	0.19	26,26,26,26	0
56	MG	1A	3197	1/1	0.93	0.12	23,23,23,23	0
56	MG	1A	3834	1/1	0.93	0.30	63,63,63,63	0
56	MG	2a	3135	1/1	0.93	0.20	73,73,73,73	0
56	MG	2a	3136	1/1	0.93	0.30	56,56,56,56	0
56	MG	1A	4048	1/1	0.93	0.11	48,48,48,48	0
56	MG	1A	3618	1/1	0.93	0.09	68,68,68,68	0
56	MG	2A	3092	1/1	0.93	0.23	48,48,48,48	0
56	MG	1A	3836	1/1	0.93	0.13	25,25,25,25	0
56	MG	1a	1807	1/1	0.93	0.14	55,55,55,55	0
56	MG	2a	3146	1/1	0.93	0.13	71,71,71,71	0
56	MG	1A	3622	1/1	0.93	0.15	36,36,36,36	0
56	MG	2a	3148	1/1	0.93	0.26	56,56,56,56	0
56	MG	1a	1810	1/1	0.93	0.18	59,59,59,59	0
56	MG	1A	3516	1/1	0.93	0.48	52,52,52,52	0
56	MG	1A	3845	1/1	0.93	0.63	35,35,35,35	0
56	MG	1a	1813	1/1	0.93	0.12	75,75,75,75	0
56	MG	2a	3154	1/1	0.93	0.19	71,71,71,71	0
56	MG	1A	3303	1/1	0.93	0.24	50,50,50,50	0
56	MG	1A	3520	1/1	0.93	0.09	61,61,61,61	0
56	MG	1A	3849	1/1	0.93	0.14	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2a	3160	1/1	0.93	0.17	61,61,61,61	0
56	MG	2a	3161	1/1	0.93	0.20	63,63,63,63	0
56	MG	1A	3352	1/1	0.93	0.20	57,57,57,57	0
56	MG	1A	3851	1/1	0.93	0.10	65,65,65,65	0
56	MG	2A	3440	1/1	0.93	0.12	50,50,50,50	0
56	MG	1A	3855	1/1	0.93	0.14	48,48,48,48	0
56	MG	1a	1624	1/1	0.93	0.12	80,80,80,80	0
56	MG	1A	3050	1/1	0.93	0.17	48,48,48,48	0
56	MG	2a	3171	1/1	0.93	0.29	46,46,46,46	0
56	MG	2A	3447	1/1	0.93	0.24	43,43,43,43	0
56	MG	2A	3448	1/1	0.93	0.12	62,62,62,62	0
56	MG	2a	3176	1/1	0.93	0.35	50,50,50,50	0
56	MG	1A	3199	1/1	0.93	0.29	44,44,44,44	0
56	MG	1A	3858	1/1	0.93	0.24	53,53,53,53	0
56	MG	2A	3453	1/1	0.93	0.12	31,31,31,31	0
56	MG	1A	3307	1/1	0.93	0.29	63,63,63,63	0
56	MG	1a	1830	1/1	0.93	0.21	68,68,68,68	0
56	MG	2a	3188	1/1	0.93	0.22	53,53,53,53	0
56	MG	1a	1833	1/1	0.93	0.29	62,62,62,62	0
56	MG	2A	3133	1/1	0.93	0.11	35,35,35,35	0
56	MG	1A	3862	1/1	0.93	0.21	45,45,45,45	0
56	MG	1A	3867	1/1	0.93	0.23	60,60,60,60	0
56	MG	2A	3471	1/1	0.93	0.23	63,63,63,63	0
56	MG	2a	3200	1/1	0.93	0.16	71,71,71,71	0
56	MG	2A	3473	1/1	0.93	0.17	41,41,41,41	0
56	MG	2A	3474	1/1	0.93	0.13	51,51,51,51	0
56	MG	2A	3141	1/1	0.93	0.40	49,49,49,49	0
56	MG	1A	3139	1/1	0.93	0.08	52,52,52,52	0
56	MG	1a	1843	1/1	0.93	0.19	55,55,55,55	0
56	MG	1A	3474	1/1	0.93	0.13	58,58,58,58	0
56	MG	2A	3147	1/1	0.93	0.07	62,62,62,62	0
56	MG	1A	3172	1/1	0.93	0.22	31,31,31,31	0
56	MG	2a	3213	1/1	0.93	0.10	71,71,71,71	0
56	MG	2A	3486	1/1	0.93	0.20	42,42,42,42	0
56	MG	1B	202	1/1	0.93	0.26	63,63,63,63	0
56	MG	2A	3489	1/1	0.93	0.10	52,52,52,52	0
56	MG	2A	3159	1/1	0.93	0.22	49,49,49,49	0
56	MG	1A	3650	1/1	0.93	0.12	28,28,28,28	0
56	MG	1A	3880	1/1	0.93	0.18	38,38,38,38	0
56	MG	1A	3883	1/1	0.93	0.13	36,36,36,36	0
56	MG	1A	3885	1/1	0.93	0.20	54,54,54,54	0
56	MG	1A	3886	1/1	0.93	0.09	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3501	1/1	0.93	0.20	37,37,37,37	0
56	MG	1A	3530	1/1	0.93	0.09	47,47,47,47	0
56	MG	1a	1872	1/1	0.93	0.13	57,57,57,57	0
56	MG	2A	3506	1/1	0.93	0.10	51,51,51,51	0
56	MG	1A	3206	1/1	0.93	0.46	45,45,45,45	0
56	MG	1A	3361	1/1	0.93	0.28	45,45,45,45	0
56	MG	2A	3519	1/1	0.93	0.13	52,52,52,52	0
56	MG	1a	1660	1/1	0.93	0.15	23,23,23,23	0
56	MG	2a	3249	1/1	0.93	0.26	36,36,36,36	0
56	MG	1B	221	1/1	0.93	0.14	30,30,30,30	0
56	MG	1a	1664	1/1	0.93	0.30	62,62,62,62	0
56	MG	1A	3661	1/1	0.93	0.08	30,30,30,30	0
56	MG	1A	3364	1/1	0.93	0.32	64,64,64,64	0
56	MG	2A	3544	1/1	0.93	0.16	48,48,48,48	0
56	MG	1A	3208	1/1	0.93	0.16	55,55,55,55	0
56	MG	1A	3270	1/1	0.93	0.31	41,41,41,41	0
56	MG	2f	201	1/1	0.93	0.19	48,48,48,48	0
56	MG	2A	3189	1/1	0.93	0.12	52,52,52,52	0
56	MG	1a	1895	1/1	0.93	0.35	59,59,59,59	0
56	MG	2l	3003	1/1	0.93	0.10	57,57,57,57	0
56	MG	2l	3004	1/1	0.93	0.10	60,60,60,60	0
56	MG	1A	3006	1/1	0.93	0.24	54,54,54,54	0
56	MG	2A	3193	1/1	0.93	0.18	37,37,37,37	0
56	MG	1a	1680	1/1	0.93	0.14	55,55,55,55	0
56	MG	1D	305	1/1	0.93	0.37	13,13,13,13	0
56	MG	2v	101	1/1	0.93	0.11	65,65,65,65	0
56	MG	1A	3682	1/1	0.93	0.23	29,29,29,29	0
56	MG	1A	3911	1/1	0.93	0.18	30,30,30,30	0
56	MG	2x	103	1/1	0.93	0.10	65,65,65,65	0
56	MG	1A	3213	1/1	0.93	0.36	44,44,44,44	0
56	MG	2A	3199	1/1	0.93	0.23	21,21,21,21	0
56	MG	1D	310	1/1	0.93	0.11	42,42,42,42	0
56	MG	1a	1690	1/1	0.93	0.10	57,57,57,57	0
56	MG	1d	503	1/1	0.93	0.19	77,77,77,77	0
56	MG	1A	3547	1/1	0.93	0.20	61,61,61,61	0
56	MG	2A	3526	1/1	0.94	0.09	50,50,50,50	0
56	MG	2A	3149	1/1	0.94	0.24	63,63,63,63	0
56	MG	2A	3535	1/1	0.94	0.06	52,52,52,52	0
56	MG	2A	3537	1/1	0.94	0.26	47,47,47,47	0
56	MG	2A	3539	1/1	0.94	0.17	57,57,57,57	0
56	MG	1A	3797	1/1	0.94	0.09	28,28,28,28	0
56	MG	2A	3542	1/1	0.94	0.12	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3800	1/1	0.94	0.14	32,32,32,32	0
56	MG	1A	3610	1/1	0.94	0.18	48,48,48,48	0
56	MG	1A	4032	1/1	0.94	0.13	38,38,38,38	0
56	MG	1a	1821	1/1	0.94	0.14	52,52,52,52	0
56	MG	2A	3162	1/1	0.94	0.13	40,40,40,40	0
56	MG	2A	3552	1/1	0.94	0.37	44,44,44,44	0
56	MG	1a	1822	1/1	0.94	0.17	56,56,56,56	0
56	MG	1A	3302	1/1	0.94	0.22	59,59,59,59	0
56	MG	2A	3555	1/1	0.94	0.34	49,49,49,49	0
56	MG	2A	3167	1/1	0.94	0.22	45,45,45,45	0
56	MG	1A	3805	1/1	0.94	0.16	49,49,49,49	0
56	MG	2A	3170	1/1	0.94	0.20	33,33,33,33	0
56	MG	2B	201	1/1	0.94	0.18	57,57,57,57	0
56	MG	1A	3806	1/1	0.94	0.12	38,38,38,38	0
56	MG	1a	1828	1/1	0.94	0.15	70,70,70,70	0
56	MG	1A	3044	1/1	0.94	0.35	60,60,60,60	0
56	MG	1A	3812	1/1	0.94	0.07	48,48,48,48	0
56	MG	1a	1614	1/1	0.94	0.10	66,66,66,66	0
56	MG	1A	3429	1/1	0.94	0.09	52,52,52,52	0
56	MG	1A	3619	1/1	0.94	0.12	56,56,56,56	0
56	MG	1A	3621	1/1	0.94	0.18	40,40,40,40	0
56	MG	2D	305	1/1	0.94	0.30	29,29,29,29	0
56	MG	1a	1839	1/1	0.94	0.24	53,53,53,53	0
56	MG	2F	301	1/1	0.94	0.18	49,49,49,49	0
56	MG	1A	3097	1/1	0.94	0.25	49,49,49,49	0
56	MG	2A	3187	1/1	0.94	0.23	40,40,40,40	0
56	MG	1a	1844	1/1	0.94	0.24	56,56,56,56	0
56	MG	1a	1848	1/1	0.94	0.23	77,77,77,77	0
56	MG	1A	3305	1/1	0.94	0.12	50,50,50,50	0
56	MG	1A	3629	1/1	0.94	0.15	33,33,33,33	0
56	MG	1A	3829	1/1	0.94	0.13	18,18,18,18	0
56	MG	1A	3831	1/1	0.94	0.13	18,18,18,18	0
56	MG	2Q	3004	1/1	0.94	0.28	41,41,41,41	0
56	MG	1A	3362	1/1	0.94	0.20	49,49,49,49	0
56	MG	1A	3833	1/1	0.94	0.11	50,50,50,50	0
56	MG	1A	3634	1/1	0.94	0.35	38,38,38,38	0
56	MG	1A	3635	1/1	0.94	0.11	50,50,50,50	0
56	MG	1a	1870	1/1	0.94	0.17	75,75,75,75	0
56	MG	2A	3200	1/1	0.94	0.20	50,50,50,50	0
56	MG	1A	3249	1/1	0.94	0.10	20,20,20,20	0
56	MG	1A	3637	1/1	0.94	0.11	43,43,43,43	0
56	MG	1a	1638	1/1	0.94	0.18	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3009	1/1	0.94	0.38	42,42,42,42	0
56	MG	1A	3519	1/1	0.94	0.18	48,48,48,48	0
56	MG	1A	4070	1/1	0.94	0.24	47,47,47,47	0
56	MG	1a	1642	1/1	0.94	0.06	58,58,58,58	0
56	MG	1A	3308	1/1	0.94	0.40	49,49,49,49	0
56	MG	2A	3216	1/1	0.94	0.45	44,44,44,44	0
56	MG	2A	3217	1/1	0.94	0.15	41,41,41,41	0
56	MG	1A	3253	1/1	0.94	0.23	32,32,32,32	0
56	MG	1a	1887	1/1	0.94	0.26	47,47,47,47	0
56	MG	1a	1646	1/1	0.94	0.30	80,80,80,80	0
56	MG	1A	3646	1/1	0.94	0.18	65,65,65,65	0
56	MG	1a	1893	1/1	0.94	0.37	69,69,69,69	0
56	MG	2A	3228	1/1	0.94	0.11	44,44,44,44	0
56	MG	2A	3229	1/1	0.94	0.21	59,59,59,59	0
56	MG	1A	3444	1/1	0.94	0.23	57,57,57,57	0
56	MG	2A	3231	1/1	0.94	0.28	57,57,57,57	0
56	MG	1A	3312	1/1	0.94	0.18	41,41,41,41	0
56	MG	2A	3234	1/1	0.94	0.11	65,65,65,65	0
56	MG	1A	3853	1/1	0.94	0.11	35,35,35,35	0
56	MG	1a	1654	1/1	0.94	0.10	45,45,45,45	0
56	MG	1A	3854	1/1	0.94	0.10	42,42,42,42	0
56	MG	2a	3032	1/1	0.94	0.27	59,59,59,59	0
56	MG	1A	3370	1/1	0.94	0.12	49,49,49,49	0
56	MG	1A	3371	1/1	0.94	0.18	46,46,46,46	0
56	MG	1A	3651	1/1	0.94	0.15	14,14,14,14	0
56	MG	1A	3149	1/1	0.94	0.39	32,32,32,32	0
56	MG	1a	1662	1/1	0.94	0.17	60,60,60,60	0
56	MG	1B	203	1/1	0.94	0.12	39,39,39,39	0
56	MG	2A	3250	1/1	0.94	0.26	30,30,30,30	0
56	MG	1A	3859	1/1	0.94	0.13	52,52,52,52	0
56	MG	1B	207	1/1	0.94	0.12	52,52,52,52	0
56	MG	1A	3374	1/1	0.94	0.27	26,26,26,26	0
56	MG	1A	3013	1/1	0.94	0.24	43,43,43,43	0
56	MG	1A	3258	1/1	0.94	0.20	63,63,63,63	0
56	MG	1a	1679	1/1	0.94	0.20	45,45,45,45	0
56	MG	2A	3259	1/1	0.94	0.13	39,39,39,39	0
56	MG	1A	3259	1/1	0.94	0.10	53,53,53,53	0
56	MG	1a	1682	1/1	0.94	0.06	47,47,47,47	0
56	MG	1A	3665	1/1	0.94	0.24	24,24,24,24	0
56	MG	1A	3070	1/1	0.94	0.45	48,48,48,48	0
56	MG	1A	3262	1/1	0.94	0.20	28,28,28,28	0
56	MG	1A	3878	1/1	0.94	0.15	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3537	1/1	0.94	0.17	53,53,53,53	0
56	MG	1A	3679	1/1	0.94	0.12	38,38,38,38	0
56	MG	1B	226	1/1	0.94	0.16	71,71,71,71	0
56	MG	1A	3539	1/1	0.94	0.11	45,45,45,45	0
56	MG	1B	229	1/1	0.94	0.12	36,36,36,36	0
56	MG	1a	1695	1/1	0.94	0.24	53,53,53,53	0
56	MG	1A	3203	1/1	0.94	0.40	47,47,47,47	0
56	MG	1D	301	1/1	0.94	0.19	32,32,32,32	0
56	MG	1A	3541	1/1	0.94	0.14	56,56,56,56	0
56	MG	2a	3074	1/1	0.94	0.36	47,47,47,47	0
56	MG	1D	303	1/1	0.94	0.18	38,38,38,38	0
56	MG	1x	103	1/1	0.94	0.17	48,48,48,48	0
56	MG	2a	3077	1/1	0.94	0.11	51,51,51,51	0
56	MG	1A	3071	1/1	0.94	0.47	37,37,37,37	0
56	MG	1x	106	1/1	0.94	0.07	42,42,42,42	0
56	MG	1A	3323	1/1	0.94	0.15	41,41,41,41	0
56	MG	2A	3296	1/1	0.94	0.29	57,57,57,57	0
56	MG	1A	3268	1/1	0.94	0.31	23,23,23,23	0
56	MG	1A	3105	1/1	0.94	0.35	47,47,47,47	0
56	MG	2a	3090	1/1	0.94	0.37	47,47,47,47	0
56	MG	2A	3302	1/1	0.94	0.18	41,41,41,41	0
56	MG	2A	3304	1/1	0.94	0.09	66,66,66,66	0
56	MG	1A	3898	1/1	0.94	0.17	52,52,52,52	0
56	MG	1A	3207	1/1	0.94	0.25	42,42,42,42	0
56	MG	2a	3097	1/1	0.94	0.29	55,55,55,55	0
56	MG	1A	3033	1/1	0.94	0.14	50,50,50,50	0
56	MG	2a	3099	1/1	0.94	0.30	41,41,41,41	0
56	MG	1A	3906	1/1	0.94	0.12	53,53,53,53	0
56	MG	1A	3110	1/1	0.94	0.26	65,65,65,65	0
56	MG	1A	3553	1/1	0.94	0.32	63,63,63,63	0
56	MG	1A	3909	1/1	0.94	0.12	46,46,46,46	0
56	MG	1A	3708	1/1	0.94	0.16	59,59,59,59	0
56	MG	1a	1728	1/1	0.94	0.15	46,46,46,46	0
56	MG	2A	3320	1/1	0.94	0.22	53,53,53,53	0
56	MG	2A	3327	1/1	0.94	0.14	44,44,44,44	0
56	MG	2a	3116	1/1	0.94	0.13	45,45,45,45	0
56	MG	1a	1729	1/1	0.94	0.17	75,75,75,75	0
56	MG	1A	3913	1/1	0.94	0.08	28,28,28,28	0
56	MG	1a	1732	1/1	0.94	0.47	63,63,63,63	0
56	MG	2A	3016	1/1	0.94	0.29	51,51,51,51	0
56	MG	2A	3017	1/1	0.94	0.35	46,46,46,46	0
56	MG	1A	3274	1/1	0.94	0.22	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3712	1/1	0.94	0.24	56,56,56,56	0
56	MG	2a	3126	1/1	0.94	0.23	60,60,60,60	0
56	MG	2a	3127	1/1	0.94	0.21	50,50,50,50	0
56	MG	1A	3919	1/1	0.94	0.10	51,51,51,51	0
56	MG	1A	3332	1/1	0.94	0.29	35,35,35,35	0
56	MG	2a	3131	1/1	0.94	0.40	48,48,48,48	0
56	MG	2A	3345	1/1	0.94	0.10	60,60,60,60	0
56	MG	1a	1740	1/1	0.94	0.20	63,63,63,63	0
56	MG	2A	3027	1/1	0.94	0.07	56,56,56,56	0
56	MG	1A	3922	1/1	0.94	0.18	25,25,25,25	0
56	MG	1A	3165	1/1	0.94	0.25	23,23,23,23	0
56	MG	1H	3001	1/1	0.94	0.26	35,35,35,35	0
56	MG	1A	3718	1/1	0.94	0.15	36,36,36,36	0
56	MG	2A	3032	1/1	0.94	0.08	62,62,62,62	0
56	MG	2A	3033	1/1	0.94	0.20	47,47,47,47	0
56	MG	1A	3215	1/1	0.94	0.21	49,49,49,49	0
56	MG	1A	3934	1/1	0.94	0.17	35,35,35,35	0
56	MG	1A	3135	1/1	0.94	0.29	30,30,30,30	0
56	MG	1A	3217	1/1	0.94	0.10	56,56,56,56	0
56	MG	1A	3561	1/1	0.94	0.09	72,72,72,72	0
56	MG	2a	3152	1/1	0.94	0.09	67,67,67,67	0
56	MG	2A	3042	1/1	0.94	0.25	46,46,46,46	0
56	MG	2A	3043	1/1	0.94	0.12	42,42,42,42	0
56	MG	2A	3376	1/1	0.94	0.17	19,19,19,19	0
56	MG	1A	3729	1/1	0.94	0.11	60,60,60,60	0
56	MG	2a	3158	1/1	0.94	0.22	65,65,65,65	0
56	MG	1A	3730	1/1	0.94	0.13	34,34,34,34	0
56	MG	1A	3733	1/1	0.94	0.26	49,49,49,49	0
56	MG	2A	3047	1/1	0.94	0.18	37,37,37,37	0
56	MG	2A	3048	1/1	0.94	0.14	45,45,45,45	0
56	MG	1A	3734	1/1	0.94	0.19	46,46,46,46	0
56	MG	1A	3010	1/1	0.94	0.12	66,66,66,66	0
56	MG	2A	3404	1/1	0.94	0.15	64,64,64,64	0
56	MG	1A	3952	1/1	0.94	0.14	40,40,40,40	0
56	MG	1A	3747	1/1	0.94	0.36	50,50,50,50	0
56	MG	1A	3748	1/1	0.94	0.21	13,13,13,13	0
56	MG	1A	3340	1/1	0.94	0.08	59,59,59,59	0
56	MG	2A	3061	1/1	0.94	0.12	29,29,29,29	0
56	MG	1A	3343	1/1	0.94	0.11	55,55,55,55	0
56	MG	1A	3752	1/1	0.94	0.11	63,63,63,63	0
56	MG	1A	3058	1/1	0.94	0.26	45,45,45,45	0
56	MG	1A	3758	1/1	0.94	0.17	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2a	3181	1/1	0.94	0.15	58,58,58,58	0
56	MG	2A	3425	1/1	0.94	0.09	48,48,48,48	0
56	MG	2a	3186	1/1	0.94	0.13	50,50,50,50	0
56	MG	2A	3066	1/1	0.94	0.20	48,48,48,48	0
56	MG	2A	3070	1/1	0.94	0.60	53,53,53,53	0
56	MG	1A	3003	1/1	0.94	0.16	44,44,44,44	0
56	MG	1A	3077	1/1	0.94	0.26	48,48,48,48	0
56	MG	1a	1766	1/1	0.94	0.16	50,50,50,50	0
56	MG	2a	3195	1/1	0.94	0.17	48,48,48,48	0
56	MG	2a	3196	1/1	0.94	0.13	70,70,70,70	0
56	MG	1T	204	1/1	0.94	0.10	50,50,50,50	0
56	MG	1a	1768	1/1	0.94	0.25	56,56,56,56	0
56	MG	1A	3985	1/1	0.94	0.16	34,34,34,34	0
56	MG	2A	3080	1/1	0.94	0.23	59,59,59,59	0
56	MG	1A	3763	1/1	0.94	0.15	42,42,42,42	0
56	MG	1a	1775	1/1	0.94	0.18	65,65,65,65	0
56	MG	1a	1776	1/1	0.94	0.19	67,67,67,67	0
56	MG	2a	3207	1/1	0.94	0.08	59,59,59,59	0
56	MG	1A	3413	1/1	0.94	0.15	60,60,60,60	0
56	MG	1A	3183	1/1	0.94	0.31	28,28,28,28	0
56	MG	1a	1779	1/1	0.94	0.22	66,66,66,66	0
56	MG	1A	3079	1/1	0.94	0.20	53,53,53,53	0
56	MG	2A	3452	1/1	0.94	0.08	60,60,60,60	0
56	MG	1A	3141	1/1	0.94	0.24	39,39,39,39	0
56	MG	1W	3001	1/1	0.94	0.22	53,53,53,53	0
56	MG	2A	3460	1/1	0.94	0.08	45,45,45,45	0
56	MG	1W	3004	1/1	0.94	0.17	40,40,40,40	0
56	MG	2a	3222	1/1	0.94	0.09	62,62,62,62	0
56	MG	1A	3419	1/1	0.94	0.39	52,52,52,52	0
56	MG	1A	3589	1/1	0.94	0.12	36,36,36,36	0
56	MG	2A	3466	1/1	0.94	0.13	45,45,45,45	0
56	MG	1A	3590	1/1	0.94	0.18	51,51,51,51	0
56	MG	2a	3227	1/1	0.94	0.12	62,62,62,62	0
56	MG	2a	3228	1/1	0.94	0.26	58,58,58,58	0
56	MG	1A	4002	1/1	0.94	0.12	65,65,65,65	0
56	MG	10	101	1/1	0.94	0.24	49,49,49,49	0
56	MG	2A	3103	1/1	0.94	0.11	46,46,46,46	0
56	MG	1A	4003	1/1	0.94	0.21	44,44,44,44	0
56	MG	1A	3420	1/1	0.94	0.16	54,54,54,54	0
56	MG	1A	4009	1/1	0.94	0.17	47,47,47,47	0
56	MG	1A	3353	1/1	0.94	0.07	40,40,40,40	0
56	MG	2A	3479	1/1	0.94	0.25	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3111	1/1	0.94	0.20	36,36,36,36	0
56	MG	2a	3247	1/1	0.94	0.30	50,50,50,50	0
56	MG	2a	3248	1/1	0.94	0.20	56,56,56,56	0
56	MG	11	101	1/1	0.94	0.20	50,50,50,50	0
56	MG	2a	3250	1/1	0.94	0.18	63,63,63,63	0
56	MG	1A	4011	1/1	0.94	0.18	68,68,68,68	0
56	MG	1A	4012	1/1	0.94	0.14	47,47,47,47	0
56	MG	2A	3487	1/1	0.94	0.10	40,40,40,40	0
56	MG	1a	1799	1/1	0.94	0.15	57,57,57,57	0
56	MG	1A	3423	1/1	0.94	0.15	42,42,42,42	0
56	MG	2A	3491	1/1	0.94	0.19	46,46,46,46	0
56	MG	1a	1801	1/1	0.94	0.12	65,65,65,65	0
56	MG	13	101	1/1	0.94	0.21	47,47,47,47	0
56	MG	1A	3080	1/1	0.94	0.07	53,53,53,53	0
56	MG	15	103	1/1	0.94	0.29	28,28,28,28	0
56	MG	2A	3497	1/1	0.94	0.16	46,46,46,46	0
56	MG	2A	3129	1/1	0.94	0.19	33,33,33,33	0
56	MG	2l	3005	1/1	0.94	0.21	44,44,44,44	0
56	MG	1A	3786	1/1	0.94	0.21	23,23,23,23	0
56	MG	2A	3132	1/1	0.94	0.11	45,45,45,45	0
56	MG	16	102	1/1	0.94	0.17	40,40,40,40	0
56	MG	2r	3001	1/1	0.94	0.15	55,55,55,55	0
56	MG	1A	3787	1/1	0.94	0.18	26,26,26,26	0
56	MG	1A	4023	1/1	0.94	0.17	52,52,52,52	0
56	MG	1A	4024	1/1	0.94	0.21	39,39,39,39	0
56	MG	1A	3144	1/1	0.94	0.34	48,48,48,48	0
56	MG	2A	3513	1/1	0.94	0.31	26,26,26,26	0
56	MG	2A	3515	1/1	0.94	0.14	55,55,55,55	0
56	MG	2A	3516	1/1	0.94	0.10	53,53,53,53	0
56	MG	1A	3239	1/1	0.94	0.14	50,50,50,50	0
56	MG	2z	8001	1/1	0.94	0.25	69,69,69,69	0
56	MG	1A	3794	1/1	0.94	0.18	19,19,19,19	0
57	ZN	1n	101	1/1	0.94	0.10	83,83,83,83	0
57	ZN	2Y	501	1/1	0.94	0.06	99,99,99,99	0
56	MG	19	104	1/1	0.94	0.16	42,42,42,42	0
56	MG	2A	3525	1/1	0.94	0.39	36,36,36,36	0
56	MG	2A	3285	1/1	0.95	0.12	33,33,33,33	0
56	MG	1a	1626	1/1	0.95	0.52	68,68,68,68	0
56	MG	1A	3445	1/1	0.95	0.12	46,46,46,46	0
56	MG	2A	3292	1/1	0.95	0.16	21,21,21,21	0
56	MG	2a	3008	1/1	0.95	0.09	53,53,53,53	0
56	MG	1A	3654	1/1	0.95	0.12	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3055	1/1	0.95	0.39	45,45,45,45	0
56	MG	1A	3098	1/1	0.95	0.18	40,40,40,40	0
56	MG	1a	1805	1/1	0.95	0.14	61,61,61,61	0
56	MG	1a	1631	1/1	0.95	0.15	44,44,44,44	0
56	MG	2A	3303	1/1	0.95	0.20	30,30,30,30	0
56	MG	1A	3658	1/1	0.95	0.13	13,13,13,13	0
56	MG	1A	3148	1/1	0.95	0.29	51,51,51,51	0
56	MG	1A	3660	1/1	0.95	0.12	24,24,24,24	0
56	MG	1A	3944	1/1	0.95	0.38	39,39,39,39	0
56	MG	1A	3945	1/1	0.95	0.26	30,30,30,30	0
56	MG	1A	3947	1/1	0.95	0.12	42,42,42,42	0
56	MG	1A	3564	1/1	0.95	0.25	36,36,36,36	0
56	MG	1a	1643	1/1	0.95	0.08	68,68,68,68	0
56	MG	1A	3565	1/1	0.95	0.31	41,41,41,41	0
56	MG	1A	3566	1/1	0.95	0.22	34,34,34,34	0
56	MG	1A	3299	1/1	0.95	0.44	59,59,59,59	0
56	MG	1A	3363	1/1	0.95	0.14	49,49,49,49	0
56	MG	1A	3810	1/1	0.95	0.17	30,30,30,30	0
56	MG	1A	3966	1/1	0.95	0.17	19,19,19,19	0
56	MG	1a	1651	1/1	0.95	0.17	62,62,62,62	0
56	MG	1a	1652	1/1	0.95	0.20	60,60,60,60	0
56	MG	1a	1824	1/1	0.95	0.09	54,54,54,54	0
56	MG	2A	3086	1/1	0.95	0.22	47,47,47,47	0
56	MG	1A	3672	1/1	0.95	0.23	29,29,29,29	0
56	MG	1A	3231	1/1	0.95	0.14	42,42,42,42	0
56	MG	1A	3971	1/1	0.95	0.12	27,27,27,27	0
56	MG	2A	3091	1/1	0.95	0.13	49,49,49,49	0
56	MG	1A	3819	1/1	0.95	0.07	43,43,43,43	0
56	MG	1a	1657	1/1	0.95	0.25	62,62,62,62	0
56	MG	2A	3349	1/1	0.95	0.07	67,67,67,67	0
56	MG	1A	3820	1/1	0.95	0.07	71,71,71,71	0
56	MG	2a	3050	1/1	0.95	0.13	86,86,86,86	0
56	MG	2A	3096	1/1	0.95	0.18	47,47,47,47	0
56	MG	1A	3976	1/1	0.95	0.21	42,42,42,42	0
56	MG	2A	3098	1/1	0.95	0.17	41,41,41,41	0
56	MG	1A	3234	1/1	0.95	0.05	46,46,46,46	0
56	MG	1E	305	1/1	0.95	0.17	14,14,14,14	0
56	MG	2A	3101	1/1	0.95	0.07	56,56,56,56	0
56	MG	1E	306	1/1	0.95	0.34	57,57,57,57	0
56	MG	1a	1666	1/1	0.95	0.17	72,72,72,72	0
56	MG	1A	3980	1/1	0.95	0.22	59,59,59,59	0
56	MG	1a	1845	1/1	0.95	0.14	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3371	1/1	0.95	0.12	52,52,52,52	0
56	MG	1a	1846	1/1	0.95	0.10	25,25,25,25	0
56	MG	2a	3066	1/1	0.95	0.38	64,64,64,64	0
56	MG	2A	3109	1/1	0.95	0.26	54,54,54,54	0
56	MG	1E	308	1/1	0.95	0.38	35,35,35,35	0
56	MG	2A	3377	1/1	0.95	0.15	33,33,33,33	0
56	MG	1A	3073	1/1	0.95	0.15	46,46,46,46	0
56	MG	2a	3073	1/1	0.95	0.10	63,63,63,63	0
56	MG	2A	3383	1/1	0.95	0.14	29,29,29,29	0
56	MG	1a	1670	1/1	0.95	0.09	50,50,50,50	0
56	MG	2A	3387	1/1	0.95	0.26	38,38,38,38	0
56	MG	1E	312	1/1	0.95	0.17	44,44,44,44	0
56	MG	2A	3115	1/1	0.95	0.16	41,41,41,41	0
56	MG	1a	1672	1/1	0.95	0.14	47,47,47,47	0
56	MG	2A	3119	1/1	0.95	0.27	35,35,35,35	0
56	MG	1F	301	1/1	0.95	0.19	30,30,30,30	0
56	MG	1a	1864	1/1	0.95	0.46	69,69,69,69	0
56	MG	2A	3405	1/1	0.95	0.13	46,46,46,46	0
56	MG	1a	1675	1/1	0.95	0.09	42,42,42,42	0
56	MG	1A	3066	1/1	0.95	0.14	56,56,56,56	0
56	MG	1A	3059	1/1	0.95	0.27	32,32,32,32	0
56	MG	2A	3411	1/1	0.95	0.18	47,47,47,47	0
56	MG	1a	1681	1/1	0.95	0.11	47,47,47,47	0
56	MG	1A	3685	1/1	0.95	0.18	16,16,16,16	0
56	MG	2A	3130	1/1	0.95	0.22	49,49,49,49	0
56	MG	1A	3457	1/1	0.95	0.07	61,61,61,61	0
56	MG	1a	1873	1/1	0.95	0.15	60,60,60,60	0
56	MG	1A	3830	1/1	0.95	0.09	34,34,34,34	0
56	MG	1a	1875	1/1	0.95	0.05	58,58,58,58	0
56	MG	2A	3427	1/1	0.95	0.33	54,54,54,54	0
56	MG	2A	3428	1/1	0.95	0.14	59,59,59,59	0
56	MG	1A	3995	1/1	0.95	0.31	54,54,54,54	0
56	MG	2A	3137	1/1	0.95	0.17	33,33,33,33	0
56	MG	2A	3138	1/1	0.95	0.23	47,47,47,47	0
56	MG	2A	3140	1/1	0.95	0.19	33,33,33,33	0
56	MG	1A	3587	1/1	0.95	0.25	42,42,42,42	0
56	MG	1a	1879	1/1	0.95	0.09	52,52,52,52	0
56	MG	1A	3997	1/1	0.95	0.18	32,32,32,32	0
56	MG	1a	1881	1/1	0.95	0.24	52,52,52,52	0
56	MG	1a	1688	1/1	0.95	0.12	61,61,61,61	0
56	MG	2A	3148	1/1	0.95	0.19	38,38,38,38	0
56	MG	1a	1689	1/1	0.95	0.15	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3068	1/1	0.95	0.25	45,45,45,45	0
56	MG	1A	3157	1/1	0.95	0.22	43,43,43,43	0
56	MG	1A	3416	1/1	0.95	0.12	66,66,66,66	0
56	MG	1A	3372	1/1	0.95	0.12	50,50,50,50	0
56	MG	1A	3470	1/1	0.95	0.11	51,51,51,51	0
56	MG	1a	1894	1/1	0.95	0.29	63,63,63,63	0
56	MG	2a	3134	1/1	0.95	0.19	55,55,55,55	0
56	MG	2A	3163	1/1	0.95	0.13	56,56,56,56	0
56	MG	2A	3455	1/1	0.95	0.15	62,62,62,62	0
56	MG	1A	3702	1/1	0.95	0.12	20,20,20,20	0
56	MG	2A	3457	1/1	0.95	0.28	46,46,46,46	0
56	MG	2a	3140	1/1	0.95	0.26	49,49,49,49	0
56	MG	1a	1898	1/1	0.95	0.16	59,59,59,59	0
56	MG	1A	4007	1/1	0.95	0.23	35,35,35,35	0
56	MG	2A	3168	1/1	0.95	0.19	33,33,33,33	0
56	MG	2A	3464	1/1	0.95	0.12	35,35,35,35	0
56	MG	1A	3705	1/1	0.95	0.11	59,59,59,59	0
56	MG	1A	3597	1/1	0.95	0.10	71,71,71,71	0
56	MG	1A	3598	1/1	0.95	0.17	30,30,30,30	0
56	MG	1A	3710	1/1	0.95	0.09	48,48,48,48	0
56	MG	2A	3174	1/1	0.95	0.17	56,56,56,56	0
56	MG	1a	1705	1/1	0.95	0.05	58,58,58,58	0
56	MG	1A	4013	1/1	0.95	0.17	42,42,42,42	0
56	MG	1A	4014	1/1	0.95	0.19	57,57,57,57	0
56	MG	2A	3179	1/1	0.95	0.34	29,29,29,29	0
56	MG	2a	3156	1/1	0.95	0.10	50,50,50,50	0
56	MG	1P	205	1/1	0.95	0.18	53,53,53,53	0
56	MG	1Q	201	1/1	0.95	0.25	33,33,33,33	0
56	MG	1A	3599	1/1	0.95	0.10	38,38,38,38	0
56	MG	1Q	205	1/1	0.95	0.15	40,40,40,40	0
56	MG	1A	4017	1/1	0.95	0.14	61,61,61,61	0
56	MG	1A	3240	1/1	0.95	0.16	32,32,32,32	0
56	MG	1a	1723	1/1	0.95	0.15	62,62,62,62	0
56	MG	1A	3602	1/1	0.95	0.09	41,41,41,41	0
56	MG	1A	3603	1/1	0.95	0.14	62,62,62,62	0
56	MG	2A	3490	1/1	0.95	0.17	66,66,66,66	0
56	MG	2A	3191	1/1	0.95	0.16	37,37,37,37	0
56	MG	2a	3169	1/1	0.95	0.18	67,67,67,67	0
56	MG	2a	3170	1/1	0.95	0.22	72,72,72,72	0
56	MG	1A	3472	1/1	0.95	0.17	53,53,53,53	0
56	MG	1A	3339	1/1	0.95	0.12	56,56,56,56	0
56	MG	1A	3720	1/1	0.95	0.17	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3606	1/1	0.95	0.21	28,28,28,28	0
56	MG	1A	3375	1/1	0.95	0.11	44,44,44,44	0
56	MG	1A	3421	1/1	0.95	0.30	38,38,38,38	0
56	MG	1A	3476	1/1	0.95	0.17	56,56,56,56	0
56	MG	2A	3500	1/1	0.95	0.10	45,45,45,45	0
56	MG	1A	3210	1/1	0.95	0.09	40,40,40,40	0
56	MG	2a	3183	1/1	0.95	0.08	60,60,60,60	0
56	MG	1A	3864	1/1	0.95	0.14	38,38,38,38	0
56	MG	1U	206	1/1	0.95	0.38	38,38,38,38	0
56	MG	1A	3341	1/1	0.95	0.11	53,53,53,53	0
56	MG	2A	3508	1/1	0.95	0.20	42,42,42,42	0
56	MG	1A	3310	1/1	0.95	0.14	52,52,52,52	0
56	MG	1A	3870	1/1	0.95	0.14	44,44,44,44	0
56	MG	1A	3740	1/1	0.95	0.28	68,68,68,68	0
56	MG	2A	3209	1/1	0.95	0.43	54,54,54,54	0
56	MG	1A	3620	1/1	0.95	0.10	55,55,55,55	0
56	MG	2A	3517	1/1	0.95	0.12	47,47,47,47	0
56	MG	1Y	502	1/1	0.95	0.12	40,40,40,40	0
56	MG	2A	3521	1/1	0.95	0.07	41,41,41,41	0
56	MG	1A	3874	1/1	0.95	0.11	28,28,28,28	0
56	MG	1x	105	1/1	0.95	0.11	64,64,64,64	0
56	MG	2a	3204	1/1	0.95	0.13	57,57,57,57	0
56	MG	1A	4039	1/1	0.95	0.08	56,56,56,56	0
56	MG	1A	4040	1/1	0.95	0.15	32,32,32,32	0
56	MG	2a	3208	1/1	0.95	0.12	65,65,65,65	0
56	MG	1A	3743	1/1	0.95	0.12	30,30,30,30	0
56	MG	2A	3533	1/1	0.95	0.20	47,47,47,47	0
56	MG	1A	3744	1/1	0.95	0.12	43,43,43,43	0
56	MG	2A	3536	1/1	0.95	0.14	42,42,42,42	0
56	MG	2A	3222	1/1	0.95	0.10	62,62,62,62	0
56	MG	1A	3745	1/1	0.95	0.09	57,57,57,57	0
56	MG	1z	8001	1/1	0.95	0.14	56,56,56,56	0
56	MG	1A	4045	1/1	0.95	0.09	23,23,23,23	0
56	MG	1A	3244	1/1	0.95	0.16	35,35,35,35	0
56	MG	2a	3220	1/1	0.95	0.25	85,85,85,85	0
56	MG	2a	3221	1/1	0.95	0.31	57,57,57,57	0
56	MG	1A	3884	1/1	0.95	0.15	58,58,58,58	0
56	MG	2A	3006	1/1	0.95	0.19	59,59,59,59	0
56	MG	1A	3483	1/1	0.95	0.16	41,41,41,41	0
56	MG	1A	3347	1/1	0.95	0.19	56,56,56,56	0
56	MG	2A	3551	1/1	0.95	0.17	32,32,32,32	0
56	MG	1A	3245	1/1	0.95	0.20	18,18,18,18	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3236	1/1	0.95	0.08	60,60,60,60	0
56	MG	1A	3889	1/1	0.95	0.17	55,55,55,55	0
56	MG	1A	3630	1/1	0.95	0.17	37,37,37,37	0
56	MG	2a	3232	1/1	0.95	0.12	54,54,54,54	0
56	MG	1A	4059	1/1	0.95	0.23	28,28,28,28	0
56	MG	1A	3891	1/1	0.95	0.26	68,68,68,68	0
56	MG	2A	3560	1/1	0.95	0.31	41,41,41,41	0
56	MG	1A	3247	1/1	0.95	0.14	35,35,35,35	0
56	MG	1A	3757	1/1	0.95	0.12	49,49,49,49	0
56	MG	2a	3243	1/1	0.95	0.26	74,74,74,74	0
56	MG	1A	3633	1/1	0.95	0.17	50,50,50,50	0
56	MG	2B	203	1/1	0.95	0.12	51,51,51,51	0
56	MG	1A	3545	1/1	0.95	0.34	50,50,50,50	0
56	MG	1A	4068	1/1	0.95	0.24	39,39,39,39	0
56	MG	1A	3761	1/1	0.95	0.19	67,67,67,67	0
56	MG	2B	207	1/1	0.95	0.09	67,67,67,67	0
56	MG	1a	1774	1/1	0.95	0.20	62,62,62,62	0
56	MG	2B	209	1/1	0.95	0.33	57,57,57,57	0
56	MG	2A	3024	1/1	0.95	0.14	55,55,55,55	0
56	MG	2D	301	1/1	0.95	0.11	49,49,49,49	0
56	MG	1A	3018	1/1	0.95	0.22	53,53,53,53	0
56	MG	1A	3902	1/1	0.95	0.15	42,42,42,42	0
56	MG	1A	3131	1/1	0.95	0.22	31,31,31,31	0
56	MG	2E	303	1/1	0.95	0.12	60,60,60,60	0
56	MG	1A	3389	1/1	0.95	0.13	56,56,56,56	0
56	MG	1A	3434	1/1	0.95	0.13	50,50,50,50	0
56	MG	1A	3284	1/1	0.95	0.11	52,52,52,52	0
56	MG	1A	4082	1/1	0.95	0.11	66,66,66,66	0
56	MG	1a	1607	1/1	0.95	0.11	60,60,60,60	0
56	MG	1A	3910	1/1	0.95	0.12	61,61,61,61	0
56	MG	2O	201	1/1	0.95	0.10	54,54,54,54	0
56	MG	1A	4085	1/1	0.95	0.58	34,34,34,34	0
56	MG	1A	3285	1/1	0.95	0.31	32,32,32,32	0
56	MG	1A	3001	1/1	0.95	0.24	31,31,31,31	0
56	MG	1A	3645	1/1	0.95	0.10	36,36,36,36	0
56	MG	1A	3164	1/1	0.95	0.14	40,40,40,40	0
56	MG	1A	3134	1/1	0.95	0.13	23,23,23,23	0
56	MG	2R	201	1/1	0.95	0.36	49,49,49,49	0
56	MG	2T	201	1/1	0.95	0.19	41,41,41,41	0
56	MG	1A	3440	1/1	0.95	0.15	39,39,39,39	0
56	MG	2Y	502	1/1	0.95	0.13	51,51,51,51	0
56	MG	1A	3776	1/1	0.95	0.18	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3278	1/1	0.95	0.27	43,43,43,43	0
56	MG	1A	3441	1/1	0.95	0.12	49,49,49,49	0
56	MG	1A	3168	1/1	0.95	0.19	35,35,35,35	0
56	MG	1A	3782	1/1	0.95	0.13	19,19,19,19	0
57	ZN	26	501	1/1	0.95	0.09	61,61,61,61	0
56	MG	1a	1625	1/1	0.95	0.12	34,34,34,34	0
56	MG	1A	4022	1/1	0.96	0.15	43,43,43,43	0
56	MG	1W	3002	1/1	0.96	0.17	35,35,35,35	0
56	MG	1W	3003	1/1	0.96	0.21	33,33,33,33	0
56	MG	1A	3171	1/1	0.96	0.29	51,51,51,51	0
56	MG	2A	3264	1/1	0.96	0.23	29,29,29,29	0
56	MG	1A	3046	1/1	0.96	0.20	45,45,45,45	0
56	MG	1A	3293	1/1	0.96	0.20	11,11,11,11	0
56	MG	1A	3727	1/1	0.96	0.16	49,49,49,49	0
56	MG	1A	3114	1/1	0.96	0.27	48,48,48,48	0
56	MG	2A	3026	1/1	0.96	0.41	49,49,49,49	0
56	MG	1A	3538	1/1	0.96	0.15	39,39,39,39	0
56	MG	1A	3379	1/1	0.96	0.34	43,43,43,43	0
56	MG	1A	3153	1/1	0.96	0.21	20,20,20,20	0
56	MG	1A	4031	1/1	0.96	0.24	66,66,66,66	0
56	MG	1A	3861	1/1	0.96	0.05	42,42,42,42	0
56	MG	1A	3627	1/1	0.96	0.19	41,41,41,41	0
56	MG	1A	3863	1/1	0.96	0.19	38,38,38,38	0
56	MG	2A	3280	1/1	0.96	0.10	58,58,58,58	0
56	MG	1A	3735	1/1	0.96	0.14	63,63,63,63	0
56	MG	1A	3865	1/1	0.96	0.19	72,72,72,72	0
56	MG	2A	3037	1/1	0.96	0.20	42,42,42,42	0
56	MG	1A	3866	1/1	0.96	0.21	42,42,42,42	0
56	MG	1A	3737	1/1	0.96	0.19	18,18,18,18	0
56	MG	1A	3739	1/1	0.96	0.18	34,34,34,34	0
56	MG	2A	3291	1/1	0.96	0.19	37,37,37,37	0
56	MG	15	102	1/1	0.96	0.17	52,52,52,52	0
56	MG	1A	3250	1/1	0.96	0.14	22,22,22,22	0
56	MG	1A	3542	1/1	0.96	0.38	63,63,63,63	0
56	MG	1A	3480	1/1	0.96	0.17	54,54,54,54	0
56	MG	2A	3300	1/1	0.96	0.12	38,38,38,38	0
56	MG	1A	3155	1/1	0.96	0.15	39,39,39,39	0
56	MG	1A	3179	1/1	0.96	0.40	22,22,22,22	0
56	MG	1A	3877	1/1	0.96	0.15	39,39,39,39	0
56	MG	1A	3746	1/1	0.96	0.09	46,46,46,46	0
56	MG	2A	3051	1/1	0.96	0.24	35,35,35,35	0
56	MG	18	3003	1/1	0.96	0.22	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3053	1/1	0.96	0.28	43,43,43,43	0
56	MG	2A	3309	1/1	0.96	0.17	37,37,37,37	0
56	MG	2A	3310	1/1	0.96	0.05	55,55,55,55	0
56	MG	1A	3879	1/1	0.96	0.11	49,49,49,49	0
56	MG	1a	1785	1/1	0.96	0.13	60,60,60,60	0
56	MG	2A	3313	1/1	0.96	0.17	46,46,46,46	0
56	MG	1A	4052	1/1	0.96	0.57	33,33,33,33	0
56	MG	2a	3027	1/1	0.96	0.22	47,47,47,47	0
56	MG	1A	3214	1/1	0.96	0.22	34,34,34,34	0
56	MG	2A	3058	1/1	0.96	0.13	51,51,51,51	0
56	MG	1a	1788	1/1	0.96	0.19	51,51,51,51	0
56	MG	1A	3881	1/1	0.96	0.07	64,64,64,64	0
56	MG	2A	3322	1/1	0.96	0.15	49,49,49,49	0
56	MG	2a	3034	1/1	0.96	0.14	43,43,43,43	0
56	MG	2A	3324	1/1	0.96	0.05	43,43,43,43	0
56	MG	2A	3325	1/1	0.96	0.11	48,48,48,48	0
56	MG	1A	3102	1/1	0.96	0.28	49,49,49,49	0
56	MG	1A	3431	1/1	0.96	0.13	43,43,43,43	0
56	MG	2A	3330	1/1	0.96	0.18	40,40,40,40	0
56	MG	1A	3638	1/1	0.96	0.20	38,38,38,38	0
56	MG	1A	3751	1/1	0.96	0.10	74,74,74,74	0
56	MG	2A	3067	1/1	0.96	0.13	49,49,49,49	0
56	MG	2A	3068	1/1	0.96	0.10	52,52,52,52	0
56	MG	1A	3487	1/1	0.96	0.13	40,40,40,40	0
56	MG	1A	3640	1/1	0.96	0.24	38,38,38,38	0
56	MG	1A	3551	1/1	0.96	0.14	55,55,55,55	0
56	MG	1a	1609	1/1	0.96	0.22	58,58,58,58	0
56	MG	2A	3344	1/1	0.96	0.27	59,59,59,59	0
56	MG	1A	4065	1/1	0.96	0.17	33,33,33,33	0
56	MG	1A	3036	1/1	0.96	0.24	40,40,40,40	0
56	MG	1a	1612	1/1	0.96	0.09	57,57,57,57	0
56	MG	2A	3079	1/1	0.96	0.08	50,50,50,50	0
56	MG	1a	1613	1/1	0.96	0.10	77,77,77,77	0
56	MG	1A	3159	1/1	0.96	0.21	36,36,36,36	0
56	MG	1a	1804	1/1	0.96	0.24	37,37,37,37	0
56	MG	1A	3160	1/1	0.96	0.15	46,46,46,46	0
56	MG	1A	3054	1/1	0.96	0.29	53,53,53,53	0
56	MG	2a	3062	1/1	0.96	0.11	81,81,81,81	0
56	MG	2a	3063	1/1	0.96	0.32	85,85,85,85	0
56	MG	1A	4073	1/1	0.96	0.42	48,48,48,48	0
56	MG	1A	4074	1/1	0.96	0.20	47,47,47,47	0
56	MG	1a	1620	1/1	0.96	0.18	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3392	1/1	0.96	0.14	33,33,33,33	0
56	MG	2A	3089	1/1	0.96	0.32	36,36,36,36	0
56	MG	1A	3126	1/1	0.96	0.11	27,27,27,27	0
56	MG	1A	3223	1/1	0.96	0.19	29,29,29,29	0
56	MG	1A	3766	1/1	0.96	0.18	37,37,37,37	0
56	MG	1A	3904	1/1	0.96	0.20	17,17,17,17	0
56	MG	1A	4081	1/1	0.96	0.25	42,42,42,42	0
56	MG	1A	3767	1/1	0.96	0.26	33,33,33,33	0
56	MG	2A	3378	1/1	0.96	0.13	41,41,41,41	0
56	MG	2a	3078	1/1	0.96	0.13	61,61,61,61	0
56	MG	1A	3224	1/1	0.96	0.17	33,33,33,33	0
56	MG	2a	3080	1/1	0.96	0.28	55,55,55,55	0
56	MG	2A	3381	1/1	0.96	0.28	41,41,41,41	0
56	MG	1A	3191	1/1	0.96	0.12	28,28,28,28	0
56	MG	2a	3084	1/1	0.96	0.20	50,50,50,50	0
56	MG	2A	3384	1/1	0.96	0.15	39,39,39,39	0
56	MG	1A	3653	1/1	0.96	0.22	48,48,48,48	0
56	MG	1A	3442	1/1	0.96	0.09	39,39,39,39	0
56	MG	2a	3089	1/1	0.96	0.09	46,46,46,46	0
56	MG	2A	3388	1/1	0.96	0.12	55,55,55,55	0
56	MG	1A	3163	1/1	0.96	0.10	32,32,32,32	0
56	MG	2A	3390	1/1	0.96	0.16	35,35,35,35	0
56	MG	1A	3773	1/1	0.96	0.31	48,48,48,48	0
56	MG	1a	1637	1/1	0.96	0.11	51,51,51,51	0
56	MG	1A	3230	1/1	0.96	0.19	35,35,35,35	0
56	MG	2A	3398	1/1	0.96	0.13	32,32,32,32	0
56	MG	2A	3399	1/1	0.96	0.34	64,64,64,64	0
56	MG	2A	3400	1/1	0.96	0.15	48,48,48,48	0
56	MG	1a	1826	1/1	0.96	0.13	59,59,59,59	0
56	MG	2a	3102	1/1	0.96	0.18	44,44,44,44	0
56	MG	2A	3402	1/1	0.96	0.28	44,44,44,44	0
56	MG	1A	3099	1/1	0.96	0.10	55,55,55,55	0
56	MG	1B	206	1/1	0.96	0.18	51,51,51,51	0
56	MG	2a	3112	1/1	0.96	0.30	53,53,53,53	0
56	MG	2A	3407	1/1	0.96	0.22	46,46,46,46	0
56	MG	1A	3918	1/1	0.96	0.12	61,61,61,61	0
56	MG	1A	3315	1/1	0.96	0.24	65,65,65,65	0
56	MG	1a	1831	1/1	0.96	0.12	84,84,84,84	0
56	MG	1A	3777	1/1	0.96	0.16	30,30,30,30	0
56	MG	1A	3921	1/1	0.96	0.10	45,45,45,45	0
56	MG	2A	3416	1/1	0.96	0.11	36,36,36,36	0
56	MG	2A	3417	1/1	0.96	0.12	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3401	1/1	0.96	0.16	30,30,30,30	0
56	MG	2A	3117	1/1	0.96	0.31	46,46,46,46	0
56	MG	2A	3118	1/1	0.96	0.40	52,52,52,52	0
56	MG	2a	3125	1/1	0.96	0.18	33,33,33,33	0
56	MG	1A	3506	1/1	0.96	0.49	75,75,75,75	0
56	MG	1A	3924	1/1	0.96	0.18	52,52,52,52	0
56	MG	2A	3423	1/1	0.96	0.08	53,53,53,53	0
56	MG	2A	3424	1/1	0.96	0.11	63,63,63,63	0
56	MG	1a	1841	1/1	0.96	0.20	52,52,52,52	0
56	MG	2A	3426	1/1	0.96	0.12	46,46,46,46	0
56	MG	1a	1842	1/1	0.96	0.37	48,48,48,48	0
56	MG	1B	215	1/1	0.96	0.20	74,74,74,74	0
56	MG	2A	3126	1/1	0.96	0.50	43,43,43,43	0
56	MG	1A	3781	1/1	0.96	0.08	24,24,24,24	0
56	MG	1A	3571	1/1	0.96	0.20	32,32,32,32	0
56	MG	1B	222	1/1	0.96	0.09	59,59,59,59	0
56	MG	1A	3931	1/1	0.96	0.09	32,32,32,32	0
56	MG	1a	1850	1/1	0.96	0.23	44,44,44,44	0
56	MG	1A	3932	1/1	0.96	0.06	59,59,59,59	0
56	MG	1A	3783	1/1	0.96	0.17	28,28,28,28	0
56	MG	1A	3784	1/1	0.96	0.19	20,20,20,20	0
56	MG	1a	1854	1/1	0.96	0.14	60,60,60,60	0
56	MG	1A	3936	1/1	0.96	0.33	33,33,33,33	0
56	MG	2A	3444	1/1	0.96	0.10	63,63,63,63	0
56	MG	1a	1856	1/1	0.96	0.11	41,41,41,41	0
56	MG	1a	1658	1/1	0.96	0.13	58,58,58,58	0
56	MG	1a	1859	1/1	0.96	0.23	59,59,59,59	0
56	MG	1A	3572	1/1	0.96	0.11	52,52,52,52	0
56	MG	2A	3143	1/1	0.96	0.03	41,41,41,41	0
56	MG	1A	3195	1/1	0.96	0.24	44,44,44,44	0
56	MG	1A	3939	1/1	0.96	0.20	19,19,19,19	0
56	MG	1A	3667	1/1	0.96	0.21	14,14,14,14	0
56	MG	1a	1663	1/1	0.96	0.13	52,52,52,52	0
56	MG	1A	3791	1/1	0.96	0.36	51,51,51,51	0
56	MG	2A	3458	1/1	0.96	0.14	54,54,54,54	0
56	MG	1a	1665	1/1	0.96	0.15	50,50,50,50	0
56	MG	1A	3792	1/1	0.96	0.07	62,62,62,62	0
56	MG	2A	3158	1/1	0.96	0.12	39,39,39,39	0
56	MG	1A	3576	1/1	0.96	0.08	65,65,65,65	0
56	MG	1A	3275	1/1	0.96	0.29	41,41,41,41	0
56	MG	1A	3673	1/1	0.96	0.09	25,25,25,25	0
56	MG	1A	3798	1/1	0.96	0.14	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3468	1/1	0.96	0.13	47,47,47,47	0
56	MG	1A	3799	1/1	0.96	0.14	20,20,20,20	0
56	MG	1A	3675	1/1	0.96	0.27	42,42,42,42	0
56	MG	2a	3174	1/1	0.96	0.17	51,51,51,51	0
56	MG	1A	3953	1/1	0.96	0.12	38,38,38,38	0
56	MG	1a	1883	1/1	0.96	0.13	53,53,53,53	0
56	MG	1a	1674	1/1	0.96	0.10	62,62,62,62	0
56	MG	1A	3801	1/1	0.96	0.17	40,40,40,40	0
56	MG	1A	3676	1/1	0.96	0.14	40,40,40,40	0
56	MG	1A	3957	1/1	0.96	0.26	34,34,34,34	0
56	MG	1A	3961	1/1	0.96	0.06	40,40,40,40	0
56	MG	2A	3173	1/1	0.96	0.15	27,27,27,27	0
56	MG	2A	3484	1/1	0.96	0.29	47,47,47,47	0
56	MG	1a	1889	1/1	0.96	0.08	42,42,42,42	0
56	MG	2A	3175	1/1	0.96	0.18	34,34,34,34	0
56	MG	2a	3190	1/1	0.96	0.11	47,47,47,47	0
56	MG	1A	3106	1/1	0.96	0.14	48,48,48,48	0
56	MG	2a	3192	1/1	0.96	0.11	61,61,61,61	0
56	MG	1a	1892	1/1	0.96	0.19	58,58,58,58	0
56	MG	1A	3166	1/1	0.96	0.16	35,35,35,35	0
56	MG	1A	3681	1/1	0.96	0.13	19,19,19,19	0
56	MG	1A	3167	1/1	0.96	0.21	25,25,25,25	0
56	MG	1a	1896	1/1	0.96	0.39	46,46,46,46	0
56	MG	2A	3493	1/1	0.96	0.11	39,39,39,39	0
56	MG	1A	3809	1/1	0.96	0.17	33,33,33,33	0
56	MG	1A	3972	1/1	0.96	0.10	41,41,41,41	0
56	MG	1a	1902	1/1	0.96	0.10	62,62,62,62	0
56	MG	1A	3454	1/1	0.96	0.22	64,64,64,64	0
56	MG	1A	3280	1/1	0.96	0.06	43,43,43,43	0
56	MG	1A	3975	1/1	0.96	0.14	44,44,44,44	0
56	MG	1a	1907	1/1	0.96	0.18	36,36,36,36	0
56	MG	1A	3515	1/1	0.96	0.55	41,41,41,41	0
56	MG	1A	3816	1/1	0.96	0.07	51,51,51,51	0
56	MG	1A	3817	1/1	0.96	0.17	40,40,40,40	0
56	MG	1A	3818	1/1	0.96	0.16	59,59,59,59	0
56	MG	1A	3410	1/1	0.96	0.11	42,42,42,42	0
56	MG	2A	3509	1/1	0.96	0.09	46,46,46,46	0
56	MG	1A	3986	1/1	0.96	0.21	49,49,49,49	0
56	MG	2A	3511	1/1	0.96	0.21	40,40,40,40	0
56	MG	2a	3216	1/1	0.96	0.10	55,55,55,55	0
56	MG	1A	3987	1/1	0.96	0.19	58,58,58,58	0
56	MG	1A	3988	1/1	0.96	0.37	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3514	1/1	0.96	0.11	71,71,71,71	0
56	MG	1h	8001	1/1	0.96	0.09	60,60,60,60	0
56	MG	1A	3021	1/1	0.96	0.24	56,56,56,56	0
56	MG	1a	1702	1/1	0.96	0.14	60,60,60,60	0
56	MG	1N	3004	1/1	0.96	0.07	26,26,26,26	0
56	MG	1a	1704	1/1	0.96	0.19	48,48,48,48	0
56	MG	1A	3822	1/1	0.96	0.21	21,21,21,21	0
56	MG	1a	1706	1/1	0.96	0.20	52,52,52,52	0
56	MG	1N	3006	1/1	0.96	0.10	55,55,55,55	0
56	MG	1a	1710	1/1	0.96	0.16	45,45,45,45	0
56	MG	2A	3527	1/1	0.96	0.22	39,39,39,39	0
56	MG	2A	3530	1/1	0.96	0.26	43,43,43,43	0
56	MG	1a	1711	1/1	0.96	0.13	62,62,62,62	0
56	MG	2A	3532	1/1	0.96	0.14	46,46,46,46	0
56	MG	1A	3991	1/1	0.96	0.41	38,38,38,38	0
56	MG	2A	3215	1/1	0.96	0.26	31,31,31,31	0
56	MG	1A	3202	1/1	0.96	0.47	50,50,50,50	0
56	MG	1A	3459	1/1	0.96	0.29	49,49,49,49	0
56	MG	2A	3538	1/1	0.96	0.20	39,39,39,39	0
56	MG	1A	3692	1/1	0.96	0.19	18,18,18,18	0
56	MG	2A	3540	1/1	0.96	0.23	46,46,46,46	0
56	MG	1A	3695	1/1	0.96	0.10	13,13,13,13	0
56	MG	1A	3521	1/1	0.96	0.07	46,46,46,46	0
56	MG	2A	3221	1/1	0.96	0.20	39,39,39,39	0
56	MG	2a	3251	1/1	0.96	0.34	43,43,43,43	0
56	MG	1A	3460	1/1	0.96	0.25	52,52,52,52	0
56	MG	1a	1721	1/1	0.96	0.07	45,45,45,45	0
56	MG	1a	1722	1/1	0.96	0.19	47,47,47,47	0
56	MG	2A	3227	1/1	0.96	0.20	38,38,38,38	0
56	MG	1A	3700	1/1	0.96	0.21	31,31,31,31	0
56	MG	1A	3462	1/1	0.96	0.18	47,47,47,47	0
56	MG	1A	3169	1/1	0.96	0.14	55,55,55,55	0
56	MG	2e	3002	1/1	0.96	0.10	64,64,64,64	0
56	MG	1A	3415	1/1	0.96	0.12	39,39,39,39	0
56	MG	1Q	208	1/1	0.96	0.10	37,37,37,37	0
56	MG	2A	3556	1/1	0.96	0.16	55,55,55,55	0
56	MG	1A	4004	1/1	0.96	0.10	49,49,49,49	0
56	MG	2A	3558	1/1	0.96	0.71	43,43,43,43	0
56	MG	1A	3706	1/1	0.96	0.10	15,15,15,15	0
56	MG	1R	203	1/1	0.96	0.15	35,35,35,35	0
56	MG	1A	3466	1/1	0.96	0.04	55,55,55,55	0
56	MG	1A	3241	1/1	0.96	0.20	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1R	206	1/1	0.96	0.19	32,32,32,32	0
56	MG	1A	3528	1/1	0.96	0.21	42,42,42,42	0
56	MG	1A	3839	1/1	0.96	0.10	18,18,18,18	0
56	MG	1A	3204	1/1	0.96	0.21	33,33,33,33	0
56	MG	2A	3245	1/1	0.96	0.23	52,52,52,52	0
56	MG	1A	3843	1/1	0.96	0.17	53,53,53,53	0
56	MG	1A	3170	1/1	0.96	0.16	25,25,25,25	0
56	MG	1a	1745	1/1	0.96	0.11	55,55,55,55	0
56	MG	1A	3531	1/1	0.96	0.09	45,45,45,45	0
56	MG	1A	3611	1/1	0.96	0.13	35,35,35,35	0
56	MG	1A	3717	1/1	0.96	0.25	55,55,55,55	0
57	ZN	15	101	1/1	0.96	0.15	54,54,54,54	0
56	MG	1A	3613	1/1	0.96	0.18	41,41,41,41	0
56	MG	1V	201	1/1	0.96	0.31	39,39,39,39	0
56	MG	2E	301	1/1	0.96	0.40	36,36,36,36	0
56	MG	2E	302	1/1	0.96	0.27	36,36,36,36	0
56	MG	1A	3288	1/1	0.96	0.44	42,42,42,42	0
56	MG	2A	3153	1/1	0.97	0.10	52,52,52,52	0
56	MG	19	105	1/1	0.97	0.19	34,34,34,34	0
56	MG	19	106	1/1	0.97	0.11	45,45,45,45	0
56	MG	1l	201	1/1	0.97	0.11	35,35,35,35	0
56	MG	1A	3407	1/1	0.97	0.44	40,40,40,40	0
56	MG	1A	3328	1/1	0.97	0.09	27,27,27,27	0
56	MG	1A	3409	1/1	0.97	0.14	42,42,42,42	0
56	MG	1A	3069	1/1	0.97	0.14	39,39,39,39	0
56	MG	2A	3395	1/1	0.97	0.24	47,47,47,47	0
56	MG	2A	3396	1/1	0.97	0.28	49,49,49,49	0
56	MG	1A	3977	1/1	0.97	0.11	31,31,31,31	0
56	MG	2A	3165	1/1	0.97	0.23	42,42,42,42	0
56	MG	1A	3623	1/1	0.97	0.17	45,45,45,45	0
56	MG	1A	3132	1/1	0.97	0.11	33,33,33,33	0
56	MG	1A	3981	1/1	0.97	0.18	42,42,42,42	0
56	MG	1B	217	1/1	0.97	0.09	38,38,38,38	0
56	MG	1B	218	1/1	0.97	0.16	34,34,34,34	0
56	MG	2A	3406	1/1	0.97	0.20	55,55,55,55	0
56	MG	1B	220	1/1	0.97	0.10	42,42,42,42	0
56	MG	1A	3871	1/1	0.97	0.10	31,31,31,31	0
56	MG	1A	3984	1/1	0.97	0.41	32,32,32,32	0
56	MG	1A	3626	1/1	0.97	0.18	45,45,45,45	0
56	MG	2a	3048	1/1	0.97	0.09	66,66,66,66	0
56	MG	1B	224	1/1	0.97	0.06	58,58,58,58	0
56	MG	2A	3412	1/1	0.97	0.23	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3507	1/1	0.97	0.08	45,45,45,45	0
56	MG	2A	3414	1/1	0.97	0.26	50,50,50,50	0
56	MG	1a	1771	1/1	0.97	0.08	48,48,48,48	0
56	MG	1a	1772	1/1	0.97	0.09	62,62,62,62	0
56	MG	1A	3181	1/1	0.97	0.15	38,38,38,38	0
56	MG	1A	3875	1/1	0.97	0.14	38,38,38,38	0
56	MG	1A	3267	1/1	0.97	0.26	22,22,22,22	0
56	MG	1A	3109	1/1	0.97	0.05	45,45,45,45	0
56	MG	1A	3790	1/1	0.97	0.20	19,19,19,19	0
56	MG	1A	3709	1/1	0.97	0.26	38,38,38,38	0
56	MG	1A	3560	1/1	0.97	0.12	63,63,63,63	0
56	MG	1D	304	1/1	0.97	0.24	34,34,34,34	0
56	MG	1A	3994	1/1	0.97	0.11	23,23,23,23	0
56	MG	2A	3001	1/1	0.97	0.18	35,35,35,35	0
56	MG	1A	3002	1/1	0.97	0.29	38,38,38,38	0
56	MG	2a	3067	1/1	0.97	0.46	57,57,57,57	0
56	MG	2A	3430	1/1	0.97	0.20	50,50,50,50	0
56	MG	1D	307	1/1	0.97	0.34	37,37,37,37	0
56	MG	1A	3111	1/1	0.97	0.34	35,35,35,35	0
56	MG	1A	3112	1/1	0.97	0.49	51,51,51,51	0
56	MG	2A	3434	1/1	0.97	0.18	42,42,42,42	0
56	MG	1A	3243	1/1	0.97	0.17	38,38,38,38	0
56	MG	1A	3377	1/1	0.97	0.31	24,24,24,24	0
56	MG	1a	1633	1/1	0.97	0.20	77,77,77,77	0
56	MG	1A	3887	1/1	0.97	0.21	45,45,45,45	0
56	MG	1A	3221	1/1	0.97	0.26	28,28,28,28	0
56	MG	1A	3222	1/1	0.97	0.12	19,19,19,19	0
56	MG	2A	3441	1/1	0.97	0.13	55,55,55,55	0
56	MG	2A	3203	1/1	0.97	0.11	43,43,43,43	0
56	MG	1E	303	1/1	0.97	0.09	31,31,31,31	0
56	MG	1A	3518	1/1	0.97	0.13	51,51,51,51	0
56	MG	2a	3085	1/1	0.97	0.12	48,48,48,48	0
56	MG	1A	3803	1/1	0.97	0.19	22,22,22,22	0
56	MG	2A	3446	1/1	0.97	0.07	55,55,55,55	0
56	MG	1A	3721	1/1	0.97	0.06	45,45,45,45	0
56	MG	1A	3894	1/1	0.97	0.15	50,50,50,50	0
56	MG	1A	3895	1/1	0.97	0.08	40,40,40,40	0
56	MG	1A	3089	1/1	0.97	0.08	52,52,52,52	0
56	MG	2A	3212	1/1	0.97	0.33	34,34,34,34	0
56	MG	1A	3725	1/1	0.97	0.12	18,18,18,18	0
56	MG	2A	3454	1/1	0.97	0.07	57,57,57,57	0
56	MG	2a	3096	1/1	0.97	0.14	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3023	1/1	0.97	0.16	45,45,45,45	0
56	MG	1A	3342	1/1	0.97	0.16	53,53,53,53	0
56	MG	1A	3808	1/1	0.97	0.13	73,73,73,73	0
56	MG	1A	4015	1/1	0.97	0.38	46,46,46,46	0
56	MG	1A	3900	1/1	0.97	0.23	39,39,39,39	0
56	MG	1F	305	1/1	0.97	0.20	40,40,40,40	0
56	MG	1A	3573	1/1	0.97	0.09	41,41,41,41	0
56	MG	2A	3463	1/1	0.97	0.32	44,44,44,44	0
56	MG	1A	3574	1/1	0.97	0.17	37,37,37,37	0
56	MG	1A	3903	1/1	0.97	0.10	71,71,71,71	0
56	MG	1A	3277	1/1	0.97	0.12	34,34,34,34	0
56	MG	1A	4021	1/1	0.97	0.15	59,59,59,59	0
56	MG	2A	3226	1/1	0.97	0.20	42,42,42,42	0
56	MG	2A	3469	1/1	0.97	0.13	49,49,49,49	0
56	MG	1A	3813	1/1	0.97	0.14	48,48,48,48	0
56	MG	1A	3344	1/1	0.97	0.14	42,42,42,42	0
56	MG	2A	3472	1/1	0.97	0.13	50,50,50,50	0
56	MG	2A	3036	1/1	0.97	0.26	30,30,30,30	0
56	MG	1A	3815	1/1	0.97	0.16	20,20,20,20	0
56	MG	1A	3731	1/1	0.97	0.11	45,45,45,45	0
56	MG	2a	3123	1/1	0.97	0.10	39,39,39,39	0
56	MG	2A	3232	1/1	0.97	0.15	47,47,47,47	0
56	MG	1A	3385	1/1	0.97	0.18	45,45,45,45	0
56	MG	1A	3309	1/1	0.97	0.18	59,59,59,59	0
56	MG	1A	3912	1/1	0.97	0.14	56,56,56,56	0
56	MG	1A	3581	1/1	0.97	0.43	54,54,54,54	0
56	MG	2a	3129	1/1	0.97	0.20	60,60,60,60	0
56	MG	1A	3652	1/1	0.97	0.22	24,24,24,24	0
56	MG	1A	3821	1/1	0.97	0.17	21,21,21,21	0
56	MG	2a	3132	1/1	0.97	0.10	57,57,57,57	0
56	MG	1A	3917	1/1	0.97	0.09	35,35,35,35	0
56	MG	1O	3002	1/1	0.97	0.15	47,47,47,47	0
56	MG	1A	3346	1/1	0.97	0.21	55,55,55,55	0
56	MG	2A	3049	1/1	0.97	0.15	56,56,56,56	0
56	MG	1A	3583	1/1	0.97	0.13	49,49,49,49	0
56	MG	1A	3190	1/1	0.97	0.07	42,42,42,42	0
56	MG	2a	3139	1/1	0.97	0.17	53,53,53,53	0
56	MG	1P	203	1/1	0.97	0.33	28,28,28,28	0
56	MG	2A	3248	1/1	0.97	0.16	35,35,35,35	0
56	MG	2A	3249	1/1	0.97	0.17	56,56,56,56	0
56	MG	2a	3144	1/1	0.97	0.14	66,66,66,66	0
56	MG	1A	3742	1/1	0.97	0.13	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3227	1/1	0.97	0.20	26,26,26,26	0
56	MG	1A	3586	1/1	0.97	0.18	33,33,33,33	0
56	MG	1Q	202	1/1	0.97	0.28	32,32,32,32	0
56	MG	1a	1832	1/1	0.97	0.15	52,52,52,52	0
56	MG	1Q	203	1/1	0.97	0.15	41,41,41,41	0
56	MG	2A	3060	1/1	0.97	0.27	40,40,40,40	0
56	MG	2A	3502	1/1	0.97	0.09	37,37,37,37	0
56	MG	2A	3503	1/1	0.97	0.05	37,37,37,37	0
56	MG	1A	3432	1/1	0.97	0.08	53,53,53,53	0
56	MG	1A	3156	1/1	0.97	0.14	50,50,50,50	0
56	MG	1A	3926	1/1	0.97	0.16	51,51,51,51	0
56	MG	1Q	207	1/1	0.97	0.35	41,41,41,41	0
56	MG	1a	1840	1/1	0.97	0.15	27,27,27,27	0
56	MG	1A	3927	1/1	0.97	0.23	66,66,66,66	0
56	MG	1A	3928	1/1	0.97	0.12	29,29,29,29	0
56	MG	2A	3267	1/1	0.97	0.35	38,38,38,38	0
56	MG	1R	201	1/1	0.97	0.18	32,32,32,32	0
56	MG	2A	3069	1/1	0.97	0.28	42,42,42,42	0
56	MG	1A	3929	1/1	0.97	0.12	29,29,29,29	0
56	MG	1A	4046	1/1	0.97	0.33	45,45,45,45	0
56	MG	1A	3391	1/1	0.97	0.11	51,51,51,51	0
56	MG	2A	3518	1/1	0.97	0.15	32,32,32,32	0
56	MG	1a	1847	1/1	0.97	0.20	53,53,53,53	0
56	MG	1A	3175	1/1	0.97	0.42	43,43,43,43	0
56	MG	2A	3075	1/1	0.97	0.30	48,48,48,48	0
56	MG	2A	3523	1/1	0.97	0.31	34,34,34,34	0
56	MG	1a	1849	1/1	0.97	0.05	38,38,38,38	0
56	MG	1A	3664	1/1	0.97	0.16	19,19,19,19	0
56	MG	2A	3078	1/1	0.97	0.07	48,48,48,48	0
56	MG	1T	201	1/1	0.97	0.07	41,41,41,41	0
56	MG	2A	3528	1/1	0.97	0.17	46,46,46,46	0
56	MG	2A	3529	1/1	0.97	0.33	53,53,53,53	0
56	MG	1A	4050	1/1	0.97	0.40	84,84,84,84	0
56	MG	1A	3591	1/1	0.97	0.19	32,32,32,32	0
56	MG	1A	3177	1/1	0.97	0.30	33,33,33,33	0
56	MG	2a	3184	1/1	0.97	0.22	53,53,53,53	0
56	MG	1A	3254	1/1	0.97	0.14	41,41,41,41	0
56	MG	1A	4055	1/1	0.97	0.17	43,43,43,43	0
56	MG	2A	3290	1/1	0.97	0.13	36,36,36,36	0
56	MG	2a	3189	1/1	0.97	0.37	76,76,76,76	0
56	MG	1a	1701	1/1	0.97	0.16	63,63,63,63	0
56	MG	1A	3837	1/1	0.97	0.12	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3294	1/1	0.97	0.32	50,50,50,50	0
56	MG	1a	1860	1/1	0.97	0.17	61,61,61,61	0
56	MG	1a	1861	1/1	0.97	0.12	51,51,51,51	0
56	MG	2A	3297	1/1	0.97	0.10	40,40,40,40	0
56	MG	1a	1863	1/1	0.97	0.12	42,42,42,42	0
56	MG	2A	3299	1/1	0.97	0.15	64,64,64,64	0
56	MG	2A	3545	1/1	0.97	0.25	53,53,53,53	0
56	MG	2a	3199	1/1	0.97	0.48	64,64,64,64	0
56	MG	2A	3546	1/1	0.97	0.21	49,49,49,49	0
56	MG	1A	3753	1/1	0.97	0.11	34,34,34,34	0
56	MG	2A	3548	1/1	0.97	0.18	38,38,38,38	0
56	MG	1a	1865	1/1	0.97	0.26	51,51,51,51	0
56	MG	1U	204	1/1	0.97	0.24	40,40,40,40	0
56	MG	2a	3205	1/1	0.97	0.29	57,57,57,57	0
56	MG	1A	3669	1/1	0.97	0.11	17,17,17,17	0
56	MG	1a	1868	1/1	0.97	0.17	44,44,44,44	0
56	MG	1A	4060	1/1	0.97	0.13	31,31,31,31	0
56	MG	1A	3840	1/1	0.97	0.18	59,59,59,59	0
56	MG	2A	3307	1/1	0.97	0.15	60,60,60,60	0
56	MG	1A	3755	1/1	0.97	0.09	26,26,26,26	0
56	MG	1A	3062	1/1	0.97	0.19	56,56,56,56	0
56	MG	1A	3256	1/1	0.97	0.72	44,44,44,44	0
56	MG	1A	3232	1/1	0.97	0.12	44,44,44,44	0
56	MG	1A	3946	1/1	0.97	0.17	24,24,24,24	0
56	MG	1A	3674	1/1	0.97	0.17	24,24,24,24	0
56	MG	1A	3233	1/1	0.97	0.24	36,36,36,36	0
56	MG	2a	3218	1/1	0.97	0.19	67,67,67,67	0
56	MG	2A	3105	1/1	0.97	0.36	28,28,28,28	0
56	MG	1A	4071	1/1	0.97	0.33	44,44,44,44	0
56	MG	1A	3211	1/1	0.97	0.39	37,37,37,37	0
56	MG	2A	3319	1/1	0.97	0.27	51,51,51,51	0
56	MG	1A	3950	1/1	0.97	0.10	64,64,64,64	0
56	MG	2A	3321	1/1	0.97	0.21	26,26,26,26	0
56	MG	1a	1882	1/1	0.97	0.13	60,60,60,60	0
56	MG	1A	3951	1/1	0.97	0.17	36,36,36,36	0
56	MG	10	102	1/1	0.97	0.05	48,48,48,48	0
56	MG	2A	3326	1/1	0.97	0.13	43,43,43,43	0
56	MG	2A	3113	1/1	0.97	0.15	29,29,29,29	0
56	MG	1a	1724	1/1	0.97	0.14	62,62,62,62	0
56	MG	2a	3231	1/1	0.97	0.23	59,59,59,59	0
56	MG	2D	304	1/1	0.97	0.14	36,36,36,36	0
56	MG	2A	3329	1/1	0.97	0.23	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3443	1/1	0.97	0.39	72,72,72,72	0
56	MG	1A	3321	1/1	0.97	0.21	33,33,33,33	0
56	MG	2a	3236	1/1	0.97	0.23	83,83,83,83	0
56	MG	2a	3237	1/1	0.97	0.11	59,59,59,59	0
56	MG	2a	3238	1/1	0.97	0.09	57,57,57,57	0
56	MG	1A	3260	1/1	0.97	0.24	31,31,31,31	0
56	MG	2A	3336	1/1	0.97	0.07	74,74,74,74	0
56	MG	1A	3543	1/1	0.97	0.14	46,46,46,46	0
56	MG	2a	3244	1/1	0.97	0.13	64,64,64,64	0
56	MG	1A	3291	1/1	0.97	0.38	41,41,41,41	0
56	MG	1a	1731	1/1	0.97	0.09	37,37,37,37	0
56	MG	2F	304	1/1	0.97	0.15	41,41,41,41	0
56	MG	1A	4080	1/1	0.97	0.65	36,36,36,36	0
56	MG	2A	3122	1/1	0.97	0.18	51,51,51,51	0
56	MG	1A	3958	1/1	0.97	0.17	40,40,40,40	0
56	MG	1a	1734	1/1	0.97	0.35	53,53,53,53	0
56	MG	2A	3125	1/1	0.97	0.18	52,52,52,52	0
56	MG	1a	1735	1/1	0.97	0.12	45,45,45,45	0
56	MG	1a	1897	1/1	0.97	0.28	84,84,84,84	0
56	MG	1A	3959	1/1	0.97	0.11	53,53,53,53	0
56	MG	1a	1737	1/1	0.97	0.46	48,48,48,48	0
56	MG	1a	1900	1/1	0.97	0.22	47,47,47,47	0
56	MG	2A	3355	1/1	0.97	0.25	45,45,45,45	0
56	MG	1a	1901	1/1	0.97	0.10	47,47,47,47	0
56	MG	2A	3357	1/1	0.97	0.31	52,52,52,52	0
56	MG	1A	3292	1/1	0.97	0.22	62,62,62,62	0
56	MG	1A	4084	1/1	0.97	0.44	32,32,32,32	0
56	MG	2A	3362	1/1	0.97	0.14	42,42,42,42	0
56	MG	2A	3134	1/1	0.97	0.10	44,44,44,44	0
56	MG	28	101	1/1	0.97	0.21	45,45,45,45	0
56	MG	1A	3962	1/1	0.97	0.22	14,14,14,14	0
56	MG	1A	3496	1/1	0.97	0.27	42,42,42,42	0
56	MG	1a	1906	1/1	0.97	0.32	45,45,45,45	0
56	MG	2A	3367	1/1	0.97	0.24	54,54,54,54	0
56	MG	1A	4087	1/1	0.97	0.44	42,42,42,42	0
56	MG	2A	3369	1/1	0.97	0.17	56,56,56,56	0
56	MG	2a	3007	1/1	0.97	0.35	40,40,40,40	0
56	MG	1A	3964	1/1	0.97	0.08	50,50,50,50	0
56	MG	1A	4090	1/1	0.97	0.24	26,26,26,26	0
56	MG	1A	3325	1/1	0.97	0.10	41,41,41,41	0
56	MG	1A	3968	1/1	0.97	0.16	26,26,26,26	0
56	MG	1A	3498	1/1	0.97	0.16	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1B	204	1/1	0.97	0.10	49,49,49,49	0
56	MG	1A	3196	1/1	0.97	0.30	37,37,37,37	0
56	MG	2a	3015	1/1	0.97	0.16	62,62,62,62	0
56	MG	1e	203	1/1	0.97	0.28	84,84,84,84	0
56	MG	1A	3295	1/1	0.97	0.19	42,42,42,42	0
56	MG	2A	3382	1/1	0.97	0.19	46,46,46,46	0
56	MG	1A	3691	1/1	0.97	0.14	54,54,54,54	0
57	ZN	29	501	1/1	0.97	0.05	66,66,66,66	0
56	MG	2A	3152	1/1	0.97	0.15	30,30,30,30	0
56	MG	1A	3226	1/1	0.98	0.22	23,23,23,23	0
56	MG	1A	3064	1/1	0.98	0.14	48,48,48,48	0
56	MG	2A	3242	1/1	0.98	0.26	22,22,22,22	0
56	MG	1A	3212	1/1	0.98	0.32	36,36,36,36	0
56	MG	1A	3869	1/1	0.98	0.18	40,40,40,40	0
56	MG	1A	3596	1/1	0.98	0.19	44,44,44,44	0
56	MG	2A	3394	1/1	0.98	0.09	54,54,54,54	0
56	MG	1a	1634	1/1	0.98	0.19	55,55,55,55	0
56	MG	2A	3008	1/1	0.98	0.15	51,51,51,51	0
56	MG	2A	3397	1/1	0.98	0.05	58,58,58,58	0
56	MG	1a	1635	1/1	0.98	0.26	56,56,56,56	0
56	MG	1A	3688	1/1	0.98	0.15	8,8,8,8	0
56	MG	1B	211	1/1	0.98	0.14	39,39,39,39	0
56	MG	1A	3176	1/1	0.98	0.08	30,30,30,30	0
56	MG	1A	3264	1/1	0.98	0.32	27,27,27,27	0
56	MG	2A	3403	1/1	0.98	0.16	57,57,57,57	0
56	MG	1A	3503	1/1	0.98	0.16	30,30,30,30	0
56	MG	2A	3254	1/1	0.98	0.17	30,30,30,30	0
56	MG	1A	3246	1/1	0.98	0.13	23,23,23,23	0
56	MG	1A	3811	1/1	0.98	0.20	28,28,28,28	0
56	MG	1A	3693	1/1	0.98	0.12	25,25,25,25	0
56	MG	2A	3258	1/1	0.98	0.37	62,62,62,62	0
56	MG	1A	3694	1/1	0.98	0.09	28,28,28,28	0
56	MG	2A	3260	1/1	0.98	0.29	39,39,39,39	0
56	MG	1B	219	1/1	0.98	0.25	62,62,62,62	0
56	MG	1a	1857	1/1	0.98	0.09	71,71,71,71	0
56	MG	1A	3130	1/1	0.98	0.15	21,21,21,21	0
56	MG	2A	3415	1/1	0.98	0.20	57,57,57,57	0
56	MG	2A	3022	1/1	0.98	0.15	46,46,46,46	0
56	MG	1U	201	1/1	0.98	0.11	26,26,26,26	0
56	MG	2a	3143	1/1	0.98	0.06	42,42,42,42	0
56	MG	1A	3696	1/1	0.98	0.26	32,32,32,32	0
56	MG	1A	3201	1/1	0.98	0.11	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3268	1/1	0.98	0.09	44,44,44,44	0
56	MG	2A	3139	1/1	0.98	0.31	35,35,35,35	0
56	MG	1A	3756	1/1	0.98	0.17	30,30,30,30	0
56	MG	1A	3698	1/1	0.98	0.04	26,26,26,26	0
56	MG	1A	3536	1/1	0.98	0.13	48,48,48,48	0
56	MG	2A	3273	1/1	0.98	0.13	53,53,53,53	0
56	MG	1A	3189	1/1	0.98	0.21	34,34,34,34	0
56	MG	1A	3760	1/1	0.98	0.13	34,34,34,34	0
56	MG	1A	3078	1/1	0.98	0.10	61,61,61,61	0
56	MG	1A	3960	1/1	0.98	0.15	28,28,28,28	0
56	MG	1A	3823	1/1	0.98	0.22	17,17,17,17	0
56	MG	2O	203	1/1	0.98	0.11	41,41,41,41	0
56	MG	1A	3569	1/1	0.98	0.20	40,40,40,40	0
56	MG	2A	3150	1/1	0.98	0.16	30,30,30,30	0
56	MG	1W	3005	1/1	0.98	0.22	42,42,42,42	0
56	MG	2Q	3003	1/1	0.98	0.18	44,44,44,44	0
56	MG	1A	3704	1/1	0.98	0.11	45,45,45,45	0
56	MG	2A	3283	1/1	0.98	0.24	35,35,35,35	0
56	MG	1A	3609	1/1	0.98	0.13	38,38,38,38	0
56	MG	2A	3154	1/1	0.98	0.29	42,42,42,42	0
56	MG	2a	3166	1/1	0.98	0.32	60,60,60,60	0
56	MG	2A	3286	1/1	0.98	0.21	47,47,47,47	0
56	MG	2A	3287	1/1	0.98	0.20	33,33,33,33	0
56	MG	2A	3155	1/1	0.98	0.17	37,37,37,37	0
56	MG	1A	3893	1/1	0.98	0.13	51,51,51,51	0
56	MG	2A	3039	1/1	0.98	0.17	38,38,38,38	0
56	MG	1a	1876	1/1	0.98	0.16	62,62,62,62	0
56	MG	1A	3967	1/1	0.98	0.27	57,57,57,57	0
56	MG	28	102	1/1	0.98	0.25	50,50,50,50	0
56	MG	1A	3570	1/1	0.98	0.13	46,46,46,46	0
56	MG	1A	3271	1/1	0.98	0.12	54,54,54,54	0
56	MG	1A	3612	1/1	0.98	0.20	23,23,23,23	0
56	MG	1A	3378	1/1	0.98	0.13	35,35,35,35	0
56	MG	1A	3482	1/1	0.98	0.14	12,12,12,12	0
56	MG	1A	3615	1/1	0.98	0.06	39,39,39,39	0
56	MG	1D	313	1/1	0.98	0.13	39,39,39,39	0
56	MG	1A	3251	1/1	0.98	0.12	31,31,31,31	0
56	MG	2a	3185	1/1	0.98	0.12	57,57,57,57	0
56	MG	1A	3154	1/1	0.98	0.50	30,30,30,30	0
56	MG	1A	3714	1/1	0.98	0.04	49,49,49,49	0
56	MG	1A	3715	1/1	0.98	0.11	9,9,9,9	0
56	MG	1a	1676	1/1	0.98	0.09	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3459	1/1	0.98	0.12	29,29,29,29	0
56	MG	1a	1890	1/1	0.98	0.21	40,40,40,40	0
56	MG	1a	1677	1/1	0.98	0.22	48,48,48,48	0
56	MG	1a	1678	1/1	0.98	0.32	51,51,51,51	0
56	MG	1A	3978	1/1	0.98	0.30	36,36,36,36	0
56	MG	13	102	1/1	0.98	0.15	46,46,46,46	0
56	MG	2A	3059	1/1	0.98	0.13	37,37,37,37	0
56	MG	1A	4056	1/1	0.98	0.12	29,29,29,29	0
56	MG	2A	3180	1/1	0.98	0.20	29,29,29,29	0
56	MG	1A	3662	1/1	0.98	0.13	30,30,30,30	0
56	MG	2a	3024	1/1	0.98	0.16	78,78,78,78	0
56	MG	1A	3905	1/1	0.98	0.25	45,45,45,45	0
56	MG	1E	309	1/1	0.98	0.04	54,54,54,54	0
56	MG	16	101	1/1	0.98	0.22	55,55,55,55	0
56	MG	2A	3185	1/1	0.98	0.21	32,32,32,32	0
56	MG	2a	3029	1/1	0.98	0.14	66,66,66,66	0
56	MG	1a	1790	1/1	0.98	0.16	62,62,62,62	0
56	MG	1A	3192	1/1	0.98	0.21	46,46,46,46	0
56	MG	2A	3475	1/1	0.98	0.11	39,39,39,39	0
56	MG	1A	3982	1/1	0.98	0.11	21,21,21,21	0
56	MG	2A	3323	1/1	0.98	0.18	43,43,43,43	0
56	MG	2a	3035	1/1	0.98	0.12	59,59,59,59	0
56	MG	16	105	1/1	0.98	0.22	44,44,44,44	0
56	MG	2a	3037	1/1	0.98	0.20	50,50,50,50	0
56	MG	17	101	1/1	0.98	0.10	26,26,26,26	0
56	MG	2A	3480	1/1	0.98	0.06	21,21,21,21	0
56	MG	1A	3577	1/1	0.98	0.20	30,30,30,30	0
56	MG	2A	3482	1/1	0.98	0.13	52,52,52,52	0
56	MG	1a	1691	1/1	0.98	0.04	66,66,66,66	0
56	MG	1A	3778	1/1	0.98	0.19	19,19,19,19	0
56	MG	1A	3043	1/1	0.98	0.16	55,55,55,55	0
56	MG	1A	3842	1/1	0.98	0.07	54,54,54,54	0
56	MG	2A	3331	1/1	0.98	0.18	45,45,45,45	0
56	MG	2A	3333	1/1	0.98	0.15	35,35,35,35	0
56	MG	1A	3359	1/1	0.98	0.09	37,37,37,37	0
56	MG	1A	3844	1/1	0.98	0.12	18,18,18,18	0
56	MG	1A	4067	1/1	0.98	0.12	21,21,21,21	0
56	MG	2A	3337	1/1	0.98	0.04	59,59,59,59	0
56	MG	1F	308	1/1	0.98	0.14	36,36,36,36	0
56	MG	1A	3580	1/1	0.98	0.21	36,36,36,36	0
56	MG	2A	3202	1/1	0.98	0.27	38,38,38,38	0
56	MG	1G	3002	1/1	0.98	0.14	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3846	1/1	0.98	0.08	66,66,66,66	0
56	MG	2a	3057	1/1	0.98	0.27	70,70,70,70	0
56	MG	1A	3915	1/1	0.98	0.14	52,52,52,52	0
56	MG	1A	3338	1/1	0.98	0.07	52,52,52,52	0
56	MG	1A	3724	1/1	0.98	0.16	38,38,38,38	0
56	MG	1A	3039	1/1	0.98	0.29	71,71,71,71	0
56	MG	2A	3347	1/1	0.98	0.06	56,56,56,56	0
56	MG	2a	3240	1/1	0.98	0.35	66,66,66,66	0
56	MG	1A	3671	1/1	0.98	0.20	27,27,27,27	0
56	MG	1a	1707	1/1	0.98	0.10	31,31,31,31	0
56	MG	2A	3350	1/1	0.98	0.14	62,62,62,62	0
56	MG	2A	3351	1/1	0.98	0.07	49,49,49,49	0
56	MG	2A	3507	1/1	0.98	0.09	38,38,38,38	0
56	MG	2A	3211	1/1	0.98	0.40	33,33,33,33	0
56	MG	1A	3108	1/1	0.98	0.11	52,52,52,52	0
56	MG	2A	3354	1/1	0.98	0.08	48,48,48,48	0
56	MG	2a	3071	1/1	0.98	0.23	72,72,72,72	0
56	MG	1A	3852	1/1	0.98	0.07	30,30,30,30	0
56	MG	1A	3628	1/1	0.98	0.10	43,43,43,43	0
56	MG	1a	1712	1/1	0.98	0.04	40,40,40,40	0
56	MG	2A	3358	1/1	0.98	0.07	60,60,60,60	0
56	MG	1A	3789	1/1	0.98	0.15	14,14,14,14	0
56	MG	2A	3360	1/1	0.98	0.25	43,43,43,43	0
56	MG	1a	1714	1/1	0.98	0.17	57,57,57,57	0
56	MG	1A	3461	1/1	0.98	0.23	48,48,48,48	0
56	MG	2A	3095	1/1	0.98	0.25	46,46,46,46	0
56	MG	2a	3081	1/1	0.98	0.33	65,65,65,65	0
56	MG	1A	4001	1/1	0.98	0.15	35,35,35,35	0
56	MG	1A	3028	1/1	0.98	0.20	50,50,50,50	0
56	MG	1A	3631	1/1	0.98	0.07	43,43,43,43	0
56	MG	1A	3677	1/1	0.98	0.07	39,39,39,39	0
56	MG	1A	4005	1/1	0.98	0.09	42,42,42,42	0
56	MG	2A	3225	1/1	0.98	0.43	58,58,58,58	0
56	MG	1a	1618	1/1	0.98	0.09	77,77,77,77	0
56	MG	1A	3463	1/1	0.98	0.11	39,39,39,39	0
56	MG	1A	3795	1/1	0.98	0.14	13,13,13,13	0
56	MG	2a	3091	1/1	0.98	0.33	46,46,46,46	0
56	MG	2A	3373	1/1	0.98	0.15	48,48,48,48	0
56	MG	1A	4008	1/1	0.98	0.10	20,20,20,20	0
56	MG	2A	3375	1/1	0.98	0.14	46,46,46,46	0
56	MG	1a	1725	1/1	0.98	0.36	51,51,51,51	0
56	MG	1A	4089	1/1	0.98	0.26	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1P	206	1/1	0.98	0.20	42,42,42,42	0
56	MG	2x	105	1/1	0.98	0.14	52,52,52,52	0
56	MG	2A	3379	1/1	0.98	0.15	35,35,35,35	0
56	MG	1A	3412	1/1	0.98	0.16	42,42,42,42	0
56	MG	1A	3680	1/1	0.98	0.25	44,44,44,44	0
57	ZN	1Y	501	1/1	0.98	0.07	62,62,62,62	0
56	MG	1A	3185	1/1	0.98	0.08	38,38,38,38	0
56	MG	1A	3365	1/1	0.98	0.08	30,30,30,30	0
56	MG	2a	3103	1/1	0.98	0.12	48,48,48,48	0
56	MG	2A	3237	1/1	0.98	0.23	37,37,37,37	0
56	MG	2A	3385	1/1	0.98	0.09	61,61,61,61	0
56	MG	2a	3109	1/1	0.98	0.31	42,42,42,42	0
56	MG	1a	1838	1/1	0.98	0.28	39,39,39,39	0
56	MG	1A	3225	1/1	0.98	0.09	21,21,21,21	0
56	MG	1A	3065	1/1	0.99	0.13	39,39,39,39	0
56	MG	1A	3668	1/1	0.99	0.16	17,17,17,17	0
56	MG	1A	3732	1/1	0.99	0.12	26,26,26,26	0
56	MG	1A	3294	1/1	0.99	0.19	55,55,55,55	0
56	MG	2A	3534	1/1	0.99	0.16	39,39,39,39	0
56	MG	1B	228	1/1	0.99	0.09	36,36,36,36	0
56	MG	1A	3600	1/1	0.99	0.10	56,56,56,56	0
56	MG	2A	3429	1/1	0.99	0.10	53,53,53,53	0
56	MG	1A	3785	1/1	0.99	0.12	26,26,26,26	0
56	MG	1a	1862	1/1	0.99	0.13	35,35,35,35	0
56	MG	2a	3105	1/1	0.99	0.09	62,62,62,62	0
56	MG	1A	3088	1/1	0.99	0.13	53,53,53,53	0
56	MG	2a	3107	1/1	0.99	0.08	57,57,57,57	0
56	MG	2a	3108	1/1	0.99	0.10	68,68,68,68	0
56	MG	2a	3172	1/1	0.99	0.08	42,42,42,42	0
56	MG	1A	4051	1/1	0.99	0.21	15,15,15,15	0
56	MG	2a	3239	1/1	0.99	0.43	55,55,55,55	0
56	MG	2a	3110	1/1	0.99	0.10	55,55,55,55	0
56	MG	2R	202	1/1	0.99	0.11	35,35,35,35	0
56	MG	1A	3736	1/1	0.99	0.20	15,15,15,15	0
56	MG	2a	3177	1/1	0.99	0.15	69,69,69,69	0
56	MG	2U	201	1/1	0.99	0.21	49,49,49,49	0
56	MG	2A	3332	1/1	0.99	0.13	42,42,42,42	0
56	MG	1A	3617	1/1	0.99	0.18	13,13,13,13	0
56	MG	1A	3956	1/1	0.99	0.18	12,12,12,12	0
56	MG	1A	3738	1/1	0.99	0.20	17,17,17,17	0
56	MG	1A	3113	1/1	0.99	0.16	35,35,35,35	0
56	MG	1A	3468	1/1	0.99	0.05	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1a	1708	1/1	0.99	0.14	67,67,67,67	0
56	MG	2A	3145	1/1	0.99	0.16	25,25,25,25	0
56	MG	1A	3655	1/1	0.99	0.11	24,24,24,24	0
56	MG	1A	3469	1/1	0.99	0.34	33,33,33,33	0
56	MG	2a	3002	1/1	0.99	0.15	58,58,58,58	0
56	MG	1A	3266	1/1	0.99	0.16	18,18,18,18	0
56	MG	1A	3592	1/1	0.99	0.13	25,25,25,25	0
56	MG	2A	3293	1/1	0.99	0.17	30,30,30,30	0
56	MG	1A	3933	1/1	0.99	0.10	46,46,46,46	0
56	MG	1A	3965	1/1	0.99	0.14	36,36,36,36	0
56	MG	2A	3450	1/1	0.99	0.09	56,56,56,56	0
56	MG	1a	1835	1/1	0.99	0.20	51,51,51,51	0
56	MG	1A	3796	1/1	0.99	0.16	24,24,24,24	0
56	MG	2A	3201	1/1	0.99	0.22	47,47,47,47	0
56	MG	2A	3108	1/1	0.99	0.05	52,52,52,52	0
56	MG	1A	3607	1/1	0.99	0.23	26,26,26,26	0
56	MG	2A	3156	1/1	0.99	0.24	23,23,23,23	0
56	MG	1A	3182	1/1	0.99	0.27	32,32,32,32	0
56	MG	1A	3722	1/1	0.99	0.08	49,49,49,49	0
56	MG	1A	3642	1/1	0.99	0.26	38,38,38,38	0
56	MG	1A	4069	1/1	0.99	0.11	47,47,47,47	0
56	MG	1A	3882	1/1	0.99	0.17	36,36,36,36	0
56	MG	1A	3625	1/1	0.99	0.11	31,31,31,31	0
56	MG	2a	3021	1/1	0.99	0.18	58,58,58,58	0
56	MG	1A	3703	1/1	0.99	0.19	18,18,18,18	0
56	MG	1E	311	1/1	0.99	0.12	40,40,40,40	0
56	MG	1a	1648	1/1	0.99	0.07	48,48,48,48	0
56	MG	1A	3594	1/1	0.99	0.14	40,40,40,40	0
56	MG	2A	3520	1/1	0.99	0.10	37,37,37,37	0
56	MG	1A	3943	1/1	0.99	0.15	44,44,44,44	0
56	MG	1A	3142	1/1	0.99	0.11	20,20,20,20	0
56	MG	1a	1808	1/1	0.99	0.14	33,33,33,33	0
57	ZN	16	103	1/1	0.99	0.16	45,45,45,45	0
57	ZN	19	103	1/1	0.99	0.12	47,47,47,47	0
56	MG	2A	3315	1/1	0.99	0.17	39,39,39,39	0
56	MG	1v	3001	1/1	0.99	0.13	41,41,41,41	0
56	MG	1A	3283	1/1	0.99	0.24	43,43,43,43	0
57	ZN	25	501	1/1	0.99	0.10	50,50,50,50	0
56	MG	1A	3082	1/1	0.99	0.06	33,33,33,33	0
56	MG	1a	1770	1/1	0.99	0.14	70,70,70,70	0
56	MG	1A	4043	1/1	0.99	0.10	26,26,26,26	0
58	SF4	1d	501	8/8	0.99	0.13	64,72,77,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	SF4	2d	501	8/8	0.99	0.10	58,72,80,87	0
56	MG	2A	3004	1/1	1.00	0.08	59,59,59,59	0

6.5 Other polymers (i)

There are no such residues in this entry.