Full wwPDB X-ray Structure Validation Report ⓘ

Jul 30, 2024 – 03:16 AM EDT

PDB ID	:	9B00
Title	:	Crystal structure of the wild-type Thermus thermophilus 70S ribosome in complex with berberine analog of chloramphenicol CAM-BER, mRNA, deacylated A- and E-site tRNAphe, and deacylated P-site tRNAmet at 2.80A resolution
Authors	:	Batool, Z.; Pavlova, J.A.; Paranjpe, M.N.; Tereshchenkov, A.G.; Lukianov, D.A.; Osterman, I.A.; Bogdanov, A.A.; Sumbatyan, N.V.; Polikanov, Y.S.
Deposited on	:	2024-03-11
Resolution	:	2.80 Å(reported)

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

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

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

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

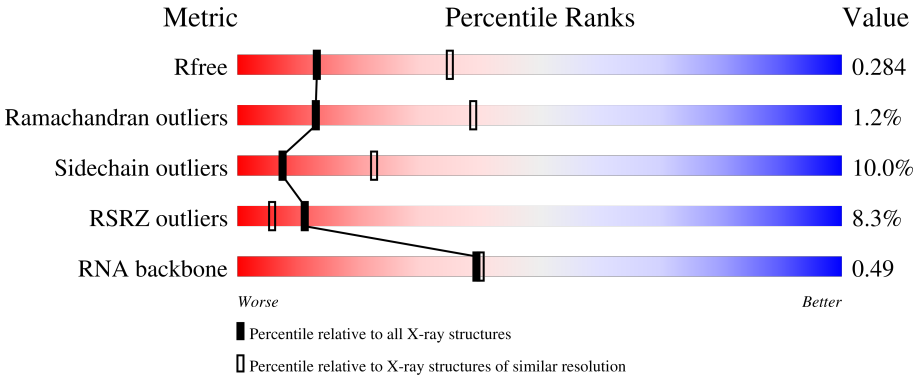
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.80 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	3140 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)
RNA backbone	3102	1227 (3.10-2.50)

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% 18%
1	2A	2915	77% 19%
2	1B	121	91% 8%
2	2B	121	74% 25%
3	1D	276	97%

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Mol	Chain	Length	Quality of chain
3	2D	276	2% 92% 8%
4	1E	206	90% 9%
4	2E	206	93% 6%
5	1F	210	2% 86% 10%
5	2F	210	14% 91% 6%
6	1G	182	90% 9%
6	2G	182	16% 89% 10%
7	1H	180	91% 6%
7	2H	180	34% 86% 11%
8	1I	148	86% 12%
8	2I	148	7% 82% 17%
9	1N	140	95% 5%
9	2N	140	4% 88% 12%
10	1O	122	95% 5%
10	2O	122	16% 96%
11	1P	150	87% 12%
11	2P	150	46% 91% 7%
12	1Q	141	2% 92% 8%
12	2Q	141	21% 94% 6%
13	1R	118	94% 6%
13	2R	118	97%
14	1S	112	93% 5%
14	2S	112	81% 17%
15	1T	146	85% 5% 10%
15	2T	146	5% 82% 8% 10%

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Mol	Chain	Length	Quality of chain
16	1U	118	97%
16	2U	118	7% 92% 7%
17	1V	101	92% 7%
17	2V	101	9% 87% 12%
18	1W	113	95%
18	2W	113	% 92% 7%
19	1X	96	96%
19	2X	96	96%
20	1Y	110	88% 9%
20	2Y	110	% 88% 9%
21	1Z	206	66% 9% 25%
21	2Z	206	3% 67% 11% 22%
22	10	85	7% 92% 6%
22	20	85	14% 92% 6%
23	11	98	% 90% 9%
23	21	98	17% 91% 8%
24	12	72	93%
24	22	72	89% 8%
25	13	60	87% 12%
25	23	60	20% 93% 5%
26	14	71	73% 23%
26	24	71	6% 80% 15%
27	15	60	93% 5%
27	25	60	92% 7%
28	16	54	2% 85% 13%

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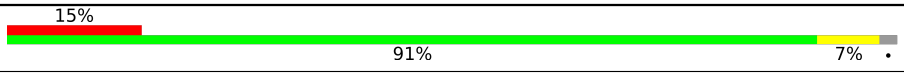
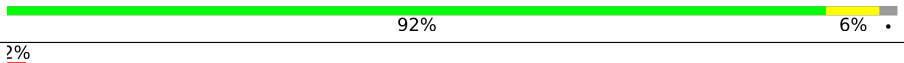
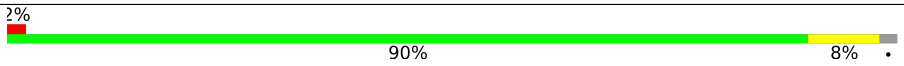
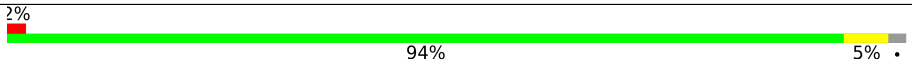
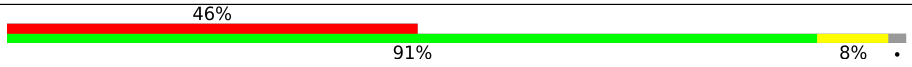
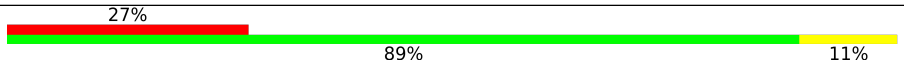
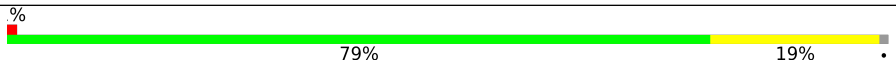
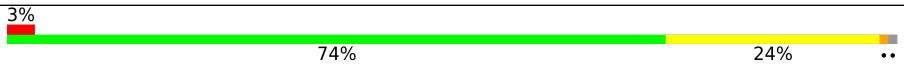
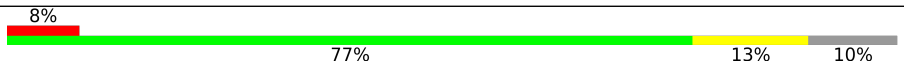
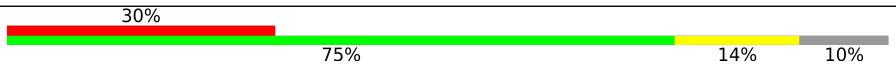
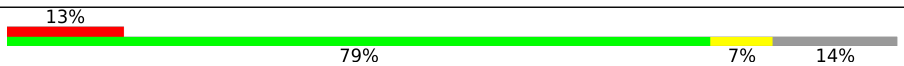
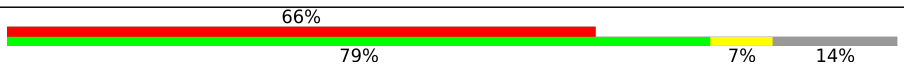
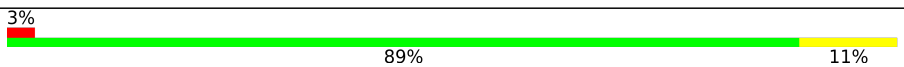
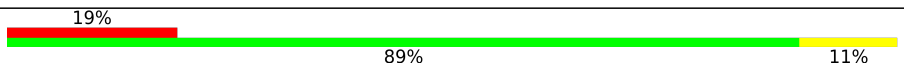
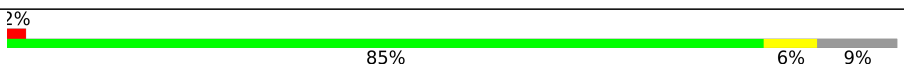
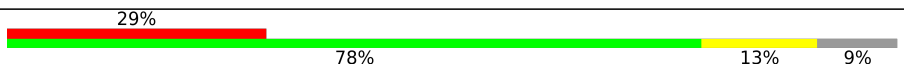
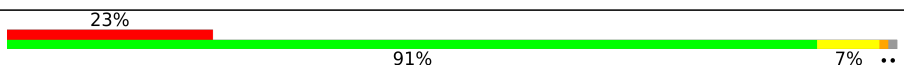
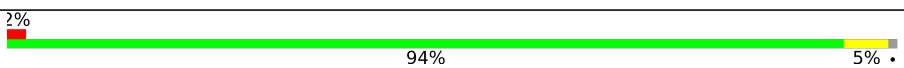
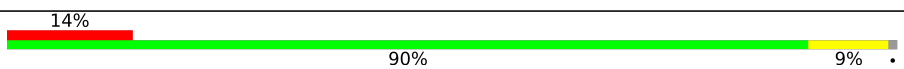
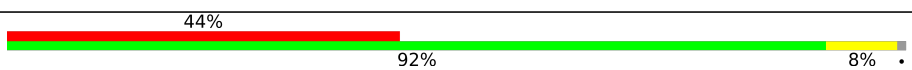
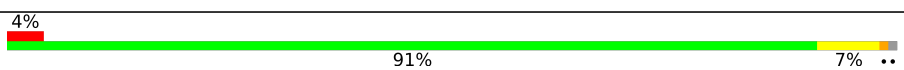
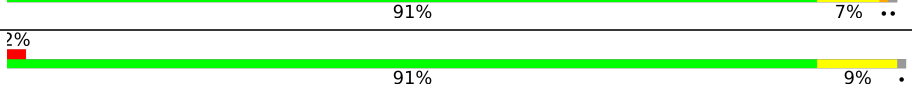
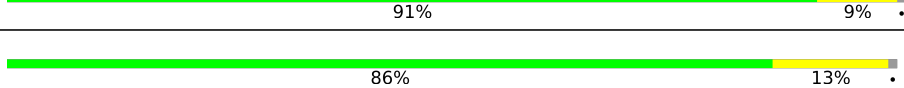
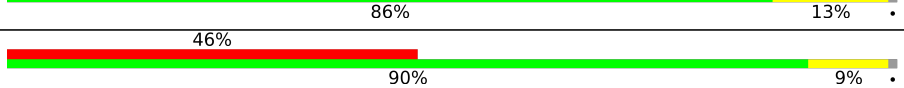
Mol	Chain	Length	Quality of chain
28	26	54	
29	17	49	
29	27	49	
30	18	65	
30	28	65	
31	19	37	
31	29	37	
32	1a	1521	
32	2a	1521	
33	1b	256	
33	2b	256	
34	1c	239	
34	2c	239	
35	1d	209	
35	2d	209	
36	1e	162	
36	2e	162	
37	1f	101	
37	2f	101	
38	1g	156	
38	2g	156	
39	1h	138	
39	2h	138	
40	1i	128	
40	2i	128	

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Mol	Chain	Length	Quality of chain
41	1j	105	% 82% 10% 8%
41	2j	105	49% 76% 14% 9%
42	1k	129	47% 81% 8% 12%
42	2k	129	36% 77% 12% 12%
43	1l	132	11% 86% 6% 8%
43	2l	132	24% 81% 11% 8%
44	1m	126	4% 86% 11%
44	2m	126	14% 83% 13%
45	1n	61	90% 8%
45	2n	61	69% 90% 8%
46	1o	89	% 92% 6%
46	2o	89	93% 6%
47	1p	88	5% 88% 6% 7%
47	2p	88	% 85% 8% 7%
48	1q	105	6% 83% 11% 6%
48	2q	105	% 82% 12% 6%
49	1r	88	49% 67% 10% 23%
49	2r	88	18% 70% 7% 23%
50	1s	93	84% 11%
50	2s	93	15% 76% 13% 11%
51	1t	106	8% 80% 10% 9%
51	2t	106	8% 84% 7% 9%
52	1u	27	81% 15%
52	2u	27	30% 74% 11% 15%
53	1v	24	12% 33% 21% 46%

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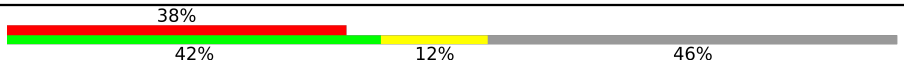
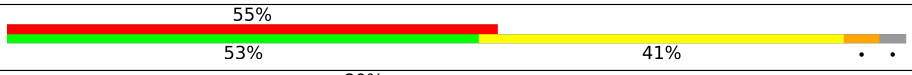
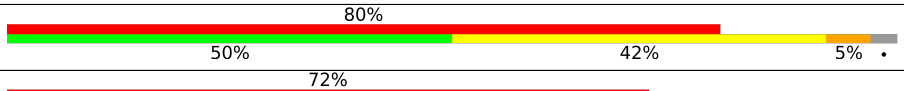
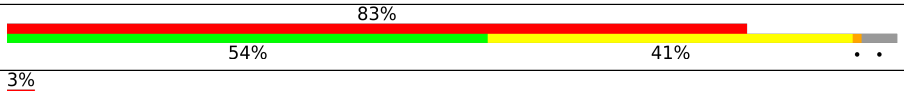
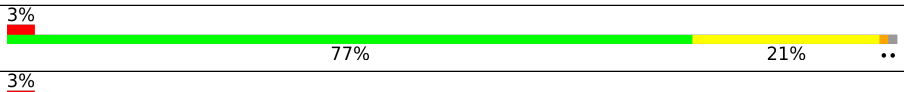
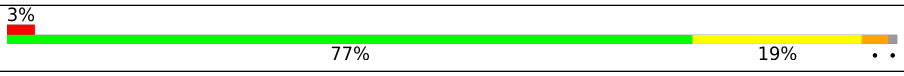
Mol	Chain	Length	Quality of chain
53	2v	24	
54	1w	76	
54	1y	76	
54	2w	76	
54	2y	76	
55	1x	77	
55	2x	77	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
54	G7M	1y	46	-	-	-	X
54	PSU	2y	32	-	-	-	X
54	G7M	2y	46	-	-	-	X
56	MG	1A	3332	-	-	-	X
56	MG	1A	3379	-	-	-	X
56	MG	1A	3509	-	-	-	X
56	MG	1B	230	-	-	-	X
56	MG	1D	306	-	-	-	X
56	MG	1a	1738	-	-	-	X
56	MG	1a	1764	-	-	-	X
56	MG	1a	1800	-	-	-	X
56	MG	2A	3044	-	-	-	X
56	MG	2A	3072	-	-	-	X
56	MG	2A	3075	-	-	-	X
56	MG	2A	3135	-	-	-	X
56	MG	2A	3165	-	-	-	X
56	MG	2A	3183	-	-	-	X
56	MG	2A	3196	-	-	-	X
56	MG	2A	3206	-	-	-	X
56	MG	2A	3228	-	-	-	X
56	MG	2A	3276	-	-	-	X
56	MG	2A	3282	-	-	-	X
56	MG	2A	3284	-	-	-	X
56	MG	2A	3285	-	-	-	X
56	MG	2A	3305	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	2A	3320	-	-	-	X
56	MG	2A	3370	-	-	-	X
56	MG	2A	3373	-	-	-	X
56	MG	2A	3376	-	-	-	X
56	MG	2A	3407	-	-	-	X
56	MG	2A	3850	-	-	-	X
56	MG	2a	3010	-	-	-	X
56	MG	2a	3048	-	-	-	X
56	MG	2a	3244	-	-	-	X

2 Entry composition (i)

There are 61 unique types of molecules in this entry. The entry contains 299897 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 23S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1A	2871	Total	C	N	O	P	0	0	0
			61852	27531	11572	19878	2871			
1	2A	2800	Total	C	N	O	P	0	0	0
			60322	26848	11284	19390	2800			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	1B	120	Total	C	N	O	P	0	0	0
			2577	1146	476	835	120			
2	2B	120	Total	C	N	O	P	0	0	0
			2575	1146	476	833	120			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	1F	203	Total	C	N	O	S	0	0	0
			1587	1011	298	276	2			
5	2F	203	Total	C	N	O	S	0	0	0
			1583	1009	297	275	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	1G	181	Total	C	N	O	S	0	0	0
			1423	913	253	253	4			
6	2G	181	Total	C	N	O	S	0	0	0
			1428	913	258	253	4			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	1I	146	Total	C	N	O	S	0	0	0
			1097	701	191	204	1			
8	2I	146	Total	C	N	O	S	0	0	0
			1064	681	186	196	1			

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	1S	110	Total 873	C 550	N 174	O 149	0	0	0
14	2S	110	Total 870	C 549	N 173	O 148	0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	1Z	154	Total	C	N	O	S	0	0	0
			1240	795	222	220	3			
21	2Z	160	Total	C	N	O	S	0	0	0
			1271	814	228	227	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	10	83	Total	C	N	O	S	0	0	0
			653	404	139	109	1			
22	20	83	Total	C	N	O	S	0	0	0
			653	404	139	109	1			

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	14	69	Total	C	N	O	S	0	0	0
			552	349	99	99	5			

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	1a	1500	Total	C	N	O	P	0	0	0
			32246	14358	5975	10413	1500			
32	2a	1503	Total	C	N	O	P	0	0	0
			32327	14396	5990	10438	1503			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	1b	231	Total	C	N	O	S	0	0	0
			1846	1179	331	331	5			
33	2b	231	Total	C	N	O	S	0	0	0
			1825	1167	326	327	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	1c	206	Total	C	N	O	S	0	0	0
			1548	973	301	273	1			
34	2c	206	Total	C	N	O	S	0	0	0
			1542	968	300	273	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	1d	208	Total	C	N	O	S	0	0	0
			1655	1038	326	284	7			
35	2d	208	Total	C	N	O	S	0	0	0
			1674	1050	333	284	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	1e	148	Total	C	N	O	S	0	0	0
			1129	714	213	198	4			
36	2e	148	Total	C	N	O	S	0	0	0
			1133	716	214	199	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	1f	100	Total	C	N	O	S	0	0	0
			810	514	144	149	3			
37	2f	100	Total	C	N	O	S	0	0	0
			816	516	146	151	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	1g	155	Total	C	N	O	S	0	0	0
			1231	766	243	216	6			
38	2g	155	Total	C	N	O	S	0	0	0
			1235	769	244	216	6			

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
40	1i	127	Total	C	N	O	0	0	0
			983	623	193	167			
40	2i	127	Total	C	N	O	0	0	0
			978	619	190	169			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
41	1j	97	Total	C	N	O	0	0	0
			709	440	138	131			
41	2j	96	Total	C	N	O	0	0	0
			714	445	138	131			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	1k	114	Total	C	N	O	S	0	0	0
			829	516	155	155	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	2k	114	Total	C	N	O	S	0	0	0
			833	519	156	155	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	1l	122	Total	C	N	O	S	0	0	0
			932	586	185	159	2			
43	2l	122	Total	C	N	O	S	0	0	0
			932	586	185	159	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	1m	123	Total	C	N	O	S	0	0	0
			958	592	198	166	2			
44	2m	122	Total	C	N	O	S	0	0	0
			950	586	197	165	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	1n	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			
45	2n	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	1p	82	Total	C	N	O	S	0	0	0
			681	433	134	113	1			
47	2p	82	Total	C	N	O	S	0	0	0
			677	430	133	113	1			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	1s	83	Total	C	N	O	S	0	0	0
			652	417	120	113	2			
50	2s	83	Total	C	N	O	S	0	0	0
			646	412	119	113	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	1t	96	Total	C	N	O	S	0	0	0
			728	446	156	124	2			
51	2t	96	Total	C	N	O	S	0	0	0
			727	446	155	124	2			

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

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

- Molecule 53 is a RNA chain called MF-mRNA.

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

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
54	1w	74	Total	C	N	O	P	S	0	0	0
			1592	713	285	518	74	2			
54	1y	74	Total	C	N	O	P	S	0	0	0
			1585	707	285	518	74	1			
54	2w	72	Total	C	N	O	P	S	0	0	0
			1544	690	278	502	72	2			
54	2y	73	Total	C	N	O	P	S	0	0	0
			1565	698	283	510	73	1			

- Molecule 55 is a RNA chain called P-site Deacylated tRNAmet.

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	1A	1083	Total	Mg	0	0
			1083	1083		
56	1B	38	Total	Mg	0	0
			38	38		
56	1D	11	Total	Mg	0	0
			11	11		
56	1E	12	Total	Mg	0	0
			12	12		
56	1F	13	Total	Mg	0	0
			13	13		
56	1G	4	Total	Mg	0	0
			4	4		
56	1H	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	1N	5	Total Mg 5 5	0	0
56	1O	3	Total Mg 3 3	0	0
56	1P	7	Total Mg 7 7	0	0
56	1Q	6	Total Mg 6 6	0	0
56	1R	5	Total Mg 5 5	0	0
56	1S	3	Total Mg 3 3	0	0
56	1T	3	Total Mg 3 3	0	0
56	1U	8	Total Mg 8 8	0	0
56	1V	8	Total Mg 8 8	0	0
56	1W	7	Total Mg 7 7	0	0
56	1X	6	Total Mg 6 6	0	0
56	1Y	3	Total Mg 3 3	0	0
56	1Z	3	Total Mg 3 3	0	0
56	10	7	Total Mg 7 7	0	0
56	11	6	Total Mg 6 6	0	0
56	12	1	Total Mg 1 1	0	0
56	13	4	Total Mg 4 4	0	0
56	14	1	Total Mg 1 1	0	0
56	15	5	Total Mg 5 5	0	0
56	16	2	Total Mg 2 2	0	0
56	17	6	Total Mg 6 6	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	18	3	Total Mg 3 3	0	0
56	19	2	Total Mg 2 2	0	0
56	1a	226	Total Mg 226 226	0	0
56	1b	1	Total Mg 1 1	0	0
56	1d	1	Total Mg 1 1	0	0
56	1e	1	Total Mg 1 1	0	0
56	1f	2	Total Mg 2 2	0	0
56	1k	1	Total Mg 1 1	0	0
56	1l	2	Total Mg 2 2	0	0
56	1m	1	Total Mg 1 1	0	0
56	1n	2	Total Mg 2 2	0	0
56	1t	1	Total Mg 1 1	0	0
56	1w	7	Total Mg 7 7	0	0
56	1x	12	Total Mg 12 12	0	0
56	1y	1	Total Mg 1 1	0	0
56	2A	849	Total Mg 849 849	0	0
56	2B	20	Total Mg 20 20	0	0
56	2D	5	Total Mg 5 5	0	0
56	2E	7	Total Mg 7 7	0	0
56	2F	7	Total Mg 7 7	0	0
56	2G	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	2N	1	Total Mg 1 1	0	0
56	2O	1	Total Mg 1 1	0	0
56	2P	1	Total Mg 1 1	0	0
56	2Q	1	Total Mg 1 1	0	0
56	2R	1	Total Mg 1 1	0	0
56	2T	4	Total Mg 4 4	0	0
56	2U	1	Total Mg 1 1	0	0
56	2V	2	Total Mg 2 2	0	0
56	2X	2	Total Mg 2 2	0	0
56	2Y	1	Total Mg 1 1	0	0
56	2Z	1	Total Mg 1 1	0	0
56	20	2	Total Mg 2 2	0	0
56	21	3	Total Mg 3 3	0	0
56	23	2	Total Mg 2 2	0	0
56	25	2	Total Mg 2 2	0	0
56	27	4	Total Mg 4 4	0	0
56	28	6	Total Mg 6 6	0	0
56	2a	246	Total Mg 246 246	0	0
56	2d	1	Total Mg 1 1	0	0
56	2e	2	Total Mg 2 2	0	0
56	2f	2	Total Mg 2 2	0	0

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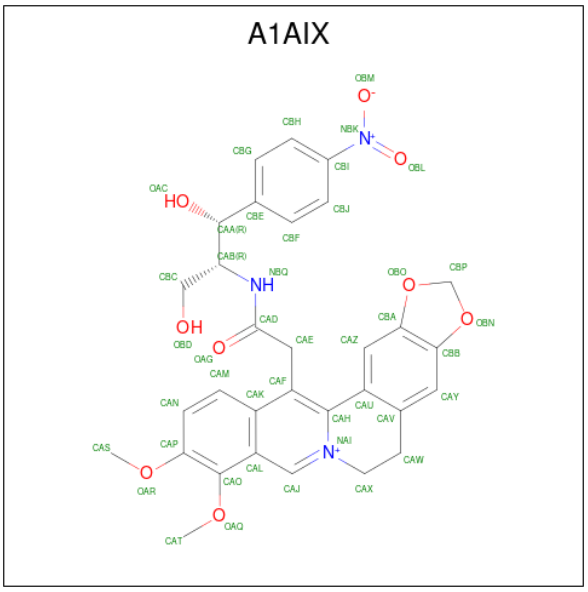
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	2g	1	Total Mg 1 1	0	0
56	2j	1	Total Mg 1 1	0	0
56	2l	4	Total Mg 4 4	0	0
56	2q	3	Total Mg 3 3	0	0
56	2t	1	Total Mg 1 1	0	0
56	2v	3	Total Mg 3 3	0	0
56	2w	1	Total Mg 1 1	0	0
56	2x	6	Total Mg 6 6	0	0
56	2y	4	Total Mg 4 4	0	0

- Molecule 57 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	1A	1	Total K 1 1	0	0
57	2A	1	Total K 1 1	0	0

- Molecule 58 is 13-(2-{[(1R,2R)-1,3-dihydroxy-1-(4-nitrophenyl)propan-2-yl]amino}-2-oxoethyl)-9,10-dimethoxy-5,6-dihydro-2H-[1,3]dioxolo[4,5-g]isoquinolino[3,2-a]isoquinolin-7-ium (three-letter code: A1AIX) (formula: $C_{31}H_{30}N_3O_9$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	1A	1	Total C N O 43 31 3 9	0	0
58	2A	1	Total C N O 43 31 3 9	0	0

- Molecule 59 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

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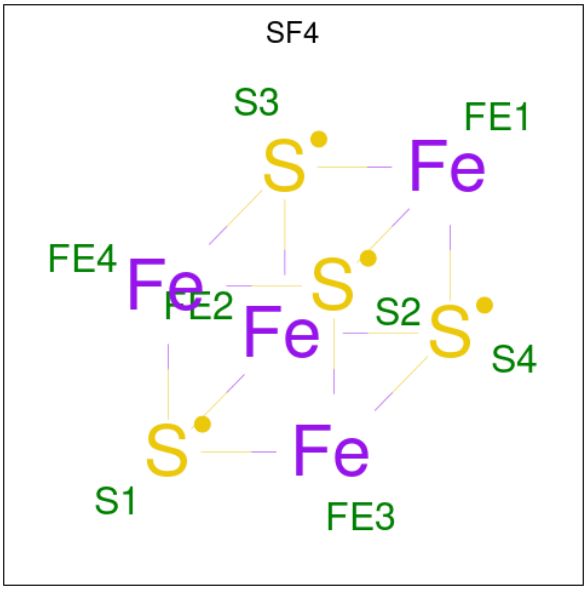
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	29	1	Total Zn 1 1	0	0
59	2n	1	Total Zn 1 1	0	0

- Molecule 60 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



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

- Molecule 61 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1A	1901	Total O 1901 1901	0	0
61	1B	57	Total O 57 57	0	0
61	1D	27	Total O 27 27	0	0
61	1E	19	Total O 19 19	0	0
61	1F	15	Total O 15 15	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1G	3	Total O 3 3	0	0
61	1N	3	Total O 3 3	0	0
61	1O	4	Total O 4 4	0	0
61	1P	21	Total O 21 21	0	0
61	1Q	8	Total O 8 8	0	0
61	1R	12	Total O 12 12	0	0
61	1S	3	Total O 3 3	0	0
61	1T	7	Total O 7 7	0	0
61	1U	11	Total O 11 11	0	0
61	1V	5	Total O 5 5	0	0
61	1W	10	Total O 10 10	0	0
61	1X	4	Total O 4 4	0	0
61	1Y	2	Total O 2 2	0	0
61	1Z	1	Total O 1 1	0	0
61	10	9	Total O 9 9	0	0
61	11	6	Total O 6 6	0	0
61	12	3	Total O 3 3	0	0
61	13	4	Total O 4 4	0	0
61	15	6	Total O 6 6	0	0
61	16	2	Total O 2 2	0	0
61	17	10	Total O 10 10	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	18	8	Total O 8 8	0	0
61	1a	364	Total O 364 364	0	0
61	1b	1	Total O 1 1	0	0
61	1d	1	Total O 1 1	0	0
61	1e	2	Total O 2 2	0	0
61	1i	1	Total O 1 1	0	0
61	1l	7	Total O 7 7	0	0
61	1o	1	Total O 1 1	0	0
61	1q	2	Total O 2 2	0	0
61	1u	1	Total O 1 1	0	0
61	1v	5	Total O 5 5	0	0
61	1w	7	Total O 7 7	0	0
61	1x	10	Total O 10 10	0	0
61	1y	1	Total O 1 1	0	0
61	2A	1097	Total O 1097 1097	0	0
61	2B	22	Total O 22 22	0	0
61	2D	19	Total O 19 19	0	0
61	2E	13	Total O 13 13	0	0
61	2F	13	Total O 13 13	0	0
61	2I	1	Total O 1 1	0	0
61	2N	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	2O	2	Total O 2 2	0	0
61	2P	11	Total O 11 11	0	0
61	2Q	1	Total O 1 1	0	0
61	2R	5	Total O 5 5	0	0
61	2T	3	Total O 3 3	0	0
61	2U	2	Total O 2 2	0	0
61	2V	1	Total O 1 1	0	0
61	2W	1	Total O 1 1	0	0
61	2X	2	Total O 2 2	0	0
61	2Y	2	Total O 2 2	0	0
61	2Z	1	Total O 1 1	0	0
61	20	6	Total O 6 6	0	0
61	21	7	Total O 7 7	0	0
61	23	1	Total O 1 1	0	0
61	26	1	Total O 1 1	0	0
61	27	2	Total O 2 2	0	0
61	28	4	Total O 4 4	0	0
61	29	1	Total O 1 1	0	0
61	2a	260	Total O 260 260	0	0
61	2c	1	Total O 1 1	0	0
61	2d	3	Total O 3 3	0	0

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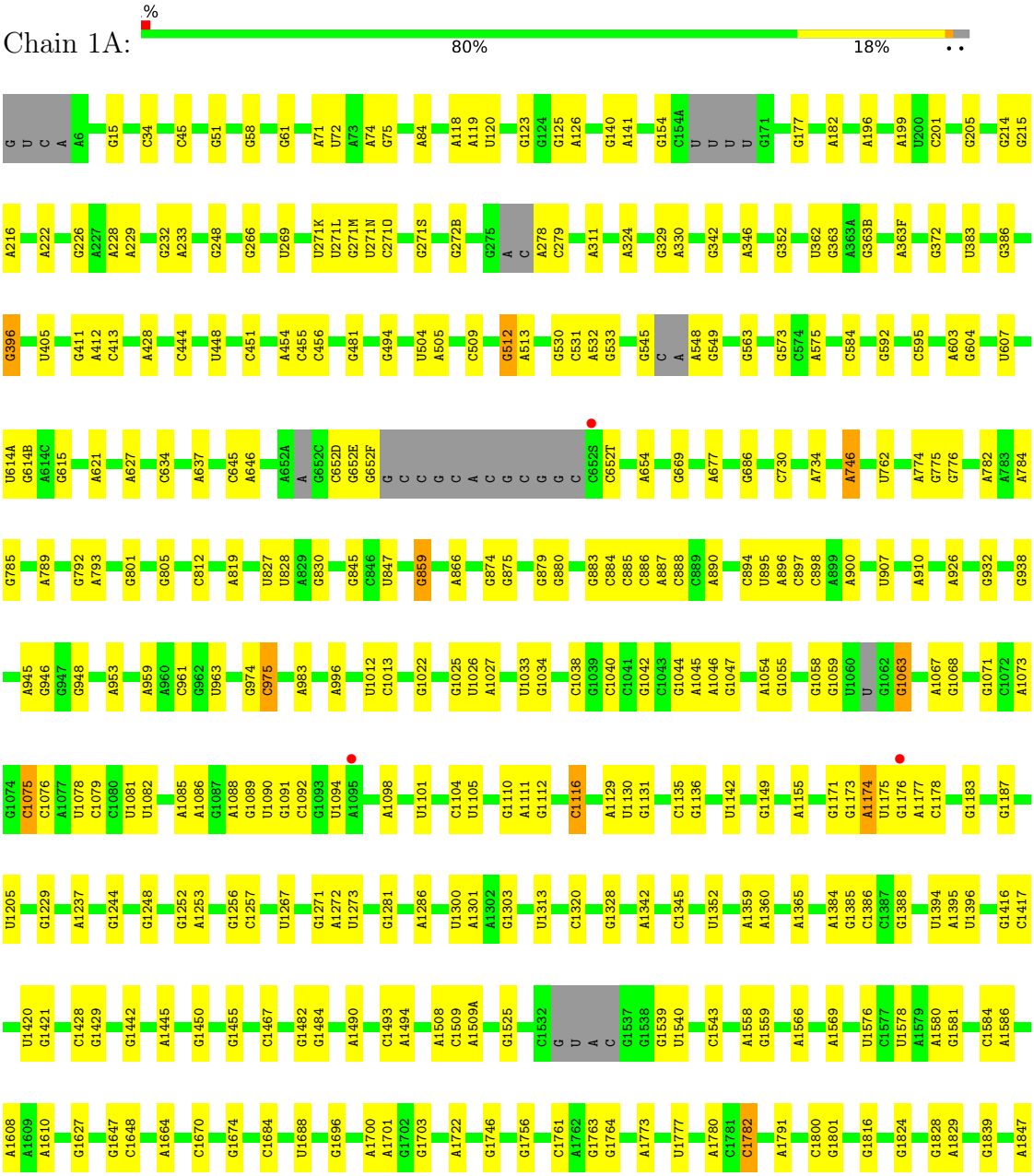
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	2e	2	Total O 2 2	0	0
61	2j	2	Total O 2 2	0	0
61	2l	2	Total O 2 2	0	0
61	2q	1	Total O 1 1	0	0
61	2r	2	Total O 2 2	0	0
61	2t	2	Total O 2 2	0	0
61	2v	2	Total O 2 2	0	0
61	2w	2	Total O 2 2	0	0
61	2x	3	Total O 3 3	0	0
61	2y	2	Total O 2 2	0	0

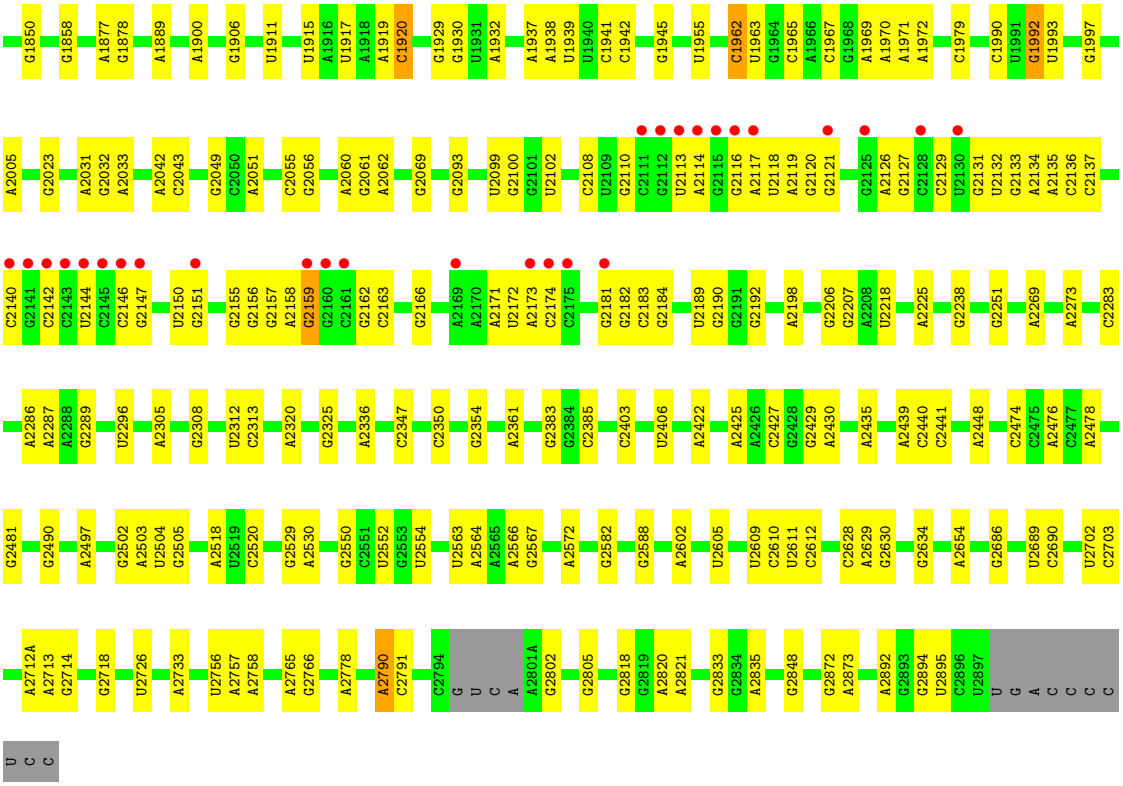
3 Residue-property plots (i)

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

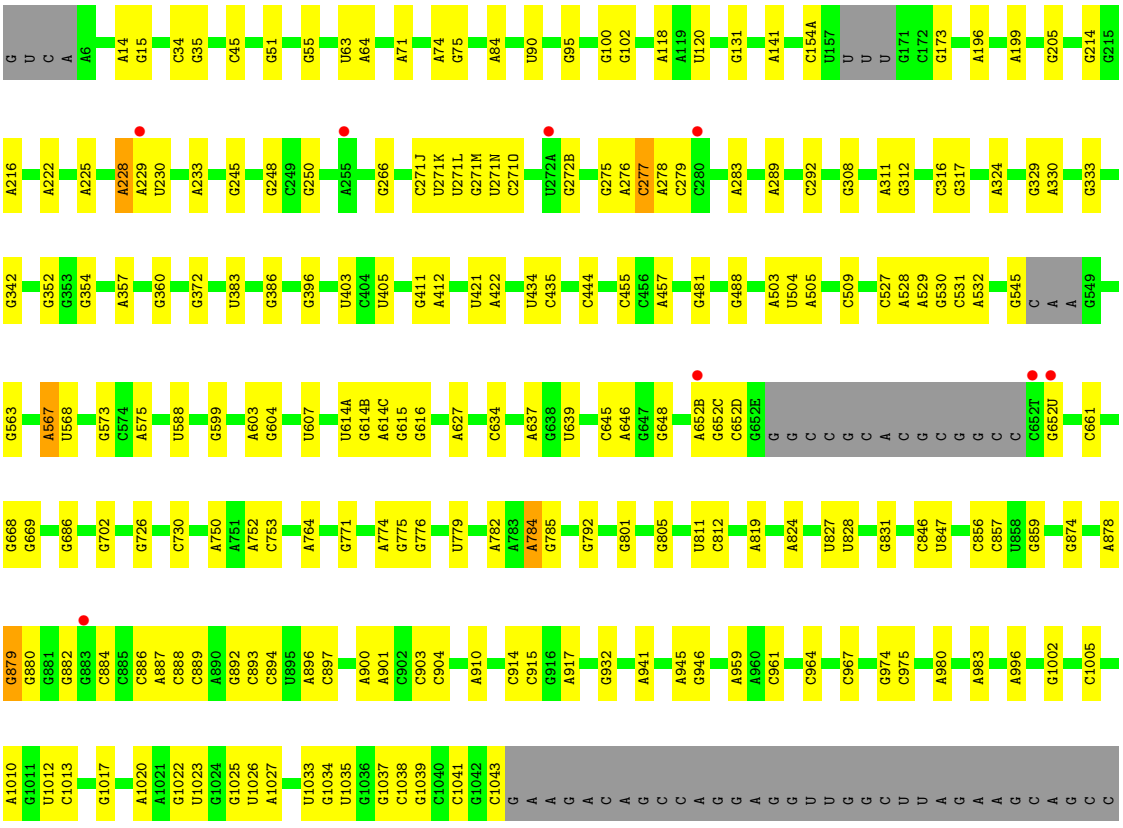
Chain 1A:

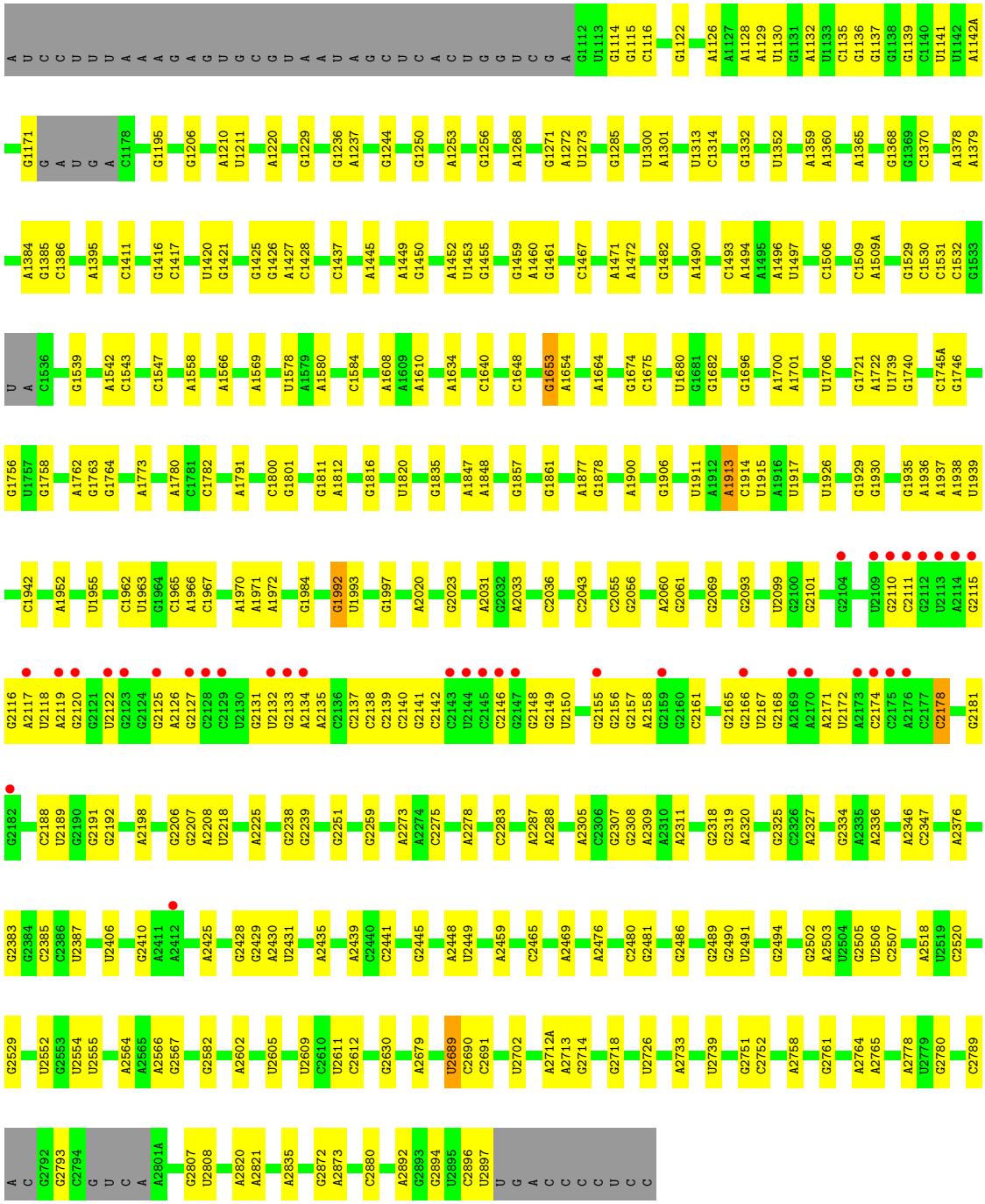




• Molecule 1: 23S Ribosomal RNA

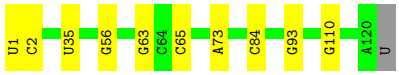
Chain 2A:





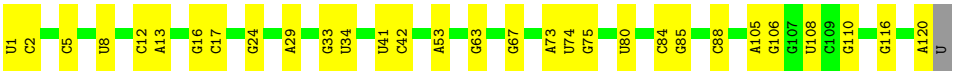
• Molecule 2: 5S Ribosomal RNA

Chain 1B:

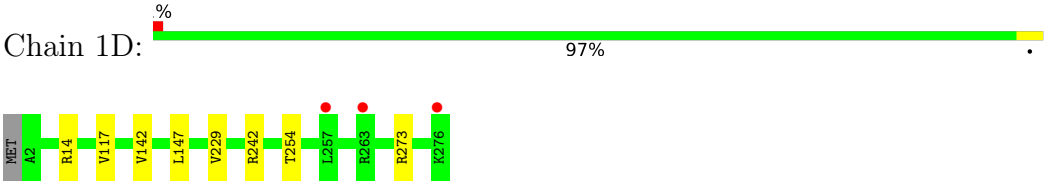


• Molecule 2: 5S Ribosomal RNA

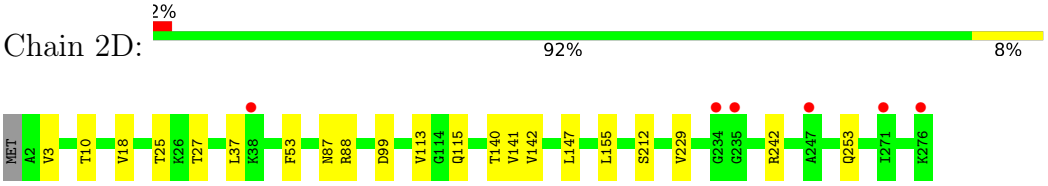
Chain 2B:



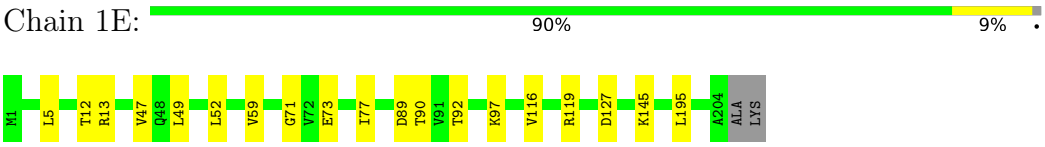
• Molecule 3: 50S ribosomal protein L2



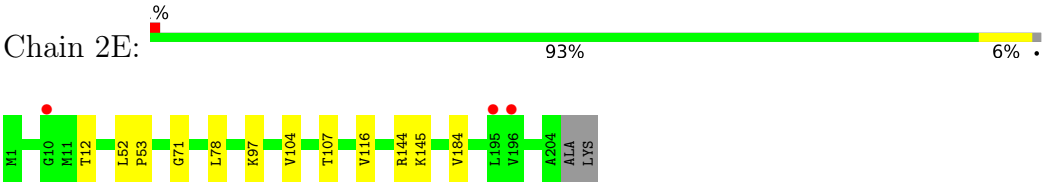
• Molecule 3: 50S ribosomal protein L2



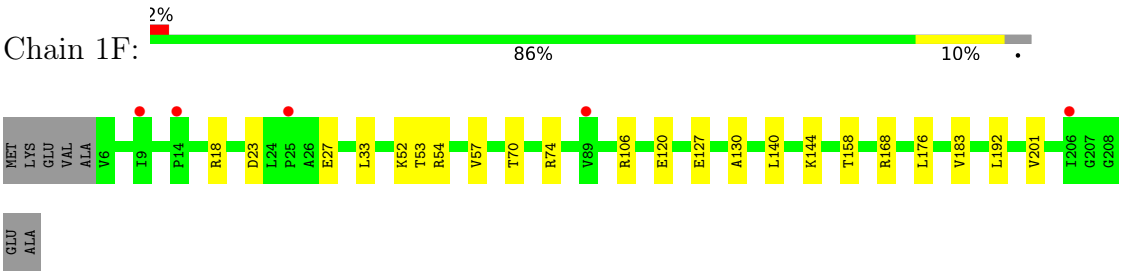
• Molecule 4: 50S ribosomal protein L3



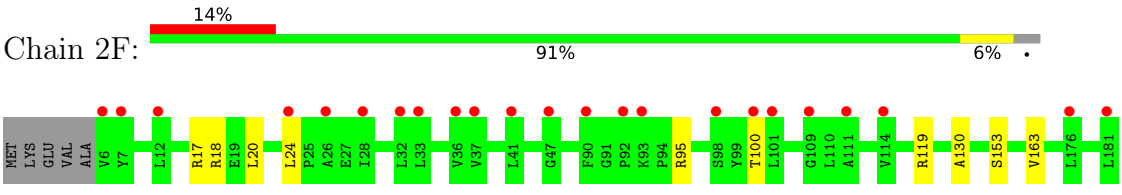
• Molecule 4: 50S ribosomal protein L3

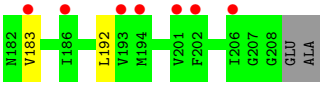


• Molecule 5: 50S ribosomal protein L4



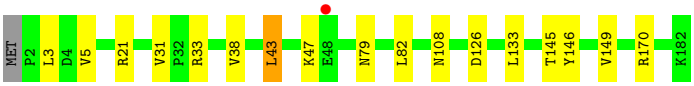
• Molecule 5: 50S ribosomal protein L4





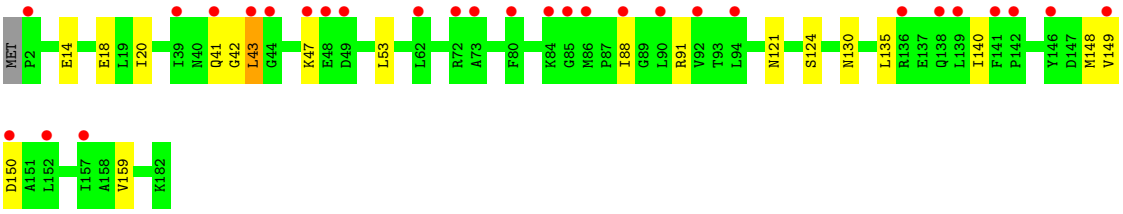
• Molecule 6: 50S ribosomal protein L5

Chain 1G:



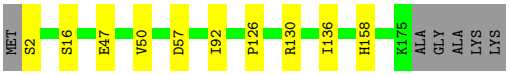
• Molecule 6: 50S ribosomal protein L5

Chain 2G:



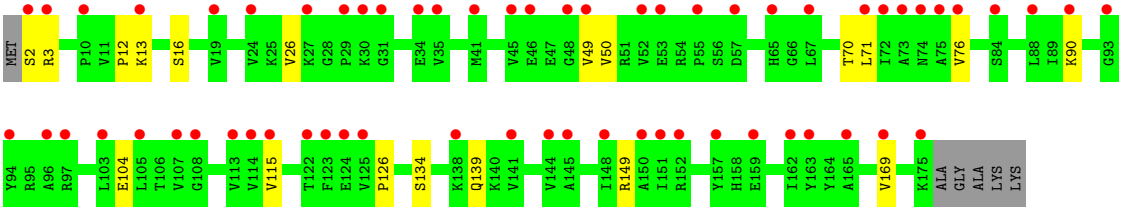
• Molecule 7: 50S ribosomal protein L6

Chain 1H:



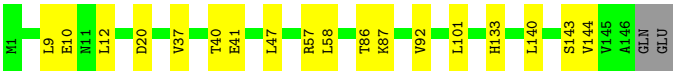
• Molecule 7: 50S ribosomal protein L6

Chain 2H:



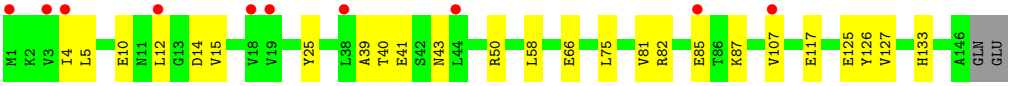
• Molecule 8: 50S ribosomal protein L9

Chain 1I:

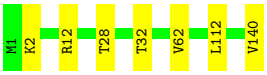


• Molecule 8: 50S ribosomal protein L9

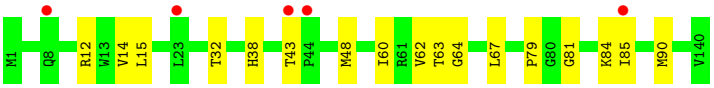
Chain 2I:



• Molecule 9: 50S ribosomal protein L13

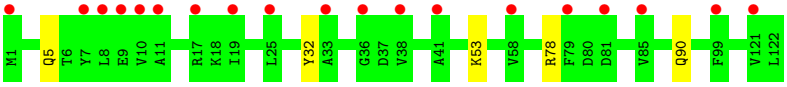


• Molecule 9: 50S ribosomal protein L13

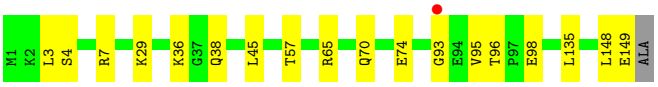


• Molecule 10: 50S ribosomal protein L14

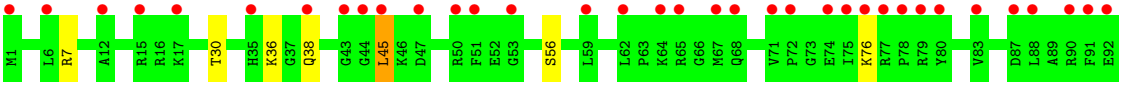
• Molecule 10: 50S ribosomal protein L14

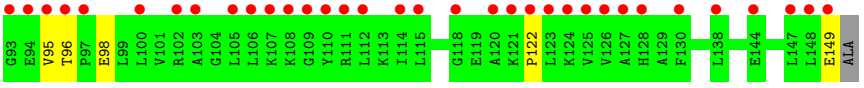


• Molecule 11: 50S ribosomal protein L15



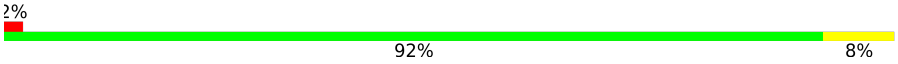
• Molecule 11: 50S ribosomal protein L15

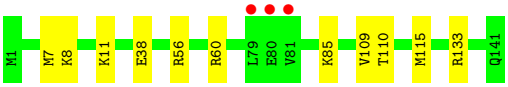




• Molecule 12: 50S ribosomal protein L16

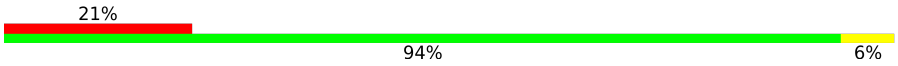
Chain 1Q:

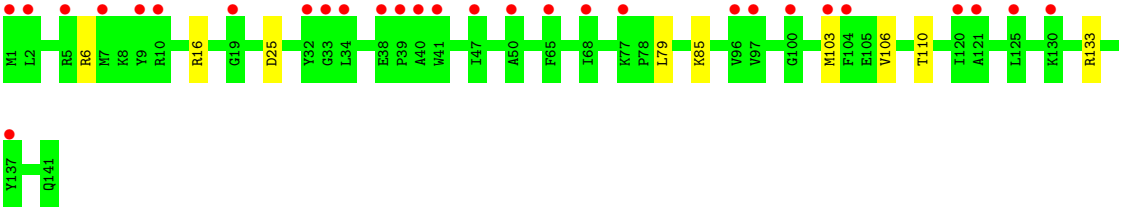




• Molecule 12: 50S ribosomal protein L16

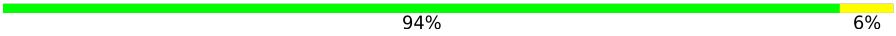
Chain 2Q:

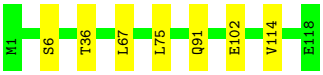




• Molecule 13: 50S ribosomal protein L17

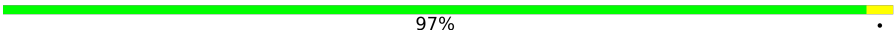
Chain 1R:

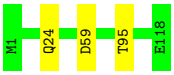




• Molecule 13: 50S ribosomal protein L17

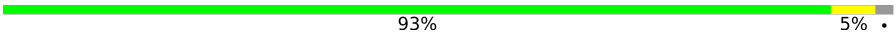
Chain 2R:





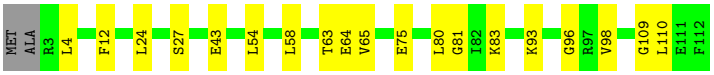
• Molecule 14: 50S ribosomal protein L18

Chain 1S:



• Molecule 14: 50S ribosomal protein L18

Chain 2S:

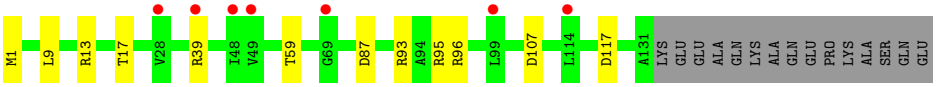


• Molecule 15: 50S ribosomal protein L19

Chain 1T:

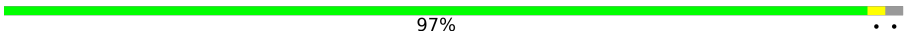
• Molecule 15: 50S ribosomal protein L19

Chain 2T:



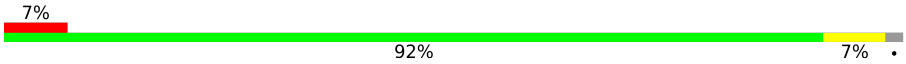
• Molecule 16: 50S ribosomal protein L20

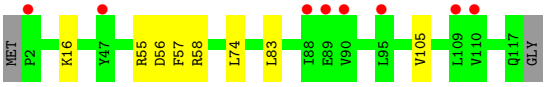
Chain 1U:



• Molecule 16: 50S ribosomal protein L20

Chain 2U:



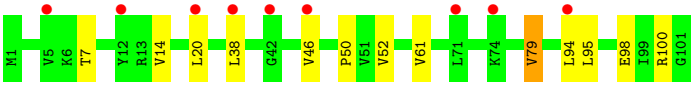


• Molecule 17: 50S ribosomal protein L21

Chain 1V:

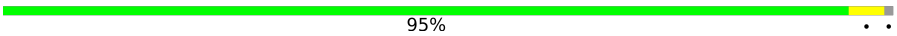
• Molecule 17: 50S ribosomal protein L21

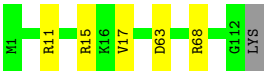
Chain 2V:



• Molecule 18: 50S ribosomal protein L22

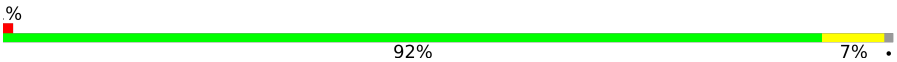
Chain 1W:

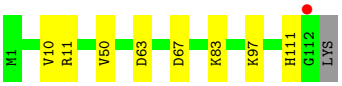




• Molecule 18: 50S ribosomal protein L22

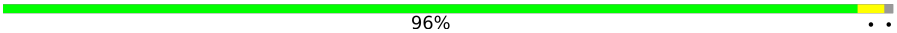
Chain 2W:





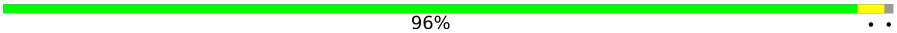
• Molecule 19: 50S ribosomal protein L23

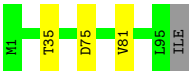
Chain 1X:



• Molecule 19: 50S ribosomal protein L23

Chain 2X:



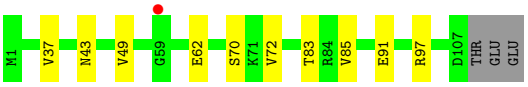


• Molecule 20: 50S ribosomal protein L24

Chain 1Y:

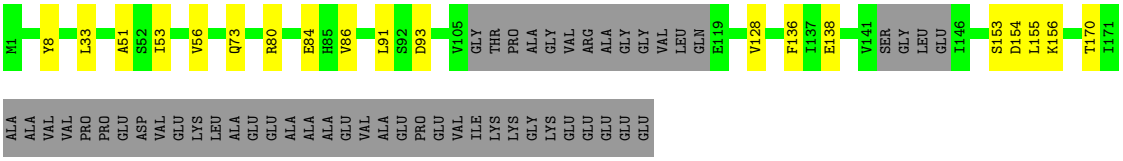
• Molecule 20: 50S ribosomal protein L24

Chain 2Y:



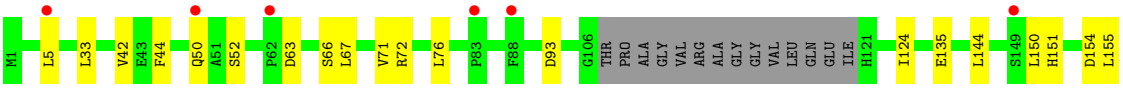
• Molecule 21: 50S ribosomal protein L25

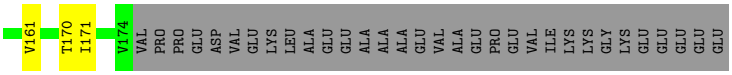
Chain 1Z:



• Molecule 21: 50S ribosomal protein L25

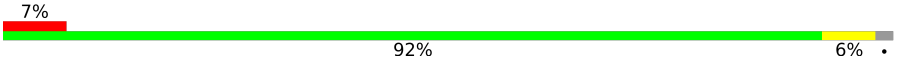
Chain 2Z:

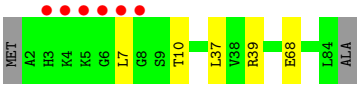




• Molecule 22: 50S ribosomal protein L27

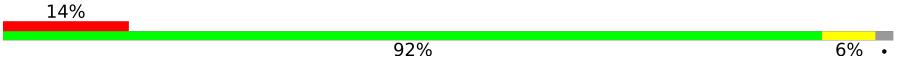
Chain 10:

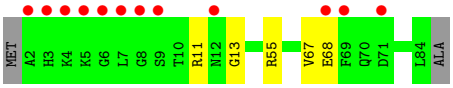




• Molecule 22: 50S ribosomal protein L27

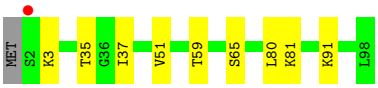
Chain 20:





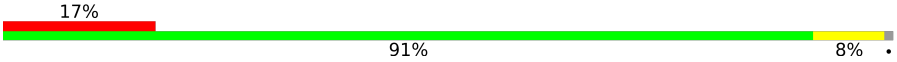
• Molecule 23: 50S ribosomal protein L28

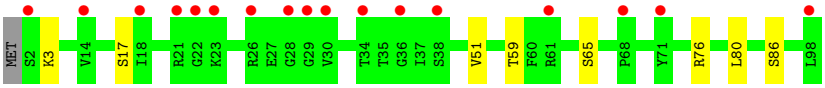
Chain 11:



• Molecule 23: 50S ribosomal protein L28

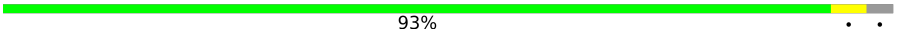
Chain 21:





• Molecule 24: 50S ribosomal protein L29

Chain 12:

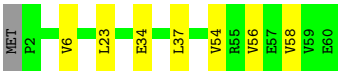


• Molecule 24: 50S ribosomal protein L29

Chain 22:

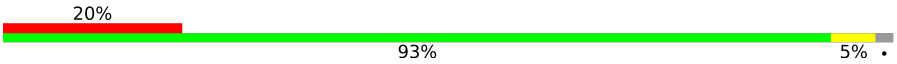
• Molecule 25: 50S ribosomal protein L30

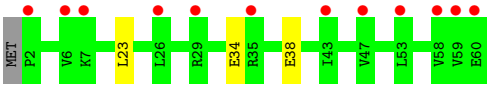
Chain 13:



• Molecule 25: 50S ribosomal protein L30

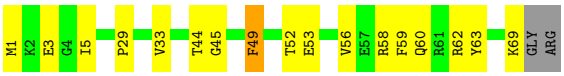
Chain 23:





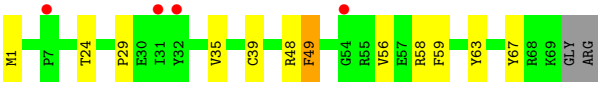
• Molecule 26: 50S ribosomal protein L31

Chain 14:



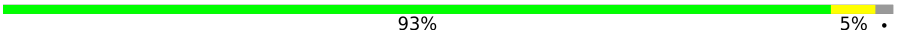
• Molecule 26: 50S ribosomal protein L31

Chain 24:



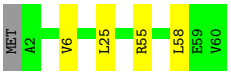
• Molecule 27: 50S ribosomal protein L32

Chain 15:



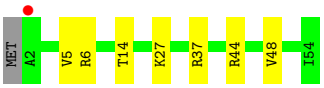
• Molecule 27: 50S ribosomal protein L32

Chain 25:



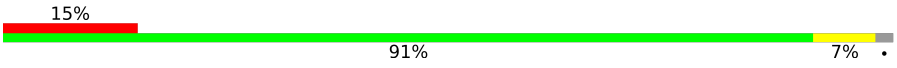
• Molecule 28: 50S ribosomal protein L33

Chain 16:



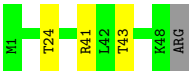
• Molecule 28: 50S ribosomal protein L33

Chain 26:



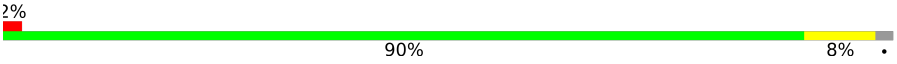
• Molecule 29: 50S ribosomal protein L34

Chain 17:



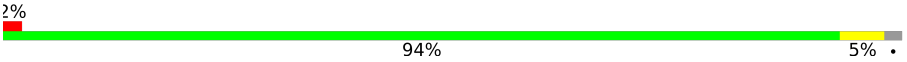
• Molecule 29: 50S ribosomal protein L34

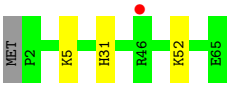
Chain 27:



• Molecule 30: 50S ribosomal protein L35

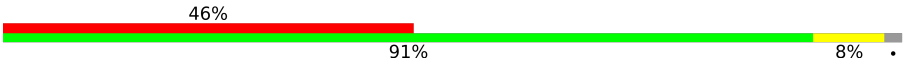
Chain 18:

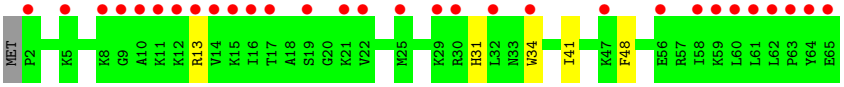




• Molecule 30: 50S ribosomal protein L35

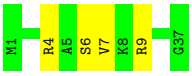
Chain 28:





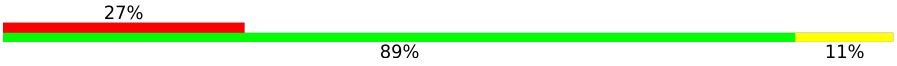
• Molecule 31: 50S ribosomal protein L36

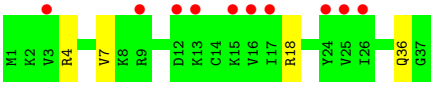
Chain 19:



• Molecule 31: 50S ribosomal protein L36

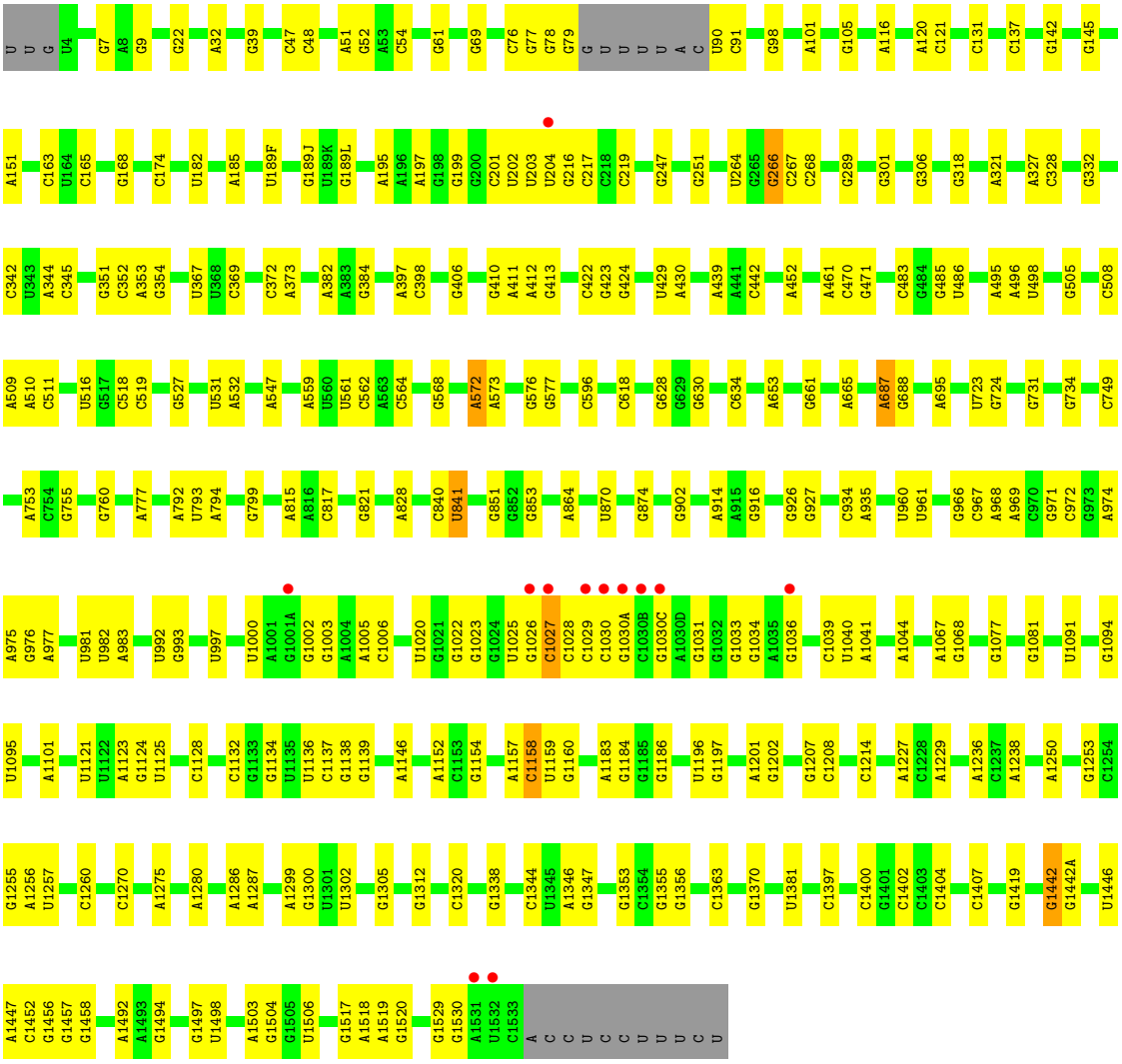
Chain 29:





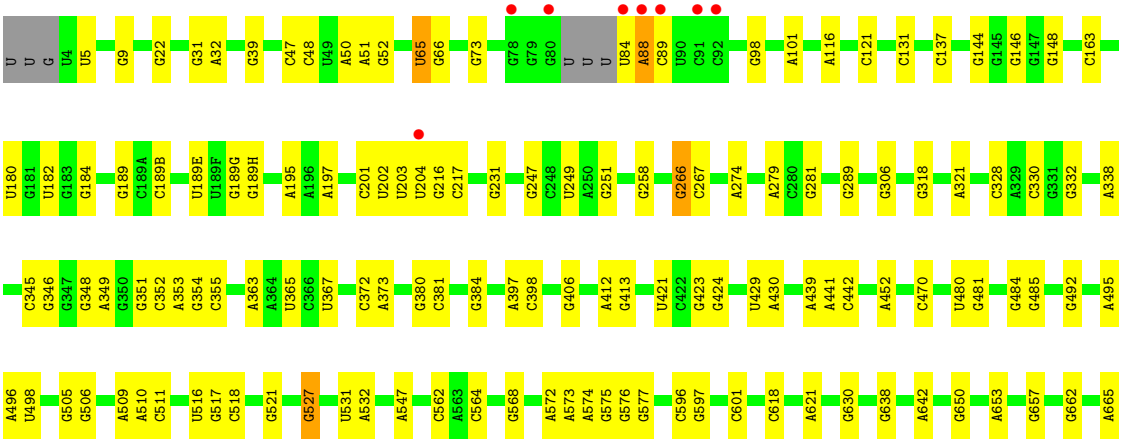
• Molecule 32: 16S Ribosomal RNA

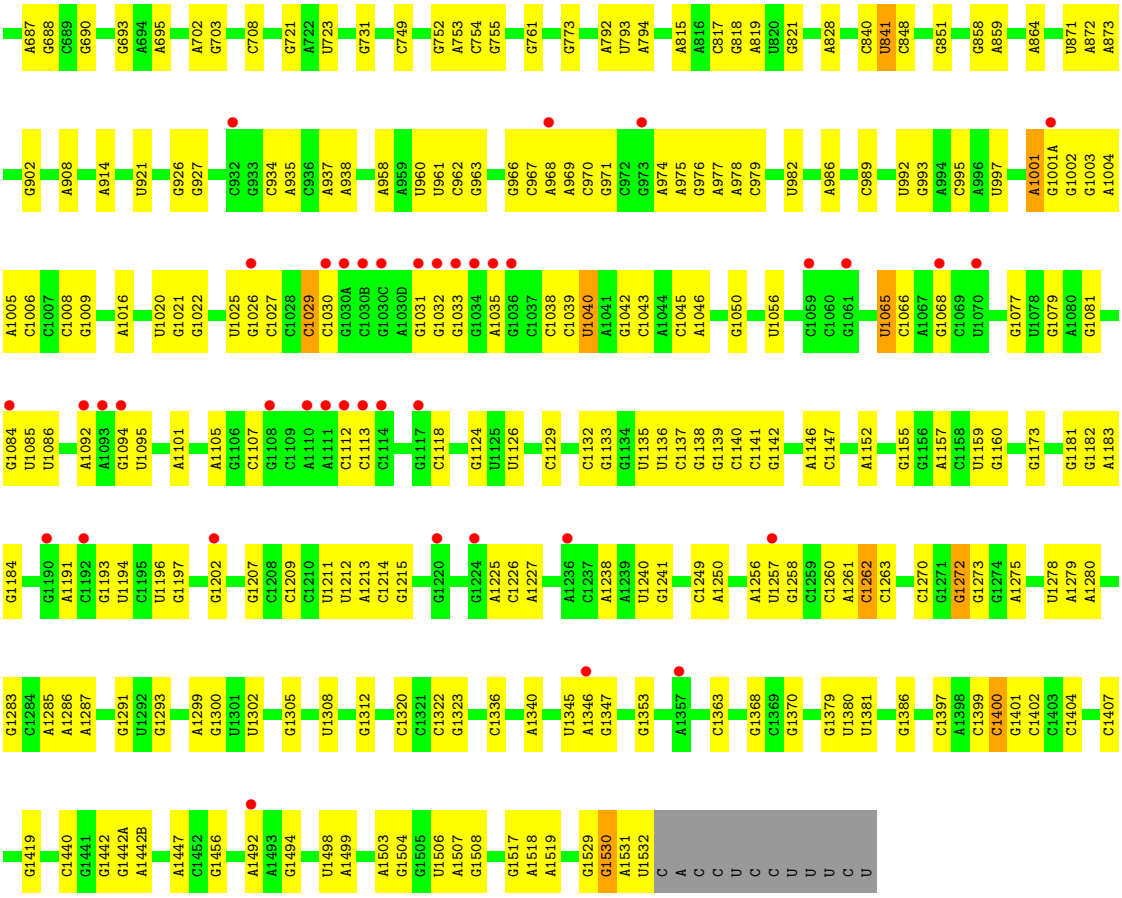
Chain 1a:



• Molecule 32: 16S Ribosomal RNA

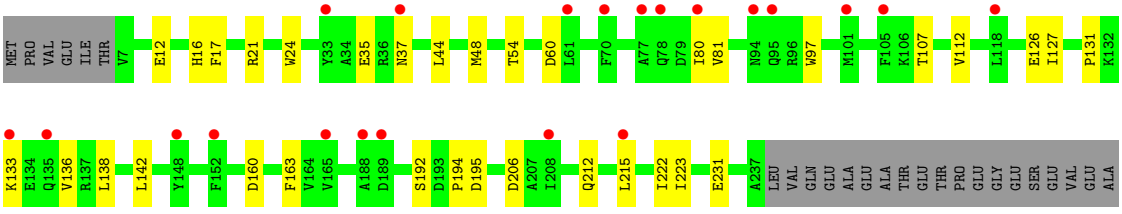
Chain 2a:





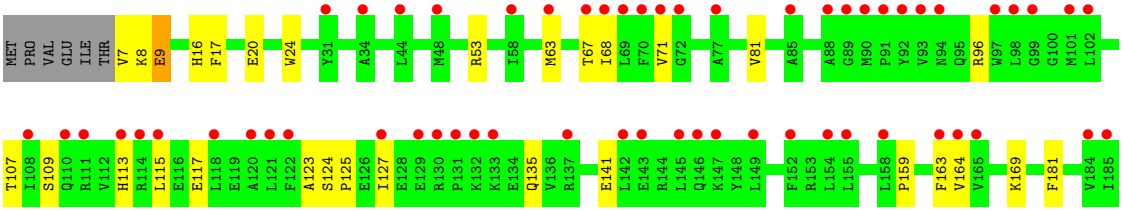
• Molecule 33: 30S ribosomal protein S2

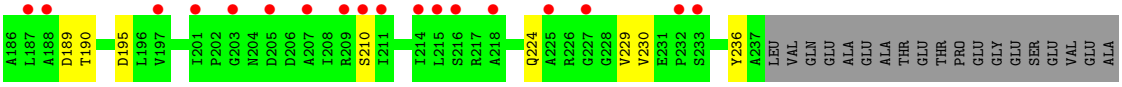
Chain 1b:



• Molecule 33: 30S ribosomal protein S2

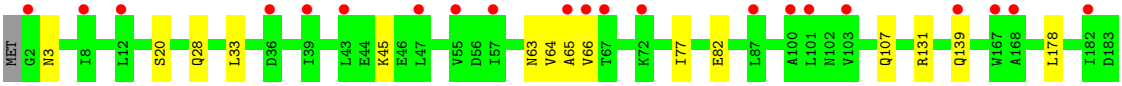
Chain 2b:

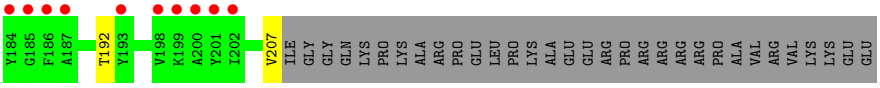




• Molecule 34: 30S ribosomal protein S3

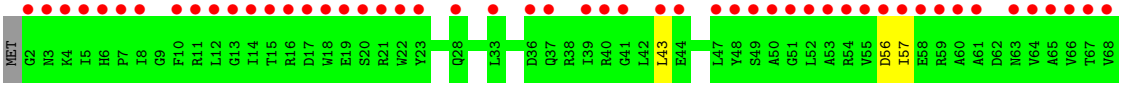
Chain 1c:

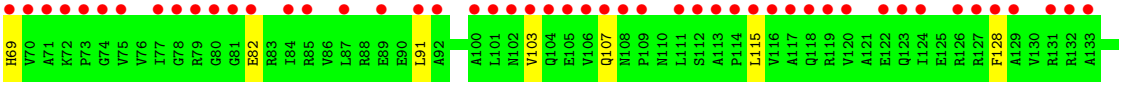


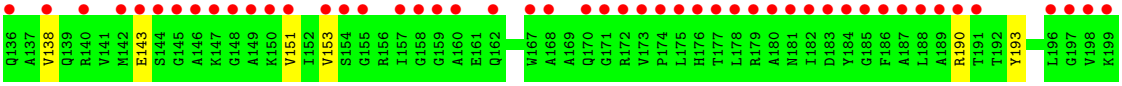


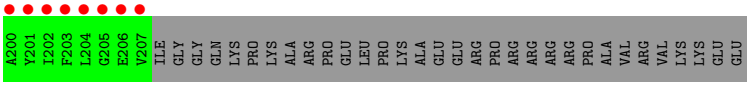
• Molecule 34: 30S ribosomal protein S3

Chain 2c:



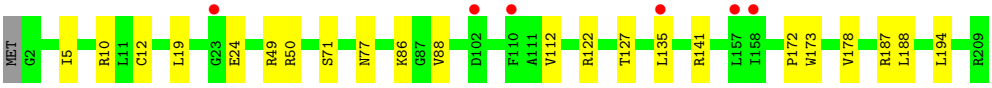






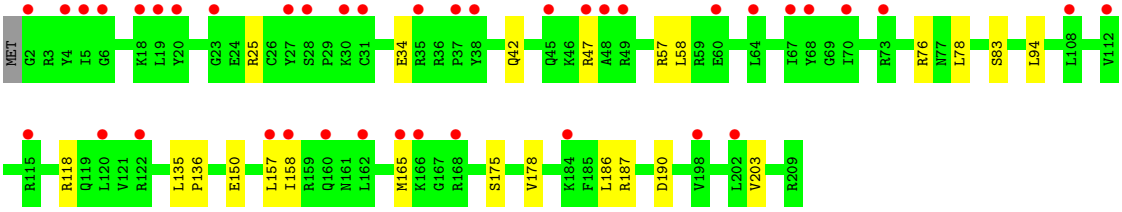
• Molecule 35: 30S ribosomal protein S4

Chain 1d:



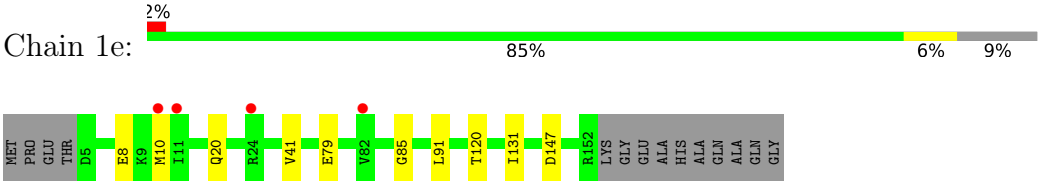
• Molecule 35: 30S ribosomal protein S4

Chain 2d:



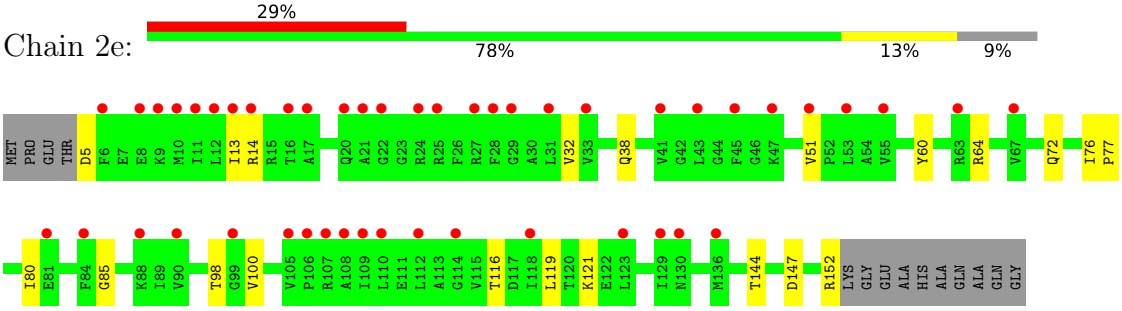
• Molecule 36: 30S ribosomal protein S5

Chain 1e:



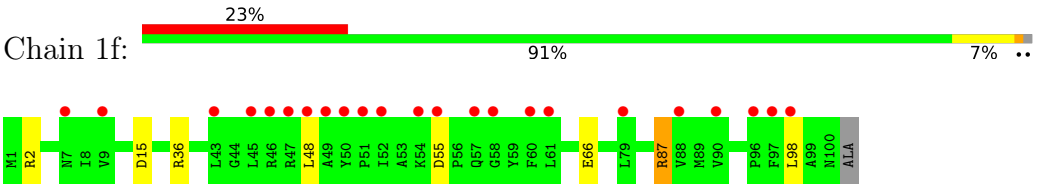
• Molecule 36: 30S ribosomal protein S5

Chain 2e:



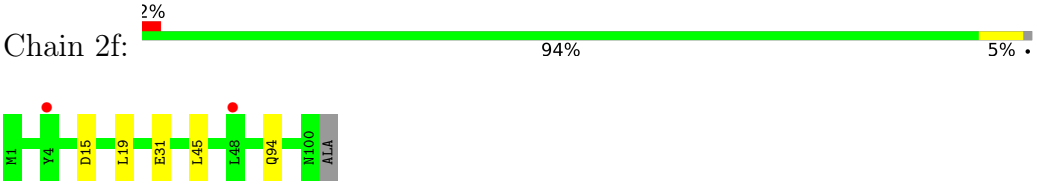
• Molecule 37: 30S ribosomal protein S6

Chain 1f:



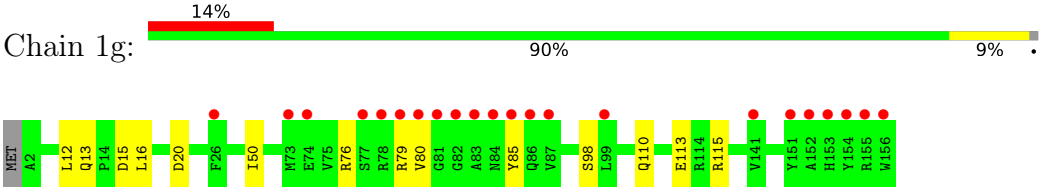
• Molecule 37: 30S ribosomal protein S6

Chain 2f:



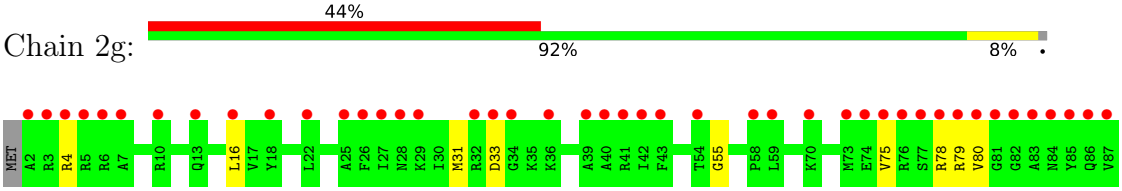
• Molecule 38: 30S ribosomal protein S7

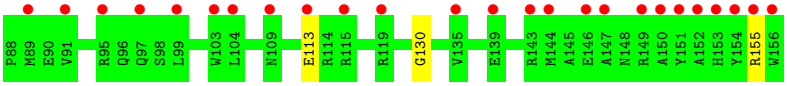
Chain 1g:



• Molecule 38: 30S ribosomal protein S7

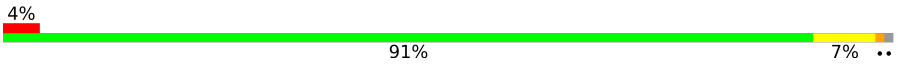
Chain 2g:

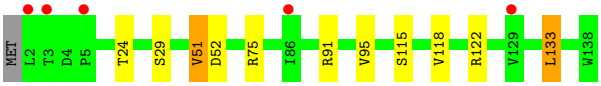




• Molecule 39: 30S ribosomal protein S8

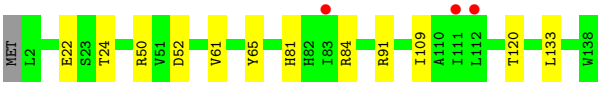
Chain 1h:





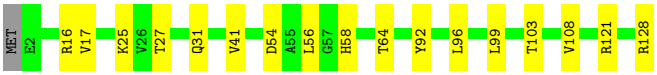
• Molecule 39: 30S ribosomal protein S8

Chain 2h:



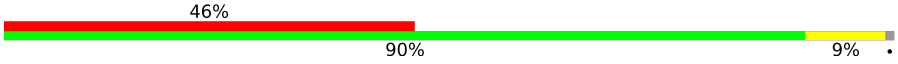
• Molecule 40: 30S ribosomal protein S9

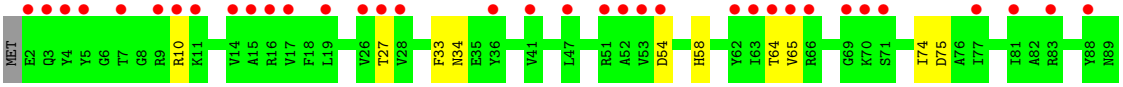
Chain 1i:

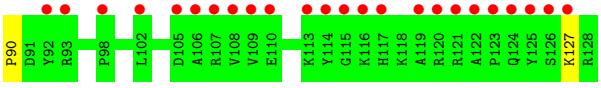


• Molecule 40: 30S ribosomal protein S9

Chain 2i:

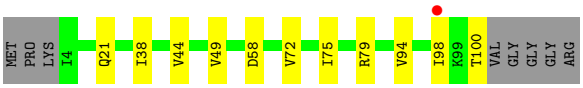






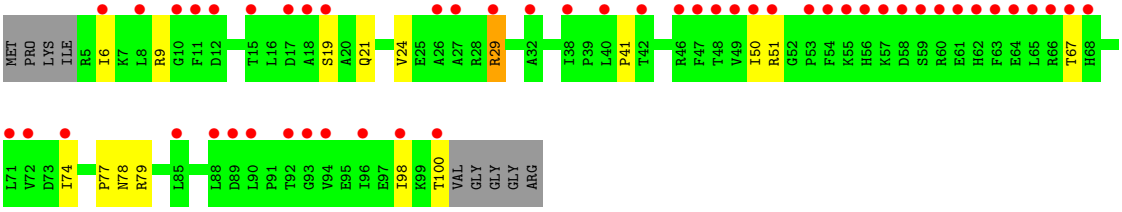
• Molecule 41: 30S ribosomal protein S10

Chain 1j:



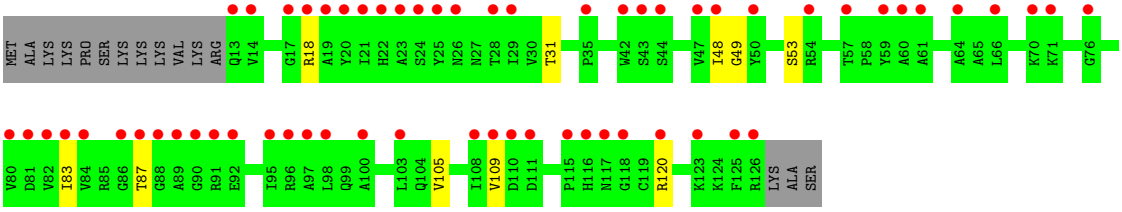
• Molecule 41: 30S ribosomal protein S10

Chain 2j:



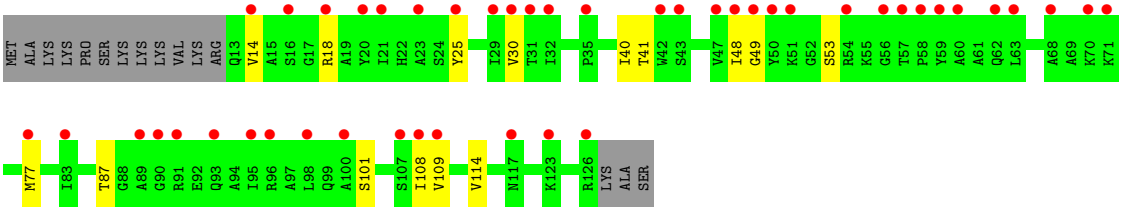
• Molecule 42: 30S ribosomal protein S11

Chain 1k:



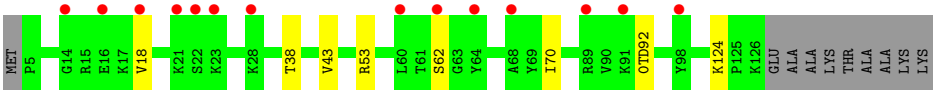
• Molecule 42: 30S ribosomal protein S11

Chain 2k:



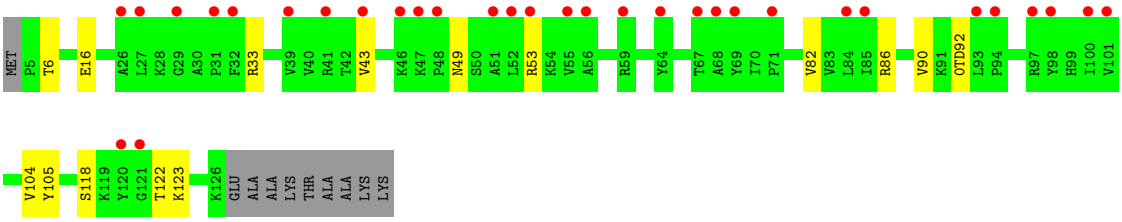
• Molecule 43: 30S ribosomal protein S12

Chain 1l:



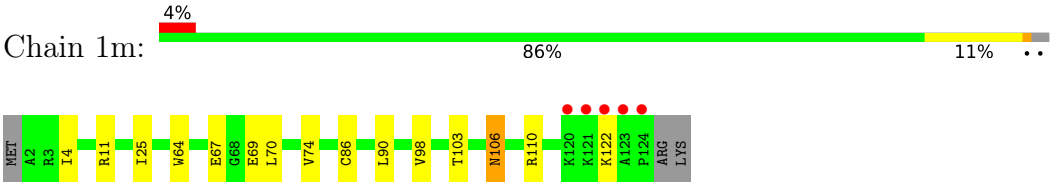
• Molecule 43: 30S ribosomal protein S12

Chain 2l:



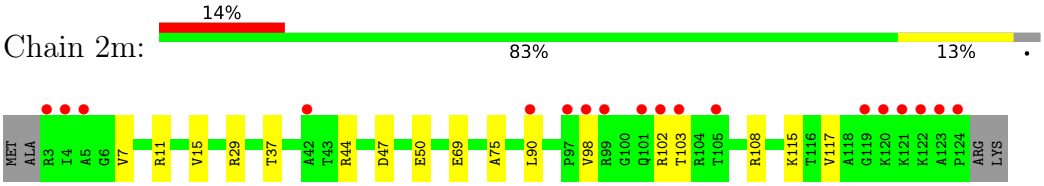
• Molecule 44: 30S ribosomal protein S13

Chain 1m:



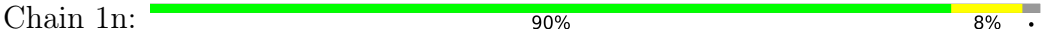
• Molecule 44: 30S ribosomal protein S13

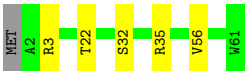
Chain 2m:



• Molecule 45: 30S ribosomal protein S14 type Z

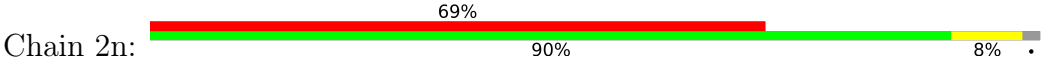
Chain 1n:

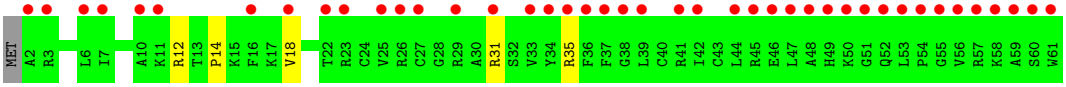




• Molecule 45: 30S ribosomal protein S14 type Z

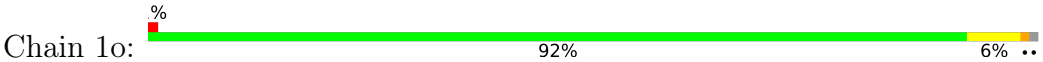
Chain 2n:

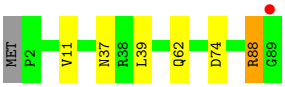




• Molecule 46: 30S ribosomal protein S15

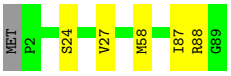
Chain 1o:





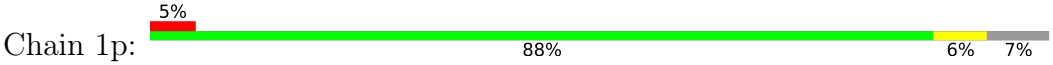
• Molecule 46: 30S ribosomal protein S15

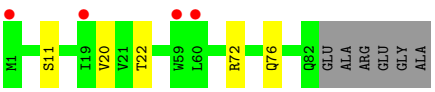
Chain 2o:



• Molecule 47: 30S ribosomal protein S16

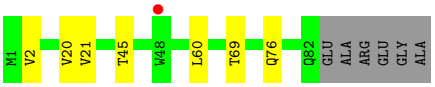
Chain 1p:





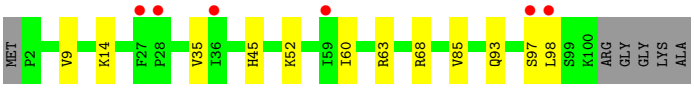
• Molecule 47: 30S ribosomal protein S16

Chain 2p:



• Molecule 48: 30S ribosomal protein S17

Chain 1q:

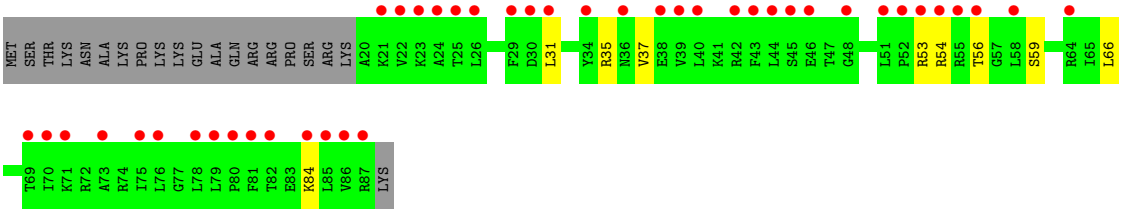


• Molecule 48: 30S ribosomal protein S17

Chain 2q:

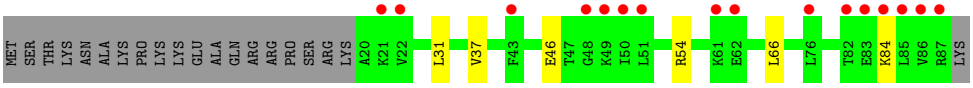
• Molecule 49: 30S ribosomal protein S18

Chain 1r:



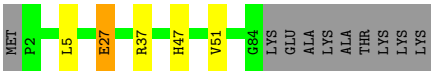
• Molecule 49: 30S ribosomal protein S18

Chain 2r:



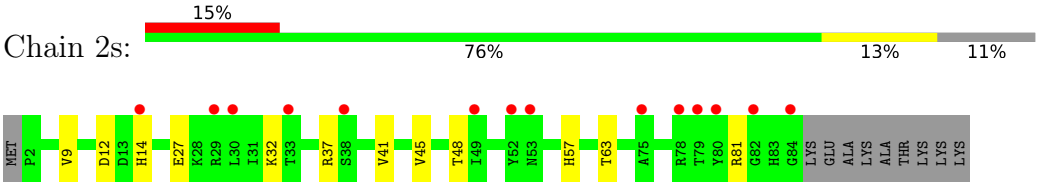
• Molecule 50: 30S ribosomal protein S19

Chain 1s:



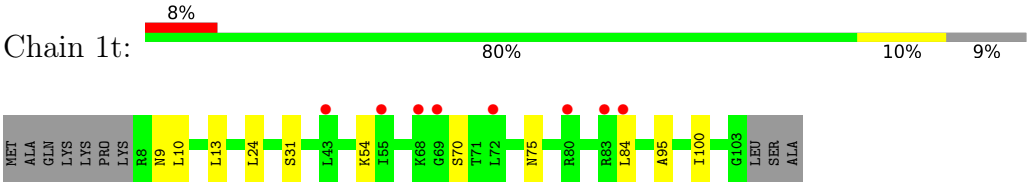
• Molecule 50: 30S ribosomal protein S19

Chain 2s:



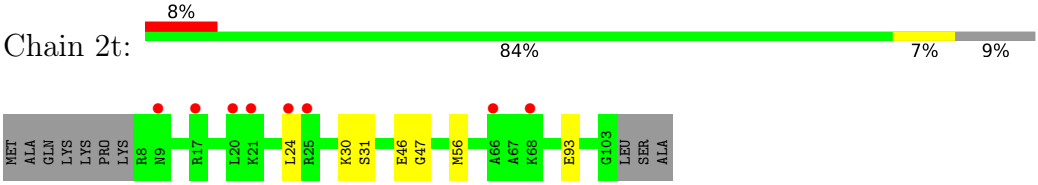
• Molecule 51: 30S ribosomal protein S20

Chain 1t:



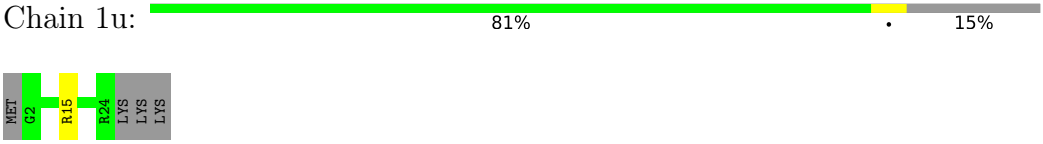
• Molecule 51: 30S ribosomal protein S20

Chain 2t:



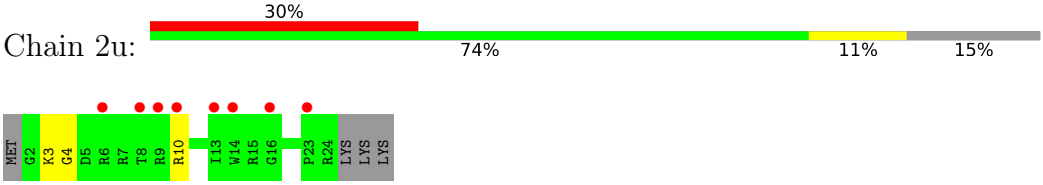
• Molecule 52: 30S ribosomal protein Thx

Chain 1u:



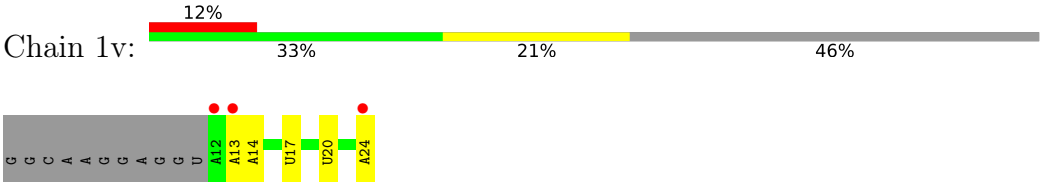
• Molecule 52: 30S ribosomal protein Thx

Chain 2u:



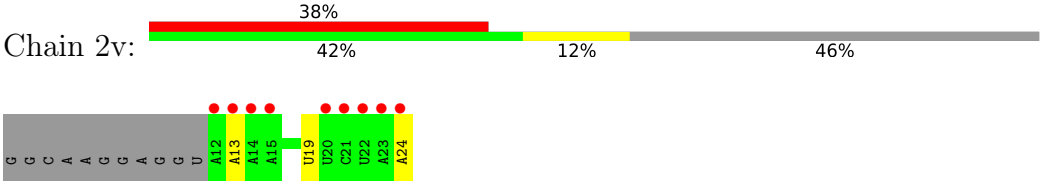
• Molecule 53: MF-mRNA

Chain 1v:



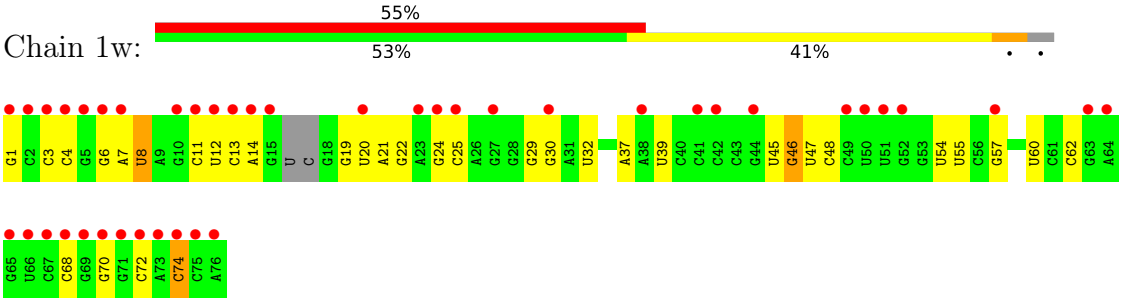
• Molecule 53: MF-mRNA

Chain 2v:



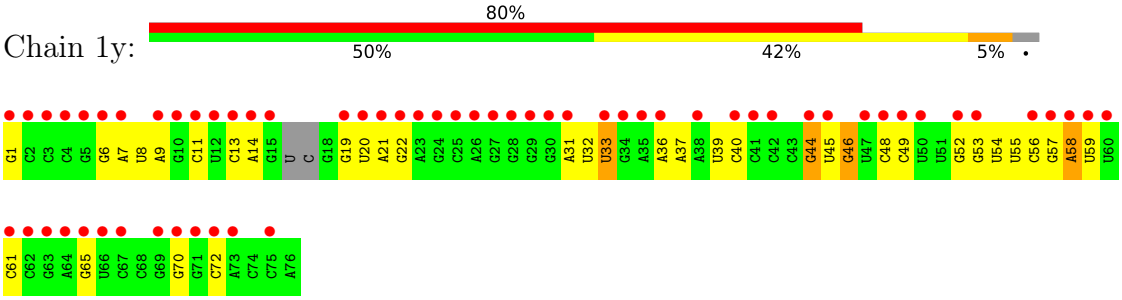
• Molecule 54: A-site and E-site Deacylated tRNAphe

Chain 1w:



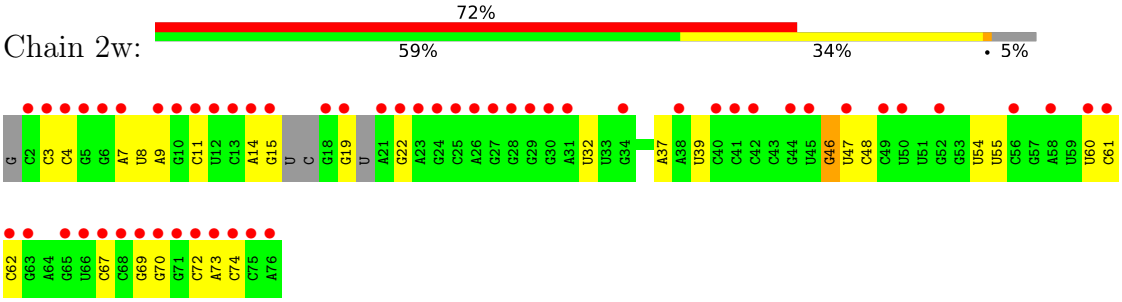
• Molecule 54: A-site and E-site Deacylated tRNAphe

Chain 1y:



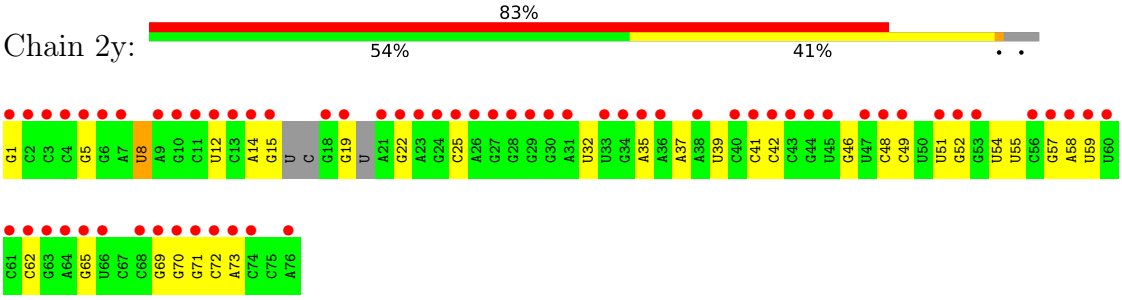
• Molecule 54: A-site and E-site Deacylated tRNAphe

Chain 2w:



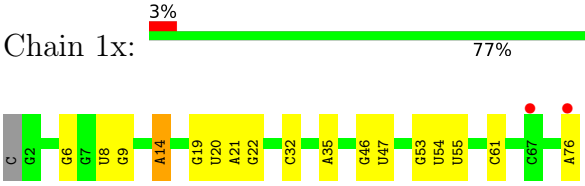
• Molecule 54: A-site and E-site Deacylated tRNAphe

Chain 2y:



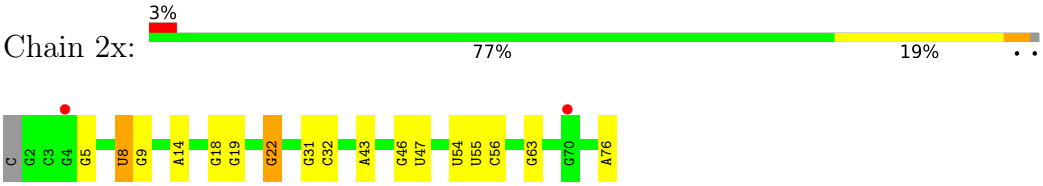
• Molecule 55: P-site Deacylated tRNAmet

Chain 1x:



• Molecule 55: P-site Deacylated tRNAmet

Chain 2x:


3%
77%
19%
C
G2
C3
G4
G5
U8
G9
A14
G18
G19
G22
G31
C32
A43
G46
U47
U54
U55
C56
G63
G70
A76

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	208.47Å 447.66Å 619.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	124.26 – 2.80 180.75 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.6 (124.26-2.80) 98.6 (180.75-2.80)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.23 (at 2.82Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.229 , 0.284 0.229 , 0.284	Depositor DCC
R_{free} test set	69396 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	60.3	Xtriage
Anisotropy	0.287	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 60.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.38$, $< L^2 > = 0.20$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	299897	wwPDB-VP
Average B, all atoms (Å^2)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.57% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, OMC, ZN, 2MA, G7M, UR3, MA6, OMU, 0TD, 4OC, 2MG, SF4, MG, M2G, A1AIX, OMG, MIA, 4SU, K, 5MC, PSU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	1A	0.55	0/69011	0.99	49/107720 (0.0%)
1	2A	0.40	0/67295	0.89	20/105042 (0.0%)
2	1B	0.49	1/2882 (0.0%)	0.95	0/4494
2	2B	0.41	1/2879 (0.0%)	0.88	1/4487 (0.0%)
3	1D	0.37	0/2186	0.57	0/2944
3	2D	0.32	0/2186	0.53	0/2944
4	1E	0.36	0/1592	0.56	0/2149
4	2E	0.31	0/1592	0.54	0/2149
5	1F	0.35	0/1622	0.52	0/2196
5	2F	0.31	0/1618	0.49	0/2191
6	1G	0.32	0/1448	0.53	0/1957
6	2G	0.29	0/1453	0.50	0/1963
7	1H	0.31	0/1356	0.51	0/1834
7	2H	0.30	0/1356	0.50	0/1834
8	1I	0.29	0/1112	0.49	0/1514
8	2I	0.29	0/1079	0.50	0/1475
9	1N	0.33	0/1144	0.50	0/1543
9	2N	0.29	0/1144	0.47	0/1543
10	1O	0.37	0/943	0.56	0/1269
10	2O	0.33	0/943	0.52	0/1269
11	1P	0.36	0/1152	0.59	0/1533
11	2P	0.30	0/1152	0.52	0/1533
12	1Q	0.38	0/1143	0.55	0/1527
12	2Q	0.31	0/1143	0.48	0/1527
13	1R	0.35	0/982	0.57	0/1312
13	2R	0.30	0/982	0.51	0/1312
14	1S	0.34	0/883	0.51	0/1176
14	2S	0.30	0/880	0.50	0/1172
15	1T	0.32	0/1105	0.50	0/1477
15	2T	0.30	0/1097	0.49	0/1468
16	1U	0.38	0/977	0.51	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
16	2U	0.29	0/977	0.43	0/1301
17	1V	0.37	0/782	0.55	0/1049
17	2V	0.31	0/782	0.52	0/1049
18	1W	0.36	0/897	0.54	0/1205
18	2W	0.32	0/897	0.49	0/1205
19	1X	0.37	0/764	0.56	0/1025
19	2X	0.31	0/764	0.52	0/1025
20	1Y	0.34	0/819	0.52	0/1095
20	2Y	0.34	0/819	0.51	0/1095
21	1Z	0.32	0/1267	0.51	0/1717
21	2Z	0.31	0/1299	0.50	0/1763
22	10	0.35	0/662	0.55	0/881
22	20	0.31	0/662	0.48	0/881
23	11	0.38	0/762	0.55	0/1014
23	21	0.31	0/762	0.50	0/1014
24	12	0.29	0/590	0.48	0/781
24	22	0.28	0/590	0.43	0/781
25	13	0.33	0/474	0.51	0/635
25	23	0.30	0/469	0.45	0/630
26	14	0.32	0/565	0.51	0/761
26	24	0.31	0/545	0.49	0/737
27	15	0.34	0/469	0.56	0/635
27	25	0.33	0/469	0.52	0/635
28	16	0.34	0/460	0.52	0/613
28	26	0.28	0/456	0.48	0/608
29	17	0.39	0/426	0.58	0/561
29	27	0.30	0/426	0.51	0/561
30	18	0.36	0/525	0.55	0/691
30	28	0.29	0/525	0.51	0/691
31	19	0.32	0/310	0.53	0/407
31	29	0.29	0/310	0.48	0/407
32	1a	0.37	0/35795	0.89	21/55864 (0.0%)
32	2a	0.37	4/35886 (0.0%)	0.91	43/56005 (0.1%)
33	1b	0.31	0/1881	0.51	0/2542
33	2b	0.32	0/1860	0.50	0/2518
34	1c	0.31	0/1572	0.52	0/2126
34	2c	0.30	0/1566	0.51	0/2119
35	1d	0.30	0/1685	0.47	0/2262
35	2d	0.29	0/1704	0.47	0/2284
36	1e	0.31	0/1145	0.52	0/1543
36	2e	0.29	0/1149	0.48	0/1548
37	1f	0.30	0/823	0.49	0/1115
37	2f	0.31	0/829	0.49	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
38	1g	0.29	0/1250	0.46	0/1679
38	2g	0.29	0/1254	0.47	0/1683
39	1h	0.29	0/1108	0.48	0/1494
39	2h	0.29	0/1108	0.48	0/1494
40	1i	0.31	0/1002	0.50	0/1346
40	2i	0.31	0/997	0.52	0/1343
41	1j	0.30	0/722	0.49	0/982
41	2j	0.30	0/727	0.51	0/988
42	1k	0.28	0/844	0.47	0/1145
42	2k	0.29	0/848	0.48	0/1149
43	1l	0.31	0/937	0.52	0/1260
43	2l	0.28	0/937	0.48	0/1260
44	1m	0.30	0/969	0.49	0/1302
44	2m	0.30	0/961	0.50	0/1291
45	1n	0.30	0/501	0.47	0/664
45	2n	0.29	0/501	0.49	0/664
46	1o	0.28	0/739	0.45	0/985
46	2o	0.27	0/739	0.43	0/985
47	1p	0.28	0/697	0.47	0/939
47	2p	0.27	0/693	0.48	0/935
48	1q	0.29	0/836	0.49	0/1117
48	2q	0.30	0/836	0.47	0/1117
49	1r	0.31	0/560	0.53	0/746
49	2r	0.29	0/560	0.46	0/746
50	1s	0.27	0/667	0.48	0/900
50	2s	0.31	0/661	0.57	0/893
51	1t	0.28	0/730	0.44	0/965
51	2t	0.27	0/729	0.41	0/965
52	1u	0.29	0/203	0.45	0/266
52	2u	0.27	0/203	0.51	0/266
53	1v	0.45	0/310	0.93	2/480 (0.4%)
53	2v	0.42	0/310	0.91	0/480
54	1w	0.52	1/1606 (0.1%)	1.11	2/2497 (0.1%)
54	1y	0.54	1/1606 (0.1%)	1.12	8/2497 (0.3%)
54	2w	0.46	0/1556	1.00	0/2418
54	2y	0.54	1/1583 (0.1%)	1.05	4/2459 (0.2%)
55	1x	0.54	1/1725 (0.1%)	1.17	18/2689 (0.7%)
55	2x	0.48	1/1725 (0.1%)	1.07	13/2689 (0.5%)
All	All	0.42	11/316696 (0.0%)	0.84	181/474135 (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
29	27	0	1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	2y	1	G	OP3-P	-10.49	1.48	1.61
54	1y	1	G	OP3-P	-10.14	1.49	1.61
2	2B	1	U	OP3-P	-10.14	1.49	1.61
2	1B	1	U	OP3-P	-10.12	1.49	1.61
54	1w	1	G	OP3-P	-10.11	1.49	1.61
32	2a	1272	G	N1-C2	-9.05	1.30	1.37
32	2a	1272	G	C6-N1	-8.25	1.33	1.39
32	2a	1263	C	N3-C4	-6.42	1.29	1.33
55	1x	22	G	N7-C5	5.51	1.42	1.39
32	2a	1272	G	C5-C4	5.22	1.42	1.38
55	2x	14	A	N7-C5	-5.05	1.36	1.39

All (181) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	2a	1263	C	N1-C2-O2	24.34	133.50	118.90
32	2a	1272	G	N3-C2-N2	21.63	135.04	119.90
32	2a	1272	G	C5-C6-O6	20.82	141.09	128.60
32	2a	1272	G	N1-C2-N2	-18.27	99.76	116.20
32	2a	1263	C	N3-C2-O2	-13.86	112.20	121.90
32	2a	1272	G	C6-N1-C2	13.18	133.01	125.10
32	2a	1263	C	C2-N3-C4	12.46	126.13	119.90
32	2a	1272	G	N1-C6-O6	-11.51	113.00	119.90
32	2a	1272	G	C5-C6-N1	-11.30	105.85	111.50
2	2B	80	U	O4'-C1'-N1	10.72	116.78	108.20
1	1A	1782	C	O5'-P-OP1	-10.23	96.50	105.70
55	1x	46	G	C6-N1-C2	-10.08	119.05	125.10
32	2a	1263	C	C5-C6-N1	9.93	125.97	121.00
55	2x	14	A	C4-C5-C6	9.39	121.70	117.00
32	2a	1263	C	C2-N1-C1'	9.29	129.01	118.80
32	2a	1029	C	N1-C2-O2	9.05	124.33	118.90
55	1x	22	G	N1-C6-O6	-8.99	114.51	119.90
55	2x	46	G	C6-N1-C2	-8.54	119.98	125.10
32	2a	841	U	C2-N1-C1'	8.42	127.80	117.70
1	1A	512	G	O4'-C1'-N9	8.29	114.83	108.20
32	2a	1263	C	C4-C5-C6	-8.23	113.29	117.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	2a	1263	C	N3-C4-N4	-8.19	112.27	118.00
32	1a	1034	G	C6-N1-C2	8.12	129.97	125.10
55	1x	14	A	C4-C5-C6	8.12	121.06	117.00
32	2a	841	U	C5-C6-N1	7.80	126.60	122.70
32	2a	1272	G	C4-N9-C1'	7.62	136.40	126.50
32	2a	1272	G	C2-N3-C4	-7.59	108.11	111.90
32	1a	90	U	N3-C2-O2	-7.51	116.94	122.20
1	1A	975	C	N1-C2-O2	-7.45	114.43	118.90
55	1x	22	G	C5-N7-C8	-7.35	100.63	104.30
1	1A	1075	C	N1-C2-O2	7.33	123.30	118.90
32	1a	90	U	C2-N1-C1'	7.33	126.49	117.70
55	1x	14	A	C5-N7-C8	7.33	107.56	103.90
32	1a	1034	G	C5-C6-O6	7.32	132.99	128.60
32	2a	1263	C	C5-C4-N4	7.25	125.28	120.20
32	2a	1272	G	C8-N9-C1'	-7.16	117.69	127.00
32	2a	1263	C	N1-C2-N3	-7.03	114.28	119.20
55	1x	22	G	C4-C5-C6	-6.92	114.65	118.80
1	1A	975	C	C2-N1-C1'	-6.90	111.21	118.80
32	2a	1029	C	C2-N1-C1'	6.83	126.31	118.80
54	1y	44	G	C5-C6-O6	-6.77	124.54	128.60
55	1x	22	G	N3-C4-N9	-6.74	121.96	126.00
32	2a	1263	C	C6-N1-C2	-6.66	117.64	120.30
54	2y	22	G	N3-C4-N9	6.62	129.97	126.00
1	2A	2178	C	N1-C2-O2	6.62	122.87	118.90
32	1a	90	U	N1-C2-O2	6.61	127.43	122.80
32	2a	1262	C	N1-C2-O2	6.51	122.81	118.90
1	2A	801	G	O5'-P-OP2	-6.50	99.85	105.70
55	2x	14	A	N1-C6-N6	6.46	122.48	118.60
55	2x	22	G	C5-N7-C8	-6.46	101.07	104.30
1	1A	51	G	O5'-P-OP2	-6.45	99.90	105.70
55	1x	14	A	C5-C6-N1	-6.43	114.49	117.70
55	2x	14	A	C5-N7-C8	6.42	107.11	103.90
1	2A	2318	G	C4-N9-C1'	6.37	134.78	126.50
32	2a	754	C	N1-C2-O2	6.37	122.72	118.90
32	2a	1263	C	C6-N1-C1'	-6.36	113.17	120.80
32	2a	754	C	C2-N1-C1'	6.33	125.76	118.80
1	1A	1086	A	N1-C6-N6	-6.25	114.85	118.60
55	1x	22	G	C8-N9-C1'	6.24	135.11	127.00
1	2A	2155	G	C6-N1-C2	6.22	128.83	125.10
1	1A	801	G	O5'-P-OP2	-6.19	100.13	105.70
1	1A	1131	G	O4'-C1'-N9	6.13	113.11	108.20
1	1A	226	G	O4'-C1'-N9	6.13	113.11	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1A	847	U	C2-N1-C1'	6.13	125.06	117.70
1	1A	372	G	O4'-C1'-N9	6.08	113.06	108.20
1	1A	1979	C	C6-N1-C2	-6.06	117.88	120.30
32	1a	841	U	C5-C6-N1	6.05	125.72	122.70
32	1a	1158	C	C2-N1-C1'	6.04	125.44	118.80
55	1x	46	G	N3-C2-N2	-5.92	115.76	119.90
55	2x	22	G	C4-C5-C6	-5.88	115.27	118.80
1	1A	845	G	O4'-C1'-N9	5.86	112.89	108.20
32	2a	1029	C	C6-N1-C1'	-5.85	113.78	120.80
1	2A	1992	G	P-O3'-C3'	5.84	126.71	119.70
32	2a	1029	C	N3-C2-O2	-5.84	117.81	121.90
1	1A	383	U	C2-N1-C1'	-5.80	110.74	117.70
1	2A	2689	U	P-O3'-C3'	5.79	126.65	119.70
1	1A	793	A	O5'-P-OP2	-5.79	100.49	105.70
1	2A	2318	G	N3-C4-C5	-5.79	125.71	128.60
1	1A	2427	C	O5'-P-OP1	-5.78	100.50	105.70
55	1x	46	G	N1-C2-N3	5.77	127.36	123.90
54	2y	22	G	C6-C5-N7	-5.77	126.94	130.40
55	2x	14	A	C5-C6-N1	-5.75	114.83	117.70
1	1A	2848	G	O4'-C1'-N9	5.74	112.80	108.20
1	2A	2155	G	C5-C6-O6	5.73	132.04	128.60
54	1y	56	C	N1-C2-O2	5.66	122.30	118.90
55	1x	46	G	N9-C4-C5	5.66	107.66	105.40
32	1a	1067	A	P-O3'-C3'	5.65	126.48	119.70
54	1w	74	C	C2-N1-C1'	5.64	125.01	118.80
32	2a	1065	U	P-O3'-C3'	5.64	126.47	119.70
54	2y	22	G	N1-C6-O6	5.62	123.27	119.90
55	2x	14	A	C8-N9-C1'	-5.61	117.60	127.70
32	1a	1442	G	C2-N3-C4	5.59	114.69	111.90
1	1A	1116	C	C2-N1-C1'	5.59	124.94	118.80
55	1x	22	G	N7-C8-N9	5.58	115.89	113.10
32	2a	1008	C	N1-C2-O2	5.56	122.24	118.90
55	1x	46	G	C5-C6-O6	-5.55	125.27	128.60
1	1A	975	C	N3-C2-O2	5.53	125.77	121.90
1	1A	948	G	O5'-P-OP1	-5.52	100.73	105.70
55	1x	22	G	C6-C5-N7	5.52	133.71	130.40
32	2a	1040	U	C5-C4-O4	5.52	129.21	125.90
1	2A	784	A	O4'-C1'-N9	5.51	112.61	108.20
1	1A	1313	U	C2-N1-C1'	5.50	124.30	117.70
1	1A	975	C	C6-N1-C1'	5.50	127.40	120.80
1	1A	383	U	O4'-C1'-N1	5.50	112.60	108.20
1	2A	567	A	O5'-P-OP1	-5.48	100.76	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1A	2155	G	C2-N3-C4	5.47	114.64	111.90
1	1A	1075	C	N3-C2-O2	-5.46	118.08	121.90
54	1y	58	A	OP1-P-O3'	5.45	117.18	105.20
55	2x	14	A	C4-N9-C1'	5.43	136.08	126.30
32	2a	1308	U	C5-C4-O4	5.41	129.15	125.90
1	2A	1913	A	P-O3'-C3'	5.40	126.18	119.70
55	1x	35	A	C5-C6-N6	5.40	128.02	123.70
1	1A	595	C	C6-N1-C2	-5.38	118.15	120.30
1	1A	1576	U	N3-C2-O2	-5.38	118.44	122.20
32	2a	841	U	N1-C2-O2	5.37	126.56	122.80
32	1a	687	A	P-O3'-C3'	5.36	126.14	119.70
54	1y	44	G	N1-C6-O6	5.36	123.12	119.90
1	1A	746	A	O4'-C1'-N9	5.34	112.47	108.20
1	2A	2318	G	N3-C4-N9	5.34	129.21	126.00
1	2A	277	C	OP2-P-O3'	5.33	116.93	105.20
1	1A	1576	U	N1-C2-O2	5.33	126.53	122.80
54	1y	33	U	C2-N1-C1'	5.33	124.10	117.70
53	1v	17	U	C5-C4-O4	5.32	129.09	125.90
54	1y	22	G	N1-C6-O6	5.32	123.09	119.90
1	1A	1174	A	OP1-P-O3'	5.31	116.89	105.20
1	1A	1824	G	O5'-P-OP2	-5.31	100.92	105.70
32	2a	841	U	C6-N1-C2	-5.30	117.82	121.00
32	1a	1002	G	C4-N9-C1'	5.30	133.39	126.50
1	2A	1653	G	P-O3'-C3'	5.27	126.03	119.70
55	1x	22	G	C5-C6-O6	5.27	131.76	128.60
32	1a	1029	C	C2-N3-C4	5.27	122.53	119.90
32	2a	1530	G	OP1-P-OP2	-5.26	111.71	119.60
1	1A	1992	G	P-O3'-C3'	5.25	126.00	119.70
54	1y	58	A	P-O3'-C3'	5.25	126.00	119.70
1	1A	1257	C	C6-N1-C2	-5.25	118.20	120.30
1	1A	2497	A	N1-C6-N6	-5.24	115.46	118.60
54	2y	22	G	C5-C6-O6	-5.24	125.46	128.60
32	1a	1158	C	N1-C2-O2	5.24	122.04	118.90
32	2a	266	G	N3-C4-C5	-5.23	125.99	128.60
1	1A	1063	G	C5-C6-O6	5.22	131.74	128.60
55	2x	22	G	N3-C4-N9	-5.22	122.86	126.00
1	1A	2005	A	OP1-P-O3'	5.22	116.69	105.20
32	1a	1027	C	C6-N1-C2	-5.22	118.21	120.30
32	1a	1229	A	C5-C6-N6	5.22	127.88	123.70
55	2x	46	G	C5-C6-N1	5.22	114.11	111.50
32	1a	1002	G	N3-C4-C5	-5.21	125.99	128.60
32	1a	266	G	P-O3'-C3'	5.21	125.95	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2A	228	A	P-O3'-C3'	5.21	125.95	119.70
1	1A	1116	C	C6-N1-C1'	-5.20	114.56	120.80
1	1A	1328	G	N3-C4-N9	5.20	129.12	126.00
1	1A	2790	A	C2-N3-C4	5.19	113.20	110.60
54	1w	4	C	C2-N3-C4	5.18	122.49	119.90
32	2a	1308	U	C2-N3-C4	5.18	130.11	127.00
32	2a	1043	C	N1-C2-O2	5.17	122.00	118.90
55	2x	46	G	N3-C2-N2	-5.15	116.29	119.90
1	1A	2159	G	N3-C4-N9	5.14	129.09	126.00
1	1A	2588	G	O5'-P-OP1	-5.14	101.07	105.70
1	2A	2155	G	N1-C2-N3	-5.14	120.82	123.90
1	1A	1313	U	N3-C2-O2	-5.14	118.60	122.20
32	1a	1442	G	N3-C4-C5	-5.13	126.03	128.60
1	2A	646	A	O4'-C1'-N9	5.13	112.30	108.20
1	2A	1313	U	C2-N1-C1'	5.13	123.85	117.70
32	1a	841	U	C6-N1-C2	-5.11	117.93	121.00
1	1A	859	G	N3-C4-C5	5.11	131.15	128.60
1	1A	396	G	N1-C6-O6	5.10	122.96	119.90
32	2a	65	U	P-O3'-C3'	5.10	125.82	119.70
32	2a	88	A	C5-C6-N1	5.10	120.25	117.70
32	2a	1001	A	N1-C6-N6	-5.10	115.54	118.60
32	2a	266	G	P-O3'-C3'	5.09	125.81	119.70
55	1x	46	G	C5-C6-N1	5.09	114.05	111.50
55	2x	14	A	C6-C5-N7	-5.08	128.74	132.30
1	2A	879	G	C4-N9-C1'	5.08	133.11	126.50
53	1v	17	U	C2-N3-C4	5.08	130.05	127.00
1	1A	1174	A	P-O3'-C3'	5.06	125.78	119.70
32	1a	572	A	N1-C6-N6	-5.06	115.57	118.60
1	1A	1187	G	N1-C6-O6	-5.03	116.88	119.90
1	1A	1969	A	OP1-P-O3'	5.03	116.26	105.20
32	1a	1002	G	N3-C4-N9	5.02	129.01	126.00
1	1A	2129	C	C2-N1-C1'	5.01	124.31	118.80
1	2A	383	U	O4'-C1'-N1	5.01	112.21	108.20
54	1y	33	U	N1-C2-O2	5.01	126.31	122.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
29	27	46	VAL	Peptide

5.2 Too-close contacts

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

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	1D	273/276 (99%)	249 (91%)	24 (9%)	0	100	100
3	2D	273/276 (99%)	247 (90%)	26 (10%)	0	100	100
4	1E	202/206 (98%)	184 (91%)	16 (8%)	2 (1%)	15	44
4	2E	202/206 (98%)	187 (93%)	12 (6%)	3 (2%)	10	33
5	1F	201/210 (96%)	196 (98%)	4 (2%)	1 (0%)	29	61
5	2F	201/210 (96%)	180 (90%)	20 (10%)	1 (0%)	29	61
6	1G	179/182 (98%)	164 (92%)	13 (7%)	2 (1%)	14	41
6	2G	179/182 (98%)	162 (90%)	14 (8%)	3 (2%)	9	29
7	1H	172/180 (96%)	158 (92%)	11 (6%)	3 (2%)	9	29
7	2H	172/180 (96%)	151 (88%)	19 (11%)	2 (1%)	13	39
8	1I	144/148 (97%)	121 (84%)	22 (15%)	1 (1%)	22	53
8	2I	144/148 (97%)	114 (79%)	27 (19%)	3 (2%)	7	23
9	1N	138/140 (99%)	129 (94%)	8 (6%)	1 (1%)	22	53
9	2N	138/140 (99%)	120 (87%)	15 (11%)	3 (2%)	6	22
10	1O	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
10	2O	120/122 (98%)	108 (90%)	11 (9%)	1 (1%)	19	49
11	1P	147/150 (98%)	126 (86%)	17 (12%)	4 (3%)	5	17
11	2P	147/150 (98%)	133 (90%)	10 (7%)	4 (3%)	5	17
12	1Q	139/141 (99%)	127 (91%)	11 (8%)	1 (1%)	22	53
12	2Q	139/141 (99%)	125 (90%)	14 (10%)	0	100	100
13	1R	116/118 (98%)	111 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
13	2R	116/118 (98%)	104 (90%)	12 (10%)	0	100 100
14	1S	108/112 (96%)	96 (89%)	12 (11%)	0	100 100
14	2S	108/112 (96%)	95 (88%)	10 (9%)	3 (3%)	5 17
15	1T	129/146 (88%)	120 (93%)	9 (7%)	0	100 100
15	2T	129/146 (88%)	118 (92%)	10 (8%)	1 (1%)	19 49
16	1U	114/118 (97%)	110 (96%)	4 (4%)	0	100 100
16	2U	114/118 (97%)	111 (97%)	3 (3%)	0	100 100
17	1V	99/101 (98%)	91 (92%)	7 (7%)	1 (1%)	15 44
17	2V	99/101 (98%)	90 (91%)	6 (6%)	3 (3%)	4 15
18	1W	110/113 (97%)	106 (96%)	4 (4%)	0	100 100
18	2W	110/113 (97%)	105 (96%)	5 (4%)	0	100 100
19	1X	93/96 (97%)	87 (94%)	5 (5%)	1 (1%)	14 41
19	2X	93/96 (97%)	83 (89%)	10 (11%)	0	100 100
20	1Y	105/110 (96%)	96 (91%)	7 (7%)	2 (2%)	8 26
20	2Y	105/110 (96%)	98 (93%)	6 (6%)	1 (1%)	15 44
21	1Z	148/206 (72%)	126 (85%)	20 (14%)	2 (1%)	11 34
21	2Z	156/206 (76%)	116 (74%)	37 (24%)	3 (2%)	8 26
22	10	81/85 (95%)	78 (96%)	3 (4%)	0	100 100
22	20	81/85 (95%)	74 (91%)	6 (7%)	1 (1%)	13 39
23	11	95/98 (97%)	91 (96%)	3 (3%)	1 (1%)	14 41
23	21	95/98 (97%)	91 (96%)	3 (3%)	1 (1%)	14 41
24	12	68/72 (94%)	65 (96%)	3 (4%)	0	100 100
24	22	68/72 (94%)	66 (97%)	2 (3%)	0	100 100
25	13	57/60 (95%)	54 (95%)	3 (5%)	0	100 100
25	23	57/60 (95%)	53 (93%)	3 (5%)	1 (2%)	8 28
26	14	67/71 (94%)	50 (75%)	12 (18%)	5 (8%)	1 2
26	24	67/71 (94%)	51 (76%)	12 (18%)	4 (6%)	1 4
27	15	57/60 (95%)	52 (91%)	5 (9%)	0	100 100
27	25	57/60 (95%)	52 (91%)	5 (9%)	0	100 100
28	16	51/54 (94%)	49 (96%)	2 (4%)	0	100 100
28	26	51/54 (94%)	44 (86%)	7 (14%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	17	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
29	27	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
30	18	62/65 (95%)	57 (92%)	5 (8%)	0	100	100
30	28	62/65 (95%)	57 (92%)	5 (8%)	0	100	100
31	19	35/37 (95%)	35 (100%)	0	0	100	100
31	29	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
33	1b	229/256 (90%)	181 (79%)	41 (18%)	7 (3%)	4	14
33	2b	229/256 (90%)	176 (77%)	47 (20%)	6 (3%)	5	18
34	1c	204/239 (85%)	178 (87%)	23 (11%)	3 (2%)	10	33
34	2c	204/239 (85%)	161 (79%)	41 (20%)	2 (1%)	15	44
35	1d	206/209 (99%)	187 (91%)	15 (7%)	4 (2%)	8	26
35	2d	206/209 (99%)	186 (90%)	19 (9%)	1 (0%)	29	61
36	1e	146/162 (90%)	126 (86%)	19 (13%)	1 (1%)	22	53
36	2e	146/162 (90%)	124 (85%)	20 (14%)	2 (1%)	11	34
37	1f	98/101 (97%)	89 (91%)	8 (8%)	1 (1%)	15	44
37	2f	98/101 (97%)	92 (94%)	6 (6%)	0	100	100
38	1g	153/156 (98%)	132 (86%)	20 (13%)	1 (1%)	22	53
38	2g	153/156 (98%)	132 (86%)	17 (11%)	4 (3%)	5	18
39	1h	135/138 (98%)	117 (87%)	15 (11%)	3 (2%)	6	22
39	2h	135/138 (98%)	119 (88%)	16 (12%)	0	100	100
40	1i	125/128 (98%)	108 (86%)	15 (12%)	2 (2%)	9	31
40	2i	125/128 (98%)	98 (78%)	24 (19%)	3 (2%)	6	20
41	1j	95/105 (90%)	79 (83%)	13 (14%)	3 (3%)	4	13
41	2j	94/105 (90%)	74 (79%)	13 (14%)	7 (7%)	1	2
42	1k	112/129 (87%)	101 (90%)	9 (8%)	2 (2%)	8	28
42	2k	112/129 (87%)	97 (87%)	14 (12%)	1 (1%)	17	46
43	1l	119/132 (90%)	108 (91%)	11 (9%)	0	100	100
43	2l	119/132 (90%)	105 (88%)	13 (11%)	1 (1%)	19	49
44	1m	121/126 (96%)	102 (84%)	17 (14%)	2 (2%)	9	29
44	2m	120/126 (95%)	99 (82%)	17 (14%)	4 (3%)	4	13
45	1n	58/61 (95%)	51 (88%)	7 (12%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
45	2n	58/61 (95%)	50 (86%)	6 (10%)	2 (3%)	3 13
46	1o	86/89 (97%)	79 (92%)	6 (7%)	1 (1%)	13 39
46	2o	86/89 (97%)	78 (91%)	7 (8%)	1 (1%)	13 39
47	1p	80/88 (91%)	67 (84%)	13 (16%)	0	100 100
47	2p	80/88 (91%)	73 (91%)	7 (9%)	0	100 100
48	1q	97/105 (92%)	84 (87%)	12 (12%)	1 (1%)	15 44
48	2q	97/105 (92%)	87 (90%)	8 (8%)	2 (2%)	7 23
49	1r	66/88 (75%)	58 (88%)	8 (12%)	0	100 100
49	2r	66/88 (75%)	60 (91%)	6 (9%)	0	100 100
50	1s	81/93 (87%)	68 (84%)	11 (14%)	2 (2%)	5 19
50	2s	81/93 (87%)	63 (78%)	17 (21%)	1 (1%)	13 39
51	1t	94/106 (89%)	81 (86%)	11 (12%)	2 (2%)	7 23
51	2t	94/106 (89%)	85 (90%)	8 (8%)	1 (1%)	14 41
52	1u	21/27 (78%)	19 (90%)	2 (10%)	0	100 100
52	2u	21/27 (78%)	16 (76%)	3 (14%)	2 (10%)	0 1
All	All	11370/12128 (94%)	10088 (89%)	1142 (10%)	140 (1%)	13 39

All (140) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	1F	130	ALA
6	1G	43	LEU
11	1P	36	LYS
11	1P	38	GLN
21	1Z	53	ILE
23	11	3	LYS
26	14	45	GLY
26	14	49	PHE
33	1b	17	PHE
33	1b	126	GLU
34	1c	66	VAL
35	1d	173	TRP
38	1g	80	VAL
41	1j	79	ARG
44	1m	67	GLU
44	1m	106	ASN
14	2S	81	GLY

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Mol	Chain	Res	Type
17	2V	100	ARG
33	2b	17	PHE
38	2g	55	GLY
38	2g	80	VAL
42	2k	49	GLY
52	2u	3	LYS
6	1G	47	LYS
7	1H	47	GLU
26	14	62	ARG
33	1b	131	PRO
33	1b	195	ASP
34	1c	65	ALA
36	1e	85	GLY
37	1f	87	ARG
39	1h	133	LEU
40	1i	54	ASP
41	1j	75	ILE
42	1k	105	VAL
48	1q	68	ARG
4	2E	71	GLY
5	2F	130	ALA
6	2G	42	GLY
7	2H	126	PRO
8	2I	10	GLU
8	2I	40	THR
9	2N	64	GLY
11	2P	36	LYS
14	2S	96	GLY
21	2Z	161	VAL
23	21	3	LYS
26	24	48	ARG
26	24	49	PHE
34	2c	107	GLN
36	2e	77	PRO
36	2e	85	GLY
43	2l	105	TYR
45	2n	14	PRO
46	2o	87	ILE
48	2q	68	ARG
4	1E	71	GLY
19	1X	67	GLY
20	1Y	78	ALA

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Mol	Chain	Res	Type
21	1Z	51	ALA
26	14	44	THR
33	1b	231	GLU
46	1o	88	ARG
4	2E	52	LEU
4	2E	144	ARG
6	2G	124	SER
8	2I	39	ALA
9	2N	79	PRO
10	2O	5	GLN
15	2T	117	ASP
26	24	39	CYS
33	2b	9	GLU
33	2b	20	GLU
34	2c	91	LEU
38	2g	4	ARG
41	2j	41	PRO
41	2j	51	ARG
41	2j	77	PRO
41	2j	79	ARG
44	2m	75	ALA
50	2s	81	ARG
4	1E	52	LEU
7	1H	92	ILE
9	1N	2	LYS
12	1Q	60	ARG
40	1i	56	LEU
6	2G	43	LEU
9	2N	81	GLY
14	2S	109	GLY
17	2V	79	VAL
20	2Y	43	ASN
21	2Z	144	LEU
25	23	38	GLU
41	2j	29	ARG
44	2m	29	ARG
44	2m	117	VAL
8	1I	12	LEU
11	1P	45	LEU
33	1b	16	HIS
34	1c	107	GLN
41	1j	58	ASP

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Mol	Chain	Res	Type
50	1s	27	GLU
50	1s	47	HIS
11	2P	38	GLN
21	2Z	52	SER
26	24	29	PRO
33	2b	113	HIS
33	2b	123	ALA
33	2b	125	PRO
40	2i	10	ARG
40	2i	58	HIS
41	2j	78	ASN
45	2n	12	ARG
48	2q	67	LYS
52	2u	4	GLY
17	1V	79	VAL
35	1d	88	VAL
39	1h	115	SER
51	1t	95	ALA
11	2P	45	LEU
35	2d	136	PRO
51	2t	47	GLY
11	1P	93	GLY
35	1d	172	PRO
7	2H	169	VAL
11	2P	122	PRO
22	20	13	GLY
38	2g	130	GLY
7	1H	126	PRO
42	1k	49	GLY
51	1t	100	ILE
41	2j	24	VAL
40	2i	90	PRO
26	14	29	PRO
33	1b	194	PRO
35	1d	50	ARG
39	1h	51	VAL
20	1Y	103	GLY
44	2m	7	VAL
17	2V	50	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%)	207 (96%)	8 (4%)	34 68
3	2D	215/218 (99%)	194 (90%)	21 (10%)	8 24
4	1E	164/166 (99%)	147 (90%)	17 (10%)	7 21
4	2E	164/166 (99%)	155 (94%)	9 (6%)	21 52
5	1F	160/166 (96%)	139 (87%)	21 (13%)	4 12
5	2F	159/166 (96%)	148 (93%)	11 (7%)	15 41
6	1G	143/156 (92%)	127 (89%)	16 (11%)	6 18
6	2G	143/156 (92%)	126 (88%)	17 (12%)	5 16
7	1H	144/148 (97%)	137 (95%)	7 (5%)	25 57
7	2H	144/148 (97%)	127 (88%)	17 (12%)	5 16
8	1I	113/124 (91%)	96 (85%)	17 (15%)	3 9
8	2I	105/124 (85%)	83 (79%)	22 (21%)	1 3
9	1N	118/119 (99%)	112 (95%)	6 (5%)	24 55
9	2N	118/119 (99%)	104 (88%)	14 (12%)	5 16
10	1O	100/100 (100%)	94 (94%)	6 (6%)	19 48
10	2O	100/100 (100%)	96 (96%)	4 (4%)	31 65
11	1P	115/116 (99%)	101 (88%)	14 (12%)	5 15
11	2P	115/116 (99%)	106 (92%)	9 (8%)	12 35
12	1Q	111/111 (100%)	101 (91%)	10 (9%)	9 28
12	2Q	111/111 (100%)	102 (92%)	9 (8%)	11 33
13	1R	101/101 (100%)	94 (93%)	7 (7%)	15 41
13	2R	101/101 (100%)	98 (97%)	3 (3%)	41 75
14	1S	86/88 (98%)	80 (93%)	6 (7%)	15 40
14	2S	85/88 (97%)	69 (81%)	16 (19%)	1 5
15	1T	115/127 (91%)	108 (94%)	7 (6%)	18 48
15	2T	113/127 (89%)	102 (90%)	11 (10%)	8 24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
16	1U	93/94 (99%)	91 (98%)	2 (2%)	52 83
16	2U	93/94 (99%)	85 (91%)	8 (9%)	10 30
17	1V	80/82 (98%)	72 (90%)	8 (10%)	7 22
17	2V	80/82 (98%)	69 (86%)	11 (14%)	3 11
18	1W	90/92 (98%)	85 (94%)	5 (6%)	21 51
18	2W	90/92 (98%)	82 (91%)	8 (9%)	9 28
19	1X	77/78 (99%)	75 (97%)	2 (3%)	46 79
19	2X	77/78 (99%)	74 (96%)	3 (4%)	32 66
20	1Y	85/91 (93%)	77 (91%)	8 (9%)	8 26
20	2Y	85/91 (93%)	76 (89%)	9 (11%)	6 20
21	1Z	135/179 (75%)	118 (87%)	17 (13%)	4 14
21	2Z	137/179 (76%)	117 (85%)	20 (15%)	3 9
22	10	65/67 (97%)	60 (92%)	5 (8%)	13 35
22	20	65/67 (97%)	61 (94%)	4 (6%)	18 47
23	11	80/83 (96%)	72 (90%)	8 (10%)	7 22
23	21	80/83 (96%)	73 (91%)	7 (9%)	10 29
24	12	65/67 (97%)	62 (95%)	3 (5%)	27 60
24	22	65/67 (97%)	59 (91%)	6 (9%)	9 27
25	13	51/52 (98%)	44 (86%)	7 (14%)	3 11
25	23	50/52 (96%)	48 (96%)	2 (4%)	31 65
26	14	59/63 (94%)	46 (78%)	13 (22%)	1 2
26	24	53/63 (84%)	44 (83%)	9 (17%)	2 6
27	15	50/52 (96%)	47 (94%)	3 (6%)	19 48
27	25	50/52 (96%)	46 (92%)	4 (8%)	12 34
28	16	51/52 (98%)	44 (86%)	7 (14%)	3 11
28	26	50/52 (96%)	46 (92%)	4 (8%)	12 34
29	17	41/42 (98%)	38 (93%)	3 (7%)	14 38
29	27	41/42 (98%)	38 (93%)	3 (7%)	14 38
30	18	54/55 (98%)	51 (94%)	3 (6%)	21 51
30	28	54/55 (98%)	49 (91%)	5 (9%)	9 26
31	19	34/34 (100%)	30 (88%)	4 (12%)	5 16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
31	29	34/34 (100%)	30 (88%)	4 (12%)	5 16
33	1b	192/220 (87%)	165 (86%)	27 (14%)	3 10
33	2b	187/220 (85%)	154 (82%)	33 (18%)	2 5
34	1c	142/188 (76%)	128 (90%)	14 (10%)	8 23
34	2c	140/188 (74%)	126 (90%)	14 (10%)	7 22
35	1d	169/181 (93%)	151 (89%)	18 (11%)	6 20
35	2d	173/181 (96%)	151 (87%)	22 (13%)	4 14
36	1e	113/123 (92%)	104 (92%)	9 (8%)	12 34
36	2e	114/123 (93%)	95 (83%)	19 (17%)	2 6
37	1f	84/90 (93%)	76 (90%)	8 (10%)	8 25
37	2f	85/90 (94%)	80 (94%)	5 (6%)	19 49
38	1g	119/127 (94%)	106 (89%)	13 (11%)	6 19
38	2g	120/127 (94%)	112 (93%)	8 (7%)	16 43
39	1h	114/119 (96%)	104 (91%)	10 (9%)	10 29
39	2h	114/119 (96%)	102 (90%)	12 (10%)	7 20
40	1i	90/99 (91%)	75 (83%)	15 (17%)	2 6
40	2i	89/99 (90%)	80 (90%)	9 (10%)	7 22
41	1j	66/92 (72%)	58 (88%)	8 (12%)	5 15
41	2j	69/92 (75%)	59 (86%)	10 (14%)	3 9
42	1k	82/99 (83%)	74 (90%)	8 (10%)	8 24
42	2k	83/99 (84%)	69 (83%)	14 (17%)	2 6
43	1l	96/108 (89%)	89 (93%)	7 (7%)	14 38
43	2l	96/108 (89%)	83 (86%)	13 (14%)	4 11
44	1m	93/101 (92%)	79 (85%)	14 (15%)	3 9
44	2m	92/101 (91%)	79 (86%)	13 (14%)	3 10
45	1n	49/50 (98%)	44 (90%)	5 (10%)	7 22
45	2n	49/50 (98%)	46 (94%)	3 (6%)	18 48
46	1o	78/80 (98%)	72 (92%)	6 (8%)	13 35
46	2o	78/80 (98%)	74 (95%)	4 (5%)	24 55
47	1p	69/74 (93%)	64 (93%)	5 (7%)	14 38
47	2p	68/74 (92%)	61 (90%)	7 (10%)	7 21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
48	1q	94/97 (97%)	83 (88%)	11 (12%)	5 16
48	2q	94/97 (97%)	83 (88%)	11 (12%)	5 16
49	1r	59/77 (77%)	50 (85%)	9 (15%)	2 8
49	2r	59/77 (77%)	53 (90%)	6 (10%)	7 22
50	1s	69/80 (86%)	65 (94%)	4 (6%)	20 50
50	2s	67/80 (84%)	56 (84%)	11 (16%)	2 7
51	1t	70/82 (85%)	61 (87%)	9 (13%)	4 13
51	2t	70/82 (85%)	64 (91%)	6 (9%)	10 30
52	1u	18/22 (82%)	17 (94%)	1 (6%)	21 51
52	2u	18/22 (82%)	17 (94%)	1 (6%)	21 51
All	All	9303/10064 (92%)	8371 (90%)	932 (10%)	7 22

All (932) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	1D	14	ARG
3	1D	117	VAL
3	1D	142	VAL
3	1D	147	LEU
3	1D	229	VAL
3	1D	242	ARG
3	1D	254	THR
3	1D	273	ARG
4	1E	5	LEU
4	1E	12	THR
4	1E	13	ARG
4	1E	47	VAL
4	1E	49	LEU
4	1E	59	VAL
4	1E	73	GLU
4	1E	77	ILE
4	1E	89	ASP
4	1E	90	THR
4	1E	92	THR
4	1E	97	LYS
4	1E	116	VAL
4	1E	119	ARG
4	1E	127	ASP

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Mol	Chain	Res	Type
4	1E	145	LYS
4	1E	195	LEU
5	1F	18	ARG
5	1F	23	ASP
5	1F	27	GLU
5	1F	33	LEU
5	1F	52	LYS
5	1F	53	THR
5	1F	54	ARG
5	1F	57	VAL
5	1F	70	THR
5	1F	74	ARG
5	1F	106	ARG
5	1F	120	GLU
5	1F	127	GLU
5	1F	140	LEU
5	1F	144	LYS
5	1F	158	THR
5	1F	168	ARG
5	1F	176	LEU
5	1F	183	VAL
5	1F	192	LEU
5	1F	201	VAL
6	1G	3	LEU
6	1G	5	VAL
6	1G	21	ARG
6	1G	31	VAL
6	1G	33	ARG
6	1G	38	VAL
6	1G	43	LEU
6	1G	79	ASN
6	1G	82	LEU
6	1G	108	ASN
6	1G	126	ASP
6	1G	133	LEU
6	1G	145	THR
6	1G	146	TYR
6	1G	149	VAL
6	1G	170	ARG
7	1H	2	SER
7	1H	16	SER
7	1H	50	VAL

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Mol	Chain	Res	Type
7	1H	57	ASP
7	1H	130	ARG
7	1H	136	ILE
7	1H	158	HIS
8	1I	9	LEU
8	1I	10	GLU
8	1I	20	ASP
8	1I	37	VAL
8	1I	40	THR
8	1I	41	GLU
8	1I	47	LEU
8	1I	57	ARG
8	1I	58	LEU
8	1I	86	THR
8	1I	87	LYS
8	1I	92	VAL
8	1I	101	LEU
8	1I	133	HIS
8	1I	140	LEU
8	1I	143	SER
8	1I	144	VAL
9	1N	12	ARG
9	1N	28	THR
9	1N	32	THR
9	1N	62	VAL
9	1N	112	LEU
9	1N	140	VAL
10	1O	21	CYS
10	1O	80	ASP
10	1O	97	ARG
10	1O	114	ILE
10	1O	117	LEU
10	1O	120	GLU
11	1P	3	LEU
11	1P	4	SER
11	1P	7	ARG
11	1P	29	LYS
11	1P	57	THR
11	1P	65	ARG
11	1P	70	GLN
11	1P	74	GLU
11	1P	95	VAL

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Mol	Chain	Res	Type
11	1P	96	THR
11	1P	98	GLU
11	1P	135	LEU
11	1P	148	LEU
11	1P	149	GLU
12	1Q	7	MET
12	1Q	8	LYS
12	1Q	11	LYS
12	1Q	38	GLU
12	1Q	56	ARG
12	1Q	85	LYS
12	1Q	109	VAL
12	1Q	110	THR
12	1Q	115	MET
12	1Q	133	ARG
13	1R	6	SER
13	1R	36	THR
13	1R	67	LEU
13	1R	75	LEU
13	1R	91	GLN
13	1R	102	GLU
13	1R	114	VAL
14	1S	12	PHE
14	1S	14	VAL
14	1S	16	ASN
14	1S	18	ILE
14	1S	25	ARG
14	1S	69	VAL
15	1T	10	VAL
15	1T	28	VAL
15	1T	40	THR
15	1T	90	GLN
15	1T	96	ARG
15	1T	108	ARG
15	1T	128	GLU
16	1U	74	LEU
16	1U	77	SER
17	1V	1	MET
17	1V	20	LEU
17	1V	32	THR
17	1V	52	VAL
17	1V	73	SER

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Mol	Chain	Res	Type
17	1V	79	VAL
17	1V	85	LYS
17	1V	100	ARG
18	1W	11	ARG
18	1W	15	ARG
18	1W	17	VAL
18	1W	63	ASP
18	1W	68	ARG
19	1X	66	LEU
19	1X	88	LYS
20	1Y	47	LYS
20	1Y	49	VAL
20	1Y	50	ARG
20	1Y	61	ILE
20	1Y	63	LYS
20	1Y	64	GLU
20	1Y	97	ARG
20	1Y	99	CYS
21	1Z	8	TYR
21	1Z	33	LEU
21	1Z	56	VAL
21	1Z	73	GLN
21	1Z	80	ARG
21	1Z	84	GLU
21	1Z	86	VAL
21	1Z	91	LEU
21	1Z	93	ASP
21	1Z	128	VAL
21	1Z	136	PHE
21	1Z	138	GLU
21	1Z	153	SER
21	1Z	154	ASP
21	1Z	155	LEU
21	1Z	156	LYS
21	1Z	170	THR
22	10	7	LEU
22	10	10	THR
22	10	37	LEU
22	10	39	ARG
22	10	68	GLU
23	11	35	THR
23	11	37	ILE

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Mol	Chain	Res	Type
23	11	51	VAL
23	11	59	THR
23	11	65	SER
23	11	80	LEU
23	11	81	LYS
23	11	91	LYS
24	12	3	LEU
24	12	40	SER
24	12	53	LEU
25	13	6	VAL
25	13	23	LEU
25	13	34	GLU
25	13	37	LEU
25	13	54	VAL
25	13	56	VAL
25	13	58	VAL
26	14	1	MET
26	14	3	GLU
26	14	5	ILE
26	14	33	VAL
26	14	49	PHE
26	14	52	THR
26	14	53	GLU
26	14	56	VAL
26	14	58	ARG
26	14	59	PHE
26	14	60	GLN
26	14	63	TYR
26	14	69	LYS
27	15	6	VAL
27	15	55	ARG
27	15	58	LEU
28	16	5	VAL
28	16	6	ARG
28	16	14	THR
28	16	27	LYS
28	16	37	ARG
28	16	44	ARG
28	16	48	VAL
29	17	24	THR
29	17	41	ARG
29	17	43	THR

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Mol	Chain	Res	Type
30	18	5	LYS
30	18	31	HIS
30	18	52	LYS
31	19	4	ARG
31	19	6	SER
31	19	7	VAL
31	19	9	ARG
33	1b	12	GLU
33	1b	21	ARG
33	1b	24	TRP
33	1b	35	GLU
33	1b	37	ASN
33	1b	44	LEU
33	1b	48	MET
33	1b	54	THR
33	1b	60	ASP
33	1b	80	ILE
33	1b	81	VAL
33	1b	97	TRP
33	1b	107	THR
33	1b	112	VAL
33	1b	127	ILE
33	1b	133	LYS
33	1b	136	VAL
33	1b	138	LEU
33	1b	142	LEU
33	1b	160	ASP
33	1b	163	PHE
33	1b	192	SER
33	1b	206	ASP
33	1b	212	GLN
33	1b	215	LEU
33	1b	222	ILE
33	1b	223	ILE
34	1c	3	ASN
34	1c	20	SER
34	1c	28	GLN
34	1c	33	LEU
34	1c	45	LYS
34	1c	63	ASN
34	1c	64	VAL
34	1c	77	ILE

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Mol	Chain	Res	Type
34	1c	82	GLU
34	1c	131	ARG
34	1c	139	GLN
34	1c	178	LEU
34	1c	192	THR
34	1c	207	VAL
35	1d	5	ILE
35	1d	10	ARG
35	1d	12	CYS
35	1d	19	LEU
35	1d	24	GLU
35	1d	49	ARG
35	1d	71	SER
35	1d	77	ASN
35	1d	86	LYS
35	1d	112	VAL
35	1d	122	ARG
35	1d	127	THR
35	1d	135	LEU
35	1d	141	ARG
35	1d	178	VAL
35	1d	187	ARG
35	1d	188	LEU
35	1d	194	LEU
36	1e	8	GLU
36	1e	10	MET
36	1e	20	GLN
36	1e	41	VAL
36	1e	79	GLU
36	1e	91	LEU
36	1e	120	THR
36	1e	131	ILE
36	1e	147	ASP
37	1f	2	ARG
37	1f	15	ASP
37	1f	36	ARG
37	1f	48	LEU
37	1f	55	ASP
37	1f	66	GLU
37	1f	87	ARG
37	1f	98	LEU
38	1g	12	LEU

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Mol	Chain	Res	Type
38	1g	13	GLN
38	1g	15	ASP
38	1g	16	LEU
38	1g	20	ASP
38	1g	50	ILE
38	1g	76	ARG
38	1g	79	ARG
38	1g	85	TYR
38	1g	98	SER
38	1g	110	GLN
38	1g	113	GLU
38	1g	115	ARG
39	1h	24	THR
39	1h	29	SER
39	1h	51	VAL
39	1h	52	ASP
39	1h	75	ARG
39	1h	91	ARG
39	1h	95	VAL
39	1h	118	VAL
39	1h	122	ARG
39	1h	133	LEU
40	1i	16	ARG
40	1i	17	VAL
40	1i	25	LYS
40	1i	27	THR
40	1i	31	GLN
40	1i	41	VAL
40	1i	58	HIS
40	1i	64	THR
40	1i	92	TYR
40	1i	96	LEU
40	1i	99	LEU
40	1i	103	THR
40	1i	108	VAL
40	1i	121	ARG
40	1i	128	ARG
41	1j	21	GLN
41	1j	38	ILE
41	1j	44	VAL
41	1j	49	VAL
41	1j	72	VAL

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Mol	Chain	Res	Type
41	1j	94	VAL
41	1j	98	ILE
41	1j	100	THR
42	1k	18	ARG
42	1k	31	THR
42	1k	48	ILE
42	1k	53	SER
42	1k	83	ILE
42	1k	87	THR
42	1k	109	VAL
42	1k	120	ARG
43	1l	18	VAL
43	1l	38	THR
43	1l	43	VAL
43	1l	53	ARG
43	1l	62	SER
43	1l	70	ILE
43	1l	124	LYS
44	1m	4	ILE
44	1m	11	ARG
44	1m	25	ILE
44	1m	64	TRP
44	1m	69	GLU
44	1m	70	LEU
44	1m	74	VAL
44	1m	86	CYS
44	1m	90	LEU
44	1m	98	VAL
44	1m	103	THR
44	1m	106	ASN
44	1m	110	ARG
44	1m	122	LYS
45	1n	3	ARG
45	1n	22	THR
45	1n	32	SER
45	1n	35	ARG
45	1n	56	VAL
46	1o	11	VAL
46	1o	37	ASN
46	1o	39	LEU
46	1o	62	GLN
46	1o	74	ASP

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Mol	Chain	Res	Type
46	1o	88	ARG
47	1p	11	SER
47	1p	20	VAL
47	1p	22	THR
47	1p	72	ARG
47	1p	76	GLN
48	1q	9	VAL
48	1q	14	LYS
48	1q	35	VAL
48	1q	45	HIS
48	1q	52	LYS
48	1q	60	ILE
48	1q	63	ARG
48	1q	85	VAL
48	1q	93	GLN
48	1q	97	SER
48	1q	98	LEU
49	1r	31	LEU
49	1r	35	ARG
49	1r	37	VAL
49	1r	53	ARG
49	1r	54	ARG
49	1r	56	THR
49	1r	59	SER
49	1r	66	LEU
49	1r	84	LYS
50	1s	5	LEU
50	1s	27	GLU
50	1s	37	ARG
50	1s	51	VAL
51	1t	9	ASN
51	1t	10	LEU
51	1t	13	LEU
51	1t	24	LEU
51	1t	31	SER
51	1t	54	LYS
51	1t	70	SER
51	1t	75	ASN
51	1t	84	LEU
52	1u	15	ARG
3	2D	3	VAL
3	2D	10	THR

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Mol	Chain	Res	Type
3	2D	18	VAL
3	2D	25	THR
3	2D	27	THR
3	2D	37	LEU
3	2D	53	PHE
3	2D	87	ASN
3	2D	88	ARG
3	2D	99	ASP
3	2D	113	VAL
3	2D	115	GLN
3	2D	140	THR
3	2D	141	VAL
3	2D	142	VAL
3	2D	147	LEU
3	2D	155	LEU
3	2D	212	SER
3	2D	229	VAL
3	2D	242	ARG
3	2D	253	GLN
4	2E	12	THR
4	2E	53	PRO
4	2E	78	LEU
4	2E	97	LYS
4	2E	104	VAL
4	2E	107	THR
4	2E	116	VAL
4	2E	145	LYS
4	2E	184	VAL
5	2F	17	ARG
5	2F	18	ARG
5	2F	20	LEU
5	2F	24	LEU
5	2F	95	ARG
5	2F	100	THR
5	2F	119	ARG
5	2F	153	SER
5	2F	163	VAL
5	2F	183	VAL
5	2F	192	LEU
6	2G	14	GLU
6	2G	18	GLU
6	2G	20	ILE

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Mol	Chain	Res	Type
6	2G	41	GLN
6	2G	43	LEU
6	2G	47	LYS
6	2G	53	LEU
6	2G	88	ILE
6	2G	91	ARG
6	2G	121	ASN
6	2G	130	ASN
6	2G	135	LEU
6	2G	140	ILE
6	2G	148	MET
6	2G	149	VAL
6	2G	150	ASP
6	2G	159	VAL
7	2H	2	SER
7	2H	3	ARG
7	2H	12	PRO
7	2H	13	LYS
7	2H	16	SER
7	2H	26	VAL
7	2H	49	VAL
7	2H	50	VAL
7	2H	70	THR
7	2H	71	LEU
7	2H	76	VAL
7	2H	90	LYS
7	2H	104	GLU
7	2H	115	VAL
7	2H	134	SER
7	2H	139	GLN
7	2H	149	ARG
8	2I	4	ILE
8	2I	5	LEU
8	2I	12	LEU
8	2I	14	ASP
8	2I	15	VAL
8	2I	25	TYR
8	2I	41	GLU
8	2I	43	ASN
8	2I	50	ARG
8	2I	58	LEU
8	2I	66	GLU

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Mol	Chain	Res	Type
8	2I	75	LEU
8	2I	81	VAL
8	2I	82	ARG
8	2I	85	GLU
8	2I	87	LYS
8	2I	107	VAL
8	2I	117	GLU
8	2I	125	GLU
8	2I	126	TYR
8	2I	127	VAL
8	2I	133	HIS
9	2N	12	ARG
9	2N	14	VAL
9	2N	15	LEU
9	2N	32	THR
9	2N	38	HIS
9	2N	43	THR
9	2N	48	MET
9	2N	60	ILE
9	2N	62	VAL
9	2N	63	THR
9	2N	67	LEU
9	2N	84	LYS
9	2N	85	ILE
9	2N	90	MET
10	2O	32	TYR
10	2O	53	LYS
10	2O	78	ARG
10	2O	90	GLN
11	2P	7	ARG
11	2P	30	THR
11	2P	45	LEU
11	2P	56	SER
11	2P	76	LYS
11	2P	95	VAL
11	2P	96	THR
11	2P	98	GLU
11	2P	149	GLU
12	2Q	6	ARG
12	2Q	16	ARG
12	2Q	25	ASP
12	2Q	79	LEU

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Mol	Chain	Res	Type
12	2Q	85	LYS
12	2Q	103	MET
12	2Q	106	VAL
12	2Q	110	THR
12	2Q	133	ARG
13	2R	24	GLN
13	2R	59	ASP
13	2R	95	THR
14	2S	4	LEU
14	2S	12	PHE
14	2S	24	LEU
14	2S	27	SER
14	2S	43	GLU
14	2S	54	LEU
14	2S	58	LEU
14	2S	63	THR
14	2S	64	GLU
14	2S	65	VAL
14	2S	75	GLU
14	2S	80	LEU
14	2S	83	LYS
14	2S	93	LYS
14	2S	98	VAL
14	2S	110	LEU
15	2T	1	MET
15	2T	9	LEU
15	2T	13	ARG
15	2T	17	THR
15	2T	39	ARG
15	2T	59	THR
15	2T	87	ASP
15	2T	93	ARG
15	2T	95	ARG
15	2T	96	ARG
15	2T	107	ASP
16	2U	16	LYS
16	2U	55	ARG
16	2U	56	ASP
16	2U	57	PHE
16	2U	58	ARG
16	2U	74	LEU
16	2U	83	LEU

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Mol	Chain	Res	Type
16	2U	105	VAL
17	2V	7	THR
17	2V	14	VAL
17	2V	20	LEU
17	2V	38	LEU
17	2V	46	VAL
17	2V	52	VAL
17	2V	61	VAL
17	2V	79	VAL
17	2V	94	LEU
17	2V	95	LEU
17	2V	98	GLU
18	2W	10	VAL
18	2W	11	ARG
18	2W	50	VAL
18	2W	63	ASP
18	2W	67	ASP
18	2W	83	LYS
18	2W	97	LYS
18	2W	111	HIS
19	2X	35	THR
19	2X	75	ASP
19	2X	81	VAL
20	2Y	37	VAL
20	2Y	49	VAL
20	2Y	62	GLU
20	2Y	70	SER
20	2Y	72	VAL
20	2Y	83	THR
20	2Y	85	VAL
20	2Y	91	GLU
20	2Y	97	ARG
21	2Z	5	LEU
21	2Z	33	LEU
21	2Z	42	VAL
21	2Z	44	PHE
21	2Z	50	GLN
21	2Z	63	ASP
21	2Z	66	SER
21	2Z	67	LEU
21	2Z	71	VAL
21	2Z	72	ARG

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Mol	Chain	Res	Type
21	2Z	76	LEU
21	2Z	93	ASP
21	2Z	124	ILE
21	2Z	135	GLU
21	2Z	150	LEU
21	2Z	151	HIS
21	2Z	154	ASP
21	2Z	155	LEU
21	2Z	170	THR
21	2Z	171	ILE
22	20	11	ARG
22	20	55	ARG
22	20	67	VAL
22	20	68	GLU
23	21	17	SER
23	21	51	VAL
23	21	59	THR
23	21	65	SER
23	21	76	ARG
23	21	80	LEU
23	21	86	SER
24	22	19	VAL
24	22	46	GLN
24	22	47	ASN
24	22	50	ILE
24	22	55	ARG
24	22	59	ARG
25	23	23	LEU
25	23	34	GLU
26	24	1	MET
26	24	24	THR
26	24	35	VAL
26	24	49	PHE
26	24	56	VAL
26	24	58	ARG
26	24	59	PHE
26	24	63	TYR
26	24	67	TYR
27	25	6	VAL
27	25	25	LEU
27	25	55	ARG
27	25	58	LEU

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Mol	Chain	Res	Type
28	26	6	ARG
28	26	9	LEU
28	26	23	THR
28	26	29	ASN
29	27	1	MET
29	27	41	ARG
29	27	47	ARG
30	28	13	ARG
30	28	31	HIS
30	28	34	TRP
30	28	41	ILE
30	28	48	PHE
31	29	4	ARG
31	29	7	VAL
31	29	18	ARG
31	29	36	GLN
33	2b	7	VAL
33	2b	8	LYS
33	2b	9	GLU
33	2b	16	HIS
33	2b	24	TRP
33	2b	53	ARG
33	2b	63	MET
33	2b	67	THR
33	2b	68	ILE
33	2b	71	VAL
33	2b	81	VAL
33	2b	96	ARG
33	2b	107	THR
33	2b	109	SER
33	2b	115	LEU
33	2b	117	GLU
33	2b	124	SER
33	2b	127	ILE
33	2b	135	GLN
33	2b	141	GLU
33	2b	159	PRO
33	2b	163	PHE
33	2b	164	VAL
33	2b	169	LYS
33	2b	181	PHE
33	2b	189	ASP

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Mol	Chain	Res	Type
33	2b	190	THR
33	2b	195	ASP
33	2b	210	SER
33	2b	224	GLN
33	2b	229	VAL
33	2b	230	VAL
33	2b	236	TYR
34	2c	43	LEU
34	2c	56	ASP
34	2c	57	ILE
34	2c	69	HIS
34	2c	82	GLU
34	2c	103	VAL
34	2c	115	LEU
34	2c	128	PHE
34	2c	138	VAL
34	2c	143	GLU
34	2c	151	VAL
34	2c	153	VAL
34	2c	190	ARG
34	2c	193	TYR
35	2d	25	ARG
35	2d	34	GLU
35	2d	42	GLN
35	2d	47	ARG
35	2d	57	ARG
35	2d	58	LEU
35	2d	76	ARG
35	2d	78	LEU
35	2d	83	SER
35	2d	94	LEU
35	2d	118	ARG
35	2d	135	LEU
35	2d	150	GLU
35	2d	157	LEU
35	2d	158	ILE
35	2d	165	MET
35	2d	175	SER
35	2d	178	VAL
35	2d	186	LEU
35	2d	187	ARG
35	2d	190	ASP

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Mol	Chain	Res	Type
35	2d	203	VAL
36	2e	5	ASP
36	2e	13	ILE
36	2e	14	ARG
36	2e	32	VAL
36	2e	38	GLN
36	2e	51	VAL
36	2e	60	TYR
36	2e	64	ARG
36	2e	72	GLN
36	2e	76	ILE
36	2e	80	ILE
36	2e	98	THR
36	2e	100	VAL
36	2e	116	THR
36	2e	119	LEU
36	2e	121	LYS
36	2e	144	THR
36	2e	147	ASP
36	2e	152	ARG
37	2f	15	ASP
37	2f	19	LEU
37	2f	31	GLU
37	2f	45	LEU
37	2f	94	GLN
38	2g	16	LEU
38	2g	31	MET
38	2g	33	ASP
38	2g	75	VAL
38	2g	78	ARG
38	2g	79	ARG
38	2g	113	GLU
38	2g	155	ARG
39	2h	22	GLU
39	2h	24	THR
39	2h	50	ARG
39	2h	52	ASP
39	2h	61	VAL
39	2h	65	TYR
39	2h	81	HIS
39	2h	84	ARG
39	2h	91	ARG

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Mol	Chain	Res	Type
39	2h	109	ILE
39	2h	120	THR
39	2h	133	LEU
40	2i	27	THR
40	2i	33	PHE
40	2i	34	ASN
40	2i	54	ASP
40	2i	64	THR
40	2i	65	VAL
40	2i	74	ILE
40	2i	75	ASP
40	2i	127	LYS
41	2j	6	ILE
41	2j	9	ARG
41	2j	19	SER
41	2j	21	GLN
41	2j	29	ARG
41	2j	50	ILE
41	2j	67	THR
41	2j	74	ILE
41	2j	98	ILE
41	2j	100	THR
42	2k	14	VAL
42	2k	18	ARG
42	2k	25	TYR
42	2k	30	VAL
42	2k	40	ILE
42	2k	41	THR
42	2k	48	ILE
42	2k	53	SER
42	2k	77	MET
42	2k	87	THR
42	2k	101	SER
42	2k	108	ILE
42	2k	109	VAL
42	2k	114	VAL
43	2l	6	THR
43	2l	16	GLU
43	2l	33	ARG
43	2l	43	VAL
43	2l	49	ASN
43	2l	53	ARG

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Mol	Chain	Res	Type
43	2l	82	VAL
43	2l	86	ARG
43	2l	90	VAL
43	2l	104	VAL
43	2l	118	SER
43	2l	122	THR
43	2l	123	LYS
44	2m	11	ARG
44	2m	15	VAL
44	2m	37	THR
44	2m	44	ARG
44	2m	47	ASP
44	2m	50	GLU
44	2m	69	GLU
44	2m	90	LEU
44	2m	98	VAL
44	2m	102	ARG
44	2m	103	THR
44	2m	108	ARG
44	2m	115	LYS
45	2n	18	VAL
45	2n	31	ARG
45	2n	35	ARG
46	2o	24	SER
46	2o	27	VAL
46	2o	58	MET
46	2o	88	ARG
47	2p	2	VAL
47	2p	20	VAL
47	2p	21	VAL
47	2p	45	THR
47	2p	60	LEU
47	2p	69	THR
47	2p	76	GLN
48	2q	5	VAL
48	2q	7	THR
48	2q	9	VAL
48	2q	24	GLU
48	2q	53	LEU
48	2q	55	ASP
48	2q	60	ILE
48	2q	65	ILE

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Mol	Chain	Res	Type
48	2q	66	SER
48	2q	90	ILE
48	2q	97	SER
49	2r	31	LEU
49	2r	37	VAL
49	2r	46	GLU
49	2r	54	ARG
49	2r	66	LEU
49	2r	84	LYS
50	2s	9	VAL
50	2s	12	ASP
50	2s	14	HIS
50	2s	27	GLU
50	2s	32	LYS
50	2s	37	ARG
50	2s	41	VAL
50	2s	45	VAL
50	2s	48	THR
50	2s	57	HIS
50	2s	63	THR
51	2t	24	LEU
51	2t	30	LYS
51	2t	31	SER
51	2t	46	GLU
51	2t	56	MET
51	2t	93	GLU
52	2u	10	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (107) such sidechains are listed below:

Mol	Chain	Res	Type
3	1D	87	ASN
3	1D	96	HIS
3	1D	115	GLN
4	1E	48	GLN
4	1E	85	ASN
5	1F	8	GLN
6	1G	26	GLN
7	1H	139	GLN
7	1H	147	ASN
12	1Q	57	HIS
12	1Q	113	GLN

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Mol	Chain	Res	Type
12	1Q	123	HIS
13	1R	13	HIS
15	1T	79	HIS
19	1X	31	HIS
19	1X	82	GLN
20	1Y	6	HIS
20	1Y	43	ASN
21	1Z	73	GLN
21	1Z	132	ASN
21	1Z	151	HIS
23	11	56	GLN
24	12	65	ASN
29	17	36	GLN
30	18	35	GLN
33	1b	78	GLN
33	1b	95	GLN
33	1b	212	GLN
34	1c	37	GLN
34	1c	162	GLN
35	1d	42	GLN
35	1d	116	GLN
35	1d	119	GLN
35	1d	123	HIS
35	1d	125	HIS
36	1e	65	ASN
36	1e	78	HIS
37	1f	57	GLN
37	1f	64	GLN
37	1f	73	ASN
37	1f	100	ASN
38	1g	13	GLN
38	1g	28	ASN
40	1i	34	ASN
40	1i	73	GLN
40	1i	124	GLN
41	1j	56	HIS
41	1j	62	HIS
44	1m	106	ASN
46	1o	9	GLN
46	1o	46	HIS
47	1p	13	HIS
47	1p	76	GLN

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Mol	Chain	Res	Type
49	1r	63	GLN
50	1s	23	ASN
50	1s	57	HIS
3	2D	115	GLN
4	2E	48	GLN
5	2F	69	HIS
5	2F	133	ASN
6	2G	26	GLN
6	2G	108	ASN
6	2G	121	ASN
7	2H	147	ASN
8	2I	74	ASN
10	2O	5	GLN
12	2Q	57	HIS
13	2R	31	HIS
13	2R	71	GLN
14	2S	38	GLN
15	2T	84	GLN
17	2V	80	GLN
20	2Y	6	HIS
20	2Y	43	ASN
21	2Z	32	HIS
21	2Z	73	GLN
21	2Z	121	HIS
23	21	56	GLN
31	29	36	GLN
33	2b	76	GLN
33	2b	95	GLN
33	2b	212	GLN
34	2c	69	HIS
34	2c	139	GLN
34	2c	162	GLN
35	2d	42	GLN
35	2d	77	ASN
35	2d	116	GLN
35	2d	119	GLN
35	2d	125	HIS
35	2d	129	ASN
35	2d	201	GLN
36	2e	20	GLN
38	2g	28	ASN
38	2g	86	GLN

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Mol	Chain	Res	Type
38	2g	148	ASN
40	2i	58	HIS
41	2j	21	GLN
42	2k	104	GLN
42	2k	117	ASN
43	2l	78	GLN
44	2m	77	ASN
46	2o	62	GLN
47	2p	13	HIS
49	2r	63	GLN
50	2s	69	HIS
50	2s	83	HIS

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2863/2915 (98%)	492 (17%)	22 (0%)
1	2A	2790/2915 (95%)	527 (18%)	22 (0%)
2	1B	119/121 (98%)	9 (7%)	0
2	2B	118/121 (97%)	28 (23%)	0
32	1a	1494/1521 (98%)	280 (18%)	0
32	2a	1498/1521 (98%)	358 (23%)	0
53	1v	12/24 (50%)	4 (33%)	0
53	2v	12/24 (50%)	3 (25%)	0
54	1w	71/76 (93%)	27 (38%)	0
54	1y	71/76 (93%)	27 (38%)	0
54	2w	68/76 (89%)	21 (30%)	0
54	2y	69/76 (90%)	24 (34%)	0
55	1x	75/77 (97%)	10 (13%)	0
55	2x	75/77 (97%)	12 (16%)	0
All	All	9335/9620 (97%)	1822 (19%)	44 (0%)

All (1822) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	15	G
1	1A	34	C
1	1A	45	C
1	1A	58	G
1	1A	61	G
1	1A	71	A

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Mol	Chain	Res	Type
1	1A	72	U
1	1A	74	A
1	1A	75	G
1	1A	84	A
1	1A	118	A
1	1A	119	A
1	1A	120	U
1	1A	123	G
1	1A	125	G
1	1A	126	A
1	1A	140	G
1	1A	141	A
1	1A	154	G
1	1A	177	G
1	1A	182	A
1	1A	196	A
1	1A	199	A
1	1A	201	C
1	1A	205	G
1	1A	214	G
1	1A	215	G
1	1A	216	A
1	1A	222	A
1	1A	228	A
1	1A	229	A
1	1A	232	G
1	1A	233	A
1	1A	248	G
1	1A	269	U
1	1A	271(K)	U
1	1A	271(L)	U
1	1A	271(M)	G
1	1A	271(N)	U
1	1A	271(O)	C
1	1A	271(S)	G
1	1A	272(B)	G
1	1A	279	C
1	1A	311	A
1	1A	324	A
1	1A	329	G
1	1A	330	A
1	1A	342	G

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Mol	Chain	Res	Type
1	1A	346	A
1	1A	352	G
1	1A	362	U
1	1A	363	G
1	1A	363(B)	G
1	1A	363(F)	A
1	1A	386	G
1	1A	396	G
1	1A	405	U
1	1A	411	G
1	1A	412	A
1	1A	413	C
1	1A	428	A
1	1A	444	C
1	1A	448	U
1	1A	451	C
1	1A	454	A
1	1A	455	C
1	1A	456	C
1	1A	481	G
1	1A	494	G
1	1A	504	U
1	1A	505	A
1	1A	509	C
1	1A	512	G
1	1A	513	A
1	1A	530	G
1	1A	531	C
1	1A	532	A
1	1A	533	G
1	1A	545	G
1	1A	549	G
1	1A	563	G
1	1A	573	G
1	1A	575	A
1	1A	584	C
1	1A	592	G
1	1A	603	A
1	1A	604	G
1	1A	607	U
1	1A	614(A)	U
1	1A	614(B)	G

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Mol	Chain	Res	Type
1	1A	615	G
1	1A	621	A
1	1A	627	A
1	1A	634	C
1	1A	637	A
1	1A	645	C
1	1A	646	A
1	1A	652(D)	C
1	1A	652(E)	G
1	1A	652(F)	G
1	1A	652(T)	C
1	1A	654	A
1	1A	669	G
1	1A	677	A
1	1A	686	G
1	1A	730	C
1	1A	734	A
1	1A	762	U
1	1A	775	G
1	1A	776	G
1	1A	782	A
1	1A	784	A
1	1A	785	G
1	1A	789	A
1	1A	792	G
1	1A	805	G
1	1A	812	C
1	1A	819	A
1	1A	827	U
1	1A	828	U
1	1A	830	G
1	1A	859	G
1	1A	866	A
1	1A	874	G
1	1A	875	G
1	1A	879	G
1	1A	880	G
1	1A	883	G
1	1A	884	C
1	1A	885	C
1	1A	886	C
1	1A	887	A

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Mol	Chain	Res	Type
1	1A	888	C
1	1A	890	A
1	1A	894	C
1	1A	895	U
1	1A	896	A
1	1A	897	C
1	1A	898	C
1	1A	900	A
1	1A	907	U
1	1A	910	A
1	1A	926	A
1	1A	932	G
1	1A	938	G
1	1A	945	A
1	1A	946	G
1	1A	953	A
1	1A	959	A
1	1A	961	C
1	1A	963	U
1	1A	974	G
1	1A	975	C
1	1A	983	A
1	1A	996	A
1	1A	1012	U
1	1A	1013	C
1	1A	1022	G
1	1A	1025	G
1	1A	1026	U
1	1A	1027	A
1	1A	1033	U
1	1A	1034	G
1	1A	1038	C
1	1A	1040	C
1	1A	1042	G
1	1A	1044	G
1	1A	1045	A
1	1A	1046	A
1	1A	1047	G
1	1A	1054	A
1	1A	1055	G
1	1A	1058	G
1	1A	1059	G

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Mol	Chain	Res	Type
1	1A	1063	G
1	1A	1068	G
1	1A	1071	G
1	1A	1073	A
1	1A	1075	C
1	1A	1076	C
1	1A	1078	U
1	1A	1079	C
1	1A	1081	U
1	1A	1082	U
1	1A	1085	A
1	1A	1088	A
1	1A	1089	G
1	1A	1090	U
1	1A	1091	G
1	1A	1092	C
1	1A	1094	U
1	1A	1098	A
1	1A	1101	U
1	1A	1104	C
1	1A	1105	U
1	1A	1110	G
1	1A	1111	A
1	1A	1112	G
1	1A	1116	C
1	1A	1129	A
1	1A	1130	U
1	1A	1135	C
1	1A	1136	G
1	1A	1142	U
1	1A	1149	G
1	1A	1155	A
1	1A	1171	G
1	1A	1173	G
1	1A	1174	A
1	1A	1175	U
1	1A	1176	G
1	1A	1177	A
1	1A	1178	C
1	1A	1183	G
1	1A	1205	U
1	1A	1229	G

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Mol	Chain	Res	Type
1	1A	1237	A
1	1A	1244	G
1	1A	1248	G
1	1A	1252	G
1	1A	1253	A
1	1A	1256	G
1	1A	1267	U
1	1A	1271	G
1	1A	1272	A
1	1A	1273	U
1	1A	1281	G
1	1A	1286	A
1	1A	1300	U
1	1A	1301	A
1	1A	1303	G
1	1A	1320	C
1	1A	1342	A
1	1A	1345	C
1	1A	1352	U
1	1A	1359	A
1	1A	1360	A
1	1A	1365	A
1	1A	1384	A
1	1A	1385	G
1	1A	1386	C
1	1A	1388	G
1	1A	1394	U
1	1A	1395	A
1	1A	1396	U
1	1A	1416	G
1	1A	1417	C
1	1A	1420	U
1	1A	1421	G
1	1A	1428	C
1	1A	1429	G
1	1A	1445	A
1	1A	1450	G
1	1A	1455	G
1	1A	1467	C
1	1A	1482	G
1	1A	1484	G
1	1A	1490	A

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Mol	Chain	Res	Type
1	1A	1493	C
1	1A	1494	A
1	1A	1509	C
1	1A	1509(A)	A
1	1A	1525	G
1	1A	1539	G
1	1A	1540	U
1	1A	1543	C
1	1A	1558	A
1	1A	1559	G
1	1A	1566	A
1	1A	1569	A
1	1A	1578	U
1	1A	1580	A
1	1A	1581	G
1	1A	1584	C
1	1A	1586	A
1	1A	1608	A
1	1A	1610	A
1	1A	1627	G
1	1A	1647	G
1	1A	1648	C
1	1A	1664	A
1	1A	1670	C
1	1A	1674	G
1	1A	1684	C
1	1A	1688	U
1	1A	1696	G
1	1A	1700	A
1	1A	1701	A
1	1A	1703	G
1	1A	1722	A
1	1A	1746	G
1	1A	1756	G
1	1A	1761	C
1	1A	1763	G
1	1A	1764	G
1	1A	1773	A
1	1A	1777	U
1	1A	1780	A
1	1A	1782	C
1	1A	1791	A

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Mol	Chain	Res	Type
1	1A	1800	C
1	1A	1801	G
1	1A	1816	G
1	1A	1828	G
1	1A	1829	A
1	1A	1839	G
1	1A	1847	A
1	1A	1850	G
1	1A	1858	G
1	1A	1877	A
1	1A	1878	G
1	1A	1889	A
1	1A	1900	A
1	1A	1906	G
1	1A	1919	A
1	1A	1920	OMC
1	1A	1929	G
1	1A	1930	G
1	1A	1932	A
1	1A	1937	A
1	1A	1938	A
1	1A	1941	C
1	1A	1945	G
1	1A	1955	U
1	1A	1962	5MC
1	1A	1963	U
1	1A	1965	C
1	1A	1967	C
1	1A	1970	A
1	1A	1971	A
1	1A	1972	A
1	1A	1990	C
1	1A	1993	U
1	1A	1997	G
1	1A	2023	G
1	1A	2031	A
1	1A	2032	G
1	1A	2033	A
1	1A	2042	A
1	1A	2043	C
1	1A	2049	G
1	1A	2051	A

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Mol	Chain	Res	Type
1	1A	2055	C
1	1A	2056	G
1	1A	2060	A
1	1A	2061	G
1	1A	2062	A
1	1A	2069	G
1	1A	2093	G
1	1A	2099	U
1	1A	2100	G
1	1A	2102	U
1	1A	2108	C
1	1A	2110	G
1	1A	2113	U
1	1A	2114	A
1	1A	2116	G
1	1A	2117	A
1	1A	2118	U
1	1A	2119	A
1	1A	2120	G
1	1A	2121	G
1	1A	2127	G
1	1A	2131	G
1	1A	2132	U
1	1A	2133	G
1	1A	2134	A
1	1A	2135	A
1	1A	2136	C
1	1A	2137	C
1	1A	2140	C
1	1A	2142	C
1	1A	2144	U
1	1A	2146	C
1	1A	2147	G
1	1A	2150	U
1	1A	2151	G
1	1A	2156	G
1	1A	2157	G
1	1A	2158	A
1	1A	2159	G
1	1A	2162	G
1	1A	2163	C
1	1A	2166	G

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Mol	Chain	Res	Type
1	1A	2171	A
1	1A	2172	U
1	1A	2173	A
1	1A	2174	C
1	1A	2181	G
1	1A	2182	G
1	1A	2183	C
1	1A	2184	G
1	1A	2189	U
1	1A	2190	G
1	1A	2192	G
1	1A	2198	A
1	1A	2206	G
1	1A	2207	G
1	1A	2218	U
1	1A	2225	A
1	1A	2238	G
1	1A	2269	A
1	1A	2273	A
1	1A	2283	C
1	1A	2286	A
1	1A	2287	A
1	1A	2289	G
1	1A	2296	U
1	1A	2305	A
1	1A	2308	G
1	1A	2312	U
1	1A	2313	C
1	1A	2320	A
1	1A	2325	G
1	1A	2336	A
1	1A	2347	C
1	1A	2350	C
1	1A	2354	G
1	1A	2361	A
1	1A	2383	G
1	1A	2385	C
1	1A	2403	C
1	1A	2406	U
1	1A	2422	A
1	1A	2425	A
1	1A	2429	G

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Mol	Chain	Res	Type
1	1A	2430	A
1	1A	2435	A
1	1A	2439	A
1	1A	2440	C
1	1A	2441	C
1	1A	2448	A
1	1A	2474	C
1	1A	2476	A
1	1A	2478	A
1	1A	2481	G
1	1A	2490	G
1	1A	2502	G
1	1A	2504	U
1	1A	2505	G
1	1A	2518	A
1	1A	2520	C
1	1A	2529	G
1	1A	2530	A
1	1A	2550	G
1	1A	2554	U
1	1A	2563	U
1	1A	2564	A
1	1A	2566	A
1	1A	2567	G
1	1A	2572	A
1	1A	2582	G
1	1A	2602	A
1	1A	2609	U
1	1A	2610	C
1	1A	2611	U
1	1A	2612	C
1	1A	2628	C
1	1A	2629	A
1	1A	2630	G
1	1A	2634	G
1	1A	2654	A
1	1A	2686	G
1	1A	2689	U
1	1A	2690	C
1	1A	2702	U
1	1A	2703	C
1	1A	2712(A)	A

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Mol	Chain	Res	Type
1	1A	2713	A
1	1A	2714	G
1	1A	2718	G
1	1A	2726	U
1	1A	2733	A
1	1A	2757	A
1	1A	2758	A
1	1A	2765	A
1	1A	2766	G
1	1A	2778	A
1	1A	2790	A
1	1A	2791	C
1	1A	2802	G
1	1A	2805	G
1	1A	2818	G
1	1A	2820	A
1	1A	2821	A
1	1A	2833	G
1	1A	2835	A
1	1A	2872	G
1	1A	2873	A
1	1A	2892	A
1	1A	2894	G
1	1A	2895	U
2	1B	2	C
2	1B	35	U
2	1B	56	G
2	1B	63	G
2	1B	65	C
2	1B	73	A
2	1B	84	C
2	1B	93	G
2	1B	110	G
32	1a	7	G
32	1a	9	G
32	1a	22	G
32	1a	32	A
32	1a	39	G
32	1a	47	C
32	1a	48	C
32	1a	51	A
32	1a	52	G

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Mol	Chain	Res	Type
32	1a	54	C
32	1a	61	G
32	1a	69	G
32	1a	76	C
32	1a	77	G
32	1a	78	G
32	1a	79	G
32	1a	91	C
32	1a	98	G
32	1a	101	A
32	1a	105	G
32	1a	116	A
32	1a	120	A
32	1a	121	C
32	1a	131	C
32	1a	137	C
32	1a	142	G
32	1a	145	G
32	1a	151	A
32	1a	163	C
32	1a	165	C
32	1a	168	G
32	1a	174	C
32	1a	182	U
32	1a	185	A
32	1a	189(F)	U
32	1a	189(J)	G
32	1a	189(L)	G
32	1a	195	A
32	1a	197	A
32	1a	199	G
32	1a	201	C
32	1a	202	U
32	1a	203	U
32	1a	204	U
32	1a	216	G
32	1a	217	C
32	1a	219	C
32	1a	247	G
32	1a	251	G
32	1a	264	U
32	1a	266	G

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Mol	Chain	Res	Type
32	1a	267	C
32	1a	268	C
32	1a	289	G
32	1a	301	G
32	1a	306	G
32	1a	318	G
32	1a	321	A
32	1a	327	A
32	1a	328	C
32	1a	332	G
32	1a	342	C
32	1a	344	A
32	1a	345	C
32	1a	351	G
32	1a	352	C
32	1a	353	A
32	1a	354	G
32	1a	367	U
32	1a	369	C
32	1a	372	C
32	1a	373	A
32	1a	382	A
32	1a	384	G
32	1a	397	A
32	1a	398	C
32	1a	406	G
32	1a	410	G
32	1a	411	A
32	1a	412	A
32	1a	413	G
32	1a	422	C
32	1a	423	G
32	1a	424	G
32	1a	429	U
32	1a	430	A
32	1a	439	A
32	1a	442	C
32	1a	452	A
32	1a	461	A
32	1a	470	C
32	1a	471	G
32	1a	483	C

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Mol	Chain	Res	Type
32	1a	485	G
32	1a	486	U
32	1a	495	A
32	1a	496	A
32	1a	498	U
32	1a	505	G
32	1a	508	C
32	1a	509	A
32	1a	510	A
32	1a	511	C
32	1a	518	C
32	1a	519	C
32	1a	531	U
32	1a	532	A
32	1a	547	A
32	1a	559	A
32	1a	561	U
32	1a	562	C
32	1a	564	C
32	1a	568	G
32	1a	572	A
32	1a	573	A
32	1a	576	G
32	1a	577	G
32	1a	596	C
32	1a	618	C
32	1a	628	G
32	1a	630	G
32	1a	634	C
32	1a	653	A
32	1a	661	G
32	1a	665	A
32	1a	687	A
32	1a	688	G
32	1a	695	A
32	1a	723	U
32	1a	724	G
32	1a	731	G
32	1a	734	G
32	1a	749	C
32	1a	753	A
32	1a	755	G

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Mol	Chain	Res	Type
32	1a	760	G
32	1a	777	A
32	1a	792	A
32	1a	793	U
32	1a	794	A
32	1a	799	G
32	1a	815	A
32	1a	817	C
32	1a	821	G
32	1a	828	A
32	1a	840	C
32	1a	841	U
32	1a	851	G
32	1a	853	G
32	1a	864	A
32	1a	870	U
32	1a	874	G
32	1a	902	G
32	1a	914	A
32	1a	916	G
32	1a	926	G
32	1a	927	G
32	1a	934	C
32	1a	935	A
32	1a	960	U
32	1a	961	U
32	1a	968	A
32	1a	969	A
32	1a	971	G
32	1a	972	C
32	1a	974	A
32	1a	975	A
32	1a	976	G
32	1a	977	A
32	1a	981	U
32	1a	982	U
32	1a	983	A
32	1a	992	U
32	1a	993	G
32	1a	997	U
32	1a	1000	U
32	1a	1003	G

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Mol	Chain	Res	Type
32	1a	1005	A
32	1a	1006	C
32	1a	1020	U
32	1a	1022	G
32	1a	1023	G
32	1a	1025	U
32	1a	1026	G
32	1a	1027	C
32	1a	1028	C
32	1a	1030	C
32	1a	1030(A)	G
32	1a	1030(C)	G
32	1a	1031	G
32	1a	1033	G
32	1a	1036	G
32	1a	1039	C
32	1a	1040	U
32	1a	1041	A
32	1a	1044	A
32	1a	1068	G
32	1a	1077	G
32	1a	1081	G
32	1a	1091	U
32	1a	1094	G
32	1a	1095	U
32	1a	1101	A
32	1a	1121	U
32	1a	1123	A
32	1a	1124	G
32	1a	1125	U
32	1a	1128	C
32	1a	1132	C
32	1a	1134	G
32	1a	1136	U
32	1a	1137	C
32	1a	1138	G
32	1a	1139	G
32	1a	1146	A
32	1a	1152	A
32	1a	1154	G
32	1a	1157	A
32	1a	1158	C

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Mol	Chain	Res	Type
32	1a	1159	U
32	1a	1160	G
32	1a	1183	A
32	1a	1184	G
32	1a	1186	G
32	1a	1196	U
32	1a	1197	G
32	1a	1201	A
32	1a	1202	G
32	1a	1208	C
32	1a	1214	C
32	1a	1227	A
32	1a	1236	A
32	1a	1238	A
32	1a	1250	A
32	1a	1253	G
32	1a	1255	G
32	1a	1256	A
32	1a	1257	U
32	1a	1260	C
32	1a	1270	C
32	1a	1275	A
32	1a	1280	A
32	1a	1286	A
32	1a	1287	A
32	1a	1299	A
32	1a	1300	G
32	1a	1302	U
32	1a	1305	G
32	1a	1312	G
32	1a	1320	C
32	1a	1338	G
32	1a	1344	C
32	1a	1346	A
32	1a	1347	G
32	1a	1353	G
32	1a	1355	G
32	1a	1356	G
32	1a	1363	C
32	1a	1370	G
32	1a	1381	U
32	1a	1397	C

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Mol	Chain	Res	Type
32	1a	1419	G
32	1a	1442	G
32	1a	1442(A)	G
32	1a	1446	U
32	1a	1447	A
32	1a	1452	C
32	1a	1456	G
32	1a	1457	G
32	1a	1458	G
32	1a	1492	A
32	1a	1494	G
32	1a	1497	G
32	1a	1503	A
32	1a	1504	G
32	1a	1506	U
32	1a	1517	G
32	1a	1520	G
32	1a	1529	G
32	1a	1530	G
53	1v	13	A
53	1v	14	A
53	1v	20	U
53	1v	24	A
54	1w	3	C
54	1w	6	G
54	1w	7	A
54	1w	8	4SU
54	1w	11	C
54	1w	12	U
54	1w	13	C
54	1w	14	A
54	1w	19	G
54	1w	20	U
54	1w	21	A
54	1w	22	G
54	1w	24	G
54	1w	25	C
54	1w	29	G
54	1w	30	G
54	1w	45	U
54	1w	46	G7M
54	1w	47	U

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Mol	Chain	Res	Type
54	1w	48	C
54	1w	57	G
54	1w	60	U
54	1w	62	C
54	1w	68	C
54	1w	70	G
54	1w	72	C
54	1w	74	C
55	1x	6	G
55	1x	9	G
55	1x	14	A
55	1x	19	G
55	1x	20	U
55	1x	21	A
55	1x	47	U
55	1x	53	G
55	1x	61	C
55	1x	76	A
54	1y	6	G
54	1y	7	A
54	1y	9	A
54	1y	11	C
54	1y	13	C
54	1y	14	A
54	1y	19	G
54	1y	20	U
54	1y	21	A
54	1y	31	A
54	1y	33	U
54	1y	36	A
54	1y	40	C
54	1y	44	G
54	1y	45	U
54	1y	46	G7M
54	1y	48	C
54	1y	49	C
54	1y	52	G
54	1y	53	G
54	1y	57	G
54	1y	58	A
54	1y	59	U
54	1y	61	C

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Mol	Chain	Res	Type
54	1y	65	G
54	1y	70	G
54	1y	72	C
1	2A	14	A
1	2A	15	G
1	2A	34	C
1	2A	35	G
1	2A	45	C
1	2A	51	G
1	2A	55	G
1	2A	63	U
1	2A	64	A
1	2A	71	A
1	2A	74	A
1	2A	75	G
1	2A	84	A
1	2A	90	U
1	2A	95	G
1	2A	100	G
1	2A	102	G
1	2A	118	A
1	2A	120	U
1	2A	131	G
1	2A	141	A
1	2A	154(A)	C
1	2A	173	G
1	2A	196	A
1	2A	199	A
1	2A	205	G
1	2A	214	G
1	2A	216	A
1	2A	222	A
1	2A	225	A
1	2A	228	A
1	2A	229	A
1	2A	230	U
1	2A	233	A
1	2A	245	G
1	2A	248	G
1	2A	250	G
1	2A	266	G
1	2A	271(J)	C

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Mol	Chain	Res	Type
1	2A	271(K)	U
1	2A	271(L)	U
1	2A	271(M)	G
1	2A	271(N)	U
1	2A	271(O)	C
1	2A	272(B)	G
1	2A	275	G
1	2A	276	A
1	2A	277	C
1	2A	278	A
1	2A	283	A
1	2A	289	A
1	2A	292	C
1	2A	308	G
1	2A	311	A
1	2A	312	G
1	2A	316	C
1	2A	317	G
1	2A	324	A
1	2A	329	G
1	2A	330	A
1	2A	333	G
1	2A	342	G
1	2A	352	G
1	2A	354	G
1	2A	357	A
1	2A	360	G
1	2A	372	G
1	2A	386	G
1	2A	396	G
1	2A	403	U
1	2A	405	U
1	2A	411	G
1	2A	412	A
1	2A	421	U
1	2A	422	A
1	2A	434	U
1	2A	435	C
1	2A	444	C
1	2A	455	C
1	2A	457	A
1	2A	481	G

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Mol	Chain	Res	Type
1	2A	488	G
1	2A	503	A
1	2A	504	U
1	2A	505	A
1	2A	509	C
1	2A	527	C
1	2A	528	A
1	2A	529	A
1	2A	530	G
1	2A	531	C
1	2A	532	A
1	2A	545	G
1	2A	563	G
1	2A	567	A
1	2A	568	U
1	2A	573	G
1	2A	575	A
1	2A	588	U
1	2A	599	G
1	2A	603	A
1	2A	604	G
1	2A	607	U
1	2A	614(A)	U
1	2A	614(B)	G
1	2A	614(C)	A
1	2A	615	G
1	2A	616	G
1	2A	627	A
1	2A	634	C
1	2A	637	A
1	2A	639	U
1	2A	645	C
1	2A	648	G
1	2A	652(B)	A
1	2A	652(C)	G
1	2A	652(D)	C
1	2A	652(U)	G
1	2A	661	C
1	2A	668	G
1	2A	669	G
1	2A	686	G
1	2A	702	G

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Mol	Chain	Res	Type
1	2A	726	G
1	2A	730	C
1	2A	750	A
1	2A	753	C
1	2A	764	A
1	2A	771	G
1	2A	774	A
1	2A	775	G
1	2A	776	G
1	2A	779	U
1	2A	782	A
1	2A	784	A
1	2A	785	G
1	2A	792	G
1	2A	805	G
1	2A	811	U
1	2A	812	C
1	2A	819	A
1	2A	824	A
1	2A	827	U
1	2A	828	U
1	2A	831	G
1	2A	846	C
1	2A	847	U
1	2A	857	C
1	2A	859	G
1	2A	874	G
1	2A	878	A
1	2A	879	G
1	2A	880	G
1	2A	882	G
1	2A	884	C
1	2A	886	C
1	2A	887	A
1	2A	888	C
1	2A	889	C
1	2A	892	G
1	2A	893	C
1	2A	894	C
1	2A	896	A
1	2A	897	C
1	2A	900	A

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Mol	Chain	Res	Type
1	2A	901	A
1	2A	903	C
1	2A	904	C
1	2A	910	A
1	2A	914	C
1	2A	915	C
1	2A	917	A
1	2A	932	G
1	2A	941	A
1	2A	945	A
1	2A	946	G
1	2A	959	A
1	2A	961	C
1	2A	964	C
1	2A	967	C
1	2A	974	G
1	2A	975	C
1	2A	980	A
1	2A	983	A
1	2A	996	A
1	2A	1002	G
1	2A	1005	C
1	2A	1010	A
1	2A	1012	U
1	2A	1013	C
1	2A	1017	G
1	2A	1020	A
1	2A	1022	G
1	2A	1023	U
1	2A	1025	G
1	2A	1026	U
1	2A	1027	A
1	2A	1033	U
1	2A	1034	G
1	2A	1035	U
1	2A	1037	G
1	2A	1038	C
1	2A	1039	G
1	2A	1041	C
1	2A	1043	C
1	2A	1114	G
1	2A	1115	G

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Mol	Chain	Res	Type
1	2A	1116	C
1	2A	1122	G
1	2A	1126	A
1	2A	1128	A
1	2A	1129	A
1	2A	1130	U
1	2A	1132	A
1	2A	1135	C
1	2A	1136	G
1	2A	1137	G
1	2A	1139	G
1	2A	1141	U
1	2A	1142(A)	A
1	2A	1171	G
1	2A	1195	G
1	2A	1206	G
1	2A	1210	A
1	2A	1211	U
1	2A	1220	A
1	2A	1229	G
1	2A	1236	G
1	2A	1237	A
1	2A	1244	G
1	2A	1250	G
1	2A	1253	A
1	2A	1256	G
1	2A	1268	A
1	2A	1271	G
1	2A	1272	A
1	2A	1273	U
1	2A	1285	G
1	2A	1300	U
1	2A	1301	A
1	2A	1314	C
1	2A	1332	G
1	2A	1352	U
1	2A	1359	A
1	2A	1360	A
1	2A	1365	A
1	2A	1368	G
1	2A	1370	C
1	2A	1378	A

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Mol	Chain	Res	Type
1	2A	1379	A
1	2A	1384	A
1	2A	1385	G
1	2A	1386	C
1	2A	1395	A
1	2A	1411	C
1	2A	1416	G
1	2A	1417	C
1	2A	1421	G
1	2A	1425	G
1	2A	1426	G
1	2A	1427	A
1	2A	1428	C
1	2A	1437	C
1	2A	1445	A
1	2A	1449	A
1	2A	1450	G
1	2A	1452	A
1	2A	1453	U
1	2A	1455	G
1	2A	1459	G
1	2A	1460	A
1	2A	1461	G
1	2A	1467	C
1	2A	1471	A
1	2A	1472	A
1	2A	1482	G
1	2A	1490	A
1	2A	1493	C
1	2A	1494	A
1	2A	1496	A
1	2A	1497	U
1	2A	1506	C
1	2A	1509	C
1	2A	1509(A)	A
1	2A	1531	C
1	2A	1532	C
1	2A	1539	G
1	2A	1542	A
1	2A	1543	C
1	2A	1547	C
1	2A	1558	A

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Mol	Chain	Res	Type
1	2A	1566	A
1	2A	1569	A
1	2A	1578	U
1	2A	1580	A
1	2A	1584	C
1	2A	1608	A
1	2A	1610	A
1	2A	1634	A
1	2A	1640	C
1	2A	1648	C
1	2A	1654	A
1	2A	1664	A
1	2A	1674	G
1	2A	1675	C
1	2A	1680	U
1	2A	1682	G
1	2A	1696	G
1	2A	1700	A
1	2A	1701	A
1	2A	1706	U
1	2A	1721	G
1	2A	1722	A
1	2A	1739	U
1	2A	1740	G
1	2A	1745(A)	C
1	2A	1746	G
1	2A	1756	G
1	2A	1758	G
1	2A	1762	A
1	2A	1763	G
1	2A	1764	G
1	2A	1773	A
1	2A	1780	A
1	2A	1782	C
1	2A	1791	A
1	2A	1800	C
1	2A	1801	G
1	2A	1811	G
1	2A	1812	A
1	2A	1816	G
1	2A	1820	U
1	2A	1835	G

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Mol	Chain	Res	Type
1	2A	1847	A
1	2A	1848	A
1	2A	1857	G
1	2A	1861	G
1	2A	1877	A
1	2A	1878	G
1	2A	1900	A
1	2A	1906	G
1	2A	1913	A
1	2A	1914	C
1	2A	1926	U
1	2A	1929	G
1	2A	1930	G
1	2A	1936	A
1	2A	1937	A
1	2A	1938	A
1	2A	1952	A
1	2A	1955	U
1	2A	1963	U
1	2A	1965	C
1	2A	1966	A
1	2A	1967	C
1	2A	1970	A
1	2A	1971	A
1	2A	1972	A
1	2A	1984	G
1	2A	1993	U
1	2A	1997	G
1	2A	2020	A
1	2A	2023	G
1	2A	2031	A
1	2A	2033	A
1	2A	2036	C
1	2A	2043	C
1	2A	2055	C
1	2A	2056	G
1	2A	2060	A
1	2A	2061	G
1	2A	2069	G
1	2A	2093	G
1	2A	2099	U
1	2A	2101	G

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Mol	Chain	Res	Type
1	2A	2110	G
1	2A	2111	C
1	2A	2115	G
1	2A	2116	G
1	2A	2117	A
1	2A	2118	U
1	2A	2119	A
1	2A	2120	G
1	2A	2122	U
1	2A	2125	G
1	2A	2126	A
1	2A	2127	G
1	2A	2131	G
1	2A	2132	U
1	2A	2133	G
1	2A	2134	A
1	2A	2135	A
1	2A	2137	C
1	2A	2138	C
1	2A	2139	C
1	2A	2140	C
1	2A	2141	G
1	2A	2142	C
1	2A	2146	C
1	2A	2148	G
1	2A	2149	G
1	2A	2150	U
1	2A	2156	G
1	2A	2157	G
1	2A	2158	A
1	2A	2161	C
1	2A	2165	G
1	2A	2166	G
1	2A	2167	U
1	2A	2168	G
1	2A	2171	A
1	2A	2172	U
1	2A	2174	C
1	2A	2178	C
1	2A	2181	G
1	2A	2188	C
1	2A	2189	U

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Mol	Chain	Res	Type
1	2A	2191	G
1	2A	2192	G
1	2A	2198	A
1	2A	2206	G
1	2A	2207	G
1	2A	2208	A
1	2A	2218	U
1	2A	2225	A
1	2A	2238	G
1	2A	2239	G
1	2A	2259	G
1	2A	2273	A
1	2A	2275	C
1	2A	2278	A
1	2A	2283	C
1	2A	2287	A
1	2A	2288	A
1	2A	2305	A
1	2A	2307	G
1	2A	2308	G
1	2A	2309	A
1	2A	2311	A
1	2A	2319	G
1	2A	2320	A
1	2A	2325	G
1	2A	2327	A
1	2A	2334	G
1	2A	2336	A
1	2A	2346	A
1	2A	2347	C
1	2A	2376	A
1	2A	2383	G
1	2A	2385	C
1	2A	2387	U
1	2A	2406	U
1	2A	2410	G
1	2A	2425	A
1	2A	2428	G
1	2A	2429	G
1	2A	2430	A
1	2A	2431	U
1	2A	2435	A

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Mol	Chain	Res	Type
1	2A	2439	A
1	2A	2441	C
1	2A	2445	G
1	2A	2448	A
1	2A	2449	U
1	2A	2459	A
1	2A	2465	C
1	2A	2469	A
1	2A	2476	A
1	2A	2480	C
1	2A	2481	G
1	2A	2486	G
1	2A	2489	G
1	2A	2490	G
1	2A	2491	U
1	2A	2494	G
1	2A	2502	G
1	2A	2505	G
1	2A	2506	U
1	2A	2507	C
1	2A	2518	A
1	2A	2520	C
1	2A	2529	G
1	2A	2554	U
1	2A	2555	U
1	2A	2564	A
1	2A	2566	A
1	2A	2567	G
1	2A	2582	G
1	2A	2602	A
1	2A	2609	U
1	2A	2611	U
1	2A	2612	C
1	2A	2630	G
1	2A	2679	A
1	2A	2689	U
1	2A	2690	C
1	2A	2691	C
1	2A	2702	U
1	2A	2712(A)	A
1	2A	2713	A
1	2A	2714	G

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Mol	Chain	Res	Type
1	2A	2718	G
1	2A	2726	U
1	2A	2733	A
1	2A	2739	U
1	2A	2751	G
1	2A	2752	C
1	2A	2758	A
1	2A	2761	G
1	2A	2764	A
1	2A	2765	A
1	2A	2778	A
1	2A	2780	G
1	2A	2789	C
1	2A	2793	G
1	2A	2807	G
1	2A	2808	U
1	2A	2820	A
1	2A	2821	A
1	2A	2835	A
1	2A	2872	G
1	2A	2873	A
1	2A	2880	C
1	2A	2892	A
1	2A	2894	G
1	2A	2896	C
1	2A	2897	U
2	2B	2	C
2	2B	5	C
2	2B	8	U
2	2B	12	C
2	2B	13	A
2	2B	16	G
2	2B	17	C
2	2B	24	G
2	2B	29	A
2	2B	33	G
2	2B	34	U
2	2B	41	U
2	2B	42	C
2	2B	53	A
2	2B	63	G
2	2B	67	G

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Mol	Chain	Res	Type
2	2B	73	A
2	2B	74	U
2	2B	75	G
2	2B	84	C
2	2B	85	G
2	2B	88	C
2	2B	105	A
2	2B	106	G
2	2B	108	U
2	2B	110	G
2	2B	116	G
2	2B	120	A
32	2a	5	U
32	2a	9	G
32	2a	22	G
32	2a	31	G
32	2a	32	A
32	2a	39	G
32	2a	47	C
32	2a	48	C
32	2a	50	A
32	2a	51	A
32	2a	52	G
32	2a	65	U
32	2a	66	G
32	2a	73	G
32	2a	88	A
32	2a	89	C
32	2a	98	G
32	2a	101	A
32	2a	116	A
32	2a	121	C
32	2a	131	C
32	2a	137	C
32	2a	144	G
32	2a	146	G
32	2a	148	G
32	2a	163	C
32	2a	180	U
32	2a	182	U
32	2a	184	G
32	2a	189	G

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Mol	Chain	Res	Type
32	2a	189(B)	C
32	2a	189(E)	U
32	2a	189(G)	G
32	2a	189(H)	G
32	2a	195	A
32	2a	197	A
32	2a	201	C
32	2a	202	U
32	2a	203	U
32	2a	204	U
32	2a	216	G
32	2a	217	C
32	2a	231	G
32	2a	247	G
32	2a	249	U
32	2a	251	G
32	2a	258	G
32	2a	266	G
32	2a	267	C
32	2a	274	A
32	2a	279	A
32	2a	281	G
32	2a	289	G
32	2a	306	G
32	2a	318	G
32	2a	321	A
32	2a	328	C
32	2a	330	C
32	2a	332	G
32	2a	338	A
32	2a	345	C
32	2a	346	G
32	2a	348	G
32	2a	349	A
32	2a	351	G
32	2a	352	C
32	2a	353	A
32	2a	354	G
32	2a	355	C
32	2a	363	A
32	2a	365	U
32	2a	367	U

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Mol	Chain	Res	Type
32	2a	372	C
32	2a	373	A
32	2a	380	G
32	2a	381	C
32	2a	384	G
32	2a	397	A
32	2a	398	C
32	2a	406	G
32	2a	412	A
32	2a	413	G
32	2a	421	U
32	2a	423	G
32	2a	424	G
32	2a	429	U
32	2a	430	A
32	2a	439	A
32	2a	441	A
32	2a	442	C
32	2a	452	A
32	2a	470	C
32	2a	480	U
32	2a	481	G
32	2a	484	G
32	2a	485	G
32	2a	492	G
32	2a	495	A
32	2a	496	A
32	2a	498	U
32	2a	505	G
32	2a	506	G
32	2a	509	A
32	2a	510	A
32	2a	511	C
32	2a	517	G
32	2a	518	C
32	2a	521	G
32	2a	527	G7M
32	2a	531	U
32	2a	532	A
32	2a	547	A
32	2a	562	C
32	2a	564	C

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Mol	Chain	Res	Type
32	2a	568	G
32	2a	572	A
32	2a	573	A
32	2a	574	A
32	2a	575	G
32	2a	576	G
32	2a	577	G
32	2a	596	C
32	2a	597	G
32	2a	601	C
32	2a	618	C
32	2a	621	A
32	2a	630	G
32	2a	638	G
32	2a	642	A
32	2a	650	G
32	2a	653	A
32	2a	657	G
32	2a	662	G
32	2a	665	A
32	2a	687	A
32	2a	688	G
32	2a	690	G
32	2a	693	G
32	2a	695	A
32	2a	702	A
32	2a	703	G
32	2a	708	C
32	2a	721	G
32	2a	723	U
32	2a	731	G
32	2a	749	C
32	2a	752	G
32	2a	753	A
32	2a	755	G
32	2a	761	G
32	2a	773	G
32	2a	792	A
32	2a	793	U
32	2a	794	A
32	2a	815	A
32	2a	817	C

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Mol	Chain	Res	Type
32	2a	818	G
32	2a	819	A
32	2a	821	G
32	2a	828	A
32	2a	840	C
32	2a	841	U
32	2a	848	C
32	2a	851	G
32	2a	858	G
32	2a	859	A
32	2a	864	A
32	2a	871	U
32	2a	872	A
32	2a	873	A
32	2a	902	G
32	2a	908	A
32	2a	914	A
32	2a	921	U
32	2a	926	G
32	2a	927	G
32	2a	934	C
32	2a	935	A
32	2a	937	A
32	2a	938	A
32	2a	958	A
32	2a	960	U
32	2a	961	U
32	2a	962	C
32	2a	963	G
32	2a	968	A
32	2a	969	A
32	2a	970	C
32	2a	971	G
32	2a	974	A
32	2a	975	A
32	2a	976	G
32	2a	977	A
32	2a	978	A
32	2a	979	C
32	2a	982	U
32	2a	986	A
32	2a	989	C

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Mol	Chain	Res	Type
32	2a	992	U
32	2a	993	G
32	2a	995	C
32	2a	997	U
32	2a	1001	A
32	2a	1001(A)	G
32	2a	1002	G
32	2a	1003	G
32	2a	1004	A
32	2a	1005	A
32	2a	1006	C
32	2a	1009	G
32	2a	1016	A
32	2a	1020	U
32	2a	1021	G
32	2a	1022	G
32	2a	1025	U
32	2a	1026	G
32	2a	1027	C
32	2a	1029	C
32	2a	1030	C
32	2a	1031	G
32	2a	1032	G
32	2a	1033	G
32	2a	1035	A
32	2a	1038	C
32	2a	1039	C
32	2a	1040	U
32	2a	1042	G
32	2a	1045	C
32	2a	1046	A
32	2a	1050	G
32	2a	1056	U
32	2a	1065	U
32	2a	1066	C
32	2a	1068	G
32	2a	1077	G
32	2a	1079	G
32	2a	1081	G
32	2a	1084	G
32	2a	1085	U
32	2a	1086	U

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Mol	Chain	Res	Type
32	2a	1092	A
32	2a	1094	G
32	2a	1095	U
32	2a	1101	A
32	2a	1105	A
32	2a	1107	C
32	2a	1112	C
32	2a	1113	C
32	2a	1118	C
32	2a	1124	G
32	2a	1126	U
32	2a	1129	C
32	2a	1132	C
32	2a	1133	G
32	2a	1135	U
32	2a	1136	U
32	2a	1137	C
32	2a	1138	G
32	2a	1139	G
32	2a	1140	C
32	2a	1141	C
32	2a	1142	G
32	2a	1146	A
32	2a	1147	C
32	2a	1152	A
32	2a	1155	G
32	2a	1157	A
32	2a	1159	U
32	2a	1160	G
32	2a	1173	G
32	2a	1181	G
32	2a	1182	G
32	2a	1183	A
32	2a	1184	G
32	2a	1191	A
32	2a	1193	G
32	2a	1194	U
32	2a	1196	U
32	2a	1197	G
32	2a	1202	G
32	2a	1209	C
32	2a	1211	U

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Mol	Chain	Res	Type
32	2a	1212	U
32	2a	1213	A
32	2a	1214	C
32	2a	1215	G
32	2a	1225	A
32	2a	1226	C
32	2a	1227	A
32	2a	1238	A
32	2a	1240	U
32	2a	1241	G
32	2a	1249	C
32	2a	1250	A
32	2a	1256	A
32	2a	1257	U
32	2a	1258	G
32	2a	1260	C
32	2a	1261	A
32	2a	1262	C
32	2a	1270	C
32	2a	1272	G
32	2a	1273	G
32	2a	1275	A
32	2a	1278	U
32	2a	1279	A
32	2a	1280	A
32	2a	1283	G
32	2a	1285	A
32	2a	1286	A
32	2a	1287	A
32	2a	1291	G
32	2a	1293	G
32	2a	1299	A
32	2a	1300	G
32	2a	1302	U
32	2a	1305	G
32	2a	1312	G
32	2a	1320	C
32	2a	1322	C
32	2a	1323	G
32	2a	1336	C
32	2a	1340	A
32	2a	1345	U

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Mol	Chain	Res	Type
32	2a	1346	A
32	2a	1347	G
32	2a	1353	G
32	2a	1363	C
32	2a	1368	G
32	2a	1370	G
32	2a	1379	G
32	2a	1380	U
32	2a	1381	U
32	2a	1386	G
32	2a	1397	C
32	2a	1399	C
32	2a	1400	5MC
32	2a	1401	G
32	2a	1419	G
32	2a	1440	C
32	2a	1442	G
32	2a	1442(A)	G
32	2a	1442(B)	A
32	2a	1447	A
32	2a	1456	G
32	2a	1492	A
32	2a	1494	G
32	2a	1499	A
32	2a	1503	A
32	2a	1504	G
32	2a	1506	U
32	2a	1507	A
32	2a	1508	G
32	2a	1517	G
32	2a	1529	G
32	2a	1530	G
32	2a	1531	A
32	2a	1532	U
53	2v	13	A
53	2v	19	U
53	2v	24	A
54	2w	3	C
54	2w	4	C
54	2w	7	A
54	2w	9	A
54	2w	11	C

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Mol	Chain	Res	Type
54	2w	14	A
54	2w	15	G
54	2w	19	G
54	2w	22	G
54	2w	46	G7M
54	2w	47	U
54	2w	48	C
54	2w	60	U
54	2w	61	C
54	2w	62	C
54	2w	67	C
54	2w	69	G
54	2w	70	G
54	2w	72	C
54	2w	73	A
54	2w	74	C
55	2x	5	G
55	2x	8	4SU
55	2x	9	G
55	2x	18	G
55	2x	19	G
55	2x	22	G
55	2x	31	G
55	2x	43	A
55	2x	47	U
55	2x	56	C
55	2x	63	G
55	2x	76	A
54	2y	5	G
54	2y	8	4SU
54	2y	12	U
54	2y	14	A
54	2y	15	G
54	2y	19	G
54	2y	25	C
54	2y	35	A
54	2y	41	C
54	2y	42	C
54	2y	48	C
54	2y	49	C
54	2y	51	U
54	2y	52	G

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Mol	Chain	Res	Type
54	2y	57	G
54	2y	58	A
54	2y	59	U
54	2y	62	C
54	2y	65	G
54	2y	69	G
54	2y	70	G
54	2y	71	G
54	2y	72	C
54	2y	73	A

All (44) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	196	A
1	1A	266	G
1	1A	278	A
1	1A	548	A
1	1A	746	A
1	1A	774	A
1	1A	827	U
1	1A	1033	U
1	1A	1067	A
1	1A	1174	A
1	1A	1176	G
1	1A	1442	G
1	1A	1508	A
1	1A	1992	G
1	1A	2126	A
1	1A	2134	A
1	1A	2181	G
1	1A	2183	C
1	1A	2406	U
1	1A	2422	A
1	1A	2439	A
1	1A	2756	U
1	2A	196	A
1	2A	228	A
1	2A	266	G
1	2A	271(M)	G
1	2A	277	C
1	2A	752	A

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Mol	Chain	Res	Type
1	2A	856	C
1	2A	1026	U
1	2A	1210	A
1	2A	1420	U
1	2A	1460	A
1	2A	1509	C
1	2A	1529	G
1	2A	1530	C
1	2A	1653	G
1	2A	1913	A
1	2A	1935	G
1	2A	1992	G
1	2A	2119	A
1	2A	2126	A
1	2A	2430	A
1	2A	2689	U

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

84 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	PSU	2w	32	54	18,21,22	1.33	2 (11%)	22,30,33	1.95	4 (18%)
1	5MU	1A	1939	1,56	19,22,23	1.54	6 (31%)	28,32,35	2.36	5 (17%)
1	PSU	2A	2605	1	18,21,22	1.39	3 (16%)	22,30,33	1.82	4 (18%)
1	PSU	1A	2605	1,56	18,21,22	1.43	4 (22%)	22,30,33	1.92	4 (18%)
54	PSU	2y	39	54	18,21,22	1.34	2 (11%)	22,30,33	1.71	3 (13%)
32	5MC	1a	1400	32	18,22,23	0.94	2 (11%)	26,32,35	1.09	2 (7%)
32	5MC	1a	1407	32	18,22,23	0.96	2 (11%)	26,32,35	1.10	2 (7%)
54	MIA	2y	37	54	18,24,32	1.14	2 (11%)	18,35,47	1.34	2 (11%)
1	5MU	2A	1915	1	19,22,23	1.46	6 (31%)	28,32,35	2.06	5 (17%)
32	UR3	1a	1498	32	19,22,23	0.99	0	26,32,35	1.46	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
54	PSU	1y	55	54	18,21,22	1.38	2 (11%)	22,30,33	1.87	3 (13%)
1	5MC	2A	1962	1,56	18,22,23	0.98	2 (11%)	26,32,35	1.18	2 (7%)
55	5MU	1x	54	55	19,22,23	1.39	5 (26%)	28,32,35	1.95	8 (28%)
54	5MU	2y	54	54	19,22,23	1.36	4 (21%)	28,32,35	1.83	7 (25%)
55	4SU	1x	8	55	18,21,22	2.03	4 (22%)	26,30,33	1.46	5 (19%)
55	5MC	2x	32	55	18,22,23	1.01	2 (11%)	26,32,35	1.27	3 (11%)
54	4SU	2y	8	54	18,21,22	1.71	4 (22%)	26,30,33	2.38	6 (23%)
1	PSU	2A	1911	1	18,21,22	1.39	2 (11%)	22,30,33	1.78	4 (18%)
1	OMC	1A	1920	1	19,22,23	0.84	0	26,31,34	0.99	1 (3%)
54	PSU	2w	55	54	18,21,22	1.35	2 (11%)	22,30,33	1.83	3 (13%)
1	5MU	1A	1915	1	19,22,23	1.44	4 (21%)	28,32,35	1.98	6 (21%)
55	5MU	2x	54	55	19,22,23	1.42	5 (26%)	28,32,35	2.10	6 (21%)
32	G7M	1a	527	32,56	20,26,27	1.28	2 (10%)	17,39,42	0.56	0
32	M2G	2a	966	32	20,27,28	1.47	3 (15%)	22,40,43	0.96	2 (9%)
54	G7M	2y	46	54	20,26,27	1.38	2 (10%)	17,39,42	0.78	0
54	PSU	1w	32	54,56	18,21,22	1.33	2 (11%)	22,30,33	1.78	3 (13%)
32	4OC	2a	1402	32,56	20,23,24	0.79	0	26,32,35	1.00	1 (3%)
55	4SU	2x	8	55	18,21,22	1.95	6 (33%)	26,30,33	1.54	6 (23%)
54	PSU	1w	39	54	18,21,22	1.30	2 (11%)	22,30,33	1.75	3 (13%)
32	UR3	2a	1498	32	19,22,23	1.04	1 (5%)	26,32,35	1.54	3 (11%)
54	5MU	1w	54	54	19,22,23	1.38	4 (21%)	28,32,35	1.90	7 (25%)
1	PSU	1A	1911	1	18,21,22	1.44	2 (11%)	22,30,33	1.89	3 (13%)
1	2MA	2A	2503	1	17,25,26	0.94	0	17,37,40	0.95	2 (11%)
54	PSU	2w	39	54	18,21,22	1.30	2 (11%)	22,30,33	1.75	3 (13%)
1	OMU	2A	2552	1,56	19,22,23	1.23	2 (10%)	26,31,34	1.71	5 (19%)
32	5MC	2a	1407	32	18,22,23	0.93	2 (11%)	26,32,35	1.13	3 (11%)
54	G7M	1w	46	54	20,26,27	1.29	1 (5%)	17,39,42	0.73	0
54	4SU	1w	8	54	18,21,22	1.73	5 (27%)	26,30,33	1.82	4 (15%)
32	M2G	1a	966	32	20,27,28	1.54	3 (15%)	22,40,43	1.02	2 (9%)
54	MIA	2w	37	53,54	20,27,32	1.86	3 (15%)	22,39,47	2.24	7 (31%)
32	MA6	1a	1519	32	18,26,27	0.80	0	19,38,41	1.53	2 (10%)
1	2MA	1A	2503	1,56	17,25,26	0.97	1 (5%)	17,37,40	1.01	2 (11%)
32	2MG	2a	1207	32	18,26,27	0.98	1 (5%)	16,38,41	0.96	1 (6%)
54	5MU	1y	54	54	19,22,23	1.38	4 (21%)	28,32,35	1.84	5 (17%)
32	MA6	1a	1518	32	18,26,27	0.79	0	19,38,41	1.41	2 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
32	5MC	2a	967	32	18,22,23	0.96	2 (11%)	26,32,35	1.13	2 (7%)
55	PSU	1x	55	55	18,21,22	1.38	2 (11%)	22,30,33	1.87	3 (13%)
43	0TD	2l	92	43	7,9,10	4.68	1 (14%)	6,11,13	7.22	2 (33%)
54	MIA	1y	37	54	18,24,32	1.17	2 (11%)	18,35,47	1.25	2 (11%)
1	5MC	1A	1962	1,56	18,22,23	0.96	2 (11%)	26,32,35	1.12	3 (11%)
32	4OC	1a	1402	32	20,23,24	0.75	0	26,32,35	0.94	1 (3%)
54	MIA	1w	37	54	24,31,32	2.10	4 (16%)	26,44,47	2.47	8 (30%)
32	5MC	2a	1400	32	18,22,23	1.01	1 (5%)	26,32,35	1.25	4 (15%)
54	PSU	1y	32	54	18,21,22	1.34	3 (16%)	22,30,33	1.81	4 (18%)
32	PSU	1a	516	32	18,21,22	1.38	2 (11%)	22,30,33	1.81	4 (18%)
1	5MU	2A	1939	1	19,22,23	1.45	5 (26%)	28,32,35	2.23	6 (21%)
54	PSU	1y	39	54	18,21,22	1.42	2 (11%)	22,30,33	1.58	2 (9%)
1	PSU	2A	1917	1	18,21,22	1.38	3 (16%)	22,30,33	1.91	3 (13%)
54	PSU	2y	32	54	18,21,22	1.35	2 (11%)	22,30,33	1.86	4 (18%)
32	5MC	2a	1404	32	18,22,23	0.97	2 (11%)	26,32,35	1.16	3 (11%)
1	OMG	1A	2251	55,1,56	18,26,27	0.95	1 (5%)	19,38,41	1.26	4 (21%)
1	PSU	1A	1917	1	18,21,22	1.35	2 (11%)	22,30,33	1.99	5 (22%)
32	MA6	2a	1518	32	18,26,27	0.82	0	19,38,41	1.46	2 (10%)
32	MA6	2a	1519	32	18,26,27	0.80	0	19,38,41	1.52	2 (10%)
32	5MC	1a	1404	32	18,22,23	0.93	2 (11%)	26,32,35	1.17	3 (11%)
32	2MG	1a	1207	32	18,26,27	1.01	1 (5%)	16,38,41	1.08	1 (6%)
55	5MC	1x	32	55	18,22,23	0.97	2 (11%)	26,32,35	1.21	2 (7%)
1	OMG	2A	2251	55,1,56	18,26,27	0.97	1 (5%)	19,38,41	1.08	2 (10%)
32	5MC	1a	967	32	18,22,23	0.97	2 (11%)	26,32,35	1.11	2 (7%)
54	4SU	1y	8	54	18,21,22	1.70	5 (27%)	26,30,33	1.70	5 (19%)
54	5MU	2w	54	54	19,22,23	1.41	4 (21%)	28,32,35	1.80	6 (21%)
43	0TD	1l	92	43	7,9,10	4.89	1 (14%)	6,11,13	5.38	2 (33%)
1	5MC	2A	1942	1	18,22,23	0.98	2 (11%)	26,32,35	1.14	3 (11%)
54	PSU	2y	55	54	18,21,22	1.35	3 (16%)	22,30,33	1.87	4 (18%)
54	G7M	2w	46	54	20,26,27	1.14	1 (5%)	17,39,42	0.96	0
55	PSU	2x	55	55	18,21,22	1.35	2 (11%)	22,30,33	1.80	3 (13%)
1	OMC	2A	1920	1	19,22,23	0.79	0	26,31,34	0.83	0
54	G7M	1y	46	54	20,26,27	1.41	2 (10%)	17,39,42	0.75	0
1	OMU	1A	2552	1,56	19,22,23	1.27	2 (10%)	26,31,34	1.78	4 (15%)
32	PSU	2a	516	32	18,21,22	1.32	2 (11%)	22,30,33	1.77	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
54	4SU	2w	8	54	18,21,22	1.60	5 (27%)	26,30,33	1.96	5 (19%)
54	PSU	1w	55	54	18,21,22	1.38	2 (11%)	22,30,33	1.80	4 (18%)
1	5MC	1A	1942	1	18,22,23	0.95	2 (11%)	26,32,35	1.24	2 (7%)
32	G7M	2a	527	32,56	20,26,27	1.19	2 (10%)	17,39,42	0.63	0

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	PSU	2w	32	54	-	0/7/25/26	0/2/2/2
1	5MU	1A	1939	1,56	-	0/7/25/26	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
1	PSU	1A	2605	1,56	-	0/7/25/26	0/2/2/2
54	PSU	2y	39	54	-	0/7/25/26	0/2/2/2
32	5MC	1a	1400	32	-	2/7/25/26	0/2/2/2
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
54	MIA	2y	37	54	-	2/3/25/34	0/3/3/3
1	5MU	2A	1915	1	-	0/7/25/26	0/2/2/2
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
54	PSU	1y	55	54	-	2/7/25/26	0/2/2/2
1	5MC	2A	1962	1,56	-	0/7/25/26	0/2/2/2
55	5MU	1x	54	55	-	0/7/25/26	0/2/2/2
54	5MU	2y	54	54	-	0/7/25/26	0/2/2/2
55	4SU	1x	8	55	-	0/7/25/26	0/2/2/2
55	5MC	2x	32	55	-	0/7/25/26	0/2/2/2
54	4SU	2y	8	54	-	4/7/25/26	0/2/2/2
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
1	OMC	1A	1920	1	-	1/9/27/28	0/2/2/2
54	PSU	2w	55	54	-	0/7/25/26	0/2/2/2
1	5MU	1A	1915	1	-	0/7/25/26	0/2/2/2
55	5MU	2x	54	55	-	0/7/25/26	0/2/2/2
32	G7M	1a	527	32,56	-	2/3/25/26	0/3/3/3
32	M2G	2a	966	32	-	0/7/29/30	0/3/3/3
54	G7M	2y	46	54	-	0/3/25/26	0/3/3/3
54	PSU	1w	32	54,56	-	0/7/25/26	0/2/2/2
32	4OC	2a	1402	32,56	-	2/9/29/30	0/2/2/2
55	4SU	2x	8	55	-	0/7/25/26	0/2/2/2
54	PSU	1w	39	54	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	UR3	2a	1498	32	-	2/7/25/26	0/2/2/2
54	5MU	1w	54	54	-	0/7/25/26	0/2/2/2
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
1	2MA	2A	2503	1	-	1/3/25/26	0/3/3/3
54	PSU	2w	39	54	-	0/7/25/26	0/2/2/2
1	OMU	2A	2552	1,56	-	0/9/27/28	0/2/2/2
32	5MC	2a	1407	32	-	0/7/25/26	0/2/2/2
54	G7M	1w	46	54	-	3/3/25/26	0/3/3/3
54	4SU	1w	8	54	-	0/7/25/26	0/2/2/2
32	M2G	1a	966	32	-	0/7/29/30	0/3/3/3
54	MIA	2w	37	53,54	-	2/7/29/34	0/3/3/3
32	MA6	1a	1519	32	-	3/7/29/30	0/3/3/3
1	2MA	1A	2503	1,56	-	1/3/25/26	0/3/3/3
32	2MG	2a	1207	32	-	2/5/27/28	0/3/3/3
54	5MU	1y	54	54	-	0/7/25/26	0/2/2/2
32	MA6	1a	1518	32	-	0/7/29/30	0/3/3/3
32	5MC	2a	967	32	-	0/7/25/26	0/2/2/2
55	PSU	1x	55	55	-	0/7/25/26	0/2/2/2
43	0TD	2l	92	43	-	2/7/12/14	-
54	MIA	1y	37	54	-	3/3/25/34	0/3/3/3
1	5MC	1A	1962	1,56	-	2/7/25/26	0/2/2/2
32	4OC	1a	1402	32	-	0/9/29/30	0/2/2/2
54	MIA	1w	37	54	-	3/11/33/34	0/3/3/3
32	5MC	2a	1400	32	-	6/7/25/26	0/2/2/2
54	PSU	1y	32	54	-	0/7/25/26	0/2/2/2
32	PSU	1a	516	32	-	0/7/25/26	0/2/2/2
1	5MU	2A	1939	1	-	0/7/25/26	0/2/2/2
54	PSU	1y	39	54	-	0/7/25/26	0/2/2/2
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
54	PSU	2y	32	54	-	0/7/25/26	0/2/2/2
32	5MC	2a	1404	32	-	0/7/25/26	0/2/2/2
1	OMG	1A	2251	55,1,56	-	1/5/27/28	0/3/3/3
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
32	MA6	2a	1518	32	-	2/7/29/30	0/3/3/3
32	MA6	2a	1519	32	-	3/7/29/30	0/3/3/3
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
32	2MG	1a	1207	32	-	0/5/27/28	0/3/3/3
55	5MC	1x	32	55	-	0/7/25/26	0/2/2/2
1	OMG	2A	2251	55,1,56	-	1/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	5MC	1a	967	32	-	2/7/25/26	0/2/2/2
54	4SU	1y	8	54	-	0/7/25/26	0/2/2/2
54	5MU	2w	54	54	-	0/7/25/26	0/2/2/2
43	0TD	1l	92	43	-	3/7/12/14	-
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
54	PSU	2y	55	54	-	1/7/25/26	0/2/2/2
54	G7M	2w	46	54	-	2/3/25/26	0/3/3/3
55	PSU	2x	55	55	-	0/7/25/26	0/2/2/2
1	OMC	2A	1920	1	-	1/9/27/28	0/2/2/2
54	G7M	1y	46	54	-	1/3/25/26	0/3/3/3
1	OMU	1A	2552	1,56	-	0/9/27/28	0/2/2/2
32	PSU	2a	516	32	-	0/7/25/26	0/2/2/2
54	4SU	2w	8	54	-	0/7/25/26	0/2/2/2
54	PSU	1w	55	54	-	0/7/25/26	0/2/2/2
1	5MC	1A	1942	1	-	0/7/25/26	0/2/2/2
32	G7M	2a	527	32,56	-	3/3/25/26	0/3/3/3

All (192) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	1l	92	0TD	CB-SB	-12.54	1.69	1.82
43	2l	92	0TD	CB-SB	-12.06	1.69	1.82
54	1w	37	MIA	C13-C14	7.22	1.53	1.32
54	2w	37	MIA	C2-S10	-6.94	1.69	1.75
54	1w	37	MIA	C2-S10	-5.14	1.71	1.75
32	1a	966	M2G	C2-N3	4.98	1.36	1.30
32	2a	966	M2G	C2-N3	4.79	1.36	1.30
55	1x	8	4SU	C4-N3	-4.67	1.32	1.37
54	2y	8	4SU	C4-S4	-4.36	1.60	1.68
54	1w	8	4SU	C4-S4	-4.34	1.60	1.68
55	2x	8	4SU	C4-N3	-4.27	1.33	1.37
54	2y	46	G7M	C5-C4	4.21	1.47	1.39
54	1y	46	G7M	C5-C4	4.17	1.47	1.39
54	1y	8	4SU	C4-S4	-4.06	1.60	1.68
55	1x	8	4SU	C4-S4	-4.05	1.60	1.68
54	1w	46	G7M	C5-C4	3.96	1.47	1.39
54	2w	8	4SU	C4-S4	-3.91	1.61	1.68
54	1w	55	PSU	C6-C5	3.90	1.39	1.35
55	2x	8	4SU	C4-S4	-3.89	1.61	1.68
32	1a	527	G7M	C5-C4	3.88	1.46	1.39
54	2y	32	PSU	C6-C5	3.87	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	1y	55	PSU	C6-C5	3.86	1.39	1.35
54	1y	39	PSU	C6-C5	3.79	1.39	1.35
55	1x	55	PSU	C6-C5	3.75	1.39	1.35
54	2w	55	PSU	C6-C5	3.65	1.39	1.35
1	1A	1911	PSU	C6-C5	3.62	1.39	1.35
54	2w	32	PSU	C6-C5	3.61	1.39	1.35
54	2w	39	PSU	C6-C5	3.60	1.39	1.35
32	2a	527	G7M	C5-C4	3.56	1.46	1.39
55	1x	8	4SU	C2-N3	-3.54	1.31	1.38
54	2y	39	PSU	C6-C5	3.54	1.39	1.35
54	2w	46	G7M	C5-C4	3.53	1.46	1.39
55	2x	55	PSU	C6-C5	3.48	1.39	1.35
54	1y	32	PSU	C6-C5	3.44	1.39	1.35
32	2a	516	PSU	C6-C5	3.39	1.39	1.35
1	2A	1911	PSU	C6-C5	3.38	1.39	1.35
1	1A	1917	PSU	C6-C5	3.34	1.39	1.35
1	1A	1939	5MU	C4-N3	-3.30	1.32	1.38
54	1w	32	PSU	C6-C5	3.30	1.39	1.35
55	2x	8	4SU	C5-C4	-3.28	1.38	1.42
1	1A	2552	OMU	C4-N3	-3.25	1.32	1.38
55	1x	8	4SU	C5-C4	-3.25	1.38	1.42
54	1w	39	PSU	C6-C5	3.24	1.39	1.35
1	2A	1917	PSU	C6-C5	3.23	1.39	1.35
1	2A	2605	PSU	C6-C5	3.20	1.39	1.35
54	1w	8	4SU	C4-N3	-3.17	1.34	1.37
32	1a	516	PSU	C6-C5	3.06	1.38	1.35
54	1y	8	4SU	C4-N3	-3.06	1.34	1.37
54	2y	55	PSU	C6-C5	3.06	1.38	1.35
55	2x	32	5MC	C6-C5	3.05	1.39	1.34
1	1A	2605	PSU	C4-N3	-3.05	1.33	1.38
1	2A	1942	5MC	C6-C5	3.04	1.39	1.34
1	2A	2605	PSU	C4-N3	-2.97	1.33	1.38
32	2a	1404	5MC	C6-C5	2.95	1.39	1.34
1	2A	1915	5MU	C6-C5	2.93	1.39	1.34
54	1y	37	MIA	C2-N3	2.91	1.36	1.32
1	2A	1939	5MU	C4-N3	-2.90	1.33	1.38
1	2A	2552	OMU	C4-N3	-2.88	1.33	1.38
54	2y	8	4SU	C2-N1	2.86	1.43	1.38
54	2w	54	5MU	C6-C5	2.85	1.39	1.34
32	1a	967	5MC	C6-C5	2.84	1.39	1.34
54	1y	39	PSU	C4-N3	-2.84	1.33	1.38
1	1A	1911	PSU	C4-N3	-2.84	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	1x	32	5MC	C6-C5	2.84	1.39	1.34
32	1a	966	M2G	C2-N2	2.83	1.40	1.35
54	1w	54	5MU	C6-C5	2.82	1.39	1.34
54	1y	37	MIA	C5-C4	2.81	1.48	1.40
32	2a	966	M2G	C2-N2	2.80	1.40	1.35
54	2y	54	5MU	C6-C5	2.80	1.39	1.34
1	2A	1915	5MU	C4-N3	-2.80	1.33	1.38
54	2y	37	MIA	C5-C4	2.79	1.48	1.40
1	1A	1942	5MC	C6-C5	2.78	1.39	1.34
1	1A	2605	PSU	C6-C5	2.77	1.38	1.35
54	2w	37	MIA	C5-C4	2.77	1.48	1.40
1	1A	1915	5MU	C6-C5	2.77	1.39	1.34
55	2x	54	5MU	C6-C5	2.76	1.39	1.34
32	2a	1400	5MC	C6-C5	2.75	1.39	1.34
32	1a	1400	5MC	C6-C5	2.75	1.39	1.34
54	1y	46	G7M	C6-N1	-2.74	1.33	1.37
1	2A	2251	OMG	C6-N1	-2.72	1.33	1.37
1	1A	1939	5MU	C6-C5	2.72	1.39	1.34
1	2A	1939	5MU	C6-N1	-2.72	1.33	1.38
54	2y	8	4SU	C5-C4	-2.71	1.39	1.42
32	1a	1207	2MG	C6-N1	-2.71	1.33	1.37
54	2y	8	4SU	C4-N3	-2.70	1.34	1.37
54	1y	54	5MU	C6-C5	2.69	1.39	1.34
55	1x	54	5MU	C4-N3	-2.69	1.33	1.38
32	1a	1407	5MC	C6-C5	2.69	1.39	1.34
32	1a	966	M2G	C6-N1	-2.69	1.33	1.37
1	1A	1917	PSU	C4-N3	-2.68	1.33	1.38
1	2A	1939	5MU	C6-C5	2.68	1.39	1.34
54	1w	8	4SU	C5-C4	-2.67	1.39	1.42
32	1a	516	PSU	C4-N3	-2.67	1.33	1.38
1	2A	1917	PSU	C4-N3	-2.67	1.33	1.38
32	2a	967	5MC	C6-C5	2.66	1.39	1.34
1	1A	2251	OMG	C6-N1	-2.63	1.34	1.37
54	2w	8	4SU	C4-N3	-2.62	1.34	1.37
1	1A	1939	5MU	C2-N3	-2.62	1.33	1.38
55	2x	8	4SU	O2-C2	2.61	1.27	1.23
1	1A	1939	5MU	C6-N1	-2.61	1.33	1.38
54	1y	8	4SU	C2-N1	2.61	1.42	1.38
1	1A	1915	5MU	C4-N3	-2.57	1.34	1.38
1	1A	1915	5MU	C2-N1	2.56	1.42	1.38
55	1x	54	5MU	C6-C5	2.55	1.38	1.34
1	2A	1911	PSU	C4-N3	-2.55	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	1w	37	MIA	C5-C4	2.55	1.47	1.40
54	2y	37	MIA	C2-N3	2.55	1.36	1.32
1	2A	1962	5MC	C6-C5	2.55	1.38	1.34
54	1y	54	5MU	C4-N3	-2.54	1.34	1.38
55	1x	54	5MU	C4-C5	2.54	1.49	1.44
1	1A	1962	5MC	C6-C5	2.54	1.38	1.34
1	2A	1915	5MU	C2-N1	2.51	1.42	1.38
54	2w	54	5MU	C4-C5	2.51	1.49	1.44
54	1w	32	PSU	C4-N3	-2.50	1.34	1.38
54	1w	54	5MU	C4-N3	-2.50	1.34	1.38
54	2y	39	PSU	C4-N3	-2.50	1.34	1.38
1	2A	1962	5MC	C6-N1	-2.50	1.33	1.38
54	1w	39	PSU	C4-N3	-2.49	1.34	1.38
55	2x	54	5MU	C4-C5	2.49	1.48	1.44
55	2x	8	4SU	C2-N1	2.49	1.42	1.38
54	2w	8	4SU	C2-N1	2.48	1.42	1.38
1	1A	2552	OMU	C2-N3	-2.47	1.33	1.38
55	2x	55	PSU	C4-N3	-2.47	1.34	1.38
54	2w	32	PSU	C4-N3	-2.45	1.34	1.38
54	1y	54	5MU	C2-N1	2.44	1.42	1.38
55	2x	54	5MU	C2-N1	2.44	1.42	1.38
54	2w	55	PSU	C4-N3	-2.43	1.34	1.38
54	1w	37	MIA	C6-N1	2.43	1.36	1.32
1	2A	2552	OMU	C2-N3	-2.41	1.33	1.38
55	2x	54	5MU	C4-N3	-2.41	1.34	1.38
54	1y	32	PSU	C4-N3	-2.41	1.34	1.38
54	2y	54	5MU	C4-N3	-2.40	1.34	1.38
54	1w	54	5MU	C4-C5	2.40	1.48	1.44
1	1A	1962	5MC	C6-N1	-2.40	1.34	1.38
54	2y	46	G7M	C6-N1	-2.40	1.34	1.37
32	2a	1407	5MC	C6-C5	2.39	1.38	1.34
54	1y	55	PSU	C4-N3	-2.39	1.34	1.38
1	1A	1915	5MU	C4-C5	2.38	1.48	1.44
1	2A	2605	PSU	C2-N3	-2.37	1.33	1.37
32	2a	516	PSU	C4-N3	-2.36	1.34	1.38
54	2y	55	PSU	C4-N3	-2.35	1.34	1.38
32	1a	1404	5MC	C6-N1	-2.33	1.34	1.38
1	1A	1942	5MC	C6-N1	-2.31	1.34	1.38
1	1A	2605	PSU	C2-N3	-2.30	1.33	1.37
55	1x	32	5MC	C6-N1	-2.30	1.34	1.38
1	1A	1939	5MU	C4-C5	2.30	1.48	1.44
54	2w	54	5MU	C2-N1	2.30	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	2a	1498	UR3	C2-N1	2.30	1.41	1.38
54	2w	8	4SU	C5-C4	-2.29	1.39	1.42
55	1x	54	5MU	C6-N1	-2.28	1.34	1.38
32	2a	1207	2MG	C6-N1	-2.28	1.34	1.37
54	2w	54	5MU	C4-N3	-2.28	1.34	1.38
32	2a	1407	5MC	C6-N1	-2.27	1.34	1.38
1	2A	1915	5MU	C4-C5	2.27	1.48	1.44
54	2y	54	5MU	C2-N1	2.26	1.42	1.38
54	1w	55	PSU	C4-N3	-2.26	1.34	1.38
54	1y	8	4SU	C5-C4	-2.26	1.39	1.42
1	2A	1939	5MU	C4-C5	2.25	1.48	1.44
32	2a	966	M2G	C6-N1	-2.24	1.34	1.37
1	2A	1939	5MU	C2-N3	-2.24	1.34	1.38
32	1a	527	G7M	C6-N1	-2.23	1.34	1.37
32	2a	527	G7M	C6-N1	-2.23	1.34	1.37
32	1a	1404	5MC	C6-C5	2.22	1.38	1.34
54	2y	54	5MU	C4-C5	2.18	1.48	1.44
1	2A	1942	5MC	C6-N1	-2.18	1.34	1.38
55	2x	8	4SU	C2-N3	-2.17	1.34	1.38
32	1a	967	5MC	C6-N1	-2.17	1.34	1.38
54	2w	39	PSU	C4-N3	-2.17	1.34	1.38
32	1a	1407	5MC	C6-N1	-2.17	1.34	1.38
32	1a	1400	5MC	C6-N1	-2.16	1.34	1.38
1	2A	1915	5MU	C2-N3	-2.15	1.34	1.38
32	2a	967	5MC	C6-N1	-2.15	1.34	1.38
32	2a	1404	5MC	C6-N1	-2.15	1.34	1.38
1	2A	1915	5MU	C6-N1	-2.14	1.34	1.38
1	1A	2503	2MA	C2-N3	2.14	1.35	1.31
55	2x	54	5MU	C6-N1	-2.13	1.34	1.38
1	1A	1939	5MU	C2-N1	2.13	1.41	1.38
54	1y	54	5MU	C4-C5	2.11	1.48	1.44
54	2y	32	PSU	C4-N3	-2.09	1.35	1.38
54	2y	55	PSU	C2-N1	-2.09	1.33	1.36
54	1w	8	4SU	C2-N3	-2.09	1.34	1.38
54	1w	54	5MU	C6-N1	-2.08	1.34	1.38
54	1w	8	4SU	C2-N1	2.08	1.41	1.38
55	1x	55	PSU	C4-N3	-2.07	1.35	1.38
55	1x	54	5MU	C2-N3	-2.06	1.34	1.38
1	2A	1917	PSU	C2-N3	-2.06	1.34	1.37
54	2w	37	MIA	C6-N1	2.06	1.35	1.32
54	1y	8	4SU	C6-C5	2.05	1.39	1.35
54	1y	32	PSU	C4-C5	2.05	1.50	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	2x	32	5MC	C6-N1	-2.03	1.34	1.38
1	1A	2605	PSU	C2-N1	-2.02	1.34	1.36
54	2w	8	4SU	C6-C5	2.01	1.39	1.35

All (269) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	2l	92	0TD	CSB-SB-CB	-17.40	70.96	102.44
43	1l	92	0TD	CSB-SB-CB	-12.61	79.62	102.44
54	1w	37	MIA	C12-C13-C14	-7.55	112.44	127.14
54	2y	8	4SU	C4-N3-C2	-6.51	121.02	127.34
54	2w	37	MIA	C11-S10-C2	-6.40	97.49	102.27
1	1A	1917	PSU	N1-C2-N3	6.27	122.24	115.13
1	2A	1917	PSU	N1-C2-N3	6.19	122.14	115.13
1	1A	1939	5MU	C4-N3-C2	-6.06	119.51	127.35
1	1A	2605	PSU	N1-C2-N3	6.03	121.97	115.13
1	1A	1911	PSU	N1-C2-N3	6.02	121.95	115.13
32	1a	1498	UR3	C4-N3-C2	-5.96	118.95	124.56
54	1y	55	PSU	N1-C2-N3	5.93	121.84	115.13
55	1x	55	PSU	N1-C2-N3	5.89	121.80	115.13
1	1A	1939	5MU	C5-C4-N3	5.86	120.31	115.31
54	2y	8	4SU	C5-C4-N3	5.84	120.11	114.69
54	2w	32	PSU	N1-C2-N3	5.84	121.74	115.13
32	2a	1498	UR3	C4-N3-C2	-5.82	119.09	124.56
32	1a	516	PSU	N1-C2-N3	5.81	121.72	115.13
55	2x	55	PSU	N1-C2-N3	5.77	121.66	115.13
54	2w	55	PSU	N1-C2-N3	5.76	121.65	115.13
54	2y	32	PSU	N1-C2-N3	5.72	121.61	115.13
1	2A	2605	PSU	N1-C2-N3	5.67	121.56	115.13
54	1w	32	PSU	N1-C2-N3	5.61	121.49	115.13
54	1w	55	PSU	N1-C2-N3	5.59	121.46	115.13
1	2A	1939	5MU	C4-N3-C2	-5.59	120.12	127.35
54	2w	8	4SU	C4-N3-C2	-5.58	121.92	127.34
54	1w	39	PSU	N1-C2-N3	5.47	121.33	115.13
54	1y	32	PSU	N1-C2-N3	5.39	121.24	115.13
54	2y	55	PSU	N1-C2-N3	5.38	121.23	115.13
1	2A	1911	PSU	N1-C2-N3	5.38	121.22	115.13
32	2a	516	PSU	N1-C2-N3	5.34	121.17	115.13
1	1A	2552	OMU	N3-C2-N1	5.28	121.90	114.89
54	2w	39	PSU	N1-C2-N3	5.27	121.10	115.13
55	2x	54	5MU	C4-N3-C2	-5.25	120.55	127.35
1	1A	1939	5MU	C5-C6-N1	-5.22	117.97	123.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	2y	39	PSU	N1-C2-N3	5.17	120.98	115.13
1	2A	1915	5MU	N3-C2-N1	5.15	121.73	114.89
1	1A	1939	5MU	N3-C2-N1	5.14	121.72	114.89
1	2A	1915	5MU	C4-N3-C2	-5.13	120.71	127.35
1	2A	1939	5MU	N3-C2-N1	5.12	121.69	114.89
54	1y	39	PSU	N1-C2-N3	5.08	120.89	115.13
54	1w	8	4SU	C5-C4-N3	5.08	119.40	114.69
1	2A	1939	5MU	C5-C6-N1	-5.05	118.14	123.34
32	2a	1518	MA6	N3-C2-N1	-4.95	120.95	128.68
1	1A	1915	5MU	C4-N3-C2	-4.86	121.05	127.35
55	2x	54	5MU	N3-C2-N1	4.83	121.30	114.89
55	1x	54	5MU	N3-C2-N1	4.81	121.27	114.89
32	1a	1519	MA6	N3-C2-N1	-4.81	121.17	128.68
1	1A	1915	5MU	N3-C2-N1	4.79	121.25	114.89
54	1w	8	4SU	C4-N3-C2	-4.76	122.72	127.34
32	2a	1519	MA6	N3-C2-N1	-4.71	121.32	128.68
54	1w	37	MIA	C2-N3-C4	4.66	121.75	115.32
54	1w	54	5MU	N3-C2-N1	4.66	121.08	114.89
1	2A	1915	5MU	C5-C4-N3	4.63	119.26	115.31
54	1w	54	5MU	C4-N3-C2	-4.62	121.37	127.35
54	1y	8	4SU	C4-N3-C2	-4.61	122.86	127.34
54	2w	8	4SU	C5-C4-N3	4.59	118.95	114.69
1	2A	2552	OMU	N3-C2-N1	4.58	120.98	114.89
54	1y	8	4SU	C5-C4-N3	4.57	118.93	114.69
55	2x	8	4SU	C1'-N1-C2	4.56	125.83	117.57
1	1A	1915	5MU	C5-C4-N3	4.56	119.20	115.31
54	1y	54	5MU	C5-C4-N3	4.55	119.19	115.31
55	1x	54	5MU	C4-N3-C2	-4.54	121.48	127.35
54	2y	8	4SU	C1'-N1-C2	4.50	125.72	117.57
1	1A	2552	OMU	C4-N3-C2	-4.50	120.65	126.58
1	2A	2552	OMU	C4-N3-C2	-4.46	120.70	126.58
32	1a	1518	MA6	N3-C2-N1	-4.42	121.76	128.68
54	2w	37	MIA	C2-N3-C4	4.41	121.40	115.32
55	2x	54	5MU	C5-C4-N3	4.40	119.07	115.31
54	1w	37	MIA	C15-C14-C13	-4.37	110.01	122.65
54	2y	8	4SU	C5-C4-S4	-4.32	118.90	124.47
54	1y	54	5MU	C4-N3-C2	-4.32	121.76	127.35
1	2A	1939	5MU	C5-C4-N3	4.31	118.99	115.31
1	1A	1917	PSU	C4-N3-C2	-4.29	120.15	126.34
54	2w	54	5MU	C4-N3-C2	-4.23	121.87	127.35
1	2A	1962	5MC	C5-C6-N1	-4.19	119.02	123.34
54	2y	54	5MU	O4-C4-C5	-4.16	120.08	124.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	2w	32	PSU	C4-N3-C2	-4.16	120.35	126.34
55	2x	54	5MU	C5-C6-N1	-4.15	119.07	123.34
54	2w	54	5MU	C5-C4-N3	4.11	118.82	115.31
55	1x	32	5MC	C5-C6-N1	-4.10	119.12	123.34
54	2y	54	5MU	C4-N3-C2	-4.04	122.12	127.35
1	1A	2605	PSU	C4-N3-C2	-4.03	120.54	126.34
55	2x	54	5MU	O4-C4-C5	-4.03	120.24	124.90
54	2y	54	5MU	C5-C4-N3	4.02	118.74	115.31
54	1w	54	5MU	C5-C4-N3	3.99	118.72	115.31
54	1y	54	5MU	O4-C4-C5	-3.99	120.28	124.90
54	2w	8	4SU	N3-C2-N1	3.96	120.14	114.89
1	1A	1942	5MC	C5-C6-N1	-3.95	119.27	123.34
54	2w	54	5MU	N3-C2-N1	3.93	120.10	114.89
54	1y	54	5MU	N3-C2-N1	3.90	120.07	114.89
1	2A	1917	PSU	C4-N3-C2	-3.90	120.72	126.34
54	2y	54	5MU	N3-C2-N1	3.90	120.07	114.89
32	2a	1404	5MC	C5-C6-N1	-3.90	119.33	123.34
1	2A	2605	PSU	C4-N3-C2	-3.84	120.81	126.34
55	2x	55	PSU	C4-N3-C2	-3.82	120.83	126.34
1	2A	1939	5MU	O4-C4-C5	-3.80	120.49	124.90
55	1x	55	PSU	O2-C2-N1	-3.79	118.61	122.79
54	2y	8	4SU	N3-C2-N1	3.78	119.90	114.89
54	2w	54	5MU	O4-C4-C5	-3.75	120.56	124.90
32	1a	516	PSU	C4-N3-C2	-3.72	120.98	126.34
1	1A	1939	5MU	O4-C4-C5	-3.71	120.60	124.90
54	2y	32	PSU	O2-C2-N1	-3.70	118.71	122.79
54	1y	55	PSU	O2-C2-N1	-3.69	118.73	122.79
54	1w	37	MIA	C5-C6-N1	-3.69	117.75	120.81
54	2y	55	PSU	C6-C5-C4	-3.68	115.62	118.20
1	2A	1915	5MU	O4-C4-C5	-3.67	120.65	124.90
32	2a	516	PSU	C4-N3-C2	-3.67	121.06	126.34
54	2w	55	PSU	C4-N3-C2	-3.67	121.06	126.34
32	1a	967	5MC	C5-C6-N1	-3.66	119.58	123.34
32	2a	1519	MA6	C4-C5-N7	-3.65	105.59	109.40
32	2a	967	5MC	C5-C6-N1	-3.64	119.59	123.34
54	1w	54	5MU	O4-C4-C5	-3.62	120.70	124.90
54	2w	39	PSU	C4-N3-C2	-3.62	121.12	126.34
1	1A	1911	PSU	C4-N3-C2	-3.62	121.13	126.34
54	1w	39	PSU	C4-N3-C2	-3.61	121.14	126.34
54	1y	32	PSU	C4-N3-C2	-3.61	121.14	126.34
1	1A	1915	5MU	O4-C4-C5	-3.60	120.73	124.90
54	2y	32	PSU	C4-N3-C2	-3.59	121.17	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	1w	37	MIA	C16-C14-C13	-3.59	112.28	122.65
54	2w	37	MIA	C5-C6-N1	-3.58	117.84	120.81
54	1w	32	PSU	C4-N3-C2	-3.57	121.19	126.34
1	2A	1911	PSU	C4-N3-C2	-3.57	121.19	126.34
55	1x	8	4SU	C6-C5-C4	-3.56	116.87	119.95
1	2A	1939	5MU	O2-C2-N1	-3.55	118.07	122.79
54	1y	55	PSU	C4-N3-C2	-3.51	121.28	126.34
55	1x	55	PSU	C4-N3-C2	-3.50	121.29	126.34
1	1A	1911	PSU	O2-C2-N1	-3.48	118.96	122.79
54	1w	55	PSU	C4-N3-C2	-3.47	121.34	126.34
54	2y	55	PSU	O2-C2-N1	-3.40	119.04	122.79
55	2x	32	5MC	C5-C6-N1	-3.40	119.84	123.34
54	2w	8	4SU	C5-C4-S4	-3.40	120.08	124.47
1	2A	1942	5MC	C5-C6-N1	-3.40	119.84	123.34
55	1x	54	5MU	C5-C6-N1	-3.40	119.84	123.34
55	1x	54	5MU	C5-C4-N3	3.37	118.19	115.31
1	2A	1915	5MU	C5-C6-N1	-3.37	119.88	123.34
32	1a	1404	5MC	C5-C6-N1	-3.32	119.92	123.34
1	2A	2552	OMU	C5-C4-N3	3.31	119.80	114.84
54	1w	32	PSU	O2-C2-N1	-3.30	119.15	122.79
54	2y	37	MIA	N3-C2-N1	-3.30	123.52	128.68
54	1y	32	PSU	O2-C2-N1	-3.30	119.16	122.79
54	1w	8	4SU	N3-C2-N1	3.29	119.26	114.89
32	1a	1407	5MC	C5-C6-N1	-3.29	119.95	123.34
32	1a	1519	MA6	C4-C5-N7	-3.29	105.97	109.40
32	2a	1407	5MC	C5-C6-N1	-3.27	119.97	123.34
1	2A	1911	PSU	O2-C2-N1	-3.24	119.22	122.79
54	2w	32	PSU	O2-C2-N1	-3.24	119.23	122.79
54	2y	39	PSU	C4-N3-C2	-3.21	121.71	126.34
54	1y	8	4SU	N3-C2-N1	3.21	119.15	114.89
1	2A	1917	PSU	O2-C2-N1	-3.19	119.28	122.79
54	1w	8	4SU	C5-C4-S4	-3.18	120.36	124.47
54	2w	54	5MU	C5-C6-N1	-3.17	120.08	123.34
55	1x	8	4SU	O2-C2-N1	3.16	126.98	122.79
32	1a	1518	MA6	C4-C5-N7	-3.12	106.14	109.40
54	1y	37	MIA	N3-C2-N1	-3.12	123.80	128.68
54	2w	37	MIA	C12-N6-C6	-3.10	120.20	122.87
54	1w	55	PSU	O2-C2-N1	-3.10	119.38	122.79
54	1w	54	5MU	C5-C6-N1	-3.09	120.16	123.34
54	2y	55	PSU	C4-N3-C2	-3.06	121.93	126.34
1	2A	2552	OMU	O2-C2-N1	-3.04	118.74	122.79
54	2y	37	MIA	C4-C5-N7	-3.04	106.23	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	1w	37	MIA	C2-N1-C6	3.03	122.61	117.19
1	1A	1962	5MC	C5-C4-N3	-3.03	118.41	121.67
55	2x	8	4SU	C6-C5-C4	-3.03	117.33	119.95
55	1x	54	5MU	C5M-C5-C4	3.01	122.08	118.77
55	1x	54	5MU	O2-C2-N1	-3.01	118.79	122.79
1	1A	1917	PSU	O2-C2-N1	-3.00	119.49	122.79
55	1x	8	4SU	C5-C4-N3	2.98	117.46	114.69
32	2a	516	PSU	O2-C2-N1	-2.98	119.52	122.79
1	1A	2552	OMU	C5-C4-N3	2.97	119.28	114.84
1	1A	1915	5MU	C5-C6-N1	-2.96	120.29	123.34
32	2a	1518	MA6	C4-C5-N7	-2.96	106.31	109.40
54	1y	54	5MU	C5-C6-N1	-2.94	120.31	123.34
54	1w	39	PSU	O2-C2-N1	-2.93	119.57	122.79
54	1y	39	PSU	C4-N3-C2	-2.93	122.12	126.34
54	2w	8	4SU	C1'-N1-C2	2.92	122.86	117.57
1	1A	2605	PSU	O2-C2-N1	-2.92	119.58	122.79
55	1x	8	4SU	C1'-N1-C2	2.91	122.84	117.57
54	2w	37	MIA	C4-C5-N7	-2.91	106.37	109.40
54	2w	39	PSU	O2-C2-N1	-2.91	119.59	122.79
55	2x	32	5MC	C5-C4-N3	-2.90	118.54	121.67
54	1w	37	MIA	N3-C2-N1	-2.89	121.67	126.98
55	2x	32	5MC	O2-C2-N3	-2.87	117.66	122.33
1	1A	1942	5MC	C5-C4-N3	-2.86	118.58	121.67
32	1a	516	PSU	O2-C2-N1	-2.85	119.66	122.79
1	1A	2251	OMG	C5-C6-N1	2.84	118.96	113.95
55	1x	54	5MU	O4-C4-C5	-2.83	121.62	124.90
55	1x	32	5MC	C5-C4-N3	-2.82	118.63	121.67
55	2x	8	4SU	C5-C4-N3	2.82	117.31	114.69
43	1l	92	0TD	OD2-CG-CB	2.82	119.24	113.15
1	2A	1942	5MC	C5-C4-N3	-2.81	118.64	121.67
54	2w	55	PSU	O2-C2-N1	-2.80	119.70	122.79
54	2y	54	5MU	C5-C6-N1	-2.79	120.47	123.34
32	2a	1407	5MC	C5-C4-N3	-2.78	118.67	121.67
54	1y	8	4SU	C5-C4-S4	-2.78	120.88	124.47
54	1w	54	5MU	O2-C2-N1	-2.75	119.13	122.79
54	1y	37	MIA	C4-C5-N7	-2.74	106.55	109.40
32	2a	1400	5MC	O2-C2-N3	-2.72	117.90	122.33
55	1x	54	5MU	C5M-C5-C6	-2.72	119.21	122.85
1	1A	1920	OMC	O2-C2-N3	-2.72	117.90	122.33
32	2a	1498	UR3	C3U-N3-C4	2.72	121.78	117.89
32	1a	1404	5MC	CM5-C5-C6	-2.70	119.24	122.85
32	2a	1400	5MC	C5-C4-N3	-2.70	118.76	121.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	2y	39	PSU	O2-C2-N1	-2.70	119.82	122.79
32	1a	1498	UR3	C3U-N3-C2	2.68	122.01	117.31
1	1A	2552	OMU	O2-C2-N1	-2.66	119.25	122.79
32	1a	1400	5MC	C5-C4-N3	-2.64	118.82	121.67
55	2x	55	PSU	O2-C2-N1	-2.64	119.88	122.79
32	1a	1400	5MC	C5-C6-N1	-2.64	120.62	123.34
1	1A	1962	5MC	C5-C6-N1	-2.63	120.64	123.34
32	1a	1207	2MG	C8-N7-C5	2.62	107.98	102.99
32	1a	1407	5MC	C5-C4-N3	-2.61	118.85	121.67
32	1a	967	5MC	C5-C4-N3	-2.57	118.90	121.67
1	2A	2251	OMG	C5-C6-N1	2.54	118.44	113.95
54	2w	37	MIA	C2-N1-C6	2.53	121.71	117.19
32	2a	1207	2MG	C8-N7-C5	2.51	107.78	102.99
32	1a	1404	5MC	C5-C4-N3	-2.47	119.00	121.67
32	2a	1404	5MC	C5-C4-N3	-2.47	119.01	121.67
32	2a	1400	5MC	C5-C6-N1	-2.44	120.83	123.34
1	1A	2503	2MA	C5-C6-N1	2.44	118.22	114.02
55	2x	8	4SU	C6-N1-C2	-2.44	117.88	120.99
54	2y	8	4SU	C1'-N1-C6	-2.43	115.53	120.84
1	1A	2503	2MA	C8-N7-C5	2.43	107.62	102.99
32	1a	966	M2G	C5-C6-N1	2.41	118.22	113.95
54	1y	8	4SU	C1'-N1-C2	2.41	121.93	117.57
1	1A	2251	OMG	C8-N7-C5	2.41	107.57	102.99
32	1a	966	M2G	C8-N7-C5	2.40	107.56	102.99
54	1y	32	PSU	C6-C5-C4	-2.37	116.54	118.20
43	2l	92	0TD	OD2-CG-CB	2.35	118.23	113.15
1	2A	2552	OMU	O4-C4-C5	-2.34	121.04	125.16
1	2A	2605	PSU	O2-C2-N3	-2.31	117.47	121.82
54	1w	37	MIA	C4-C5-N7	-2.28	107.02	109.40
32	2a	967	5MC	C5-C4-N3	-2.28	119.22	121.67
32	1a	1402	4OC	C6-C5-C4	2.25	119.72	116.96
54	2y	54	5MU	C1'-N1-C2	2.25	121.64	117.57
55	2x	8	4SU	O2-C2-N1	2.24	125.76	122.79
32	2a	966	M2G	C8-N7-C5	2.23	107.23	102.99
1	2A	2503	2MA	C8-N7-C5	2.22	107.22	102.99
1	2A	2503	2MA	C5-C6-N1	2.22	117.84	114.02
1	2A	1911	PSU	C6-C5-C4	-2.21	116.66	118.20
32	2a	966	M2G	C5-C6-N1	2.20	117.84	113.95
1	1A	1962	5MC	CM5-C5-C6	-2.19	119.92	122.85
32	2a	516	PSU	O4'-C1'-C2'	2.19	108.23	105.14
1	2A	2605	PSU	C5-C6-N1	-2.19	118.83	122.11
55	2x	54	5MU	O2-C2-N1	-2.18	119.89	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	2a	1498	UR3	C1'-N1-C2	2.17	120.65	116.99
1	1A	2605	PSU	C5-C6-N1	-2.15	118.88	122.11
1	2A	2251	OMG	C8-N7-C5	2.15	107.09	102.99
1	2A	1962	5MC	C5-C4-N3	-2.15	119.36	121.67
1	1A	2251	OMG	CM2-O2'-C2'	-2.13	108.94	114.52
32	2a	1400	5MC	C1'-N1-C6	-2.13	117.58	121.12
1	1A	1917	PSU	C5-C6-N1	-2.10	118.96	122.11
55	2x	8	4SU	C1'-N1-C6	-2.10	116.27	120.84
54	2y	54	5MU	C1'-N1-C6	-2.10	117.63	121.12
54	2w	37	MIA	N3-C2-N1	-2.10	123.13	126.98
54	2y	32	PSU	O4'-C1'-C2'	2.09	108.09	105.14
32	2a	1402	4OC	C6-C5-C4	2.08	119.50	116.96
1	2A	1942	5MC	O2-C2-N3	-2.08	118.95	122.33
55	1x	8	4SU	O2-C2-N3	-2.08	117.64	121.50
1	1A	1915	5MU	C5M-C5-C4	2.07	121.05	118.77
54	2w	32	PSU	C6-C5-C4	-2.07	116.75	118.20
54	2w	54	5MU	C5M-C5-C4	2.06	121.03	118.77
54	1w	55	PSU	C6-C5-C4	-2.06	116.76	118.20
1	1A	1917	PSU	O4'-C1'-C2'	2.05	108.04	105.14
32	2a	1404	5MC	O2-C2-N3	-2.05	119.00	122.33
32	2a	1407	5MC	CM5-C5-C6	-2.03	120.14	122.85
54	1w	54	5MU	C5M-C5-C4	2.03	121.00	118.77
32	1a	516	PSU	O4'-C1'-C2'	2.03	108.00	105.14
1	1A	2251	OMG	O6-C6-C5	-2.01	120.44	124.37

There are no chirality outliers.

All (65) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
43	1l	92	0TD	CG-CB-SB-CSB
54	1w	37	MIA	N1-C2-S10-C11
54	1w	37	MIA	N3-C2-S10-C11
54	1w	37	MIA	C12-C13-C14-C16
1	2A	2251	OMG	C1'-C2'-O2'-CM2
32	2a	527	G7M	C3'-C4'-C5'-O5'
32	2a	1207	2MG	N1-C2-N2-CM2
32	2a	1207	2MG	N3-C2-N2-CM2
32	2a	1400	5MC	O4'-C4'-C5'-O5'
32	2a	1400	5MC	C2'-C1'-N1-C2
32	2a	1400	5MC	C2'-C1'-N1-C6
32	2a	1518	MA6	O4'-C4'-C5'-O5'
32	2a	1518	MA6	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
32	2a	1519	MA6	O4'-C4'-C5'-O5'
54	2w	37	MIA	N1-C2-S10-C11
54	2w	37	MIA	N3-C2-S10-C11
54	2w	46	G7M	O4'-C4'-C5'-O5'
54	2w	46	G7M	C3'-C4'-C5'-O5'
32	2a	1498	UR3	O4'-C4'-C5'-O5'
32	2a	1498	UR3	C3'-C4'-C5'-O5'
32	2a	1519	MA6	C3'-C4'-C5'-O5'
54	2y	37	MIA	C3'-C4'-C5'-O5'
32	1a	967	5MC	O4'-C4'-C5'-O5'
32	1a	1519	MA6	O4'-C4'-C5'-O5'
32	2a	1400	5MC	C3'-C4'-C5'-O5'
32	1a	527	G7M	C3'-C4'-C5'-O5'
32	2a	527	G7M	O4'-C4'-C5'-O5'
32	1a	1519	MA6	C3'-C4'-C5'-O5'
54	1w	46	G7M	O4'-C4'-C5'-O5'
54	1w	46	G7M	C3'-C4'-C5'-O5'
54	2y	37	MIA	O4'-C4'-C5'-O5'
32	2a	1400	5MC	O4'-C1'-N1-C6
54	1y	37	MIA	C3'-C4'-C5'-O5'
32	2a	1400	5MC	O4'-C1'-N1-C2
32	1a	527	G7M	O4'-C4'-C5'-O5'
54	1y	46	G7M	C4'-C5'-O5'-P
43	1l	92	0TD	SB-CB-CG-OD1
43	2l	92	0TD	SB-CB-CG-OD1
32	2a	527	G7M	C4'-C5'-O5'-P
32	2a	1519	MA6	C4'-C5'-O5'-P
54	2y	8	4SU	C2'-C1'-N1-C6
32	2a	1402	4OC	O4'-C4'-C5'-O5'
54	1y	37	MIA	C4'-C5'-O5'-P
54	2y	8	4SU	C2'-C1'-N1-C2
54	1w	46	G7M	C4'-C5'-O5'-P
32	1a	967	5MC	C3'-C4'-C5'-O5'
1	2A	2503	2MA	O4'-C4'-C5'-O5'
54	2y	8	4SU	C3'-C4'-C5'-O5'
54	1y	55	PSU	O4'-C1'-C5-C4
43	1l	92	0TD	CA-CB-SB-CSB
32	1a	1400	5MC	O4'-C4'-C5'-O5'
54	1y	37	MIA	O4'-C4'-C5'-O5'
54	2y	8	4SU	O4'-C4'-C5'-O5'
54	1y	55	PSU	O4'-C1'-C5-C6
43	2l	92	0TD	CG-CB-SB-CSB

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Mol	Chain	Res	Type	Atoms
54	2y	55	PSU	O4'-C1'-C5-C6
1	1A	1920	OMC	C2'-C1'-N1-C2
1	2A	1920	OMC	C2'-C1'-N1-C2
1	1A	2251	OMG	C4'-C5'-O5'-P
1	1A	2503	2MA	O4'-C4'-C5'-O5'
32	1a	1400	5MC	C3'-C4'-C5'-O5'
32	2a	1402	4OC	C3'-C4'-C5'-O5'
1	1A	1962	5MC	C2'-C1'-N1-C6
32	1a	1519	MA6	C4'-C5'-O5'-P
1	1A	1962	5MC	O4'-C1'-N1-C6

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 2741 ligands modelled in this entry, 2737 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
60	SF4	2d	302	35	0,12,12	-	-	-		
58	A1AIX	1A	4085	-	47,48,48	2.68	12 (25%)	60,70,70	1.63	13 (21%)
58	A1AIX	2A	3851	-	47,48,48	3.68	12 (25%)	60,70,70	1.80	13 (21%)
60	SF4	1d	302	35	0,12,12	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
60	SF4	2d	302	35	-	-	0/6/5/5
58	A1AIX	1A	4085	-	-	2/24/41/41	0/6/6/6
58	A1AIX	2A	3851	-	-	4/24/41/41	0/6/6/6
60	SF4	1d	302	35	-	-	0/6/5/5

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	2A	3851	A1AIX	OBL-NBK	18.40	1.54	1.22
58	1A	4085	A1AIX	OBL-NBK	9.03	1.38	1.22
58	2A	3851	A1AIX	CBE-CAA	-8.70	1.39	1.51
58	1A	4085	A1AIX	CBE-CAA	-8.04	1.40	1.51
58	2A	3851	A1AIX	CAW-CAV	-8.01	1.37	1.51
58	1A	4085	A1AIX	CAW-CAV	-7.81	1.37	1.51
58	2A	3851	A1AIX	CAJ-NAI	6.69	1.38	1.33
58	1A	4085	A1AIX	CAJ-NAI	5.18	1.37	1.33
58	2A	3851	A1AIX	CBI-NBK	-4.78	1.33	1.45
58	1A	4085	A1AIX	CBI-NBK	-4.16	1.35	1.45
58	1A	4085	A1AIX	CAU-CAH	-4.03	1.40	1.46
58	2A	3851	A1AIX	CAU-CAH	-3.92	1.41	1.46
58	2A	3851	A1AIX	CAE-CAF	-3.31	1.41	1.51
58	1A	4085	A1AIX	CAZ-CBA	-3.19	1.32	1.38
58	1A	4085	A1AIX	CAE-CAF	-3.11	1.42	1.51
58	2A	3851	A1AIX	CAZ-CBA	-3.10	1.33	1.38
58	1A	4085	A1AIX	CAY-CBB	-2.99	1.33	1.38
58	2A	3851	A1AIX	CAY-CBB	-2.86	1.33	1.38
58	1A	4085	A1AIX	CBB-CBA	-2.37	1.33	1.39
58	2A	3851	A1AIX	CAL-CAK	-2.33	1.39	1.43
58	1A	4085	A1AIX	CAO-CAL	-2.23	1.38	1.43
58	2A	3851	A1AIX	CAO-CAL	-2.20	1.38	1.43
58	2A	3851	A1AIX	CBB-CBA	-2.19	1.33	1.39
58	1A	4085	A1AIX	CAL-CAK	-2.13	1.39	1.43

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
58	2A	3851	A1AIX	CAS-OAR-CAP	-6.21	108.16	117.53
58	2A	3851	A1AIX	CAX-CAW-CAV	-6.18	102.73	109.79
58	1A	4085	A1AIX	CAX-CAW-CAV	-4.91	104.18	109.79
58	1A	4085	A1AIX	CAS-OAR-CAP	-4.06	111.40	117.53
58	1A	4085	A1AIX	CAX-NAI-CAJ	-3.93	115.33	118.30
58	1A	4085	A1AIX	CAU-CAH-NAI	-3.57	112.56	116.80
58	2A	3851	A1AIX	CAU-CAH-NAI	-3.55	112.59	116.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
58	2A	3851	A1AIX	CAL-CAJ-NAI	-3.52	119.56	121.82
58	1A	4085	A1AIX	CAL-CAJ-NAI	-3.39	119.65	121.82
58	2A	3851	A1AIX	CBC-CAB-NBQ	3.22	114.40	109.27
58	1A	4085	A1AIX	CAJ-CAL-CAO	-3.11	119.39	121.62
58	1A	4085	A1AIX	CAZ-CAU-CAV	-3.04	115.11	119.14
58	2A	3851	A1AIX	CAZ-CAU-CAV	-2.80	115.43	119.14
58	2A	3851	A1AIX	CAE-CAF-CAK	-2.78	114.95	121.49
58	1A	4085	A1AIX	CAX-NAI-CAH	2.70	121.88	118.60
58	1A	4085	A1AIX	CBP-OBO-CBA	-2.47	102.14	105.34
58	2A	3851	A1AIX	CBE-CAA-CAB	-2.46	107.31	111.64
58	2A	3851	A1AIX	CBP-OBO-CBA	-2.34	102.30	105.34
58	2A	3851	A1AIX	CBP-OBN-CBB	-2.34	102.31	105.34
58	2A	3851	A1AIX	CAX-NAI-CAJ	-2.20	116.64	118.30
58	1A	4085	A1AIX	OBO-CBP-OBN	-2.18	104.59	108.08
58	1A	4085	A1AIX	CBH-CBI-NBK	2.17	121.01	119.38
58	1A	4085	A1AIX	CBJ-CBI-NBK	2.17	121.01	119.38
58	1A	4085	A1AIX	CAE-CAF-CAK	-2.17	116.38	121.49
58	2A	3851	A1AIX	CAJ-CAL-CAO	-2.12	120.10	121.62
58	2A	3851	A1AIX	OBO-CBP-OBN	-2.04	104.83	108.08

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	1A	4085	A1AIX	NBQ-CAB-CBC-OBD
58	2A	3851	A1AIX	CAO-CAP-OAR-CAS
58	1A	4085	A1AIX	CAA-CAB-CBC-OBD
58	2A	3851	A1AIX	CAN-CAP-OAR-CAS
58	2A	3851	A1AIX	NBQ-CAB-CBC-OBD
58	2A	3851	A1AIX	CAA-CAB-CBC-OBD

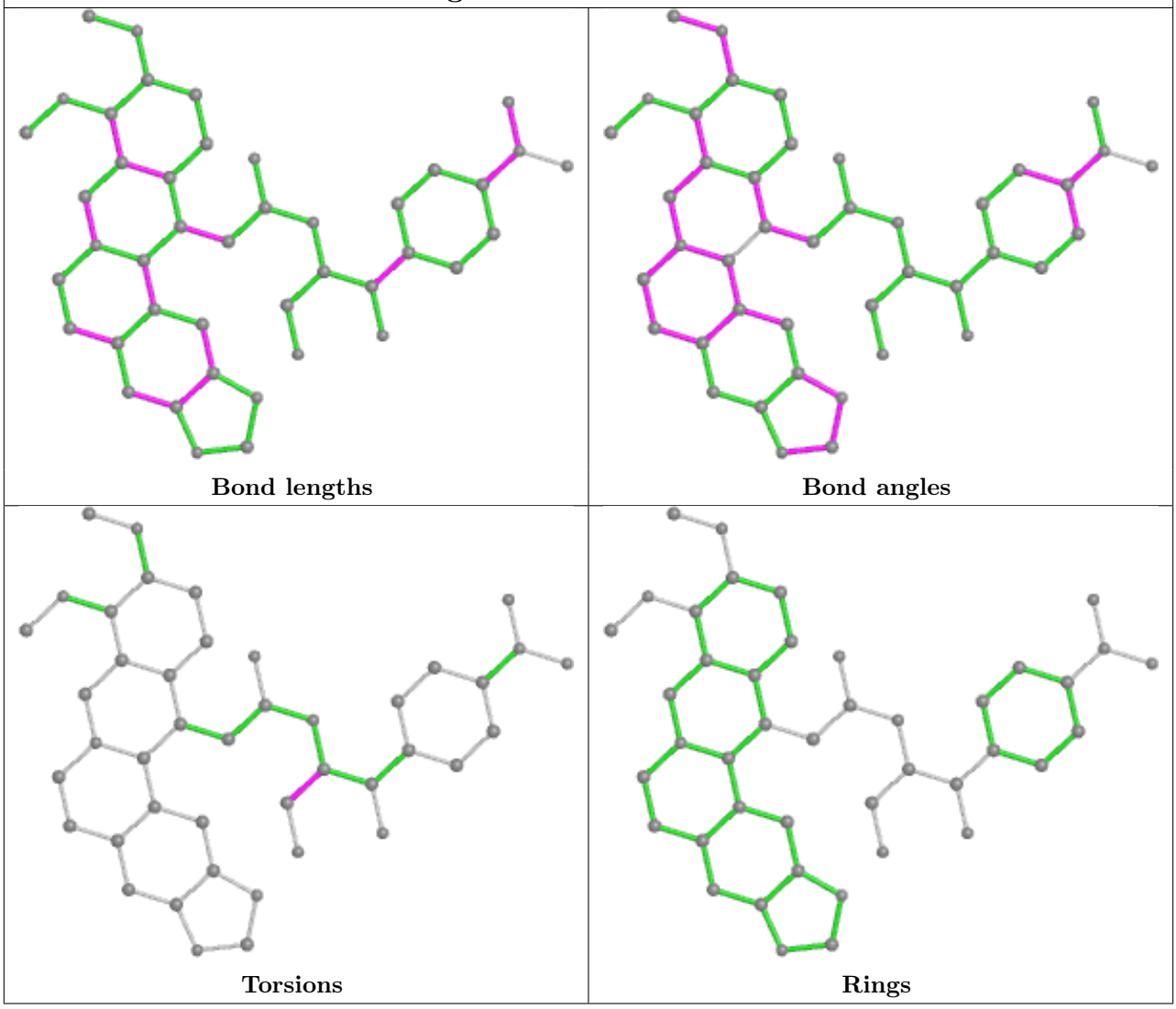
There are no ring outliers.

No monomer is involved in short contacts.

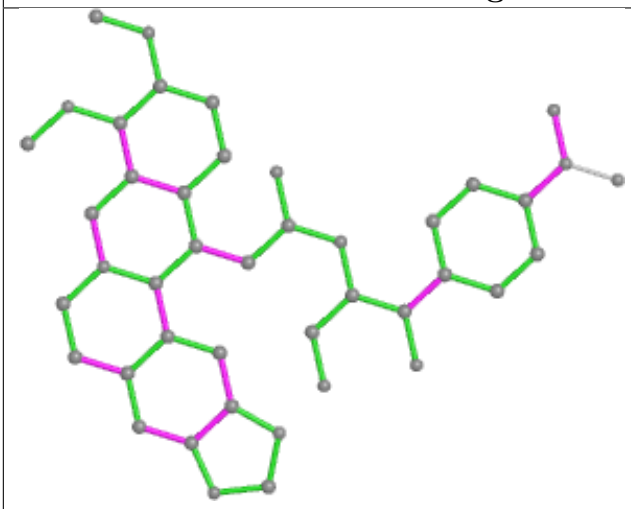
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

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

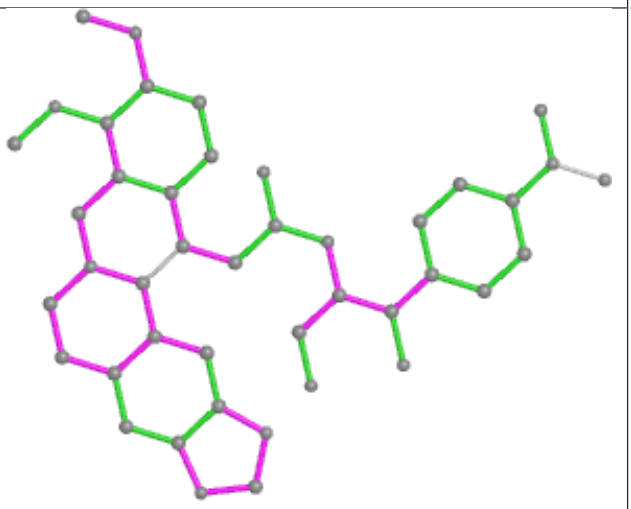
Ligand A1AIX 1A 4085



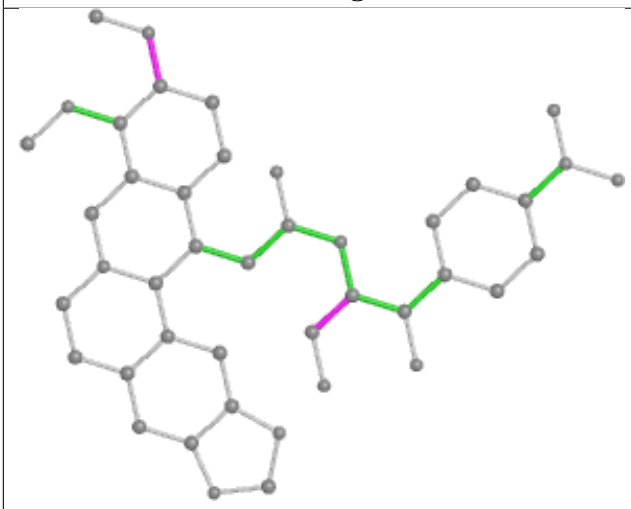
Ligand A1AIX 2A 3851



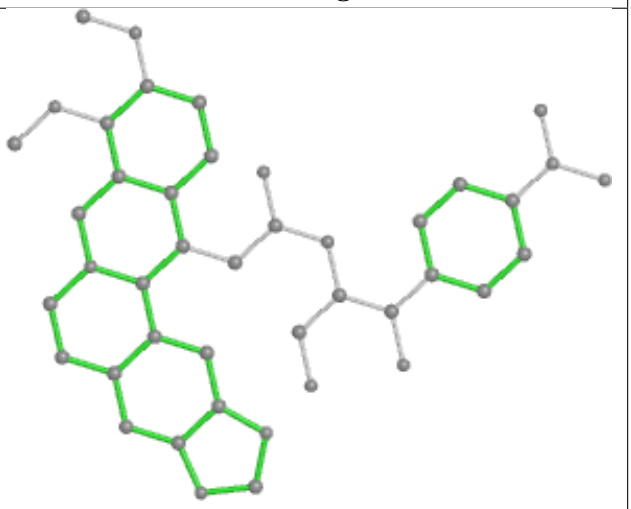
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	1A	2860/2915 (98%)	0.17	31 (1%) 80 75	16, 36, 96, 109	0
1	2A	2789/2915 (95%)	0.21	44 (1%) 72 66	33, 60, 93, 107	0
2	1B	120/121 (99%)	-0.01	0 100 100	25, 45, 60, 87	0
2	2B	120/121 (99%)	-0.40	0 100 100	62, 82, 91, 100	0
3	1D	275/276 (99%)	0.26	3 (1%) 80 75	18, 36, 51, 70	0
3	2D	275/276 (99%)	0.44	6 (2%) 62 52	35, 54, 67, 78	0
4	1E	204/206 (99%)	-0.07	0 100 100	19, 42, 61, 69	0
4	2E	204/206 (99%)	0.21	3 (1%) 73 68	35, 61, 72, 83	0
5	1F	203/210 (96%)	0.37	5 (2%) 57 47	19, 43, 68, 84	0
5	2F	203/210 (96%)	1.06	30 (14%) 2 1	34, 67, 78, 83	0
6	1G	181/182 (99%)	-0.11	1 (0%) 89 86	36, 55, 70, 86	0
6	2G	181/182 (99%)	0.50	29 (16%) 1 1	71, 81, 87, 90	0
7	1H	174/180 (96%)	-0.13	0 100 100	34, 53, 67, 72	0
7	2H	174/180 (96%)	1.72	62 (35%) 0 0	67, 81, 90, 98	0
8	1I	146/148 (98%)	-0.06	0 100 100	45, 72, 80, 87	0
8	2I	146/148 (98%)	0.32	10 (6%) 17 10	58, 75, 83, 89	0
9	1N	140/140 (100%)	-0.06	0 100 100	26, 39, 59, 72	0
9	2N	140/140 (100%)	0.35	5 (3%) 42 32	42, 67, 76, 82	0
10	1O	122/122 (100%)	0.34	0 100 100	26, 41, 57, 63	0
10	2O	122/122 (100%)	1.16	19 (15%) 2 1	47, 60, 69, 76	0
11	1P	149/150 (99%)	0.26	1 (0%) 87 84	21, 46, 69, 80	0
11	2P	149/150 (99%)	2.07	69 (46%) 0 0	40, 69, 81, 89	0
12	1Q	141/141 (100%)	0.27	3 (2%) 63 54	27, 40, 53, 73	0
12	2Q	141/141 (100%)	1.22	29 (20%) 1 0	49, 68, 78, 86	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	1R	118/118 (100%)	-0.08	0 100 100	26, 35, 51, 57	0
13	2R	118/118 (100%)	0.05	0 100 100	41, 52, 64, 73	0
14	1S	110/112 (98%)	-0.27	0 100 100	33, 46, 58, 66	0
14	2S	110/112 (98%)	-0.40	0 100 100	62, 74, 82, 87	0
15	1T	131/146 (89%)	0.05	0 100 100	33, 47, 66, 75	0
15	2T	131/146 (89%)	0.61	7 (5%) 26 17	49, 62, 75, 82	0
16	1U	116/118 (98%)	0.13	0 100 100	20, 32, 49, 64	0
16	2U	116/118 (98%)	0.50	8 (6%) 16 10	44, 65, 76, 88	0
17	1V	101/101 (100%)	-0.10	0 100 100	20, 42, 57, 68	0
17	2V	101/101 (100%)	0.62	9 (8%) 9 5	48, 72, 80, 84	0
18	1W	112/113 (99%)	-0.06	0 100 100	23, 32, 52, 76	0
18	2W	112/113 (99%)	0.21	1 (0%) 84 80	38, 51, 68, 92	0
19	1X	95/96 (98%)	-0.08	0 100 100	21, 36, 58, 82	0
19	2X	95/96 (98%)	0.00	0 100 100	44, 60, 69, 71	0
20	1Y	107/110 (97%)	-0.13	0 100 100	36, 51, 69, 77	0
20	2Y	107/110 (97%)	0.17	1 (0%) 84 80	62, 73, 82, 89	0
21	1Z	154/206 (74%)	-0.06	0 100 100	40, 58, 79, 85	0
21	2Z	160/206 (77%)	0.35	6 (3%) 40 30	68, 80, 87, 94	0
22	10	83/85 (97%)	0.66	6 (7%) 15 8	27, 38, 61, 81	0
22	20	83/85 (97%)	0.93	12 (14%) 2 1	53, 64, 78, 84	0
23	11	97/98 (98%)	0.22	1 (1%) 82 77	22, 43, 67, 70	0
23	21	97/98 (98%)	0.88	17 (17%) 1 1	41, 58, 75, 83	0
24	12	70/72 (97%)	-0.07	0 100 100	32, 48, 60, 71	0
24	22	70/72 (97%)	-0.27	0 100 100	58, 69, 76, 85	0
25	13	59/60 (98%)	0.02	0 100 100	26, 35, 62, 70	0
25	23	59/60 (98%)	1.12	12 (20%) 1 0	51, 67, 81, 90	0
26	14	69/71 (97%)	-0.41	0 100 100	46, 70, 86, 87	0
26	24	69/71 (97%)	0.11	4 (5%) 23 15	75, 87, 95, 104	0
27	15	59/60 (98%)	0.00	0 100 100	20, 34, 53, 65	0
27	25	59/60 (98%)	0.06	0 100 100	34, 53, 67, 77	0
28	16	53/54 (98%)	0.38	1 (1%) 66 59	29, 39, 51, 57	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
28	26	53/54 (98%)	1.03	8 (15%) 2 1	50, 62, 68, 75	0
29	17	48/49 (97%)	0.03	0 100 100	22, 26, 50, 62	0
29	27	48/49 (97%)	0.36	1 (2%) 63 54	32, 42, 58, 68	0
30	18	64/65 (98%)	0.44	1 (1%) 72 66	24, 33, 41, 49	0
30	28	64/65 (98%)	2.09	30 (46%) 0 0	47, 56, 65, 72	0
31	19	37/37 (100%)	0.17	0 100 100	31, 40, 53, 62	0
31	29	37/37 (100%)	1.31	10 (27%) 0 0	62, 71, 84, 90	0
32	1a	1488/1521 (97%)	-0.03	12 (0%) 86 81	34, 69, 93, 106	0
32	2a	1491/1521 (98%)	0.17	48 (3%) 47 37	59, 82, 98, 107	0
33	1b	231/256 (90%)	0.63	21 (9%) 9 5	61, 78, 85, 89	0
33	2b	231/256 (90%)	1.57	76 (32%) 0 0	73, 87, 92, 97	0
34	1c	206/239 (86%)	0.79	31 (15%) 2 1	62, 72, 82, 88	0
34	2c	206/239 (86%)	3.67	157 (76%) 0 0	74, 85, 92, 94	0
35	1d	208/209 (99%)	0.24	6 (2%) 51 41	58, 72, 80, 86	0
35	2d	208/209 (99%)	1.01	40 (19%) 1 0	65, 76, 84, 88	0
36	1e	148/162 (91%)	0.47	4 (2%) 54 44	53, 65, 74, 86	0
36	2e	148/162 (91%)	1.34	47 (31%) 0 0	71, 81, 87, 90	0
37	1f	100/101 (99%)	1.02	23 (23%) 0 0	54, 67, 77, 82	0
37	2f	100/101 (99%)	0.17	2 (2%) 65 56	66, 75, 82, 90	0
38	1g	155/156 (99%)	0.98	22 (14%) 2 1	55, 70, 82, 100	0
38	2g	155/156 (99%)	2.11	69 (44%) 0 0	70, 82, 89, 93	0
39	1h	137/138 (99%)	0.38	5 (3%) 42 32	52, 68, 74, 78	0
39	2h	137/138 (99%)	-0.17	3 (2%) 62 52	71, 81, 86, 90	0
40	1i	127/128 (99%)	-0.17	0 100 100	51, 74, 83, 89	0
40	2i	127/128 (99%)	2.00	59 (46%) 0 0	78, 86, 92, 94	0
41	1j	97/105 (92%)	0.06	1 (1%) 82 77	57, 76, 85, 88	0
41	2j	96/105 (91%)	2.55	51 (53%) 0 0	73, 86, 92, 100	0
42	1k	114/129 (88%)	2.21	61 (53%) 0 0	47, 65, 76, 82	0
42	2k	114/129 (88%)	1.69	46 (40%) 0 0	68, 78, 84, 86	0
43	1l	121/132 (91%)	0.65	14 (11%) 4 2	48, 58, 68, 76	0
43	2l	121/132 (91%)	1.42	32 (26%) 0 0	60, 72, 81, 85	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
44	1m	123/126 (97%)	-0.28	5 (4%) 37 27	55, 68, 76, 81	0
44	2m	122/126 (96%)	0.77	18 (14%) 2 1	69, 83, 88, 92	0
45	1n	60/61 (98%)	0.10	0 100 100	62, 68, 74, 76	0
45	2n	60/61 (98%)	3.19	42 (70%) 0 0	79, 87, 92, 94	0
46	1o	88/89 (98%)	0.16	1 (1%) 80 75	52, 64, 74, 82	0
46	2o	88/89 (98%)	-0.16	0 100 100	62, 77, 83, 85	0
47	1p	82/88 (93%)	0.34	4 (4%) 29 20	61, 73, 81, 86	0
47	2p	82/88 (93%)	-0.01	1 (1%) 79 73	56, 70, 81, 82	0
48	1q	99/105 (94%)	0.52	6 (6%) 21 13	53, 66, 73, 76	0
48	2q	99/105 (94%)	0.01	1 (1%) 82 77	66, 74, 82, 87	0
49	1r	68/88 (77%)	2.69	43 (63%) 0 0	57, 68, 78, 83	0
49	2r	68/88 (77%)	1.12	16 (23%) 0 0	68, 77, 82, 87	0
50	1s	83/93 (89%)	-0.40	0 100 100	60, 71, 80, 91	0
50	2s	83/93 (89%)	0.76	14 (16%) 1 1	78, 86, 92, 94	0
51	1t	96/106 (90%)	0.51	8 (8%) 11 6	60, 70, 78, 88	0
51	2t	96/106 (90%)	0.61	8 (8%) 11 6	57, 72, 82, 86	0
52	1u	23/27 (85%)	-0.14	0 100 100	59, 65, 71, 74	0
52	2u	23/27 (85%)	1.69	8 (34%) 0 0	78, 81, 86, 91	0
53	1v	13/24 (54%)	1.59	3 (23%) 0 0	48, 68, 90, 99	0
53	2v	13/24 (54%)	2.43	9 (69%) 0 0	78, 89, 99, 99	0
54	1w	67/76 (88%)	3.03	42 (62%) 0 0	66, 94, 103, 107	0
54	1y	67/76 (88%)	3.63	61 (91%) 0 0	46, 96, 102, 104	0
54	2w	65/76 (85%)	3.80	55 (84%) 0 0	75, 98, 104, 107	0
54	2y	66/76 (86%)	4.03	63 (95%) 0 0	63, 99, 104, 106	0
55	1x	72/77 (93%)	0.38	2 (2%) 53 43	34, 60, 77, 89	0
55	2x	72/77 (93%)	0.70	2 (2%) 53 43	60, 81, 92, 94	0
All	All	20875/21748 (95%)	0.44	1727 (8%) 11 6	16, 65, 91, 109	0

All (1727) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
22	10	6	GLY	11.8
54	1w	71	G	11.2

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Mol	Chain	Res	Type	RSRZ
38	1g	81	GLY	10.8
38	2g	80	VAL	10.8
34	2c	185	GLY	10.6
38	2g	82	GLY	10.3
54	2w	70	G	9.9
44	2m	124	PRO	9.7
34	2c	184	TYR	9.6
54	2y	34	G	9.5
54	2w	71	G	9.3
22	10	7	LEU	9.3
44	2m	123	ALA	9.0
38	1g	80	VAL	8.9
45	2n	34	TYR	8.9
38	2g	84	ASN	8.7
54	2y	36	A	8.4
33	2b	165	VAL	8.4
40	2i	125	TYR	8.3
41	2j	65	LEU	8.3
54	1w	70	G	8.3
34	2c	57	ILE	8.2
34	2c	101	LEU	8.2
34	2c	53	ALA	8.1
50	2s	82	GLY	8.0
54	2w	4	C	8.0
34	2c	21	ARG	7.9
34	2c	52	LEU	7.9
34	2c	58	GLU	7.8
34	2c	189	ALA	7.8
49	1r	78	LEU	7.7
34	2c	205	GLY	7.7
34	2c	51	GLY	7.7
34	2c	183	ASP	7.7
41	2j	47	PHE	7.7
38	1g	156	TRP	7.6
54	2w	76	A	7.5
45	2n	53	LEU	7.5
38	1g	84	ASN	7.5
54	1y	36	A	7.5
34	2c	182	ILE	7.5
34	2c	60	ALA	7.5
34	2c	91	LEU	7.4
34	2c	49	SER	7.3

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Mol	Chain	Res	Type	RSRZ
22	10	5	LYS	7.3
54	2w	72	C	7.3
25	23	60	GLU	7.3
34	2c	200	ALA	7.2
22	10	4	LYS	7.1
38	1g	82	GLY	7.1
54	1w	3	C	7.0
34	2c	80	GLY	6.9
54	1w	73	A	6.9
34	2c	204	LEU	6.8
34	2c	17	ASP	6.8
38	1g	154	TYR	6.7
38	1g	153	HIS	6.7
54	1y	24	G	6.7
54	1y	35	A	6.6
11	2P	149	GLU	6.6
12	2Q	104	PHE	6.6
54	1y	14	A	6.6
34	2c	202	ILE	6.6
40	2i	14	VAL	6.6
54	2y	27	G	6.5
41	2j	93	GLY	6.5
11	2P	123	LEU	6.5
34	2c	159	GLY	6.5
42	1k	92	GLU	6.5
22	20	7	LEU	6.5
54	1w	72	C	6.4
44	2m	121	LYS	6.4
38	2g	86	GLN	6.4
38	2g	85	TYR	6.4
54	2w	73	A	6.4
54	2w	14	A	6.3
42	1k	13	GLN	6.3
54	1w	67	C	6.3
11	2P	68	GLN	6.3
38	2g	78	ARG	6.3
34	2c	8	ILE	6.3
38	1g	79	ARG	6.2
34	2c	186	PHE	6.2
33	2b	187	LEU	6.2
45	2n	25	VAL	6.1
34	2c	124	ILE	6.1

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Mol	Chain	Res	Type	RSRZ
7	2H	165	ALA	6.1
34	1c	87	LEU	6.1
54	2y	33	U	6.1
40	2i	17	VAL	6.1
30	28	16	ILE	6.1
49	1r	22	VAL	6.1
34	2c	201	TYR	6.1
54	1w	69	G	6.1
34	2c	56	ASP	6.0
54	1w	1	G	6.0
34	2c	171	GLY	6.0
38	2g	152	ALA	6.0
54	2y	22	G	6.0
34	2c	160	ALA	6.0
34	2c	55	VAL	6.0
41	2j	55	LYS	6.0
38	2g	156	TRP	6.0
34	2c	188	LEU	5.9
41	2j	62	HIS	5.9
38	2g	83	ALA	5.9
45	2n	57	ARG	5.9
34	2c	81	GLY	5.9
45	2n	39	LEU	5.9
54	2y	6	G	5.9
34	2c	158	GLY	5.8
36	2e	13	ILE	5.8
54	2y	28	G	5.8
45	2n	29	ARG	5.8
54	2y	65	G	5.8
54	2w	75	C	5.8
30	28	15	LYS	5.8
44	2m	122	LYS	5.8
45	2n	49	HIS	5.8
12	2Q	121	ALA	5.7
44	2m	103	THR	5.7
7	2H	107	VAL	5.7
34	2c	65	ALA	5.7
34	2c	108	ASN	5.7
43	2l	27	LEU	5.7
42	2k	90	GLY	5.7
37	1f	48	LEU	5.7
42	2k	32	ILE	5.7

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Mol	Chain	Res	Type	RSRZ
49	1r	40	LEU	5.7
22	10	8	GLY	5.7
33	2b	214	ILE	5.6
38	1g	78	ARG	5.6
33	2b	71	VAL	5.6
38	2g	81	GLY	5.6
54	2y	26	A	5.6
34	2c	6	HIS	5.6
43	2l	64	TYR	5.6
34	2c	170	GLN	5.6
44	2m	120	LYS	5.6
34	2c	67	THR	5.5
54	2y	23	A	5.5
54	2w	13	C	5.5
11	2P	79	ARG	5.5
54	1y	12	U	5.5
34	2c	19	GLU	5.5
38	1g	85	TYR	5.5
45	2n	47	LEU	5.5
38	1g	155	ARG	5.5
45	2n	56	VAL	5.5
54	1w	76	A	5.5
54	2y	38	A	5.5
41	2j	89	ASP	5.5
7	2H	94	TYR	5.4
34	2c	199	LYS	5.4
54	1w	4	C	5.4
54	2y	29	G	5.4
49	1r	54	ARG	5.4
54	2w	3	C	5.4
34	2c	77	ILE	5.4
38	2g	26	PHE	5.4
54	2w	10	G	5.4
54	1w	13	C	5.4
41	2j	48	THR	5.4
34	2c	149	ALA	5.4
42	1k	82	VAL	5.4
33	2b	130	ARG	5.4
54	1y	2	C	5.4
11	2P	45	LEU	5.4
54	1w	10	G	5.3
54	1y	3	C	5.3

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Mol	Chain	Res	Type	RSRZ
11	2P	95	VAL	5.3
43	2l	68	ALA	5.3
49	1r	71	LYS	5.3
34	2c	187	ALA	5.3
42	2k	25	TYR	5.3
7	2H	76	VAL	5.3
54	1y	25	C	5.3
23	21	22	GLY	5.3
41	2j	58	ASP	5.3
33	2b	118	LEU	5.2
40	2i	114	TYR	5.2
34	2c	10	PHE	5.2
41	2j	51	ARG	5.2
54	1w	75	C	5.2
54	1y	6	G	5.2
41	2j	96	ILE	5.2
45	2n	55	GLY	5.2
38	2g	154	TYR	5.2
11	2P	78	PRO	5.2
34	2c	103	VAL	5.2
44	2m	102	ARG	5.2
35	2d	2	GLY	5.1
33	2b	233	SER	5.1
38	1g	83	ALA	5.1
42	1k	83	ILE	5.1
23	21	26	ARG	5.1
54	2w	74	C	5.1
34	2c	44	GLU	5.1
54	2y	24	G	5.1
54	1y	62	C	5.1
34	2c	172	ARG	5.1
54	1y	63	G	5.1
45	2n	36	PHE	5.1
34	2c	145	GLY	5.1
34	2c	181	ASN	5.0
33	2b	163	PHE	5.0
30	28	64	TYR	5.0
50	2s	79	THR	5.0
49	1r	87	ARG	5.0
34	2c	107	GLN	5.0
41	2j	56	HIS	5.0
41	2j	8	LEU	5.0

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Mol	Chain	Res	Type	RSRZ
30	28	63	PRO	5.0
54	1y	56	C	5.0
34	2c	33	LEU	5.0
35	2d	49	ARG	5.0
43	2l	39	VAL	5.0
33	2b	152	PHE	4.9
42	1k	108	ILE	4.9
36	2e	12	LEU	4.9
53	1v	12	A	4.9
34	2c	59	ARG	4.9
54	2y	12	U	4.9
34	2c	64	VAL	4.9
54	2w	31	A	4.9
49	1r	85	LEU	4.9
54	2y	52	G	4.9
54	2w	40	C	4.9
38	2g	79	ARG	4.9
54	2w	38	A	4.9
54	2w	15	G	4.9
35	2d	4	TYR	4.8
45	2n	50	LYS	4.8
34	2c	115	LEU	4.8
22	20	6	GLY	4.8
54	2w	5	G	4.8
22	20	2	ALA	4.8
34	2c	50	ALA	4.8
38	2g	32	ARG	4.8
54	1y	21	A	4.8
42	2k	59	TYR	4.8
54	2w	24	G	4.8
34	2c	198	VAL	4.8
34	2c	23	TYR	4.8
33	2b	132	LYS	4.8
34	2c	206	GLU	4.8
5	2F	181	LEU	4.8
54	2y	48	C	4.7
34	2c	14	ILE	4.7
34	2c	13	GLY	4.7
45	2n	51	GLY	4.7
41	2j	63	PHE	4.7
54	1y	23	A	4.7
54	1y	64	A	4.7

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Mol	Chain	Res	Type	RSRZ
23	21	2	SER	4.7
49	1r	75	ILE	4.7
41	2j	54	PHE	4.7
54	2y	72	C	4.7
54	2y	73	A	4.7
34	2c	5	ILE	4.7
54	1y	22	G	4.7
54	2y	2	C	4.7
54	2y	70	G	4.7
1	2A	652(B)	A	4.6
34	2c	147	LYS	4.6
34	2c	100	ALA	4.6
45	2n	42	ILE	4.6
54	2w	69	G	4.6
54	2y	53	G	4.6
54	1y	33	U	4.6
49	1r	44	LEU	4.6
34	2c	167	TRP	4.6
41	2j	92	THR	4.6
54	1w	15	G	4.6
54	2y	1	G	4.6
36	2e	31	LEU	4.6
50	2s	84	GLY	4.6
54	2y	64	A	4.6
54	2y	63	G	4.6
43	2l	56	ALA	4.6
34	2c	15	THR	4.6
34	2c	196	LEU	4.6
49	2r	87	ARG	4.6
11	2P	105	LEU	4.5
49	1r	79	LEU	4.5
45	2n	6	LEU	4.5
42	1k	126	ARG	4.5
34	2c	66	VAL	4.5
49	1r	39	VAL	4.5
54	1y	27	G	4.5
43	2l	43	VAL	4.5
54	2w	2	C	4.5
33	2b	120	ALA	4.5
41	2j	66	ARG	4.5
35	2d	23	GLY	4.5
54	1y	13	C	4.5

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Mol	Chain	Res	Type	RSRZ
54	1y	20	U	4.5
54	1w	74	C	4.5
1	1A	2141	G	4.5
7	2H	35	VAL	4.5
8	2I	3	VAL	4.5
41	2j	59	SER	4.5
37	1f	58	GLY	4.5
34	2c	207	VAL	4.5
40	2i	36	TYR	4.5
49	1r	21	LYS	4.5
22	20	4	LYS	4.4
38	2g	4	ARG	4.4
5	2F	6	VAL	4.4
40	2i	5	TYR	4.4
45	2n	2	ALA	4.4
54	1y	29	G	4.4
53	2v	24	A	4.4
34	2c	22	TRP	4.4
34	2c	87	LEU	4.4
42	2k	31	THR	4.4
54	1w	6	G	4.4
34	2c	142	MET	4.4
54	2y	35	A	4.4
22	10	3	HIS	4.4
54	1y	34	G	4.4
33	2b	210	SER	4.4
34	2c	154	SER	4.4
40	2i	126	SER	4.4
42	1k	89	ALA	4.4
38	2g	73	MET	4.4
11	2P	108	LYS	4.4
1	2A	2112	G	4.4
40	2i	7	THR	4.4
34	2c	74	GLY	4.4
43	2l	26	ALA	4.3
34	2c	178	LEU	4.3
35	2d	37	PRO	4.3
34	2c	4	LYS	4.3
33	2b	69	LEU	4.3
40	2i	124	GLN	4.3
54	2y	15	G	4.3
54	2y	57	G	4.3

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Mol	Chain	Res	Type	RSRZ
54	2w	50	U	4.3
7	2H	114	VAL	4.3
41	2j	10	GLY	4.3
34	2c	20	SER	4.3
37	1f	54	LYS	4.3
35	2d	198	VAL	4.3
41	2j	72	VAL	4.3
1	1A	2145	C	4.3
34	2c	157	ILE	4.3
30	28	61	LEU	4.2
36	2e	109	ILE	4.2
37	1f	46	ARG	4.2
54	1y	48	C	4.2
42	1k	87	THR	4.2
45	2n	37	PHE	4.2
54	2w	45	U	4.2
53	1v	24	A	4.2
54	1w	25	C	4.2
54	2w	56	C	4.2
38	2g	155	ARG	4.2
12	2Q	103	MET	4.2
41	2j	6	ILE	4.2
34	1c	65	ALA	4.2
36	2e	20	GLN	4.2
17	2V	74	LYS	4.2
41	2j	71	LEU	4.2
54	1w	2	C	4.2
40	2i	66	ARG	4.2
41	2j	85	LEU	4.2
43	1l	68	ALA	4.2
32	2a	1030(B)	C	4.2
34	2c	105	GLU	4.2
45	2n	41	ARG	4.2
33	2b	97	TRP	4.2
37	1f	43	LEU	4.2
34	2c	16	ARG	4.2
54	2y	4	C	4.2
54	2y	21	A	4.2
41	2j	50	ILE	4.1
34	2c	47	LEU	4.1
22	20	9	SER	4.1
34	2c	173	VAL	4.1

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Mol	Chain	Res	Type	RSRZ
42	1k	21	ILE	4.1
1	2A	2146	C	4.1
5	2F	24	LEU	4.1
54	2w	9	A	4.1
42	1k	117	ASN	4.1
42	1k	91	ARG	4.1
5	2F	90	PHE	4.1
54	2y	7	A	4.1
34	2c	102	ASN	4.1
33	1b	77	ALA	4.1
34	2c	162	GLN	4.1
54	2y	9	A	4.1
11	2P	91	PHE	4.1
43	2l	32	PHE	4.1
11	2P	122	PRO	4.1
34	2c	40	ARG	4.1
49	1r	51	LEU	4.1
38	2g	150	ALA	4.1
54	1y	47	U	4.1
26	24	54	GLY	4.1
45	2n	22	THR	4.1
1	1A	2112	G	4.1
54	1y	1	G	4.1
42	1k	109	VAL	4.0
33	2b	70	PHE	4.0
35	2d	48	ALA	4.0
44	1m	123	ALA	4.0
52	2u	14	TRP	4.0
54	1w	5	G	4.0
54	2y	25	C	4.0
41	2j	26	ALA	4.0
53	2v	23	A	4.0
38	2g	59	LEU	4.0
34	2c	109	PRO	4.0
34	2c	18	TRP	4.0
54	2w	23	A	4.0
32	2a	1030(A)	G	4.0
34	2c	111	LEU	4.0
49	1r	56	THR	4.0
34	1c	100	ALA	4.0
44	2m	42	ALA	4.0
7	2H	24	VAL	4.0

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Mol	Chain	Res	Type	RSRZ
17	2V	5	VAL	4.0
35	2d	47	ARG	4.0
40	2i	4	TYR	4.0
42	1k	42	TRP	4.0
33	2b	149	LEU	4.0
33	2b	184	VAL	4.0
34	1c	198	VAL	4.0
54	2y	47	U	4.0
6	2G	150	ASP	4.0
30	28	11	LYS	4.0
33	2b	131	PRO	4.0
41	2j	60	ARG	4.0
42	1k	61	ALA	4.0
40	2i	16	ARG	3.9
40	2i	123	PRO	3.9
11	2P	6	LEU	3.9
54	1y	71	G	3.9
34	2c	75	VAL	3.9
23	21	23	LYS	3.9
33	2b	93	VAL	3.9
40	2i	127	LYS	3.9
42	1k	64	ALA	3.9
43	1l	64	TYR	3.9
43	1l	89	ARG	3.9
41	2j	17	ASP	3.9
16	2U	88	ILE	3.9
54	2y	13	C	3.9
34	2c	153	VAL	3.9
41	2j	61	GLU	3.9
34	2c	71	ALA	3.9
16	2U	90	VAL	3.9
38	2g	6	ARG	3.9
41	2j	12	ASP	3.9
33	2b	155	LEU	3.9
40	2i	19	LEU	3.9
54	2y	5	G	3.9
34	2c	78	GLY	3.8
42	1k	111	ASP	3.8
11	2P	100	LEU	3.8
53	2v	14	A	3.8
54	1w	14	A	3.8
45	2n	58	LYS	3.8

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Mol	Chain	Res	Type	RSRZ
51	2t	66	ALA	3.8
38	2g	153	HIS	3.8
54	2y	74	C	3.8
34	1c	57	ILE	3.8
35	2d	160	GLN	3.8
43	2l	31	PRO	3.8
54	1y	7	A	3.8
11	2P	124	LYS	3.8
11	2P	127	ALA	3.8
34	2c	179	ARG	3.8
38	2g	13	GLN	3.8
33	2b	122	PHE	3.8
3	1D	276	LYS	3.8
32	1a	1027	C	3.8
36	2e	33	VAL	3.8
40	2i	117	HIS	3.8
42	1k	25	TYR	3.8
54	2y	61	C	3.8
49	1r	31	LEU	3.8
16	2U	89	GLU	3.8
44	2m	97	PRO	3.8
54	1y	15	G	3.8
6	2G	41	GLN	3.8
35	1d	23	GLY	3.8
42	1k	80	VAL	3.8
11	2P	112	LEU	3.8
30	28	12	LYS	3.8
34	2c	2	GLY	3.8
28	26	54	ILE	3.8
54	1y	53	G	3.8
40	2i	98	PRO	3.8
6	2G	149	VAL	3.8
8	2I	12	LEU	3.8
49	2r	85	LEU	3.8
35	2d	28	SER	3.8
45	2n	31	ARG	3.8
1	2A	2174	C	3.7
6	2G	44	GLY	3.7
34	2c	37	GLN	3.7
43	2l	51	ALA	3.7
49	1r	81	PHE	3.7
33	2b	68	ILE	3.7

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Mol	Chain	Res	Type	RSRZ
12	2Q	10	ARG	3.7
33	2b	67	THR	3.7
40	2i	83	ARG	3.7
10	2O	1	MET	3.7
54	2y	14	A	3.7
7	2H	162	ILE	3.7
54	2w	6	G	3.7
34	2c	54	ARG	3.7
51	1t	69	GLY	3.7
45	2n	10	ALA	3.7
10	2O	19	ILE	3.7
6	2G	138	GLN	3.7
10	2O	10	VAL	3.7
49	1r	55	ARG	3.7
35	2d	120	LEU	3.7
49	2r	49	LYS	3.7
33	2b	99	GLY	3.7
42	2k	49	GLY	3.7
7	2H	138	LYS	3.7
5	2F	176	LEU	3.7
7	2H	52	VAL	3.7
34	2c	82	GLU	3.7
41	2j	88	LEU	3.7
54	1w	11	C	3.7
54	2w	42	C	3.7
54	2y	45	U	3.7
37	1f	50	TYR	3.7
48	1q	28	PRO	3.7
54	2y	18	G	3.7
23	21	29	GLY	3.7
22	20	5	LYS	3.7
43	2l	48	PRO	3.7
33	2b	115	LEU	3.7
33	2b	197	VAL	3.7
30	28	25	MET	3.6
43	2l	59	ARG	3.6
1	2A	229	A	3.6
22	20	3	HIS	3.6
34	1c	66	VAL	3.6
34	2c	7	PRO	3.6
49	1r	58	LEU	3.6
33	2b	101	MET	3.6

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Mol	Chain	Res	Type	RSRZ
45	2n	26	ARG	3.6
54	1y	11	C	3.6
54	2w	11	C	3.6
34	2c	203	PHE	3.6
34	2c	176	HIS	3.6
11	2P	80	TYR	3.6
54	1y	70	G	3.6
54	2w	30	G	3.6
34	2c	180	ALA	3.6
54	2w	67	C	3.6
34	2c	69	HIS	3.6
30	28	2	PRO	3.6
45	2n	18	VAL	3.6
45	2n	35	ARG	3.6
11	2P	64	LYS	3.6
32	1a	1030(B)	C	3.6
34	2c	113	ALA	3.6
40	2i	9	ARG	3.6
45	2n	59	ALA	3.6
49	1r	29	PHE	3.6
11	2P	125	VAL	3.6
33	1b	165	VAL	3.6
54	1y	72	C	3.6
54	2y	40	C	3.6
34	2c	150	LYS	3.6
30	28	9	GLY	3.6
38	2g	75	VAL	3.6
33	2b	225	ALA	3.6
7	2H	55	PRO	3.6
38	2g	95	ARG	3.6
45	2n	52	GLN	3.6
50	2s	80	TYR	3.5
54	1w	12	U	3.5
8	2I	85	GLU	3.5
34	2c	197	GLY	3.5
23	11	2	SER	3.5
33	2b	121	LEU	3.5
38	2g	3	ARG	3.5
7	2H	19	VAL	3.5
40	2i	81	ILE	3.5
43	1l	62	SER	3.5
40	2i	70	LYS	3.5

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Mol	Chain	Res	Type	RSRZ
42	2k	30	VAL	3.5
36	2e	45	PHE	3.5
33	2b	90	MET	3.5
33	2b	215	LEU	3.5
7	2H	148	ILE	3.5
9	2N	8	GLN	3.5
1	1A	2117	A	3.5
38	1g	151	TYR	3.5
54	1y	67	C	3.5
38	1g	99	LEU	3.5
42	1k	14	VAL	3.5
49	2r	50	ILE	3.5
38	1g	86	GLN	3.5
40	2i	119	ALA	3.5
42	1k	60	ALA	3.5
49	1r	24	ALA	3.5
5	2F	36	VAL	3.5
42	1k	84	VAL	3.5
54	2w	66	U	3.5
11	2P	126	VAL	3.5
34	2c	143	GLU	3.5
38	2g	77	SER	3.5
22	20	8	GLY	3.5
36	2e	110	LEU	3.5
11	2P	92	GLU	3.5
41	2j	98	ILE	3.5
11	2P	65	ARG	3.5
38	2g	41	ARG	3.5
7	2H	103	LEU	3.5
34	2c	146	ALA	3.5
37	1f	98	LEU	3.5
42	1k	23	ALA	3.5
42	2k	50	TYR	3.5
1	1A	2174	C	3.5
49	1r	43	PHE	3.5
54	1y	65	G	3.5
33	2b	113	HIS	3.4
38	2g	16	LEU	3.4
34	2c	61	ALA	3.4
5	2F	183	VAL	3.4
54	1y	75	C	3.4
54	2w	68	C	3.4

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Mol	Chain	Res	Type	RSRZ
42	1k	43	SER	3.4
54	2y	58	A	3.4
32	1a	1030(A)	G	3.4
54	1w	20	U	3.4
54	2w	44	G	3.4
34	2c	68	VAL	3.4
42	1k	20	TYR	3.4
54	2y	3	C	3.4
28	26	28	ARG	3.4
54	1y	26	A	3.4
1	1A	2115	G	3.4
11	2P	83	VAL	3.4
43	2l	85	ILE	3.4
49	1r	82	THR	3.4
45	2n	27	CYS	3.4
38	2g	33	ASP	3.4
36	2e	108	ALA	3.4
34	2c	70	VAL	3.4
54	2w	19	G	3.4
37	1f	60	PHE	3.4
32	2a	1257	U	3.4
11	2P	147	LEU	3.4
45	2n	11	LYS	3.4
11	2P	75	ILE	3.4
42	2k	89	ALA	3.4
42	1k	47	VAL	3.4
54	2y	10	G	3.4
53	2v	22	U	3.4
51	2t	24	LEU	3.4
36	2e	21	ALA	3.4
7	2H	34	GLU	3.4
7	2H	159	GLU	3.4
41	2j	49	VAL	3.4
49	2r	43	PHE	3.4
34	2c	104	GLN	3.4
37	1f	57	GLN	3.4
54	2y	62	C	3.4
1	2A	2110	G	3.4
32	2a	1034	G	3.4
54	2w	28	G	3.4
54	2y	71	G	3.4
7	2H	115	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
34	2c	155	GLY	3.4
40	2i	28	VAL	3.4
43	2l	55	VAL	3.4
34	2c	119	ARG	3.3
36	2e	25	ARG	3.3
38	2g	103	TRP	3.4
30	28	32	LEU	3.3
31	29	17	ILE	3.3
33	2b	216	SER	3.3
11	2P	77	ARG	3.3
34	2c	126	ARG	3.3
54	1w	66	U	3.3
54	2y	31	A	3.3
6	2G	142	PRO	3.3
7	2H	29	PRO	3.3
11	2P	109	GLY	3.3
42	2k	108	ILE	3.3
42	2k	42	TRP	3.3
36	2e	129	ILE	3.3
8	2I	18	VAL	3.3
33	2b	188	ALA	3.3
36	2e	90	VAL	3.3
54	1w	7	A	3.3
30	28	29	LYS	3.3
35	2d	115	ARG	3.3
33	2b	227	GLY	3.3
34	2c	117	ALA	3.3
35	2d	18	LYS	3.3
40	2i	26	VAL	3.3
45	2n	45	ARG	3.3
47	1p	1	MET	3.3
34	2c	144	SER	3.3
35	2d	27	TYR	3.3
7	2H	48	GLY	3.3
36	2e	29	GLY	3.3
52	2u	10	ARG	3.3
54	2w	27	G	3.3
7	2H	141	VAL	3.3
34	2c	128	PHE	3.3
36	2e	8	GLU	3.3
42	1k	110	ASP	3.3
38	2g	2	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
42	2k	57	THR	3.3
36	2e	10	MET	3.3
5	2F	101	LEU	3.3
54	2w	7	A	3.3
42	1k	17	GLY	3.3
44	1m	124	PRO	3.3
42	2k	63	LEU	3.3
38	2g	151	TYR	3.3
51	1t	55	ILE	3.3
6	2G	62	LEU	3.3
49	1r	30	ASP	3.3
12	2Q	100	GLY	3.3
34	2c	148	GLY	3.3
40	2i	110	GLU	3.2
30	28	58	ILE	3.2
30	28	59	LYS	3.2
53	2v	13	A	3.2
54	1w	23	A	3.2
34	1c	55	VAL	3.2
49	1r	52	PRO	3.2
11	2P	148	LEU	3.2
17	2V	38	LEU	3.2
7	2H	145	ALA	3.2
23	21	68	PRO	3.2
34	2c	174	PRO	3.2
34	2c	12	LEU	3.2
49	1r	76	LEU	3.2
42	1k	29	ILE	3.2
51	2t	9	ASN	3.2
54	1y	10	G	3.2
6	2G	90	LEU	3.2
11	2P	90	ARG	3.2
36	2e	24	ARG	3.2
49	1r	42	ARG	3.2
36	2e	11	ILE	3.2
11	2P	1	MET	3.2
54	1w	65	G	3.2
54	2w	41	C	3.2
34	2c	39	ILE	3.2
7	2H	90	LYS	3.2
42	2k	107	SER	3.2
11	2P	59	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
40	2i	69	GLY	3.2
21	2Z	62	PRO	3.2
35	2d	162	LEU	3.2
42	2k	98	LEU	3.2
8	2I	4	ILE	3.2
11	2P	50	ARG	3.2
33	2b	209	ARG	3.2
35	2d	38	TYR	3.2
42	1k	86	GLY	3.2
49	1r	80	PRO	3.2
54	1w	68	C	3.2
5	2F	7	TYR	3.2
15	2T	99	LEU	3.2
54	2w	49	C	3.2
40	2i	41	VAL	3.1
5	2F	194	MET	3.1
3	2D	276	LYS	3.1
11	2P	38	GLN	3.1
11	2P	53	GLY	3.1
18	2W	112	GLY	3.1
45	2n	38	GLY	3.1
11	2P	110	TYR	3.1
34	1c	201	TYR	3.1
34	2c	48	TYR	3.1
1	2A	2123	G	3.1
7	2H	123	PHE	3.1
33	2b	77	ALA	3.1
41	2j	68	HIS	3.1
33	1b	70	PHE	3.1
40	2i	120	ARG	3.1
1	1A	2113	U	3.1
34	2c	175	LEU	3.1
1	1A	1095	A	3.1
30	28	10	ALA	3.1
38	2g	40	ALA	3.1
40	2i	15	ALA	3.1
49	1r	38	GLU	3.1
7	2H	41	MET	3.1
44	2m	4	ILE	3.1
36	2e	88	LYS	3.1
37	1f	88	VAL	3.1
49	1r	86	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
7	2H	152	ARG	3.1
1	2A	2115	G	3.1
1	2A	2147	G	3.1
11	2P	35	HIS	3.1
54	1w	49	C	3.1
40	2i	64	THR	3.1
33	2b	111	ARG	3.1
40	2i	122	ALA	3.1
54	1y	49	C	3.1
54	2y	11	C	3.1
38	1g	73	MET	3.1
6	2G	72	ARG	3.1
42	1k	24	SER	3.1
12	2Q	97	VAL	3.1
34	2c	120	VAL	3.1
10	2O	17	ARG	3.1
32	2a	1030	C	3.1
6	2G	48	GLU	3.1
32	1a	1001(A)	G	3.1
32	2a	1068	G	3.1
6	2G	80	PHE	3.0
34	2c	43	LEU	3.0
1	1A	2114	A	3.0
32	1a	1531	A	3.0
42	1k	96	ARG	3.0
38	2g	42	ILE	3.0
40	2i	27	THR	3.0
11	2P	76	LYS	3.0
32	1a	1036	G	3.0
7	2H	71	LEU	3.0
42	1k	54	ARG	3.0
1	1A	2143	C	3.0
33	2b	185	ILE	3.0
54	2w	61	C	3.0
42	1k	19	ALA	3.0
7	2H	175	LYS	3.0
10	2O	81	ASP	3.0
42	1k	81	ASP	3.0
42	1k	116	HIS	3.0
45	2n	7	ILE	3.0
5	2F	193	VAL	3.0
54	2w	58	A	3.0

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Mol	Chain	Res	Type	RSRZ
45	2n	44	LEU	3.0
38	2g	36	LYS	3.0
36	1e	10	MET	3.0
37	1f	9	VAL	3.0
42	2k	54	ARG	3.0
32	2a	1114	C	3.0
1	2A	2109	U	3.0
22	20	68	GLU	3.0
54	1y	5	G	3.0
10	2O	11	ALA	3.0
11	2P	72	PRO	3.0
38	2g	147	ALA	3.0
1	2A	2144	U	3.0
49	1r	84	LYS	3.0
54	1y	38	A	3.0
54	2w	21	A	3.0
41	1j	98	ILE	3.0
1	2A	2166	G	3.0
10	2O	41	ALA	3.0
26	24	32	TYR	3.0
30	28	65	GLU	3.0
43	2l	69	TYR	3.0
30	28	60	LEU	3.0
38	2g	99	LEU	3.0
7	2H	84	SER	3.0
41	2j	46	ARG	3.0
36	2e	51	VAL	3.0
49	2r	22	VAL	3.0
5	2F	32	LEU	3.0
11	2P	88	LEU	3.0
12	2Q	34	LEU	3.0
49	1r	64	ARG	3.0
34	2c	72	LYS	3.0
43	2l	94	PRO	2.9
32	2a	1112	C	2.9
7	2H	169	VAL	2.9
12	2Q	96	VAL	2.9
25	23	59	VAL	2.9
34	2c	106	VAL	2.9
11	2P	51	PHE	2.9
36	2e	17	ALA	2.9
36	2e	114	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	2A	2128	C	2.9
35	1d	158	ILE	2.9
40	2i	77	ILE	2.9
54	1y	19	G	2.9
54	2y	69	G	2.9
36	2e	41	VAL	2.9
33	1b	188	ALA	2.9
53	1v	13	A	2.9
54	1y	31	A	2.9
7	2H	163	TYR	2.9
54	1y	60	U	2.9
36	2e	63	ARG	2.9
41	2j	57	LYS	2.9
54	1y	40	C	2.9
23	21	30	VAL	2.9
25	23	58	VAL	2.9
42	2k	100	ALA	2.9
54	2w	34	G	2.9
40	2i	62	TYR	2.9
5	2F	186	ILE	2.9
7	2H	151	ILE	2.9
33	2b	137	ARG	2.9
44	2m	105	THR	2.9
48	1q	27	PHE	2.9
7	2H	108	GLY	2.9
35	2d	19	LEU	2.9
32	2a	1108	G	2.9
54	2w	65	G	2.9
54	2y	66	U	2.9
12	2Q	9	TYR	2.9
31	29	13	LYS	2.9
7	2H	125	VAL	2.9
41	2j	94	VAL	2.9
54	2y	56	C	2.9
34	2c	133	ALA	2.9
5	2F	93	LYS	2.9
11	2P	17	LYS	2.9
43	2l	71	PRO	2.9
54	1y	45	U	2.9
5	1F	89	VAL	2.9
45	2n	61	TRP	2.9
38	2g	5	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
7	2H	72	ILE	2.9
37	1f	52	ILE	2.9
12	2Q	130	LYS	2.9
54	2w	22	G	2.9
42	1k	118	GLY	2.9
44	2m	90	LEU	2.9
32	2a	1192	C	2.9
34	2c	114	PRO	2.9
42	1k	115	PRO	2.9
10	2O	7	TYR	2.9
30	28	21	LYS	2.9
32	2a	1092	A	2.9
44	2m	119	GLY	2.9
32	2a	1033	G	2.9
54	1y	30	G	2.9
1	1A	2142	C	2.8
1	2A	2175	C	2.8
41	2j	15	THR	2.8
42	1k	28	THR	2.8
42	1k	57	THR	2.8
34	2c	116	VAL	2.8
34	2c	190	ARG	2.8
38	2g	143	ARG	2.8
42	2k	56	GLY	2.8
51	2t	25	ARG	2.8
5	2F	111	ALA	2.8
6	2G	152	LEU	2.8
43	1l	60	LEU	2.8
54	1w	44	G	2.8
35	2d	31	CYS	2.8
54	2y	41	C	2.8
10	2O	85	VAL	2.8
35	1d	110	PHE	2.8
36	2e	84	PHE	2.8
42	2k	109	VAL	2.8
49	1r	26	LEU	2.8
34	1c	199	LYS	2.8
1	1A	2140	C	2.8
54	1w	27	G	2.8
52	2u	16	GLY	2.8
11	2P	138	LEU	2.8
34	2c	3	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
34	2c	151	VAL	2.8
36	2e	123	LEU	2.8
1	2A	2412	A	2.8
15	2T	39	ARG	2.8
44	2m	99	ARG	2.8
45	2n	23	ARG	2.8
5	1F	14	PRO	2.8
54	1y	73	A	2.8
41	2j	42	THR	2.8
54	1y	42	C	2.8
54	2w	25	C	2.8
54	2y	42	C	2.8
32	2a	1220	G	2.8
40	2i	102	LEU	2.8
43	2l	52	LEU	2.8
34	2c	118	GLN	2.8
45	2n	46	GLU	2.8
6	2G	85	GLY	2.8
9	2N	23	LEU	2.8
7	2H	124	GLU	2.8
12	1Q	80	GLU	2.8
32	2a	1036	G	2.8
54	1y	52	G	2.8
31	29	15	LYS	2.8
23	21	36	GLY	2.8
34	2c	73	PRO	2.8
42	2k	29	ILE	2.8
37	1f	55	ASP	2.8
41	2j	67	THR	2.8
43	1l	98	TYR	2.8
33	1b	78	GLN	2.8
38	2g	7	ALA	2.8
54	2w	52	G	2.8
17	2V	71	LEU	2.8
34	2c	138	VAL	2.8
38	2g	139	GLU	2.8
28	26	8	LYS	2.8
42	2k	20	TYR	2.8
15	2T	69	GLY	2.8
32	2a	1030(C)	G	2.8
32	2a	1190	G	2.8
11	2P	94	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
11	2P	107	LYS	2.8
12	1Q	79	LEU	2.8
35	2d	20	TYR	2.8
40	2i	3	GLN	2.8
42	2k	60	ALA	2.8
53	2v	12	A	2.7
53	2v	21	C	2.8
34	1c	2	GLY	2.7
16	2U	110	VAL	2.7
33	2b	98	LEU	2.7
38	2g	22	LEU	2.7
41	2j	18	ALA	2.7
25	23	7	LYS	2.7
36	2e	14	ARG	2.7
43	2l	41	ARG	2.7
22	20	69	PHE	2.7
10	2O	8	LEU	2.7
33	2b	145	LEU	2.7
35	2d	112	VAL	2.7
38	1g	77	SER	2.7
1	2A	2145	C	2.7
12	2Q	7	MET	2.7
12	2Q	19	GLY	2.7
36	2e	130	ASN	2.7
54	1y	61	C	2.7
11	2P	106	LEU	2.7
38	2g	91	VAL	2.7
39	1h	129	VAL	2.7
45	2n	60	SER	2.7
32	1a	204	U	2.7
49	1r	70	ILE	2.7
54	1y	59	U	2.7
54	1y	58	A	2.7
55	1x	76	A	2.7
41	2j	40	LEU	2.7
50	2s	30	LEU	2.7
41	2j	29	ARG	2.7
43	1l	22	SER	2.7
43	2l	97	ARG	2.7
43	2l	98	TYR	2.7
1	1A	2130	U	2.7
32	1a	1030(C)	G	2.7

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Mol	Chain	Res	Type	RSRZ
32	2a	89	C	2.7
6	2G	49	ASP	2.7
7	2H	105	LEU	2.7
25	23	2	PRO	2.7
33	1b	95	GLN	2.7
38	2g	104	LEU	2.7
33	2b	203	GLY	2.7
38	2g	34	GLY	2.7
7	2H	157	TYR	2.7
33	2b	201	ILE	2.7
35	2d	35	ARG	2.7
42	2k	96	ARG	2.7
43	2l	67	THR	2.7
52	2u	6	ARG	2.7
1	1A	2111	C	2.7
43	1l	16	GLU	2.7
1	1A	2159	G	2.7
54	2w	63	G	2.7
45	2n	48	ALA	2.7
1	1A	2144	U	2.7
37	2f	4	TYR	2.7
41	2j	38	ILE	2.7
33	2b	44	LEU	2.7
49	1r	46	GLU	2.7
26	24	7	PRO	2.7
38	2g	39	ALA	2.7
33	2b	127	ILE	2.6
6	2G	43	LEU	2.6
15	2T	114	LEU	2.6
34	1c	47	LEU	2.6
40	2i	116	LYS	2.6
10	2O	58	VAL	2.6
36	1e	82	VAL	2.6
11	2P	43	GLY	2.6
20	2Y	59	GLY	2.6
11	2P	74	GLU	2.6
32	2a	80	G	2.6
39	1h	86	ILE	2.6
1	1A	2169	A	2.6
32	2a	1236	A	2.6
5	2F	114	VAL	2.6
34	2c	11	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
38	2g	10	ARG	2.6
40	2i	93	ARG	2.6
49	2r	84	LYS	2.6
12	2Q	68	ILE	2.6
34	2c	28	GLN	2.6
54	1w	24	G	2.6
7	2H	113	VAL	2.6
17	2V	42	GLY	2.6
30	28	14	VAL	2.6
31	29	16	VAL	2.6
32	2a	1110	A	2.6
36	2e	107	ARG	2.6
42	2k	123	LYS	2.6
34	1c	186	PHE	2.6
36	2e	28	PHE	2.6
54	2y	49	C	2.6
12	2Q	120	ILE	2.6
8	2I	38	LEU	2.6
36	2e	53	LEU	2.6
5	2F	37	VAL	2.6
1	1A	2121	G	2.6
30	28	5	LYS	2.6
32	2a	973	G	2.6
32	2a	1093	A	2.6
36	2e	9	LYS	2.6
41	2j	32	ALA	2.6
42	1k	35	PRO	2.6
52	2u	23	PRO	2.6
38	2g	43	PHE	2.6
15	2T	48	ILE	2.6
42	1k	22	HIS	2.6
32	2a	84	U	2.6
38	2g	135	VAL	2.6
11	2P	12	ALA	2.6
40	2i	2	GLU	2.6
40	2i	52	ALA	2.6
42	2k	117	ASN	2.6
1	2A	2159	G	2.6
32	1a	1026	G	2.6
1	1A	2146	C	2.6
6	2G	86	MET	2.6
9	2N	85	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
33	2b	48	MET	2.6
36	2e	118	ILE	2.6
54	1y	41	C	2.6
11	2P	93	GLY	2.6
34	2c	112	SER	2.6
34	2c	92	ALA	2.6
1	2A	2170	A	2.6
36	2e	16	THR	2.6
32	2a	1061	G	2.6
32	2a	1346	A	2.6
38	1g	87	VAL	2.6
42	1k	120	ARG	2.6
42	2k	91	ARG	2.6
35	2d	6	GLY	2.6
1	1A	2151	G	2.6
54	2y	30	G	2.6
25	23	6	VAL	2.6
31	29	12	ASP	2.6
37	1f	90	VAL	2.6
42	1k	44	SER	2.6
38	2g	29	LYS	2.6
42	1k	97	ALA	2.6
1	2A	2113	U	2.5
1	2A	2122	U	2.5
1	1A	2161	C	2.5
22	20	71	ASP	2.5
40	2i	105	ASP	2.5
42	1k	59	TYR	2.5
11	2P	103	ALA	2.5
41	2j	11	PHE	2.5
41	2j	53	PRO	2.5
33	1b	135	GLN	2.5
42	1k	88	GLY	2.5
12	2Q	125	LEU	2.5
35	1d	157	LEU	2.5
33	2b	133	LYS	2.5
36	1e	24	ARG	2.5
38	2g	149	ARG	2.5
42	1k	18	ARG	2.5
42	2k	51	LYS	2.5
1	2A	2114	A	2.5
1	2A	2133	G	2.5

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Mol	Chain	Res	Type	RSRZ
54	1w	63	G	2.5
34	2c	63	ASN	2.5
34	2c	123	GLN	2.5
44	2m	101	GLN	2.5
33	2b	211	ILE	2.5
42	1k	90	GLY	2.5
42	2k	95	ILE	2.5
5	2F	33	LEU	2.5
34	2c	85	ARG	2.5
7	2H	57	ASP	2.5
54	2w	62	C	2.5
32	2a	1224	G	2.5
25	23	26	LEU	2.5
25	23	53	LEU	2.5
43	2l	84	LEU	2.5
28	26	5	VAL	2.5
42	2k	47	VAL	2.5
11	2P	128	HIS	2.5
36	2e	6	PHE	2.5
45	2n	54	PRO	2.5
30	28	62	LEU	2.5
37	2f	48	LEU	2.5
49	2r	76	LEU	2.5
1	2A	2127	G	2.5
4	2E	196	VAL	2.5
38	2g	144	MET	2.5
54	1w	30	G	2.5
45	2n	33	VAL	2.5
54	1y	66	U	2.5
54	2y	51	U	2.5
45	2n	16	PHE	2.5
33	2b	218	ALA	2.5
34	2c	79	ARG	2.5
34	2c	41	GLY	2.5
49	2r	48	GLY	2.5
5	1F	25	PRO	2.5
5	2F	206	ILE	2.5
37	1f	45	LEU	2.5
7	2H	13	LYS	2.5
55	2x	70	G	2.5
11	2P	111	ARG	2.5
35	2d	168	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
49	1r	53	ARG	2.5
33	2b	92	TYR	2.5
42	2k	93	GLN	2.5
11	2P	97	PRO	2.5
34	1c	43	LEU	2.5
42	1k	103	LEU	2.5
54	2y	68	C	2.5
43	1l	28	LYS	2.5
51	2t	21	LYS	2.5
54	1y	9	A	2.5
43	1l	18	VAL	2.5
21	2Z	88	PHE	2.5
35	1d	102	ASP	2.5
35	2d	122	ARG	2.5
38	1g	74	GLU	2.5
40	2i	121	ARG	2.5
23	21	28	GLY	2.5
43	2l	46	LYS	2.5
5	2F	41	LEU	2.5
33	2b	58	ILE	2.5
8	2I	107	VAL	2.5
40	2i	53	VAL	2.5
50	2s	29	ARG	2.5
33	2b	205	ASP	2.5
7	2H	150	ALA	2.5
40	2i	106	ALA	2.5
40	2i	113	LYS	2.5
1	2A	2125	G	2.5
5	1F	206	ILE	2.5
33	2b	91	PRO	2.4
37	1f	79	LEU	2.5
42	1k	48	ILE	2.5
48	1q	36	ILE	2.5
50	2s	49	ILE	2.5
54	1y	28	G	2.5
39	1h	5	PRO	2.4
50	2s	53	ASN	2.4
33	1b	189	ASP	2.4
35	2d	30	LYS	2.4
5	2F	109	GLY	2.4
43	2l	29	GLY	2.4
54	1w	64	A	2.4

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Mol	Chain	Res	Type	RSRZ
52	2u	8	THR	2.4
6	2G	139	LEU	2.4
11	2P	102	ARG	2.4
33	2b	31	TYR	2.4
37	1f	96	PRO	2.4
1	2A	652(T)	C	2.4
1	2A	2132	U	2.4
30	28	22	VAL	2.4
33	2b	63	MET	2.4
37	1f	97	PHE	2.4
54	2w	47	U	2.4
40	2i	115	GLY	2.4
32	2a	1357	A	2.4
35	2d	158	ILE	2.4
51	1t	83	ARG	2.4
1	2A	2129	C	2.4
28	26	20	ASN	2.4
32	2a	1117	G	2.4
42	2k	77	MET	2.4
5	2F	26	ALA	2.4
34	2c	89	GLU	2.4
36	2e	81	GLU	2.4
30	28	8	LYS	2.4
33	2b	158	LEU	2.4
21	2Z	83	PRO	2.4
33	1b	148	TYR	2.4
11	2P	130	PHE	2.4
36	2e	136	MET	2.4
7	2H	97	ARG	2.4
54	2y	43	C	2.4
32	2a	1084	G	2.4
17	2V	20	LEU	2.4
35	2d	108	LEU	2.4
1	2A	2117	A	2.4
1	2A	2176	A	2.4
33	2b	164	VAL	2.4
3	1D	263	ARG	2.4
54	2w	12	U	2.4
36	2e	47	LYS	2.4
32	2a	1059	C	2.4
1	1A	2147	G	2.4
16	2U	95	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
32	2a	78	G	2.4
32	2a	1032	G	2.4
34	1c	202	ILE	2.4
12	2Q	33	GLY	2.4
34	1c	72	LYS	2.4
34	2c	122	GLU	2.4
43	2l	47	LYS	2.4
34	1c	200	ALA	2.4
32	2a	92	C	2.4
23	21	98	LEU	2.4
37	1f	61	LEU	2.4
42	2k	21	ILE	2.4
37	1f	47	ARG	2.4
7	2H	53	GLU	2.4
38	2g	74	GLU	2.4
1	2A	2173	A	2.4
34	2c	36	ASP	2.4
28	16	2	ALA	2.4
10	2O	25	LEU	2.4
17	2V	94	LEU	2.4
31	29	9	ARG	2.4
33	1b	133	LYS	2.4
42	2k	126	ARG	2.4
6	2G	2	PRO	2.4
7	2H	10	PRO	2.4
12	2Q	39	PRO	2.4
38	2g	87	VAL	2.4
46	1o	89	GLY	2.4
1	2A	2182	G	2.4
29	27	1	MET	2.4
1	1A	2173	A	2.4
1	2A	2169	A	2.4
50	2s	75	ALA	2.4
54	2w	26	A	2.4
30	28	47	LYS	2.4
33	1b	80	ILE	2.4
36	1e	11	ILE	2.4
5	2F	202	PHE	2.3
36	2e	67	VAL	2.3
38	1g	141	VAL	2.3
6	2G	136	ARG	2.3
54	1y	57	G	2.3

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Mol	Chain	Res	Type	RSRZ
12	2Q	41	TRP	2.3
28	26	7	ILE	2.3
34	1c	8	ILE	2.3
30	28	56	GLU	2.3
55	1x	67	C	2.3
44	1m	121	LYS	2.3
36	2e	27	ARG	2.3
12	2Q	2	LEU	2.3
1	1A	2116	G	2.3
1	2A	2120	G	2.3
23	21	18	ILE	2.3
34	1c	39	ILE	2.3
34	1c	182	ILE	2.3
52	2u	13	ILE	2.3
34	1c	103	VAL	2.3
1	2A	272(A)	U	2.3
40	2i	10	ARG	2.3
12	2Q	50	ALA	2.3
3	2D	271	ILE	2.3
6	2G	39	ILE	2.3
11	2P	144	GLU	2.3
21	2Z	5	LEU	2.3
34	2c	191	THR	2.3
42	1k	98	LEU	2.3
6	2G	141	PHE	2.3
49	2r	61	LYS	2.3
42	2k	62	GLN	2.3
44	2m	98	VAL	2.3
52	2u	9	ARG	2.3
7	2H	75	ALA	2.3
11	2P	67	MET	2.3
34	2c	129	ALA	2.3
11	2P	114	ILE	2.3
26	24	31	ILE	2.3
33	2b	142	LEU	2.3
38	2g	27	ILE	2.3
43	2l	93	LEU	2.3
49	2r	51	LEU	2.3
42	2k	70	LYS	2.3
23	21	38	SER	2.3
42	2k	43	SER	2.3
51	1t	80	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
10	2O	38	VAL	2.3
12	1Q	81	VAL	2.3
40	2i	65	VAL	2.3
1	2A	883	G	2.3
32	1a	1532	U	2.3
41	2j	64	GLU	2.3
54	2y	60	U	2.3
49	1r	23	LYS	2.3
42	2k	83	ILE	2.3
47	1p	19	ILE	2.3
33	1b	37	ASN	2.3
34	2c	140	ARG	2.3
49	1r	36	ASN	2.3
6	1G	48	GLU	2.3
50	2s	14	HIS	2.3
1	2A	2111	C	2.3
35	2d	184	LYS	2.3
1	2A	2155	G	2.3
54	1y	4	C	2.3
11	2P	62	LEU	2.3
23	21	71	TYR	2.3
33	2b	85	ALA	2.3
43	2l	120	TYR	2.3
54	2w	29	G	2.3
30	28	13	ARG	2.3
33	2b	114	ARG	2.3
43	1l	14	GLY	2.3
33	2b	110	GLN	2.3
7	2H	144	VAL	2.3
7	2H	46	GLU	2.3
42	2k	71	LYS	2.3
44	1m	120	LYS	2.3
16	2U	2	PRO	2.3
32	2a	204	U	2.3
1	1A	2175	C	2.3
1	2A	2119	A	2.3
32	2a	1492	A	2.3
33	1b	61	LEU	2.3
34	2c	132	ARG	2.3
33	2b	72	GLY	2.3
40	2i	63	ILE	2.3
42	1k	95	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
31	29	3	VAL	2.3
35	2d	60	GLU	2.3
11	2P	87	ASP	2.3
9	2N	44	PRO	2.3
38	2g	76	ARG	2.3
3	2D	234	GLY	2.3
3	2D	247	ALA	2.3
5	2F	12	LEU	2.3
7	2H	67	LEU	2.3
34	2c	168	ALA	2.3
11	2P	121	LYS	2.3
51	1t	68	LYS	2.3
54	1w	52	G	2.3
5	2F	100	THR	2.2
6	2G	92	VAL	2.2
7	2H	45	VAL	2.2
34	1c	67	THR	2.2
53	2v	20	U	2.2
4	2E	195	LEU	2.2
8	2I	1	MET	2.2
8	2I	44	LEU	2.2
33	2b	147	LYS	2.2
35	2d	166	LYS	2.2
38	2g	18	TYR	2.2
10	2O	121	VAL	2.2
40	2i	109	VAL	2.2
1	2A	652(U)	G	2.2
49	1r	25	THR	2.2
42	1k	123	LYS	2.2
43	1l	21	LYS	2.2
11	2P	44	GLY	2.2
34	1c	187	ALA	2.2
38	2g	25	ALA	2.2
12	2Q	32	TYR	2.2
16	2U	47	TYR	2.2
40	2i	88	TYR	2.2
7	2H	49	VAL	2.2
34	2c	127	ARG	2.2
34	2c	131	ARG	2.2
43	2l	101	VAL	2.2
51	2t	17	ARG	2.2
7	2H	122	THR	2.2

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Mol	Chain	Res	Type	RSRZ
7	2H	96	ALA	2.2
12	2Q	40	ALA	2.2
34	1c	12	LEU	2.2
35	2d	157	LEU	2.2
41	2j	90	LEU	2.2
10	2O	79	PHE	2.2
35	2d	67	ILE	2.2
17	2V	12	TYR	2.2
23	21	21	ARG	2.2
49	1r	34	TYR	2.2
6	2G	47	LYS	2.2
15	2T	28	VAL	2.2
49	1r	45	SER	2.2
6	2G	73	ALA	2.2
12	2Q	38	GLU	2.2
49	2r	62	GLU	2.2
54	2w	60	U	2.2
36	2e	106	PRO	2.2
1	1A	2125	G	2.2
1	1A	2160	G	2.2
11	2P	15	ARG	2.2
32	2a	1094	G	2.2
33	1b	101	MET	2.2
33	1b	33	TYR	2.2
43	1l	91	LYS	2.2
15	2T	49	VAL	2.2
7	2H	74	ASN	2.2
11	2P	118	GLY	2.2
33	2b	89	GLY	2.2
42	1k	26	ASN	2.2
11	2P	96	THR	2.2
32	2a	88	A	2.2
34	2c	84	ILE	2.2
38	2g	54	THR	2.2
40	2i	47	LEU	2.2
35	2d	165	MET	2.2
37	1f	51	PRO	2.2
38	2g	58	PRO	2.2
42	1k	70	LYS	2.2
50	2s	52	TYR	2.2
54	2w	18	G	2.2
1	2A	280	C	2.2

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Mol	Chain	Res	Type	RSRZ
7	2H	27	LYS	2.2
30	28	30	ARG	2.2
30	28	17	THR	2.2
33	2b	207	ALA	2.2
37	1f	49	ALA	2.2
32	2a	1035	A	2.2
30	28	34	TRP	2.2
32	2a	1001(A)	G	2.2
38	2g	113	GLU	2.2
32	1a	1030	C	2.2
38	2g	70	LYS	2.2
16	2U	109	LEU	2.2
33	2b	102	LEU	2.2
34	1c	101	LEU	2.2
40	2i	54	ASP	2.2
47	1p	60	LEU	2.2
10	2O	33	ALA	2.2
33	1b	152	PHE	2.2
54	1w	50	U	2.2
54	2y	59	U	2.2
30	28	19	SER	2.2
31	29	26	ILE	2.2
33	1b	208	ILE	2.2
33	2b	108	ILE	2.2
33	2b	232	PRO	2.2
35	2d	45	GLN	2.2
41	2j	19	SER	2.2
50	2s	33	THR	2.2
8	2I	19	VAL	2.2
12	2Q	77	LYS	2.2
34	1c	193	TYR	2.2
48	2q	10	VAL	2.2
34	1c	185	GLY	2.2
40	2i	107	ARG	2.2
51	2t	68	LYS	2.2
10	2O	99	PHE	2.2
11	2P	115	LEU	2.2
51	1t	43	LEU	2.2
38	2g	28	ASN	2.2
54	1w	51	U	2.2
5	2F	98	SER	2.2
7	2H	65	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
42	2k	35	PRO	2.2
10	2O	9	GLU	2.2
43	1l	23	LYS	2.2
33	1b	105	PHE	2.1
35	2d	64	LEU	2.1
36	2e	43	LEU	2.1
42	1k	66	LEU	2.1
47	2p	48	TRP	2.1
6	2G	88	ILE	2.1
32	2a	932	C	2.1
34	1c	139	GLN	2.1
1	1A	2181	G	2.1
1	2A	2104	G	2.1
42	2k	58	PRO	2.1
54	1y	69	G	2.1
23	21	61	ARG	2.1
36	2e	105	VAL	2.1
1	2A	255	A	2.1
28	26	36	LEU	2.1
48	1q	98	LEU	2.1
5	1F	9	ILE	2.1
5	2F	28	ILE	2.1
7	2H	30	LYS	2.1
42	1k	100	ALA	2.1
1	1A	2128	C	2.1
35	2d	73	ARG	2.1
40	2i	51	ARG	2.1
32	2a	1026	G	2.1
11	1P	93	GLY	2.1
31	29	25	VAL	2.1
41	2j	100	THR	2.1
42	2k	14	VAL	2.1
7	2H	73	ALA	2.1
33	2b	146	GLN	2.1
35	2d	5	ILE	2.1
38	2g	97	GLN	2.1
54	2y	76	A	2.1
44	2m	3	ARG	2.1
44	2m	5	ALA	2.1
38	2g	89	MET	2.1
54	1w	57	G	2.1
3	1D	257	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
40	2i	92	TYR	2.1
7	2H	3	ARG	2.1
11	2P	47	ASP	2.1
25	23	29	ARG	2.1
34	2c	136	GLN	2.1
39	2h	111	ILE	2.1
41	2j	27	ALA	2.1
43	2l	100	ILE	2.1
1	2A	2143	C	2.1
4	2E	10	GLY	2.1
5	2F	92	PRO	2.1
32	2a	1113	C	2.1
7	2H	2	SER	2.1
42	1k	71	LYS	2.1
38	2g	115	ARG	2.1
49	2r	83	GLU	2.1
51	1t	72	LEU	2.1
54	1y	44	G	2.1
54	2y	19	G	2.1
55	2x	4	G	2.1
12	2Q	47	ILE	2.1
41	2j	74	ILE	2.1
42	2k	23	ALA	2.1
42	2k	68	ALA	2.1
3	2D	38	LYS	2.1
3	2D	235	GLY	2.1
33	1b	94	ASN	2.1
38	2g	109	ASN	2.1
5	2F	201	VAL	2.1
23	21	14	VAL	2.1
54	1w	42	C	2.1
12	2Q	5	ARG	2.1
9	2N	43	THR	2.1
35	1d	135	LEU	2.1
35	2d	202	LEU	2.1
38	2g	146	GLU	2.1
39	1h	3	THR	2.1
42	1k	125	PHE	2.1
6	2G	157	ILE	2.1
25	23	43	ILE	2.1
28	26	17	LYS	2.1
34	1c	168	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
54	2y	44	G	2.1
5	2F	47	GLY	2.1
10	2O	36	GLY	2.1
32	2a	968	A	2.1
38	2g	119	ARG	2.1
45	2n	3	ARG	2.1
53	2v	15	A	2.1
34	1c	167	TRP	2.1
38	1g	26	PHE	2.1
34	1c	184	TYR	2.1
42	1k	50	TYR	2.1
49	1r	69	THR	2.1
48	1q	59	ILE	2.1
54	1y	50	U	2.1
36	2e	22	GLY	2.1
32	2a	1202	G	2.1
33	2b	94	ASN	2.1
36	2e	112	LEU	2.1
51	2t	20	LEU	2.1
30	18	46	ARG	2.1
25	23	47	VAL	2.1
1	1A	1176	G	2.1
50	2s	38	SER	2.0
54	1w	38	A	2.0
11	2P	120	ALA	2.0
12	2Q	137	TYR	2.0
23	21	34	THR	2.0
25	23	35	ARG	2.0
34	2c	177	THR	2.0
50	2s	78	ARG	2.0
49	1r	48	GLY	2.0
12	2Q	1	MET	2.0
36	2e	55	VAL	2.0
1	1A	652(S)	C	2.0
40	2i	71	SER	2.0
42	2k	16	SER	2.0
42	2k	18	ARG	2.0
33	2b	34	ALA	2.0
35	2d	70	ILE	2.0
38	1g	152	ALA	2.0
42	2k	48	ILE	2.0
6	2G	84	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
42	1k	76	GLY	2.0
43	2l	121	GLY	2.0
47	1p	59	TRP	2.0
49	1r	73	ALA	2.0
49	2r	82	THR	2.0
40	2i	108	VAL	2.0
7	2H	88	LEU	2.0
33	1b	118	LEU	2.0
39	2h	112	LEU	2.0
51	1t	84	LEU	2.0
43	2l	53	ARG	2.0
44	1m	122	LYS	2.0
7	2H	93	GLY	2.0
21	2Z	149	SER	2.0
32	1a	1029	C	2.0
48	1q	97	SER	2.0
32	2a	1031	G	2.0
32	2a	1111	A	2.0
11	2P	71	VAL	2.0
17	2V	46	VAL	2.0
49	2r	86	VAL	2.0
6	2G	94	LEU	2.0
33	1b	215	LEU	2.0
33	2b	154	LEU	2.0
37	1f	7	ASN	2.0
39	1h	2	LEU	2.0
40	2i	11	LYS	2.0
7	2H	31	GLY	2.0
33	2b	129	GLU	2.0
33	2b	143	GLU	2.0
34	1c	36	ASP	2.0
33	2b	88	ALA	2.0
36	2e	99	GLY	2.0
39	2h	83	ILE	2.0
6	2G	146	TYR	2.0
31	29	24	TYR	2.0
32	2a	91	C	2.0
32	2a	1070	U	2.0
35	2d	68	TYR	2.0
54	1w	41	C	2.0
1	2A	2134	A	2.0
12	2Q	65	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
21	2Z	50	GLN	2.0
49	2r	21	LYS	2.0
22	20	12	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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	PSU	1y	55	20/21	0.73	0.37	87,96,109,113	0
54	PSU	2y	32	20/21	0.74	0.51	86,96,102,112	0
54	G7M	2y	46	24/25	0.74	0.46	94,102,109,118	0
54	PSU	2y	55	20/21	0.76	0.39	93,99,105,111	0
54	5MU	1y	54	21/22	0.78	0.40	85,94,101,105	0
54	4SU	1y	8	20/21	0.79	0.36	94,98,110,117	0
54	G7M	1y	46	24/25	0.80	0.43	91,101,105,120	0
54	G7M	2w	46	24/25	0.80	0.34	85,95,104,116	0
54	PSU	2w	55	20/21	0.80	0.34	81,94,101,107	0
54	PSU	1w	55	20/21	0.81	0.30	78,90,93,96	0
54	PSU	1y	32	20/21	0.81	0.56	82,91,106,106	0
54	PSU	2y	39	20/21	0.82	0.52	89,97,108,118	0
54	G7M	1w	46	24/25	0.83	0.24	83,93,109,114	0
54	4SU	2y	8	20/21	0.83	0.34	83,102,109,114	0
54	PSU	1y	39	20/21	0.84	0.47	79,90,97,97	0
54	5MU	2w	54	21/22	0.84	0.24	78,90,94,98	0
55	4SU	2x	8	20/21	0.85	0.18	79,87,104,106	0
54	4SU	2w	8	20/21	0.85	0.32	87,101,105,107	0
54	MIA	1y	37	22/30	0.85	0.41	79,88,96,113	0
54	MIA	2w	37	25/30	0.86	0.38	81,91,93,97	0
54	5MU	2y	54	21/22	0.87	0.55	88,98,104,112	0
54	MIA	2y	37	22/30	0.87	0.42	81,92,105,113	0
54	PSU	2w	39	20/21	0.88	0.47	79,89,93,93	0
32	2MG	2a	1207	24/25	0.88	0.20	80,87,94,98	0
32	5MC	2a	1400	21/22	0.88	0.30	76,82,87,90	0
32	4OC	2a	1402	22/23	0.89	0.20	66,75,79,80	0
54	4SU	1w	8	20/21	0.89	0.22	86,91,98,106	0
54	PSU	2w	32	20/21	0.89	0.52	89,94,104,108	0
32	5MC	2a	967	21/22	0.89	0.19	68,76,86,92	0
55	PSU	2x	55	20/21	0.90	0.19	72,78,91,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	5MU	2A	1915	21/22	0.90	0.16	74,82,91,95	0
32	PSU	2a	516	20/21	0.91	0.18	82,87,94,99	0
32	M2G	2a	966	25/26	0.92	0.23	66,73,95,101	0
43	0TD	1l	92	10/11	0.92	0.26	54,59,65,77	0
32	G7M	2a	527	24/25	0.92	0.19	65,73,80,82	0
1	PSU	2A	1911	20/21	0.93	0.22	55,69,77,78	0
55	5MU	2x	54	21/22	0.93	0.20	70,81,89,95	0
55	PSU	1x	55	20/21	0.94	0.14	55,61,68,74	0
55	5MC	2x	32	21/22	0.94	0.22	70,77,80,85	0
32	5MC	2a	1404	21/22	0.94	0.22	64,69,75,78	0
32	5MC	2a	1407	21/22	0.94	0.21	65,72,76,77	0
54	PSU	1w	32	20/21	0.94	0.25	75,81,89,94	0
54	MIA	1w	37	29/30	0.94	0.31	58,71,76,76	0
54	PSU	1w	39	20/21	0.94	0.28	68,78,83,84	0
1	5MU	1A	1915	21/22	0.94	0.18	54,63,67,75	0
54	5MU	1w	54	21/22	0.94	0.25	72,79,87,93	0
32	PSU	1a	516	20/21	0.94	0.11	61,68,73,79	0
55	5MU	1x	54	21/22	0.94	0.16	54,61,69,72	0
32	UR3	2a	1498	21/22	0.95	0.18	57,67,72,83	0
32	MA6	2a	1519	24/25	0.95	0.28	61,71,76,77	0
43	0TD	2l	92	10/11	0.95	0.31	63,71,75,77	0
32	5MC	1a	1404	21/22	0.95	0.24	34,48,54,60	0
1	PSU	2A	1917	20/21	0.95	0.15	60,73,83,84	0
1	OMC	2A	1920	21/22	0.95	0.19	64,72,74,74	0
55	4SU	1x	8	20/21	0.95	0.18	56,61,73,73	0
32	5MC	1a	1400	21/22	0.96	0.17	42,52,57,58	0
32	G7M	1a	527	24/25	0.96	0.17	46,53,60,64	0
55	5MC	1x	32	21/22	0.96	0.18	55,59,64,67	0
32	MA6	2a	1518	24/25	0.96	0.20	60,69,74,75	0
32	2MG	1a	1207	24/25	0.96	0.13	63,70,73,75	0
1	5MC	2A	1942	21/22	0.96	0.18	39,59,62,70	0
1	5MC	2A	1962	21/22	0.96	0.21	45,57,64,68	0
1	PSU	2A	2605	20/21	0.96	0.17	36,41,48,48	0
1	OMG	2A	2251	24/25	0.97	0.19	38,45,48,51	0
32	4OC	1a	1402	22/23	0.97	0.20	47,49,54,61	0
1	PSU	1A	1911	20/21	0.97	0.19	37,53,62,62	0
32	5MC	1a	1407	21/22	0.97	0.21	30,46,50,53	0
32	MA6	1a	1518	24/25	0.97	0.22	38,41,47,49	0
32	MA6	1a	1519	24/25	0.97	0.27	36,43,49,51	0
1	PSU	1A	1917	20/21	0.97	0.17	44,57,61,63	0
32	M2G	1a	966	25/26	0.97	0.16	40,54,58,61	0
32	5MC	1a	967	21/22	0.97	0.15	48,57,64,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	5MC	1A	1942	21/22	0.97	0.21	32,39,43,52	0
1	5MC	1A	1962	21/22	0.97	0.23	33,40,44,52	0
1	PSU	1A	2605	20/21	0.98	0.22	25,31,36,39	0
1	OMC	1A	1920	21/22	0.98	0.23	35,49,55,58	0
1	5MU	2A	1939	21/22	0.98	0.19	33,41,45,48	0
1	5MU	1A	1939	21/22	0.98	0.23	25,29,36,42	0
1	OMG	1A	2251	24/25	0.98	0.19	12,27,34,36	0
32	UR3	1a	1498	21/22	0.98	0.23	38,41,46,48	0
1	2MA	2A	2503	23/24	0.98	0.22	35,39,42,49	0
1	OMU	2A	2552	21/22	0.98	0.19	37,42,51,53	0
1	2MA	1A	2503	23/24	0.98	0.21	18,24,28,29	0
1	OMU	1A	2552	21/22	0.98	0.20	21,26,34,41	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	1800	1/1	0.43	0.48	81,81,81,81	0
56	MG	2A	3731	1/1	0.46	0.15	84,84,84,84	0
56	MG	2a	3223	1/1	0.49	0.16	82,82,82,82	0
56	MG	2a	3042	1/1	0.56	0.26	75,75,75,75	0
56	MG	1A	3566	1/1	0.58	0.18	40,40,40,40	0
56	MG	1a	1748	1/1	0.58	0.18	65,65,65,65	0
56	MG	1a	1795	1/1	0.59	0.14	78,78,78,78	0
56	MG	1A	3237	1/1	0.59	0.18	70,70,70,70	0
56	MG	2a	3048	1/1	0.59	0.54	76,76,76,76	0
56	MG	2a	3157	1/1	0.59	0.16	80,80,80,80	0
56	MG	2A	3183	1/1	0.59	0.56	83,83,83,83	0
56	MG	2A	3237	1/1	0.60	0.25	63,63,63,63	0
56	MG	1A	4018	1/1	0.60	0.36	83,83,83,83	0
56	MG	2A	3135	1/1	0.61	0.48	53,53,53,53	0
56	MG	2a	3089	1/1	0.63	0.10	69,69,69,69	0
56	MG	2a	3108	1/1	0.63	0.11	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3389	1/1	0.64	0.23	67,67,67,67	0
56	MG	2A	3305	1/1	0.64	0.40	61,61,61,61	0
56	MG	2a	3229	1/1	0.64	0.07	87,87,87,87	0
56	MG	1a	1711	1/1	0.65	0.18	61,61,61,61	0
56	MG	2a	3143	1/1	0.65	0.12	70,70,70,70	0
56	MG	1A	4019	1/1	0.65	0.25	49,49,49,49	0
56	MG	2A	3369	1/1	0.65	0.28	65,65,65,65	0
56	MG	1a	1662	1/1	0.65	0.11	73,73,73,73	0
56	MG	2A	3634	1/1	0.66	0.18	66,66,66,66	0
56	MG	1A	3509	1/1	0.66	0.69	51,51,51,51	0
56	MG	1A	3755	1/1	0.66	0.11	33,33,33,33	0
56	MG	1a	1625	1/1	0.66	0.19	68,68,68,68	0
56	MG	1a	1764	1/1	0.66	0.60	75,75,75,75	0
56	MG	2y	103	1/1	0.66	0.12	79,79,79,79	0
56	MG	1a	1775	1/1	0.67	0.21	86,86,86,86	0
56	MG	2A	3680	1/1	0.67	0.14	75,75,75,75	0
56	MG	2A	3295	1/1	0.68	0.14	80,80,80,80	0
56	MG	2a	3166	1/1	0.68	0.17	52,52,52,52	0
56	MG	1a	1788	1/1	0.68	0.09	73,73,73,73	0
56	MG	1A	3465	1/1	0.68	0.26	65,65,65,65	0
56	MG	1A	3982	1/1	0.68	0.12	30,30,30,30	0
56	MG	1A	3919	1/1	0.69	0.11	66,66,66,66	0
56	MG	2A	3076	1/1	0.69	0.27	64,64,64,64	0
56	MG	1B	226	1/1	0.69	0.21	63,63,63,63	0
56	MG	2a	3135	1/1	0.69	0.33	76,76,76,76	0
56	MG	2v	102	1/1	0.69	0.19	74,74,74,74	0
56	MG	2A	3407	1/1	0.69	0.51	73,73,73,73	0
56	MG	2a	3118	1/1	0.70	0.09	72,72,72,72	0
56	MG	2a	3127	1/1	0.70	0.29	66,66,66,66	0
56	MG	2A	3196	1/1	0.70	0.55	58,58,58,58	0
56	MG	2A	3253	1/1	0.70	0.18	48,48,48,48	0
56	MG	2A	3282	1/1	0.70	0.45	57,57,57,57	0
56	MG	2A	3165	1/1	0.71	0.42	65,65,65,65	0
56	MG	2a	3112	1/1	0.71	0.28	62,62,62,62	0
56	MG	1A	3373	1/1	0.71	0.30	62,62,62,62	0
56	MG	2A	3462	1/1	0.71	0.15	43,43,43,43	0
56	MG	2A	3582	1/1	0.71	0.20	33,33,33,33	0
56	MG	2A	3072	1/1	0.71	0.49	60,60,60,60	0
56	MG	2A	3323	1/1	0.72	0.16	63,63,63,63	0
56	MG	2a	3020	1/1	0.72	0.23	69,69,69,69	0
56	MG	1A	3948	1/1	0.72	0.24	77,77,77,77	0
56	MG	1a	1755	1/1	0.72	0.13	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2a	3065	1/1	0.72	0.20	65,65,65,65	0
56	MG	1A	3379	1/1	0.72	0.44	57,57,57,57	0
56	MG	2a	3010	1/1	0.73	0.72	72,72,72,72	0
56	MG	2A	3352	1/1	0.73	0.23	60,60,60,60	0
56	MG	2A	3177	1/1	0.73	0.21	58,58,58,58	0
56	MG	2A	3039	1/1	0.73	0.17	75,75,75,75	0
56	MG	2a	3147	1/1	0.73	0.32	92,92,92,92	0
56	MG	2a	3151	1/1	0.73	0.10	67,67,67,67	0
56	MG	2a	3051	1/1	0.73	0.24	77,77,77,77	0
56	MG	2A	3397	1/1	0.73	0.11	63,63,63,63	0
56	MG	2a	3084	1/1	0.73	0.20	81,81,81,81	0
56	MG	2A	3041	1/1	0.73	0.29	55,55,55,55	0
56	MG	2A	3850	1/1	0.73	0.41	81,81,81,81	0
56	MG	2y	102	1/1	0.73	0.23	81,81,81,81	0
56	MG	2B	216	1/1	0.73	0.13	69,69,69,69	0
56	MG	1a	1799	1/1	0.74	0.13	79,79,79,79	0
56	MG	1A	3332	1/1	0.74	1.22	44,44,44,44	0
56	MG	2a	3069	1/1	0.74	0.14	73,73,73,73	0
56	MG	2A	3266	1/1	0.74	0.19	65,65,65,65	0
56	MG	2A	3337	1/1	0.74	0.19	65,65,65,65	0
56	MG	2a	3006	1/1	0.74	0.20	66,66,66,66	0
56	MG	2A	3001	1/1	0.74	0.40	47,47,47,47	0
56	MG	2a	3235	1/1	0.74	0.22	76,76,76,76	0
56	MG	2A	3618	1/1	0.74	0.35	61,61,61,61	0
56	MG	2A	3285	1/1	0.74	0.60	64,64,64,64	0
56	MG	2A	3653	1/1	0.74	0.18	43,43,43,43	0
56	MG	1A	3673	1/1	0.75	0.29	66,66,66,66	0
56	MG	2A	3474	1/1	0.75	0.17	46,46,46,46	0
56	MG	2A	3521	1/1	0.75	0.17	45,45,45,45	0
56	MG	2a	3106	1/1	0.75	0.21	74,74,74,74	0
56	MG	1A	3829	1/1	0.75	0.12	55,55,55,55	0
56	MG	2a	3222	1/1	0.75	0.14	83,83,83,83	0
56	MG	2a	3110	1/1	0.75	0.13	70,70,70,70	0
56	MG	2A	3741	1/1	0.75	0.09	44,44,44,44	0
56	MG	2a	3230	1/1	0.75	0.12	66,66,66,66	0
56	MG	2A	3799	1/1	0.75	0.22	73,73,73,73	0
56	MG	2a	3122	1/1	0.75	0.12	60,60,60,60	0
56	MG	2x	104	1/1	0.75	0.20	72,72,72,72	0
56	MG	2A	3845	1/1	0.75	0.26	78,78,78,78	0
56	MG	2A	3373	1/1	0.75	0.52	65,65,65,65	0
56	MG	2A	3228	1/1	0.76	1.00	66,66,66,66	0
56	MG	2A	3835	1/1	0.76	0.11	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3578	1/1	0.76	0.19	66,66,66,66	0
56	MG	2A	3376	1/1	0.76	0.41	65,65,65,65	0
56	MG	2a	3099	1/1	0.76	0.38	69,69,69,69	0
56	MG	2A	3007	1/1	0.76	0.36	62,62,62,62	0
56	MG	1A	3171	1/1	0.76	0.16	66,66,66,66	0
56	MG	1a	1772	1/1	0.76	0.08	71,71,71,71	0
56	MG	2A	3437	1/1	0.76	0.36	62,62,62,62	0
56	MG	2A	3716	1/1	0.76	0.18	90,90,90,90	0
56	MG	1A	3306	1/1	0.76	0.36	48,48,48,48	0
56	MG	2w	101	1/1	0.76	0.24	74,74,74,74	0
56	MG	1A	3783	1/1	0.76	0.15	61,61,61,61	0
56	MG	2a	3064	1/1	0.76	0.12	61,61,61,61	0
56	MG	2a	3136	1/1	0.76	0.20	71,71,71,71	0
56	MG	2a	3160	1/1	0.77	0.11	69,69,69,69	0
56	MG	2A	3111	1/1	0.77	0.16	67,67,67,67	0
56	MG	2a	3209	1/1	0.77	0.12	76,76,76,76	0
56	MG	1A	3263	1/1	0.77	0.18	67,67,67,67	0
56	MG	1B	232	1/1	0.77	0.17	55,55,55,55	0
56	MG	2B	208	1/1	0.77	0.15	64,64,64,64	0
56	MG	2A	3075	1/1	0.77	0.86	55,55,55,55	0
56	MG	2A	3692	1/1	0.77	0.17	48,48,48,48	0
56	MG	2a	3244	1/1	0.77	0.64	90,90,90,90	0
56	MG	2l	202	1/1	0.77	0.28	70,70,70,70	0
56	MG	2A	3318	1/1	0.77	0.23	49,49,49,49	0
56	MG	2A	3539	1/1	0.77	0.15	60,60,60,60	0
56	MG	2x	103	1/1	0.77	0.22	66,66,66,66	0
56	MG	2A	3320	1/1	0.77	0.49	73,73,73,73	0
56	MG	2a	3152	1/1	0.77	0.18	66,66,66,66	0
56	MG	1S	203	1/1	0.77	0.25	57,57,57,57	0
56	MG	2A	3284	1/1	0.78	0.85	57,57,57,57	0
56	MG	1A	3981	1/1	0.78	0.10	39,39,39,39	0
56	MG	2A	3506	1/1	0.78	0.16	36,36,36,36	0
56	MG	1A	3563	1/1	0.78	0.17	53,53,53,53	0
56	MG	1a	1781	1/1	0.78	0.15	70,70,70,70	0
56	MG	1V	207	1/1	0.78	0.14	48,48,48,48	0
56	MG	2a	3153	1/1	0.78	0.05	76,76,76,76	0
56	MG	1A	3988	1/1	0.78	0.15	33,33,33,33	0
56	MG	2A	3585	1/1	0.78	0.26	49,49,49,49	0
56	MG	1a	1632	1/1	0.78	0.13	60,60,60,60	0
56	MG	1A	3383	1/1	0.78	0.29	68,68,68,68	0
56	MG	1a	1803	1/1	0.78	0.20	77,77,77,77	0
56	MG	2A	3662	1/1	0.78	0.23	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	3206	1/1	0.78	0.46	67,67,67,67	0
56	MG	1A	3048	1/1	0.78	0.17	32,32,32,32	0
56	MG	1A	4030	1/1	0.78	0.18	99,99,99,99	0
56	MG	2A	3727	1/1	0.78	0.11	60,60,60,60	0
56	MG	1a	1753	1/1	0.78	0.07	69,69,69,69	0
56	MG	1A	3371	1/1	0.78	0.30	58,58,58,58	0
56	MG	2A	3271	1/1	0.78	0.26	57,57,57,57	0
56	MG	2a	3113	1/1	0.78	0.10	77,77,77,77	0
56	MG	2A	3811	1/1	0.78	0.17	49,49,49,49	0
56	MG	1B	230	1/1	0.78	0.49	76,76,76,76	0
56	MG	2A	3454	1/1	0.78	0.26	54,54,54,54	0
56	MG	1D	306	1/1	0.79	0.47	35,35,35,35	0
56	MG	2a	3145	1/1	0.79	0.08	91,91,91,91	0
56	MG	2a	3027	1/1	0.79	0.26	69,69,69,69	0
56	MG	2a	3148	1/1	0.79	0.10	86,86,86,86	0
56	MG	2A	3370	1/1	0.79	0.42	62,62,62,62	0
56	MG	2A	3250	1/1	0.79	0.21	74,74,74,74	0
56	MG	2A	3044	1/1	0.79	0.47	69,69,69,69	0
56	MG	1a	1703	1/1	0.79	0.27	69,69,69,69	0
56	MG	1Q	204	1/1	0.79	0.17	67,67,67,67	0
56	MG	2A	3276	1/1	0.79	0.47	52,52,52,52	0
56	MG	2a	3170	1/1	0.79	0.14	79,79,79,79	0
56	MG	1a	1791	1/1	0.79	0.22	56,56,56,56	0
56	MG	2A	3097	1/1	0.79	0.37	70,70,70,70	0
56	MG	1a	1722	1/1	0.79	0.24	58,58,58,58	0
56	MG	1A	3990	1/1	0.79	0.15	41,41,41,41	0
56	MG	1a	1749	1/1	0.79	0.16	56,56,56,56	0
56	MG	2A	3515	1/1	0.79	0.16	40,40,40,40	0
56	MG	1A	3991	1/1	0.79	0.15	43,43,43,43	0
56	MG	1a	1622	1/1	0.79	0.30	65,65,65,65	0
56	MG	2a	3115	1/1	0.79	0.23	74,74,74,74	0
56	MG	2A	3544	1/1	0.79	0.17	35,35,35,35	0
56	MG	2B	213	1/1	0.79	0.23	69,69,69,69	0
56	MG	1A	3896	1/1	0.79	0.11	68,68,68,68	0
56	MG	2A	3027	1/1	0.79	0.17	64,64,64,64	0
56	MG	1A	3356	1/1	0.79	0.17	40,40,40,40	0
56	MG	1A	3970	1/1	0.80	0.10	50,50,50,50	0
56	MG	1a	1738	1/1	0.80	0.70	78,78,78,78	0
56	MG	1A	3017	1/1	0.80	0.18	38,38,38,38	0
56	MG	10	105	1/1	0.80	0.14	48,48,48,48	0
56	MG	1a	1812	1/1	0.80	0.13	58,58,58,58	0
56	MG	1A	3637	1/1	0.80	0.11	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3504	1/1	0.80	0.25	48,48,48,48	0
56	MG	1A	3530	1/1	0.80	0.16	59,59,59,59	0
56	MG	2a	3172	1/1	0.80	0.08	82,82,82,82	0
56	MG	2a	3186	1/1	0.80	0.21	80,80,80,80	0
56	MG	1A	3503	1/1	0.80	0.18	57,57,57,57	0
56	MG	1A	3944	1/1	0.80	0.22	34,34,34,34	0
56	MG	2A	3236	1/1	0.80	0.20	59,59,59,59	0
56	MG	2A	3347	1/1	0.80	0.18	64,64,64,64	0
56	MG	2A	3573	1/1	0.80	0.12	51,51,51,51	0
56	MG	1a	1689	1/1	0.80	0.68	57,57,57,57	0
56	MG	1a	1696	1/1	0.80	0.15	55,55,55,55	0
56	MG	2B	220	1/1	0.80	0.20	77,77,77,77	0
56	MG	1a	1784	1/1	0.80	0.11	62,62,62,62	0
56	MG	2A	3591	1/1	0.80	0.10	66,66,66,66	0
56	MG	2A	3265	1/1	0.80	0.19	59,59,59,59	0
56	MG	1A	3770	1/1	0.80	0.27	43,43,43,43	0
56	MG	2a	3036	1/1	0.80	0.22	70,70,70,70	0
56	MG	1Q	205	1/1	0.80	0.22	57,57,57,57	0
56	MG	2A	3514	1/1	0.81	0.15	34,34,34,34	0
56	MG	2A	3218	1/1	0.81	0.17	63,63,63,63	0
56	MG	1a	1786	1/1	0.81	0.18	56,56,56,56	0
56	MG	2A	3235	1/1	0.81	0.25	72,72,72,72	0
56	MG	2A	3340	1/1	0.81	0.58	74,74,74,74	0
56	MG	2A	3346	1/1	0.81	0.14	65,65,65,65	0
56	MG	2a	3150	1/1	0.81	0.11	78,78,78,78	0
56	MG	1A	3473	1/1	0.81	0.43	63,63,63,63	0
56	MG	2A	3350	1/1	0.81	0.19	53,53,53,53	0
56	MG	1a	1789	1/1	0.81	0.08	63,63,63,63	0
56	MG	1A	3403	1/1	0.81	0.50	59,59,59,59	0
56	MG	1A	3962	1/1	0.81	0.13	56,56,56,56	0
56	MG	1A	3421	1/1	0.81	0.22	48,48,48,48	0
56	MG	2A	3375	1/1	0.81	0.85	65,65,65,65	0
56	MG	2a	3171	1/1	0.81	0.12	73,73,73,73	0
56	MG	2a	3053	1/1	0.81	0.27	73,73,73,73	0
56	MG	1a	1671	1/1	0.81	0.20	65,65,65,65	0
56	MG	2A	3674	1/1	0.81	0.14	80,80,80,80	0
56	MG	2A	3677	1/1	0.81	0.18	59,59,59,59	0
56	MG	1A	3977	1/1	0.81	0.21	60,60,60,60	0
56	MG	1A	3199	1/1	0.81	0.59	52,52,52,52	0
56	MG	2A	3277	1/1	0.81	0.34	51,51,51,51	0
56	MG	2a	3231	1/1	0.81	0.23	70,70,70,70	0
56	MG	2A	3416	1/1	0.81	0.26	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2a	3239	1/1	0.81	0.08	69,69,69,69	0
56	MG	1a	1774	1/1	0.81	0.09	60,60,60,60	0
56	MG	2A	3178	1/1	0.81	1.03	62,62,62,62	0
56	MG	2A	3794	1/1	0.81	0.15	56,56,56,56	0
56	MG	1A	4033	1/1	0.81	0.68	81,81,81,81	0
56	MG	1A	3555	1/1	0.81	0.19	40,40,40,40	0
56	MG	2A	3205	1/1	0.81	0.42	48,48,48,48	0
56	MG	2A	3838	1/1	0.81	0.22	60,60,60,60	0
56	MG	1a	1608	1/1	0.81	0.21	53,53,53,53	0
56	MG	2A	3698	1/1	0.82	0.38	75,75,75,75	0
56	MG	2A	3058	1/1	0.82	0.38	68,68,68,68	0
56	MG	1A	3665	1/1	0.82	0.21	34,34,34,34	0
56	MG	2A	3729	1/1	0.82	0.14	87,87,87,87	0
56	MG	2A	3258	1/1	0.82	0.46	60,60,60,60	0
56	MG	1A	3532	1/1	0.82	0.32	60,60,60,60	0
56	MG	2A	3764	1/1	0.82	0.11	47,47,47,47	0
56	MG	2A	3781	1/1	0.82	0.27	87,87,87,87	0
56	MG	2A	3414	1/1	0.82	0.12	63,63,63,63	0
56	MG	1a	1724	1/1	0.82	0.14	52,52,52,52	0
56	MG	1A	3723	1/1	0.82	0.17	41,41,41,41	0
56	MG	2A	3820	1/1	0.82	0.28	77,77,77,77	0
56	MG	2A	3821	1/1	0.82	0.32	60,60,60,60	0
56	MG	1A	3368	1/1	0.82	0.30	60,60,60,60	0
56	MG	2A	3122	1/1	0.82	0.28	57,57,57,57	0
56	MG	1A	3968	1/1	0.82	0.13	55,55,55,55	0
56	MG	1A	4056	1/1	0.82	0.29	69,69,69,69	0
56	MG	2A	3167	1/1	0.82	0.26	65,65,65,65	0
56	MG	2A	3289	1/1	0.82	0.42	73,73,73,73	0
56	MG	1A	3218	1/1	0.82	0.32	47,47,47,47	0
56	MG	1a	1757	1/1	0.82	0.16	64,64,64,64	0
56	MG	28	101	1/1	0.82	0.73	66,66,66,66	0
56	MG	2A	3306	1/1	0.82	0.28	68,68,68,68	0
56	MG	1a	1656	1/1	0.82	0.30	62,62,62,62	0
56	MG	2A	3194	1/1	0.82	0.43	72,72,72,72	0
56	MG	2A	3004	1/1	0.82	0.20	61,61,61,61	0
56	MG	2A	3580	1/1	0.82	0.16	44,44,44,44	0
56	MG	2A	3328	1/1	0.82	0.45	60,60,60,60	0
56	MG	2A	3204	1/1	0.82	0.34	66,66,66,66	0
56	MG	1A	3333	1/1	0.82	0.92	43,43,43,43	0
56	MG	2a	3234	1/1	0.82	0.10	73,73,73,73	0
56	MG	1A	3601	1/1	0.82	0.15	22,22,22,22	0
56	MG	2A	3028	1/1	0.82	0.39	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	3224	1/1	0.82	0.22	41,41,41,41	0
56	MG	2g	201	1/1	0.82	0.33	74,74,74,74	0
56	MG	1A	3838	1/1	0.82	0.17	16,16,16,16	0
56	MG	2v	101	1/1	0.82	0.38	78,78,78,78	0
56	MG	2a	3080	1/1	0.82	0.24	57,57,57,57	0
56	MG	2A	3672	1/1	0.82	0.17	43,43,43,43	0
56	MG	1A	3865	1/1	0.82	0.15	60,60,60,60	0
56	MG	1A	3107	1/1	0.82	0.51	46,46,46,46	0
56	MG	2A	3050	1/1	0.82	0.20	55,55,55,55	0
56	MG	2A	3247	1/1	0.82	0.38	51,51,51,51	0
56	MG	2a	3123	1/1	0.83	0.10	66,66,66,66	0
56	MG	1A	3394	1/1	0.83	0.73	55,55,55,55	0
56	MG	1A	3367	1/1	0.83	0.22	56,56,56,56	0
56	MG	1A	3547	1/1	0.83	0.43	45,45,45,45	0
56	MG	2A	3593	1/1	0.83	0.17	48,48,48,48	0
56	MG	19	101	1/1	0.83	0.14	53,53,53,53	0
56	MG	1A	3411	1/1	0.83	0.16	55,55,55,55	0
56	MG	2E	302	1/1	0.83	0.17	55,55,55,55	0
56	MG	2F	307	1/1	0.83	0.19	56,56,56,56	0
56	MG	2A	3641	1/1	0.83	0.37	66,66,66,66	0
56	MG	28	105	1/1	0.83	0.26	65,65,65,65	0
56	MG	1A	3418	1/1	0.83	0.24	56,56,56,56	0
56	MG	2a	3009	1/1	0.83	0.33	69,69,69,69	0
56	MG	2a	3159	1/1	0.83	0.17	69,69,69,69	0
56	MG	2A	3264	1/1	0.83	0.25	57,57,57,57	0
56	MG	2a	3163	1/1	0.83	0.15	79,79,79,79	0
56	MG	1A	3994	1/1	0.83	0.12	40,40,40,40	0
56	MG	1A	3997	1/1	0.83	0.11	45,45,45,45	0
56	MG	1a	1652	1/1	0.83	1.09	46,46,46,46	0
56	MG	2a	3040	1/1	0.83	0.20	56,56,56,56	0
56	MG	1a	1655	1/1	0.83	0.15	63,63,63,63	0
56	MG	2A	3687	1/1	0.83	0.54	73,73,73,73	0
56	MG	2a	3221	1/1	0.83	0.17	62,62,62,62	0
56	MG	1A	3874	1/1	0.83	0.11	47,47,47,47	0
56	MG	2A	3695	1/1	0.83	0.20	41,41,41,41	0
56	MG	1A	3879	1/1	0.83	0.08	68,68,68,68	0
56	MG	1A	3302	1/1	0.83	0.13	47,47,47,47	0
56	MG	1A	3453	1/1	0.83	0.40	58,58,58,58	0
56	MG	2a	3073	1/1	0.83	0.14	72,72,72,72	0
56	MG	1A	3921	1/1	0.83	0.12	38,38,38,38	0
56	MG	1A	4084	1/1	0.83	0.19	45,45,45,45	0
56	MG	2A	3298	1/1	0.83	0.18	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	1A	3463	1/1	0.83	0.16	54,54,54,54	0
56	MG	1A	3023	1/1	0.83	0.15	37,37,37,37	0
56	MG	2q	203	1/1	0.83	0.16	62,62,62,62	0
56	MG	1A	3256	1/1	0.83	0.15	32,32,32,32	0
56	MG	1B	234	1/1	0.83	0.44	79,79,79,79	0
56	MG	2A	3213	1/1	0.83	0.62	61,61,61,61	0
56	MG	1a	1741	1/1	0.83	0.18	78,78,78,78	0
56	MG	1A	3002	1/1	0.83	0.95	44,44,44,44	0
56	MG	1A	3731	1/1	0.83	0.10	36,36,36,36	0
56	MG	1A	3283	1/1	0.83	0.43	45,45,45,45	0
56	MG	2a	3082	1/1	0.84	0.15	63,63,63,63	0
56	MG	1a	1804	1/1	0.84	0.09	63,63,63,63	0
56	MG	2A	3349	1/1	0.84	0.27	45,45,45,45	0
56	MG	1a	1808	1/1	0.84	0.13	58,58,58,58	0
56	MG	1A	3552	1/1	0.84	0.17	45,45,45,45	0
56	MG	2A	3363	1/1	0.84	0.33	59,59,59,59	0
56	MG	1a	1826	1/1	0.84	0.21	49,49,49,49	0
56	MG	1x	102	1/1	0.84	0.14	60,60,60,60	0
56	MG	2A	3372	1/1	0.84	0.49	54,54,54,54	0
56	MG	1x	108	1/1	0.84	0.15	53,53,53,53	0
56	MG	1a	1718	1/1	0.84	0.12	54,54,54,54	0
56	MG	1E	303	1/1	0.84	0.45	39,39,39,39	0
56	MG	2A	3735	1/1	0.84	0.36	73,73,73,73	0
56	MG	2A	3384	1/1	0.84	0.11	60,60,60,60	0
56	MG	1A	3828	1/1	0.84	0.13	51,51,51,51	0
56	MG	2A	3392	1/1	0.84	0.32	48,48,48,48	0
56	MG	1A	3094	1/1	0.84	0.19	38,38,38,38	0
56	MG	1A	3194	1/1	0.84	0.17	57,57,57,57	0
56	MG	2A	3251	1/1	0.84	0.38	65,65,65,65	0
56	MG	1A	3847	1/1	0.84	0.11	63,63,63,63	0
56	MG	2A	3428	1/1	0.84	0.25	58,58,58,58	0
56	MG	2A	3826	1/1	0.84	0.31	54,54,54,54	0
56	MG	2A	3256	1/1	0.84	0.18	55,55,55,55	0
56	MG	1A	3119	1/1	0.84	0.09	75,75,75,75	0
56	MG	14	101	1/1	0.84	0.18	57,57,57,57	0
56	MG	2A	3046	1/1	0.84	0.26	69,69,69,69	0
56	MG	2B	207	1/1	0.84	0.08	65,65,65,65	0
56	MG	2A	3493	1/1	0.84	0.12	49,49,49,49	0
56	MG	1A	3588	1/1	0.84	0.10	23,23,23,23	0
56	MG	2a	3169	1/1	0.84	0.05	74,74,74,74	0
56	MG	2B	215	1/1	0.84	0.18	69,69,69,69	0
56	MG	2A	3268	1/1	0.84	0.30	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3323	1/1	0.84	0.22	42,42,42,42	0
56	MG	2A	3064	1/1	0.84	0.46	56,56,56,56	0
56	MG	2a	3193	1/1	0.84	0.11	65,65,65,65	0
56	MG	2a	3200	1/1	0.84	0.14	70,70,70,70	0
56	MG	2F	304	1/1	0.84	0.15	42,42,42,42	0
56	MG	2A	3520	1/1	0.84	0.16	41,41,41,41	0
56	MG	1A	4011	1/1	0.84	0.21	44,44,44,44	0
56	MG	1a	1770	1/1	0.84	0.30	64,64,64,64	0
56	MG	2a	3005	1/1	0.84	0.15	67,67,67,67	0
56	MG	1A	3635	1/1	0.84	0.20	27,27,27,27	0
56	MG	2A	3553	1/1	0.84	0.10	63,63,63,63	0
56	MG	1A	3905	1/1	0.84	0.08	42,42,42,42	0
56	MG	1A	3201	1/1	0.84	0.29	59,59,59,59	0
56	MG	1A	3514	1/1	0.84	0.29	49,49,49,49	0
56	MG	2a	3241	1/1	0.84	0.19	64,64,64,64	0
56	MG	1A	3930	1/1	0.84	0.20	25,25,25,25	0
56	MG	2A	3143	1/1	0.84	0.13	63,63,63,63	0
56	MG	1A	3374	1/1	0.84	0.27	47,47,47,47	0
56	MG	1a	1665	1/1	0.84	0.24	64,64,64,64	0
56	MG	1A	3430	1/1	0.84	0.12	62,62,62,62	0
56	MG	1a	1673	1/1	0.84	0.12	66,66,66,66	0
56	MG	2v	103	1/1	0.84	0.23	72,72,72,72	0
56	MG	1A	3540	1/1	0.84	0.40	55,55,55,55	0
56	MG	1A	3543	1/1	0.84	0.17	35,35,35,35	0
56	MG	2A	3661	1/1	0.84	0.14	56,56,56,56	0
56	MG	1A	3274	1/1	0.84	0.43	44,44,44,44	0
56	MG	1a	1705	1/1	0.84	0.37	51,51,51,51	0
56	MG	1a	1649	1/1	0.85	0.12	85,85,85,85	0
56	MG	1a	1650	1/1	0.85	0.07	78,78,78,78	0
56	MG	1A	3522	1/1	0.85	0.46	32,32,32,32	0
56	MG	2A	3518	1/1	0.85	0.10	52,52,52,52	0
56	MG	2a	3138	1/1	0.85	0.17	76,76,76,76	0
56	MG	2a	3141	1/1	0.85	0.20	73,73,73,73	0
56	MG	1A	3599	1/1	0.85	0.10	45,45,45,45	0
56	MG	2A	3332	1/1	0.85	0.18	66,66,66,66	0
56	MG	1A	3527	1/1	0.85	0.30	50,50,50,50	0
56	MG	1A	3624	1/1	0.85	0.09	44,44,44,44	0
56	MG	2A	3548	1/1	0.85	0.11	55,55,55,55	0
56	MG	2A	3550	1/1	0.85	0.12	46,46,46,46	0
56	MG	1A	3378	1/1	0.85	0.20	55,55,55,55	0
56	MG	1A	3438	1/1	0.85	0.78	62,62,62,62	0
56	MG	2A	3240	1/1	0.85	0.45	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	3341	1/1	0.85	0.32	43,43,43,43	0
56	MG	1A	3028	1/1	0.85	0.16	28,28,28,28	0
56	MG	1A	3722	1/1	0.85	0.11	31,31,31,31	0
56	MG	1A	3917	1/1	0.85	0.13	52,52,52,52	0
56	MG	2A	3085	1/1	0.85	0.16	76,76,76,76	0
56	MG	2A	3090	1/1	0.85	0.09	77,77,77,77	0
56	MG	1A	3999	1/1	0.85	0.14	49,49,49,49	0
56	MG	2A	3374	1/1	0.85	0.22	53,53,53,53	0
56	MG	1Y	202	1/1	0.85	0.11	47,47,47,47	0
56	MG	2A	3655	1/1	0.85	0.35	74,74,74,74	0
56	MG	1A	3322	1/1	0.85	0.15	56,56,56,56	0
56	MG	2a	3208	1/1	0.85	0.23	60,60,60,60	0
56	MG	2A	3380	1/1	0.85	0.08	63,63,63,63	0
56	MG	1a	1801	1/1	0.85	0.18	80,80,80,80	0
56	MG	12	101	1/1	0.85	0.20	40,40,40,40	0
56	MG	1a	1723	1/1	0.85	0.37	63,63,63,63	0
56	MG	1A	3724	1/1	0.85	0.13	56,56,56,56	0
56	MG	2A	3402	1/1	0.85	0.17	44,44,44,44	0
56	MG	2A	3171	1/1	0.85	0.29	65,65,65,65	0
56	MG	2A	3410	1/1	0.85	0.35	43,43,43,43	0
56	MG	1a	1729	1/1	0.85	0.12	62,62,62,62	0
56	MG	2A	3712	1/1	0.85	0.14	50,50,50,50	0
56	MG	2A	3713	1/1	0.85	0.10	60,60,60,60	0
56	MG	1A	3191	1/1	0.85	0.21	41,41,41,41	0
56	MG	2d	301	1/1	0.85	0.20	58,58,58,58	0
56	MG	2A	3720	1/1	0.85	0.23	54,54,54,54	0
56	MG	2A	3424	1/1	0.85	0.36	51,51,51,51	0
56	MG	2q	201	1/1	0.85	0.19	61,61,61,61	0
56	MG	1A	4027	1/1	0.85	0.31	45,45,45,45	0
56	MG	2A	3435	1/1	0.85	0.17	55,55,55,55	0
56	MG	1A	3104	1/1	0.85	0.64	44,44,44,44	0
56	MG	1A	3131	1/1	0.85	0.16	46,46,46,46	0
56	MG	1A	3337	1/1	0.85	0.16	50,50,50,50	0
56	MG	1a	1633	1/1	0.85	0.14	58,58,58,58	0
56	MG	2A	3478	1/1	0.85	0.15	35,35,35,35	0
56	MG	2A	3308	1/1	0.85	0.27	54,54,54,54	0
56	MG	2A	3311	1/1	0.85	0.15	57,57,57,57	0
59	ZN	24	501	1/1	0.85	0.04	127,127,127,127	0
56	MG	2A	3192	1/1	0.86	0.22	68,68,68,68	0
56	MG	1a	1773	1/1	0.86	0.20	72,72,72,72	0
56	MG	2A	3784	1/1	0.86	0.17	49,49,49,49	0
56	MG	1a	1695	1/1	0.86	0.16	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	3795	1/1	0.86	0.21	69,69,69,69	0
56	MG	1A	3971	1/1	0.86	0.26	61,61,61,61	0
56	MG	2A	3032	1/1	0.86	0.40	47,47,47,47	0
56	MG	2A	3034	1/1	0.86	0.10	34,34,34,34	0
56	MG	1A	3721	1/1	0.86	0.23	33,33,33,33	0
56	MG	1a	1601	1/1	0.86	0.13	59,59,59,59	0
56	MG	1A	3113	1/1	0.86	0.47	56,56,56,56	0
56	MG	2A	3546	1/1	0.86	0.23	61,61,61,61	0
56	MG	1A	3232	1/1	0.86	0.37	46,46,46,46	0
56	MG	2A	3232	1/1	0.86	0.20	48,48,48,48	0
56	MG	2A	3233	1/1	0.86	0.21	49,49,49,49	0
56	MG	2A	3557	1/1	0.86	0.13	44,44,44,44	0
56	MG	2A	3562	1/1	0.86	0.23	39,39,39,39	0
56	MG	1A	3984	1/1	0.86	0.09	49,49,49,49	0
56	MG	1A	3603	1/1	0.86	0.26	61,61,61,61	0
56	MG	1a	1794	1/1	0.86	0.17	52,52,52,52	0
56	MG	1A	3325	1/1	0.86	0.70	48,48,48,48	0
56	MG	2A	3244	1/1	0.86	0.16	47,47,47,47	0
56	MG	1A	3507	1/1	0.86	0.74	43,43,43,43	0
56	MG	2A	3249	1/1	0.86	0.37	70,70,70,70	0
56	MG	1a	1733	1/1	0.86	0.20	56,56,56,56	0
56	MG	2A	3633	1/1	0.86	0.11	51,51,51,51	0
56	MG	2A	3082	1/1	0.86	0.16	61,61,61,61	0
56	MG	2A	3083	1/1	0.86	0.18	64,64,64,64	0
56	MG	1A	3565	1/1	0.86	0.09	23,23,23,23	0
56	MG	2a	3012	1/1	0.86	0.20	76,76,76,76	0
56	MG	2a	3015	1/1	0.86	0.35	77,77,77,77	0
56	MG	1O	202	1/1	0.86	0.56	67,67,67,67	0
56	MG	2a	3023	1/1	0.86	0.31	54,54,54,54	0
56	MG	2A	3391	1/1	0.86	0.31	55,55,55,55	0
56	MG	1A	3922	1/1	0.86	0.12	56,56,56,56	0
56	MG	2A	3100	1/1	0.86	0.21	39,39,39,39	0
56	MG	2A	3103	1/1	0.86	0.20	45,45,45,45	0
56	MG	2A	3406	1/1	0.86	0.22	60,60,60,60	0
56	MG	1A	3649	1/1	0.86	0.14	20,20,20,20	0
56	MG	1a	1660	1/1	0.86	0.27	54,54,54,54	0
56	MG	2A	3689	1/1	0.86	0.23	49,49,49,49	0
56	MG	2A	3690	1/1	0.86	0.22	70,70,70,70	0
56	MG	1A	3177	1/1	0.86	0.40	54,54,54,54	0
56	MG	2A	3140	1/1	0.86	0.41	57,57,57,57	0
56	MG	1w	105	1/1	0.86	0.26	78,78,78,78	0
56	MG	1A	3419	1/1	0.86	0.16	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1x	104	1/1	0.86	0.12	66,66,66,66	0
56	MG	1x	107	1/1	0.86	0.14	60,60,60,60	0
56	MG	2A	3441	1/1	0.86	0.13	63,63,63,63	0
56	MG	2A	3175	1/1	0.86	0.27	50,50,50,50	0
56	MG	1A	3679	1/1	0.86	0.18	46,46,46,46	0
56	MG	1A	3703	1/1	0.86	0.32	65,65,65,65	0
56	MG	1A	3715	1/1	0.86	0.18	15,15,15,15	0
56	MG	2A	3184	1/1	0.86	0.61	55,55,55,55	0
56	MG	2A	3744	1/1	0.86	0.15	44,44,44,44	0
56	MG	1A	3683	1/1	0.87	0.17	66,66,66,66	0
56	MG	1A	3830	1/1	0.87	0.38	60,60,60,60	0
56	MG	1A	3952	1/1	0.87	0.13	24,24,24,24	0
56	MG	2A	3343	1/1	0.87	0.10	63,63,63,63	0
56	MG	1a	1670	1/1	0.87	0.14	52,52,52,52	0
56	MG	2A	3042	1/1	0.87	0.16	58,58,58,58	0
56	MG	1A	3468	1/1	0.87	0.20	41,41,41,41	0
56	MG	1A	3153	1/1	0.87	0.40	57,57,57,57	0
56	MG	2a	3128	1/1	0.87	0.12	82,82,82,82	0
56	MG	2A	3825	1/1	0.87	0.40	65,65,65,65	0
56	MG	1A	3485	1/1	0.87	0.43	47,47,47,47	0
56	MG	2A	3362	1/1	0.87	0.31	48,48,48,48	0
56	MG	1a	1692	1/1	0.87	0.45	59,59,59,59	0
56	MG	2A	3364	1/1	0.87	0.16	56,56,56,56	0
56	MG	2A	3847	1/1	0.87	0.58	73,73,73,73	0
56	MG	1A	3429	1/1	0.87	0.34	43,43,43,43	0
56	MG	1A	4038	1/1	0.87	0.20	64,64,64,64	0
56	MG	1a	1702	1/1	0.87	0.12	50,50,50,50	0
56	MG	1A	3629	1/1	0.87	0.18	20,20,20,20	0
56	MG	1A	3891	1/1	0.87	0.20	55,55,55,55	0
56	MG	1a	1709	1/1	0.87	0.19	55,55,55,55	0
56	MG	2A	3620	1/1	0.87	0.34	55,55,55,55	0
56	MG	2a	3158	1/1	0.87	0.20	80,80,80,80	0
56	MG	2D	302	1/1	0.87	0.21	42,42,42,42	0
56	MG	1B	205	1/1	0.87	0.30	51,51,51,51	0
56	MG	1B	217	1/1	0.87	0.06	41,41,41,41	0
56	MG	1A	3399	1/1	0.87	0.29	58,58,58,58	0
56	MG	2T	204	1/1	0.87	0.22	67,67,67,67	0
56	MG	1a	1626	1/1	0.87	0.28	61,61,61,61	0
56	MG	1B	229	1/1	0.87	0.15	71,71,71,71	0
56	MG	1a	1728	1/1	0.87	0.13	61,61,61,61	0
56	MG	1A	3361	1/1	0.87	0.10	41,41,41,41	0
56	MG	2a	3191	1/1	0.87	0.09	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	2a	3008	1/1	0.87	0.28	62,62,62,62	0
56	MG	2a	3199	1/1	0.87	0.13	85,85,85,85	0
56	MG	1e	3101	1/1	0.87	0.24	69,69,69,69	0
56	MG	2a	3207	1/1	0.87	0.14	66,66,66,66	0
56	MG	1a	1645	1/1	0.87	0.14	54,54,54,54	0
56	MG	2A	3273	1/1	0.87	0.52	64,64,64,64	0
56	MG	1w	107	1/1	0.87	0.12	66,66,66,66	0
56	MG	2a	3016	1/1	0.87	0.24	50,50,50,50	0
56	MG	2A	3686	1/1	0.87	0.19	61,61,61,61	0
56	MG	1x	101	1/1	0.87	0.22	51,51,51,51	0
56	MG	1a	1648	1/1	0.87	0.50	53,53,53,53	0
56	MG	2a	3034	1/1	0.87	0.14	74,74,74,74	0
56	MG	2A	3170	1/1	0.87	0.59	68,68,68,68	0
56	MG	1A	3439	1/1	0.87	0.34	48,48,48,48	0
56	MG	1A	3761	1/1	0.87	0.08	39,39,39,39	0
56	MG	2A	3291	1/1	0.87	0.38	55,55,55,55	0
56	MG	2a	3243	1/1	0.87	0.21	68,68,68,68	0
56	MG	2a	3049	1/1	0.87	0.10	80,80,80,80	0
56	MG	1A	3303	1/1	0.87	0.17	38,38,38,38	0
56	MG	1x	110	1/1	0.87	0.21	65,65,65,65	0
56	MG	1A	3134	1/1	0.87	0.12	30,30,30,30	0
56	MG	2l	203	1/1	0.87	0.69	72,72,72,72	0
56	MG	2A	3003	1/1	0.87	0.28	60,60,60,60	0
56	MG	1A	3329	1/1	0.87	0.33	40,40,40,40	0
56	MG	1a	1756	1/1	0.87	0.15	71,71,71,71	0
56	MG	2A	3312	1/1	0.87	0.16	58,58,58,58	0
56	MG	2A	3023	1/1	0.87	0.15	52,52,52,52	0
56	MG	2A	3202	1/1	0.87	0.24	45,45,45,45	0
56	MG	1a	1657	1/1	0.87	0.47	60,60,60,60	0
56	MG	2a	3096	1/1	0.87	0.38	78,78,78,78	0
56	MG	2A	3752	1/1	0.87	0.14	41,41,41,41	0
56	MG	2A	3760	1/1	0.87	0.10	53,53,53,53	0
59	ZN	14	102	1/1	0.87	0.06	98,98,98,98	0
56	MG	1a	1659	1/1	0.87	0.66	66,66,66,66	0
56	MG	1A	3940	1/1	0.88	0.10	40,40,40,40	0
56	MG	1A	3110	1/1	0.88	0.39	38,38,38,38	0
56	MG	2a	3022	1/1	0.88	0.16	62,62,62,62	0
56	MG	2A	3081	1/1	0.88	0.17	47,47,47,47	0
56	MG	1A	3704	1/1	0.88	0.23	39,39,39,39	0
56	MG	2a	3033	1/1	0.88	0.15	59,59,59,59	0
56	MG	2A	3571	1/1	0.88	0.27	40,40,40,40	0
56	MG	2A	3297	1/1	0.88	0.12	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3707	1/1	0.88	0.09	64,64,64,64	0
56	MG	1A	3377	1/1	0.88	0.10	42,42,42,42	0
56	MG	2a	3043	1/1	0.88	0.13	63,63,63,63	0
56	MG	2a	3044	1/1	0.88	0.39	59,59,59,59	0
56	MG	1a	1615	1/1	0.88	0.11	57,57,57,57	0
56	MG	1A	3146	1/1	0.88	0.15	57,57,57,57	0
56	MG	2A	3310	1/1	0.88	0.10	56,56,56,56	0
56	MG	1A	3550	1/1	0.88	0.91	42,42,42,42	0
56	MG	1A	3449	1/1	0.88	0.28	33,33,33,33	0
56	MG	1a	1777	1/1	0.88	0.16	50,50,50,50	0
56	MG	2a	3067	1/1	0.88	0.09	67,67,67,67	0
56	MG	1a	1779	1/1	0.88	0.09	60,60,60,60	0
56	MG	1A	3024	1/1	0.88	0.23	41,41,41,41	0
56	MG	2A	3639	1/1	0.88	0.11	64,64,64,64	0
56	MG	1A	3381	1/1	0.88	0.56	38,38,38,38	0
56	MG	1A	3734	1/1	0.88	0.11	20,20,20,20	0
56	MG	2a	3085	1/1	0.88	0.07	59,59,59,59	0
56	MG	2A	3335	1/1	0.88	0.41	69,69,69,69	0
56	MG	2A	3163	1/1	0.88	0.27	50,50,50,50	0
56	MG	1A	3744	1/1	0.88	0.08	40,40,40,40	0
56	MG	2a	3100	1/1	0.88	0.56	80,80,80,80	0
56	MG	1A	3745	1/1	0.88	0.12	43,43,43,43	0
56	MG	2A	3345	1/1	0.88	0.12	71,71,71,71	0
56	MG	1A	3464	1/1	0.88	0.13	51,51,51,51	0
56	MG	1A	3169	1/1	0.88	0.15	32,32,32,32	0
56	MG	1A	3385	1/1	0.88	0.16	35,35,35,35	0
56	MG	1A	3780	1/1	0.88	0.16	54,54,54,54	0
56	MG	1A	3594	1/1	0.88	0.18	21,21,21,21	0
56	MG	2A	3353	1/1	0.88	0.14	48,48,48,48	0
56	MG	1A	3790	1/1	0.88	0.16	34,34,34,34	0
56	MG	1A	3598	1/1	0.88	0.16	40,40,40,40	0
56	MG	2A	3185	1/1	0.88	0.16	57,57,57,57	0
56	MG	2A	3187	1/1	0.88	0.11	43,43,43,43	0
56	MG	1a	1661	1/1	0.88	0.24	52,52,52,52	0
56	MG	1A	3387	1/1	0.88	0.16	37,37,37,37	0
56	MG	2A	3719	1/1	0.88	0.13	58,58,58,58	0
56	MG	1A	3389	1/1	0.88	0.41	33,33,33,33	0
56	MG	2A	3722	1/1	0.88	0.41	67,67,67,67	0
56	MG	2A	3198	1/1	0.88	0.17	69,69,69,69	0
56	MG	1a	1823	1/1	0.88	0.13	53,53,53,53	0
56	MG	1A	3491	1/1	0.88	0.45	54,54,54,54	0
56	MG	1d	301	1/1	0.88	0.12	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	4032	1/1	0.88	0.21	70,70,70,70	0
56	MG	2A	3211	1/1	0.88	0.26	57,57,57,57	0
56	MG	1a	1672	1/1	0.88	0.25	64,64,64,64	0
56	MG	1A	3840	1/1	0.88	0.07	33,33,33,33	0
56	MG	1A	3620	1/1	0.88	0.14	25,25,25,25	0
56	MG	2A	3766	1/1	0.88	0.20	37,37,37,37	0
56	MG	2A	3770	1/1	0.88	0.10	46,46,46,46	0
56	MG	2A	3779	1/1	0.88	0.11	56,56,56,56	0
56	MG	2a	3168	1/1	0.88	0.12	73,73,73,73	0
56	MG	1A	3848	1/1	0.88	0.20	51,51,51,51	0
56	MG	2A	3403	1/1	0.88	0.35	57,57,57,57	0
56	MG	1A	4063	1/1	0.88	0.10	68,68,68,68	0
56	MG	1A	4071	1/1	0.88	0.13	65,65,65,65	0
56	MG	2a	3180	1/1	0.88	0.14	57,57,57,57	0
56	MG	1A	3863	1/1	0.88	0.25	26,26,26,26	0
56	MG	1A	3298	1/1	0.88	0.28	30,30,30,30	0
56	MG	2A	3819	1/1	0.88	0.19	74,74,74,74	0
56	MG	1a	1704	1/1	0.88	0.10	49,49,49,49	0
56	MG	2A	3238	1/1	0.88	0.18	56,56,56,56	0
56	MG	2A	3425	1/1	0.88	0.10	44,44,44,44	0
56	MG	1A	3212	1/1	0.88	0.22	53,53,53,53	0
56	MG	2A	3430	1/1	0.88	0.21	49,49,49,49	0
56	MG	2A	3432	1/1	0.88	0.17	42,42,42,42	0
56	MG	1A	3878	1/1	0.88	0.23	41,41,41,41	0
56	MG	2A	3246	1/1	0.88	0.39	44,44,44,44	0
56	MG	1A	3049	1/1	0.88	0.17	42,42,42,42	0
56	MG	2A	3449	1/1	0.88	0.17	54,54,54,54	0
56	MG	1a	1715	1/1	0.88	0.12	58,58,58,58	0
56	MG	1a	1717	1/1	0.88	0.27	60,60,60,60	0
56	MG	2B	214	1/1	0.88	0.16	67,67,67,67	0
56	MG	2A	3472	1/1	0.88	0.20	57,57,57,57	0
56	MG	1A	3225	1/1	0.88	0.15	56,56,56,56	0
56	MG	2a	3242	1/1	0.88	0.25	64,64,64,64	0
56	MG	1A	3894	1/1	0.88	0.12	59,59,59,59	0
56	MG	2A	3480	1/1	0.88	0.17	57,57,57,57	0
56	MG	2A	3490	1/1	0.88	0.12	39,39,39,39	0
56	MG	1A	3517	1/1	0.88	0.54	43,43,43,43	0
56	MG	1A	3901	1/1	0.88	0.10	51,51,51,51	0
56	MG	1A	3904	1/1	0.88	0.07	30,30,30,30	0
56	MG	1A	3657	1/1	0.88	0.19	49,49,49,49	0
56	MG	28	102	1/1	0.88	0.12	56,56,56,56	0
56	MG	28	104	1/1	0.88	0.06	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	3316	1/1	0.88	0.13	35,35,35,35	0
56	MG	1A	3174	1/1	0.88	0.21	42,42,42,42	0
56	MG	2A	3049	1/1	0.88	0.09	58,58,58,58	0
56	MG	1A	3678	1/1	0.88	0.10	48,48,48,48	0
56	MG	2A	3052	1/1	0.88	0.13	64,64,64,64	0
56	MG	1A	3092	1/1	0.88	0.84	59,59,59,59	0
56	MG	2a	3011	1/1	0.88	0.11	73,73,73,73	0
56	MG	1A	3324	1/1	0.88	0.19	42,42,42,42	0
56	MG	1A	3933	1/1	0.88	0.13	23,23,23,23	0
56	MG	2A	3248	1/1	0.89	0.17	62,62,62,62	0
56	MG	1A	3888	1/1	0.89	0.14	12,12,12,12	0
56	MG	1A	3053	1/1	0.89	0.12	33,33,33,33	0
56	MG	1a	1675	1/1	0.89	0.14	55,55,55,55	0
56	MG	1a	1681	1/1	0.89	0.20	39,39,39,39	0
56	MG	2A	3255	1/1	0.89	0.11	60,60,60,60	0
56	MG	1a	1682	1/1	0.89	0.18	57,57,57,57	0
56	MG	2A	3257	1/1	0.89	0.39	61,61,61,61	0
56	MG	2A	3524	1/1	0.89	0.17	50,50,50,50	0
56	MG	2A	3530	1/1	0.89	0.15	51,51,51,51	0
56	MG	1a	1687	1/1	0.89	0.21	55,55,55,55	0
56	MG	1A	3172	1/1	0.89	0.19	23,23,23,23	0
56	MG	1A	4061	1/1	0.89	0.25	60,60,60,60	0
56	MG	2A	3547	1/1	0.89	0.19	45,45,45,45	0
56	MG	1A	3895	1/1	0.89	0.05	77,77,77,77	0
56	MG	1A	3054	1/1	0.89	0.22	45,45,45,45	0
56	MG	2A	3552	1/1	0.89	0.14	47,47,47,47	0
56	MG	2A	3270	1/1	0.89	0.09	63,63,63,63	0
56	MG	2a	3038	1/1	0.89	0.07	64,64,64,64	0
56	MG	1A	4082	1/1	0.89	0.19	57,57,57,57	0
56	MG	1A	3900	1/1	0.89	0.15	60,60,60,60	0
56	MG	2A	3563	1/1	0.89	0.16	77,77,77,77	0
56	MG	1B	204	1/1	0.89	0.12	32,32,32,32	0
56	MG	2a	3047	1/1	0.89	0.27	73,73,73,73	0
56	MG	1A	3231	1/1	0.89	0.19	50,50,50,50	0
56	MG	2A	3576	1/1	0.89	0.16	40,40,40,40	0
56	MG	2A	3040	1/1	0.89	0.24	66,66,66,66	0
56	MG	1B	214	1/1	0.89	0.35	45,45,45,45	0
56	MG	2a	3061	1/1	0.89	0.13	66,66,66,66	0
56	MG	1A	3451	1/1	0.89	0.34	46,46,46,46	0
56	MG	1A	3106	1/1	0.89	0.30	38,38,38,38	0
56	MG	1a	1716	1/1	0.89	0.12	59,59,59,59	0
56	MG	2a	3068	1/1	0.89	0.12	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	1A	3913	1/1	0.89	0.18	19,19,19,19	0
56	MG	1A	3916	1/1	0.89	0.15	59,59,59,59	0
56	MG	1a	1720	1/1	0.89	0.17	58,58,58,58	0
56	MG	2A	3622	1/1	0.89	0.13	40,40,40,40	0
56	MG	2A	3300	1/1	0.89	0.28	66,66,66,66	0
56	MG	2A	3057	1/1	0.89	0.15	52,52,52,52	0
56	MG	2a	3087	1/1	0.89	0.20	58,58,58,58	0
56	MG	1A	3457	1/1	0.89	0.53	32,32,32,32	0
56	MG	1A	3458	1/1	0.89	0.41	58,58,58,58	0
56	MG	2A	3649	1/1	0.89	0.15	68,68,68,68	0
56	MG	2A	3652	1/1	0.89	0.23	37,37,37,37	0
56	MG	2A	3069	1/1	0.89	0.30	42,42,42,42	0
56	MG	1A	3725	1/1	0.89	0.16	35,35,35,35	0
56	MG	1a	1726	1/1	0.89	0.25	55,55,55,55	0
56	MG	1A	3233	1/1	0.89	0.13	42,42,42,42	0
56	MG	1F	308	1/1	0.89	0.15	42,42,42,42	0
56	MG	1a	1732	1/1	0.89	0.10	62,62,62,62	0
56	MG	1A	3924	1/1	0.89	0.27	58,58,58,58	0
56	MG	1a	1734	1/1	0.89	0.09	41,41,41,41	0
56	MG	2A	3681	1/1	0.89	0.11	69,69,69,69	0
56	MG	1A	3733	1/1	0.89	0.13	43,43,43,43	0
56	MG	1A	3568	1/1	0.89	0.17	29,29,29,29	0
56	MG	1A	3935	1/1	0.89	0.11	25,25,25,25	0
56	MG	1A	3186	1/1	0.89	0.72	35,35,35,35	0
56	MG	2A	3105	1/1	0.89	0.30	46,46,46,46	0
56	MG	1a	1750	1/1	0.89	0.08	61,61,61,61	0
56	MG	2A	3113	1/1	0.89	0.41	55,55,55,55	0
56	MG	2A	3704	1/1	0.89	0.18	35,35,35,35	0
56	MG	1W	203	1/1	0.89	0.24	64,64,64,64	0
56	MG	1Y	201	1/1	0.89	0.16	49,49,49,49	0
56	MG	1A	3248	1/1	0.89	0.53	46,46,46,46	0
56	MG	2A	3718	1/1	0.89	0.11	51,51,51,51	0
56	MG	1A	3386	1/1	0.89	0.16	39,39,39,39	0
56	MG	2A	3355	1/1	0.89	0.14	63,63,63,63	0
56	MG	1A	3759	1/1	0.89	0.10	19,19,19,19	0
56	MG	1A	3253	1/1	0.89	0.81	31,31,31,31	0
56	MG	1a	1771	1/1	0.89	0.09	54,54,54,54	0
56	MG	1A	3476	1/1	0.89	0.15	45,45,45,45	0
56	MG	1A	3143	1/1	0.89	0.27	27,27,27,27	0
56	MG	2a	3165	1/1	0.89	0.09	66,66,66,66	0
56	MG	2A	3739	1/1	0.89	0.17	67,67,67,67	0
56	MG	1a	1604	1/1	0.89	0.10	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3392	1/1	0.89	0.10	47,47,47,47	0
56	MG	1a	1614	1/1	0.89	0.83	49,49,49,49	0
56	MG	2A	3180	1/1	0.89	0.28	60,60,60,60	0
56	MG	1A	3492	1/1	0.89	0.25	32,32,32,32	0
56	MG	1A	3978	1/1	0.89	0.07	45,45,45,45	0
56	MG	1A	3804	1/1	0.89	0.19	22,22,22,22	0
56	MG	2a	3189	1/1	0.89	0.10	91,91,91,91	0
56	MG	2A	3387	1/1	0.89	0.29	57,57,57,57	0
56	MG	1A	3496	1/1	0.89	0.16	41,41,41,41	0
56	MG	2A	3782	1/1	0.89	0.12	45,45,45,45	0
56	MG	1a	1629	1/1	0.89	0.14	53,53,53,53	0
56	MG	2A	3785	1/1	0.89	0.14	43,43,43,43	0
56	MG	1A	3632	1/1	0.89	0.16	25,25,25,25	0
56	MG	1A	3070	1/1	0.89	0.33	52,52,52,52	0
56	MG	2a	3211	1/1	0.89	0.10	73,73,73,73	0
56	MG	2a	3220	1/1	0.89	0.15	71,71,71,71	0
56	MG	1A	3989	1/1	0.89	0.16	33,33,33,33	0
56	MG	2A	3805	1/1	0.89	0.15	58,58,58,58	0
56	MG	1A	3831	1/1	0.89	0.23	26,26,26,26	0
56	MG	2a	3224	1/1	0.89	0.12	52,52,52,52	0
56	MG	1A	3835	1/1	0.89	0.17	40,40,40,40	0
56	MG	1A	3993	1/1	0.89	0.11	21,21,21,21	0
56	MG	1A	3081	1/1	0.89	0.16	38,38,38,38	0
56	MG	2a	3233	1/1	0.89	0.15	53,53,53,53	0
56	MG	2A	3411	1/1	0.89	0.25	53,53,53,53	0
56	MG	2A	3210	1/1	0.89	0.78	54,54,54,54	0
56	MG	2a	3236	1/1	0.89	0.42	60,60,60,60	0
56	MG	2a	3237	1/1	0.89	0.10	63,63,63,63	0
56	MG	1a	1653	1/1	0.89	0.07	64,64,64,64	0
56	MG	2A	3836	1/1	0.89	0.11	61,61,61,61	0
56	MG	1A	3275	1/1	0.89	0.14	41,41,41,41	0
56	MG	1A	3406	1/1	0.89	0.15	49,49,49,49	0
56	MG	1A	3022	1/1	0.89	0.58	26,26,26,26	0
56	MG	2A	3227	1/1	0.89	0.27	61,61,61,61	0
56	MG	1a	1813	1/1	0.89	0.17	56,56,56,56	0
56	MG	1a	1658	1/1	0.89	0.46	65,65,65,65	0
56	MG	1A	4013	1/1	0.89	0.12	46,46,46,46	0
56	MG	2A	3439	1/1	0.89	0.21	59,59,59,59	0
56	MG	2A	3234	1/1	0.89	0.21	51,51,51,51	0
56	MG	1A	4016	1/1	0.89	0.19	26,26,26,26	0
56	MG	2B	218	1/1	0.89	0.15	63,63,63,63	0
56	MG	2A	3452	1/1	0.89	0.12	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3290	1/1	0.89	0.45	42,42,42,42	0
56	MG	1n	102	1/1	0.89	0.15	54,54,54,54	0
56	MG	1t	201	1/1	0.89	0.09	49,49,49,49	0
56	MG	1A	3296	1/1	0.89	0.26	53,53,53,53	0
56	MG	1A	3202	1/1	0.89	0.21	50,50,50,50	0
56	MG	2y	104	1/1	0.89	0.15	60,60,60,60	0
57	K	2A	3399	1/1	0.89	0.15	73,73,73,73	0
56	MG	1A	3301	1/1	0.89	0.21	42,42,42,42	0
56	MG	1A	3702	1/1	0.89	0.12	23,23,23,23	0
56	MG	1a	1792	1/1	0.90	0.17	69,69,69,69	0
56	MG	2a	3018	1/1	0.90	0.15	60,60,60,60	0
56	MG	1A	3545	1/1	0.90	0.28	55,55,55,55	0
56	MG	2a	3021	1/1	0.90	0.34	56,56,56,56	0
56	MG	2A	3608	1/1	0.90	0.10	49,49,49,49	0
56	MG	2A	3616	1/1	0.90	0.09	48,48,48,48	0
56	MG	1A	3345	1/1	0.90	1.12	37,37,37,37	0
56	MG	1A	3882	1/1	0.90	0.13	43,43,43,43	0
56	MG	1A	4031	1/1	0.90	0.08	58,58,58,58	0
56	MG	1A	3886	1/1	0.90	0.11	45,45,45,45	0
56	MG	2a	3037	1/1	0.90	0.20	70,70,70,70	0
56	MG	1A	3549	1/1	0.90	0.12	49,49,49,49	0
56	MG	2A	3638	1/1	0.90	0.13	62,62,62,62	0
56	MG	1A	3889	1/1	0.90	0.22	20,20,20,20	0
56	MG	1A	3469	1/1	0.90	0.32	42,42,42,42	0
56	MG	2A	3648	1/1	0.90	0.15	71,71,71,71	0
56	MG	2a	3046	1/1	0.90	0.14	60,60,60,60	0
56	MG	1A	3420	1/1	0.90	0.17	59,59,59,59	0
56	MG	1A	3348	1/1	0.90	0.22	41,41,41,41	0
56	MG	2A	3186	1/1	0.90	0.10	47,47,47,47	0
56	MG	1a	1822	1/1	0.90	0.13	48,48,48,48	0
56	MG	2A	3188	1/1	0.90	0.25	50,50,50,50	0
56	MG	1A	3557	1/1	0.90	0.18	30,30,30,30	0
56	MG	2A	3367	1/1	0.90	0.24	62,62,62,62	0
56	MG	1a	1824	1/1	0.90	0.34	52,52,52,52	0
56	MG	1A	4073	1/1	0.90	0.29	45,45,45,45	0
56	MG	2A	3197	1/1	0.90	0.50	62,62,62,62	0
56	MG	1A	3720	1/1	0.90	0.15	29,29,29,29	0
56	MG	2A	3682	1/1	0.90	0.15	57,57,57,57	0
56	MG	2A	3685	1/1	0.90	0.13	46,46,46,46	0
56	MG	1A	3560	1/1	0.90	0.24	49,49,49,49	0
56	MG	1k	201	1/1	0.90	0.10	55,55,55,55	0
56	MG	1A	3354	1/1	0.90	0.20	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3486	1/1	0.90	0.19	58,58,58,58	0
56	MG	2A	3382	1/1	0.90	0.13	38,38,38,38	0
56	MG	2A	3693	1/1	0.90	0.12	47,47,47,47	0
56	MG	1A	3911	1/1	0.90	0.12	26,26,26,26	0
56	MG	1A	3142	1/1	0.90	0.34	26,26,26,26	0
56	MG	1B	219	1/1	0.90	0.18	34,34,34,34	0
56	MG	1a	1698	1/1	0.90	0.26	69,69,69,69	0
56	MG	1B	222	1/1	0.90	0.23	68,68,68,68	0
56	MG	2a	3111	1/1	0.90	0.34	74,74,74,74	0
56	MG	1A	3914	1/1	0.90	0.27	45,45,45,45	0
56	MG	2A	3717	1/1	0.90	0.20	57,57,57,57	0
56	MG	1A	3434	1/1	0.90	0.21	50,50,50,50	0
56	MG	1A	3359	1/1	0.90	0.14	51,51,51,51	0
56	MG	2A	3404	1/1	0.90	0.20	61,61,61,61	0
56	MG	1A	3732	1/1	0.90	0.15	65,65,65,65	0
56	MG	2A	3002	1/1	0.90	0.35	44,44,44,44	0
56	MG	2A	3408	1/1	0.90	0.58	55,55,55,55	0
56	MG	1a	1710	1/1	0.90	0.20	47,47,47,47	0
56	MG	2A	3734	1/1	0.90	0.49	60,60,60,60	0
56	MG	1A	3095	1/1	0.90	0.43	27,27,27,27	0
56	MG	1A	3441	1/1	0.90	0.19	51,51,51,51	0
56	MG	2A	3022	1/1	0.90	0.15	70,70,70,70	0
56	MG	1A	3736	1/1	0.90	0.15	26,26,26,26	0
56	MG	2A	3745	1/1	0.90	0.13	59,59,59,59	0
56	MG	2A	3746	1/1	0.90	0.13	54,54,54,54	0
56	MG	2A	3748	1/1	0.90	0.11	63,63,63,63	0
56	MG	1A	3508	1/1	0.90	0.35	42,42,42,42	0
56	MG	2A	3427	1/1	0.90	0.17	64,64,64,64	0
56	MG	1F	312	1/1	0.90	0.23	54,54,54,54	0
56	MG	1A	3445	1/1	0.90	0.22	52,52,52,52	0
56	MG	1A	3751	1/1	0.90	0.16	18,18,18,18	0
56	MG	2A	3775	1/1	0.90	0.10	63,63,63,63	0
56	MG	2A	3777	1/1	0.90	0.08	58,58,58,58	0
56	MG	1A	3272	1/1	0.90	0.20	52,52,52,52	0
56	MG	1A	3756	1/1	0.90	0.12	57,57,57,57	0
56	MG	1A	3606	1/1	0.90	0.12	34,34,34,34	0
56	MG	1A	3001	1/1	0.90	0.08	40,40,40,40	0
56	MG	1A	3519	1/1	0.90	0.20	44,44,44,44	0
56	MG	2A	3788	1/1	0.90	0.13	54,54,54,54	0
56	MG	1A	3963	1/1	0.90	0.21	72,72,72,72	0
56	MG	2A	3453	1/1	0.90	0.15	56,56,56,56	0
56	MG	2A	3796	1/1	0.90	0.13	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	1A	3964	1/1	0.90	0.10	49,49,49,49	0
56	MG	1A	3777	1/1	0.90	0.16	38,38,38,38	0
56	MG	2A	3469	1/1	0.90	0.09	49,49,49,49	0
56	MG	2A	3261	1/1	0.90	0.26	54,54,54,54	0
56	MG	2a	3194	1/1	0.90	0.14	71,71,71,71	0
56	MG	2a	3197	1/1	0.90	0.10	66,66,66,66	0
56	MG	1A	3152	1/1	0.90	0.14	43,43,43,43	0
56	MG	1A	3372	1/1	0.90	0.31	48,48,48,48	0
56	MG	2a	3201	1/1	0.90	0.10	74,74,74,74	0
56	MG	2a	3203	1/1	0.90	0.29	71,71,71,71	0
56	MG	1A	3976	1/1	0.90	0.15	46,46,46,46	0
56	MG	2A	3060	1/1	0.90	0.19	39,39,39,39	0
56	MG	2A	3833	1/1	0.90	0.23	49,49,49,49	0
56	MG	2A	3063	1/1	0.90	0.10	48,48,48,48	0
56	MG	2a	3213	1/1	0.90	0.10	64,64,64,64	0
56	MG	2A	3499	1/1	0.90	0.21	25,25,25,25	0
56	MG	2A	3500	1/1	0.90	0.20	32,32,32,32	0
56	MG	2A	3843	1/1	0.90	0.16	46,46,46,46	0
56	MG	1A	3528	1/1	0.90	0.19	53,53,53,53	0
56	MG	1A	3032	1/1	0.90	0.15	38,38,38,38	0
56	MG	2A	3274	1/1	0.90	0.11	58,58,58,58	0
56	MG	1A	3815	1/1	0.90	0.12	36,36,36,36	0
56	MG	1A	3638	1/1	0.90	0.10	31,31,31,31	0
56	MG	1A	3648	1/1	0.90	0.18	32,32,32,32	0
56	MG	1A	3284	1/1	0.90	0.16	42,42,42,42	0
56	MG	1A	3656	1/1	0.90	0.18	14,14,14,14	0
56	MG	1A	3533	1/1	0.90	0.35	56,56,56,56	0
56	MG	1A	3663	1/1	0.90	0.30	63,63,63,63	0
56	MG	2a	3238	1/1	0.90	0.19	74,74,74,74	0
56	MG	1A	3315	1/1	0.90	0.20	40,40,40,40	0
56	MG	2a	3240	1/1	0.90	0.15	62,62,62,62	0
56	MG	2A	3296	1/1	0.90	0.07	72,72,72,72	0
56	MG	1a	1641	1/1	0.90	0.24	41,41,41,41	0
56	MG	2E	307	1/1	0.90	0.07	59,59,59,59	0
56	MG	2F	303	1/1	0.90	0.53	46,46,46,46	0
56	MG	1a	1643	1/1	0.90	0.23	61,61,61,61	0
56	MG	2f	202	1/1	0.90	0.13	51,51,51,51	0
56	MG	2F	305	1/1	0.90	0.09	61,61,61,61	0
56	MG	2A	3102	1/1	0.90	0.19	41,41,41,41	0
56	MG	2O	201	1/1	0.90	0.60	58,58,58,58	0
56	MG	2l	204	1/1	0.90	0.17	55,55,55,55	0
56	MG	1A	3844	1/1	0.90	0.24	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	3666	1/1	0.90	0.25	46,46,46,46	0
56	MG	2A	3554	1/1	0.90	0.11	74,74,74,74	0
56	MG	1A	3667	1/1	0.90	0.27	33,33,33,33	0
56	MG	1A	4004	1/1	0.90	0.22	55,55,55,55	0
56	MG	28	106	1/1	0.90	0.14	72,72,72,72	0
56	MG	2A	3115	1/1	0.90	0.11	50,50,50,50	0
56	MG	1A	3854	1/1	0.90	0.15	37,37,37,37	0
56	MG	1A	3672	1/1	0.90	0.16	69,69,69,69	0
56	MG	1a	1654	1/1	0.90	0.12	63,63,63,63	0
56	MG	2A	3322	1/1	0.90	0.52	63,63,63,63	0
57	K	1A	3497	1/1	0.90	0.16	67,67,67,67	0
56	MG	1A	3288	1/1	0.90	0.18	43,43,43,43	0
56	MG	1A	3544	1/1	0.90	0.22	43,43,43,43	0
56	MG	2A	3164	1/1	0.90	0.16	50,50,50,50	0
56	MG	1A	3925	1/1	0.91	0.15	60,60,60,60	0
56	MG	1A	3786	1/1	0.91	0.12	57,57,57,57	0
56	MG	1A	3788	1/1	0.91	0.11	50,50,50,50	0
56	MG	1A	3498	1/1	0.91	0.19	43,43,43,43	0
56	MG	2a	3024	1/1	0.91	0.25	61,61,61,61	0
56	MG	1A	3792	1/1	0.91	0.06	56,56,56,56	0
56	MG	1A	3677	1/1	0.91	0.18	33,33,33,33	0
56	MG	2A	3656	1/1	0.91	0.15	49,49,49,49	0
56	MG	2A	3658	1/1	0.91	0.08	46,46,46,46	0
56	MG	1A	3155	1/1	0.91	0.32	36,36,36,36	0
56	MG	1A	3951	1/1	0.91	0.10	44,44,44,44	0
56	MG	2a	3039	1/1	0.91	0.30	76,76,76,76	0
56	MG	1A	3241	1/1	0.91	0.25	42,42,42,42	0
56	MG	2a	3041	1/1	0.91	0.24	74,74,74,74	0
56	MG	1A	3244	1/1	0.91	0.19	37,37,37,37	0
56	MG	2A	3675	1/1	0.91	0.14	53,53,53,53	0
56	MG	1B	233	1/1	0.91	0.16	52,52,52,52	0
56	MG	2a	3045	1/1	0.91	0.19	66,66,66,66	0
56	MG	2A	3678	1/1	0.91	0.13	60,60,60,60	0
56	MG	1A	3690	1/1	0.91	0.09	60,60,60,60	0
56	MG	1A	3569	1/1	0.91	0.23	17,17,17,17	0
56	MG	1a	1701	1/1	0.91	0.21	55,55,55,55	0
56	MG	1D	310	1/1	0.91	0.28	46,46,46,46	0
56	MG	1A	3393	1/1	0.91	0.54	32,32,32,32	0
56	MG	2a	3056	1/1	0.91	0.17	77,77,77,77	0
56	MG	2a	3057	1/1	0.91	0.12	60,60,60,60	0
56	MG	1F	303	1/1	0.91	0.64	29,29,29,29	0
56	MG	1x	109	1/1	0.91	0.49	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3214	1/1	0.91	1.16	68,68,68,68	0
56	MG	2A	3394	1/1	0.91	0.17	61,61,61,61	0
56	MG	1F	305	1/1	0.91	0.12	47,47,47,47	0
56	MG	2A	3398	1/1	0.91	0.36	42,42,42,42	0
56	MG	2A	3222	1/1	0.91	0.20	46,46,46,46	0
56	MG	2a	3078	1/1	0.91	0.18	64,64,64,64	0
56	MG	1a	1707	1/1	0.91	0.08	63,63,63,63	0
56	MG	2A	3706	1/1	0.91	0.26	48,48,48,48	0
56	MG	1A	3446	1/1	0.91	0.16	40,40,40,40	0
56	MG	1A	3596	1/1	0.91	0.15	24,24,24,24	0
56	MG	2a	3086	1/1	0.91	0.11	50,50,50,50	0
56	MG	1A	3025	1/1	0.91	0.71	57,57,57,57	0
56	MG	1P	205	1/1	0.91	0.14	42,42,42,42	0
56	MG	2a	3095	1/1	0.91	0.14	68,68,68,68	0
56	MG	1Q	203	1/1	0.91	0.14	39,39,39,39	0
56	MG	1A	3719	1/1	0.91	0.19	29,29,29,29	0
56	MG	1A	3397	1/1	0.91	0.99	44,44,44,44	0
56	MG	2a	3105	1/1	0.91	0.17	67,67,67,67	0
56	MG	1A	3187	1/1	0.91	0.25	70,70,70,70	0
56	MG	2A	3417	1/1	0.91	0.41	52,52,52,52	0
56	MG	2A	3418	1/1	0.91	0.15	46,46,46,46	0
56	MG	2A	3420	1/1	0.91	0.13	50,50,50,50	0
56	MG	2A	3031	1/1	0.91	0.21	53,53,53,53	0
56	MG	1A	3525	1/1	0.91	0.39	62,62,62,62	0
56	MG	1A	3189	1/1	0.91	0.32	36,36,36,36	0
56	MG	2a	3117	1/1	0.91	0.13	69,69,69,69	0
56	MG	2A	3037	1/1	0.91	0.32	68,68,68,68	0
56	MG	1A	3867	1/1	0.91	0.07	60,60,60,60	0
56	MG	1A	3261	1/1	0.91	0.09	41,41,41,41	0
56	MG	10	103	1/1	0.91	0.15	50,50,50,50	0
56	MG	1A	3058	1/1	0.91	0.22	37,37,37,37	0
56	MG	2a	3132	1/1	0.91	0.20	65,65,65,65	0
56	MG	2a	3133	1/1	0.91	0.05	67,67,67,67	0
56	MG	1A	3727	1/1	0.91	0.16	17,17,17,17	0
56	MG	2A	3757	1/1	0.91	0.09	43,43,43,43	0
56	MG	2A	3758	1/1	0.91	0.14	33,33,33,33	0
56	MG	2A	3045	1/1	0.91	0.10	55,55,55,55	0
56	MG	2A	3446	1/1	0.91	0.37	53,53,53,53	0
56	MG	1A	3414	1/1	0.91	0.25	35,35,35,35	0
56	MG	2A	3047	1/1	0.91	0.14	63,63,63,63	0
56	MG	2A	3772	1/1	0.91	0.10	56,56,56,56	0
56	MG	1A	3192	1/1	0.91	0.14	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	3536	1/1	0.91	0.12	46,46,46,46	0
56	MG	2A	3259	1/1	0.91	0.13	61,61,61,61	0
56	MG	1A	3998	1/1	0.91	0.12	44,44,44,44	0
56	MG	2A	3056	1/1	0.91	0.21	66,66,66,66	0
56	MG	1a	1746	1/1	0.91	0.15	51,51,51,51	0
56	MG	1a	1606	1/1	0.91	0.12	66,66,66,66	0
56	MG	1A	3096	1/1	0.91	0.55	37,37,37,37	0
56	MG	2A	3269	1/1	0.91	0.18	69,69,69,69	0
56	MG	1A	3307	1/1	0.91	0.14	43,43,43,43	0
56	MG	2A	3494	1/1	0.91	0.10	65,65,65,65	0
56	MG	2a	3167	1/1	0.91	0.08	75,75,75,75	0
56	MG	2A	3797	1/1	0.91	0.14	47,47,47,47	0
56	MG	1A	4008	1/1	0.91	0.09	34,34,34,34	0
56	MG	1a	1617	1/1	0.91	0.43	64,64,64,64	0
56	MG	2A	3806	1/1	0.91	0.16	61,61,61,61	0
56	MG	2A	3808	1/1	0.91	0.38	71,71,71,71	0
56	MG	2a	3175	1/1	0.91	0.12	58,58,58,58	0
56	MG	2A	3809	1/1	0.91	0.10	44,44,44,44	0
56	MG	1A	3310	1/1	0.91	0.15	39,39,39,39	0
56	MG	2A	3074	1/1	0.91	1.18	48,48,48,48	0
56	MG	2A	3511	1/1	0.91	0.16	51,51,51,51	0
56	MG	2A	3512	1/1	0.91	0.12	43,43,43,43	0
56	MG	1A	3384	1/1	0.91	0.31	67,67,67,67	0
56	MG	1a	1762	1/1	0.91	0.09	59,59,59,59	0
56	MG	2A	3828	1/1	0.91	0.20	52,52,52,52	0
56	MG	1A	3481	1/1	0.91	0.33	44,44,44,44	0
56	MG	1a	1628	1/1	0.91	0.20	59,59,59,59	0
56	MG	1A	3753	1/1	0.91	0.13	21,21,21,21	0
56	MG	2A	3084	1/1	0.91	0.09	47,47,47,47	0
56	MG	2A	3840	1/1	0.91	0.13	60,60,60,60	0
56	MG	1A	3061	1/1	0.91	0.49	51,51,51,51	0
56	MG	1A	3658	1/1	0.91	0.11	27,27,27,27	0
56	MG	2A	3846	1/1	0.91	0.25	68,68,68,68	0
56	MG	2a	3214	1/1	0.91	0.12	75,75,75,75	0
56	MG	2A	3540	1/1	0.91	0.14	38,38,38,38	0
56	MG	1A	3757	1/1	0.91	0.09	40,40,40,40	0
56	MG	2B	204	1/1	0.91	0.10	70,70,70,70	0
56	MG	1A	3432	1/1	0.91	0.12	31,31,31,31	0
56	MG	1A	3488	1/1	0.91	0.25	49,49,49,49	0
56	MG	2B	212	1/1	0.91	0.17	64,64,64,64	0
56	MG	1a	1646	1/1	0.91	0.05	69,69,69,69	0
56	MG	1a	1647	1/1	0.91	0.15	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3106	1/1	0.91	0.19	49,49,49,49	0
56	MG	1a	1783	1/1	0.91	0.27	59,59,59,59	0
56	MG	2A	3112	1/1	0.91	0.23	52,52,52,52	0
56	MG	1A	3279	1/1	0.91	0.14	51,51,51,51	0
56	MG	2A	3316	1/1	0.91	0.11	46,46,46,46	0
56	MG	2A	3317	1/1	0.91	0.68	43,43,43,43	0
56	MG	2E	303	1/1	0.91	0.12	47,47,47,47	0
56	MG	2A	3569	1/1	0.91	0.13	43,43,43,43	0
56	MG	2F	301	1/1	0.91	0.57	43,43,43,43	0
56	MG	1A	4037	1/1	0.91	0.19	49,49,49,49	0
56	MG	1A	3773	1/1	0.91	0.15	34,34,34,34	0
56	MG	2A	3321	1/1	0.91	0.22	34,34,34,34	0
56	MG	1A	4039	1/1	0.91	0.84	65,65,65,65	0
56	MG	2G	201	1/1	0.91	0.19	62,62,62,62	0
56	MG	1A	4047	1/1	0.91	0.12	40,40,40,40	0
56	MG	1A	4049	1/1	0.91	0.50	41,41,41,41	0
56	MG	20	101	1/1	0.91	0.21	60,60,60,60	0
56	MG	27	103	1/1	0.91	0.25	53,53,53,53	0
56	MG	2A	3145	1/1	0.91	0.14	71,71,71,71	0
56	MG	2A	3147	1/1	0.91	0.11	49,49,49,49	0
56	MG	1a	1793	1/1	0.91	0.09	60,60,60,60	0
56	MG	2A	3603	1/1	0.91	0.24	61,61,61,61	0
56	MG	2A	3605	1/1	0.91	0.10	50,50,50,50	0
56	MG	1A	3435	1/1	0.91	0.27	46,46,46,46	0
56	MG	1A	4058	1/1	0.91	0.29	60,60,60,60	0
56	MG	1A	3669	1/1	0.91	0.16	57,57,57,57	0
56	MG	1A	3920	1/1	0.91	0.17	52,52,52,52	0
56	MG	1A	3782	1/1	0.91	0.20	50,50,50,50	0
56	MG	2A	3623	1/1	0.91	0.16	64,64,64,64	0
56	MG	1A	3437	1/1	0.91	0.39	43,43,43,43	0
56	MG	1A	4077	1/1	0.91	0.14	37,37,37,37	0
56	MG	1A	3923	1/1	0.91	0.21	59,59,59,59	0
56	MG	1A	3785	1/1	0.91	0.16	34,34,34,34	0
56	MG	1n	101	1/1	0.92	0.31	60,60,60,60	0
56	MG	1A	3200	1/1	0.92	0.55	34,34,34,34	0
56	MG	2E	304	1/1	0.92	0.17	51,51,51,51	0
56	MG	2E	306	1/1	0.92	0.13	40,40,40,40	0
56	MG	1A	4001	1/1	0.92	0.24	40,40,40,40	0
56	MG	1A	3433	1/1	0.92	0.28	51,51,51,51	0
56	MG	1A	3833	1/1	0.92	0.08	24,24,24,24	0
56	MG	1A	3006	1/1	0.92	0.24	38,38,38,38	0
56	MG	2A	3537	1/1	0.92	0.15	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	3252	1/1	0.92	0.17	61,61,61,61	0
56	MG	1A	3521	1/1	0.92	0.15	40,40,40,40	0
56	MG	2N	201	1/1	0.92	0.16	69,69,69,69	0
56	MG	2A	3543	1/1	0.92	0.09	65,65,65,65	0
56	MG	2P	201	1/1	0.92	0.85	51,51,51,51	0
56	MG	2T	202	1/1	0.92	0.20	52,52,52,52	0
56	MG	1A	3018	1/1	0.92	0.20	35,35,35,35	0
56	MG	1A	3841	1/1	0.92	0.13	21,21,21,21	0
56	MG	23	101	1/1	0.92	0.13	42,42,42,42	0
56	MG	1A	3523	1/1	0.92	0.40	54,54,54,54	0
56	MG	1A	3436	1/1	0.92	0.16	31,31,31,31	0
56	MG	2A	3549	1/1	0.92	0.14	49,49,49,49	0
56	MG	1A	3210	1/1	0.92	0.38	28,28,28,28	0
56	MG	2A	3551	1/1	0.92	0.09	61,61,61,61	0
56	MG	1A	3066	1/1	0.92	0.09	18,18,18,18	0
56	MG	2A	3262	1/1	0.92	0.13	60,60,60,60	0
56	MG	1A	3179	1/1	0.92	0.26	50,50,50,50	0
56	MG	1A	3380	1/1	0.92	0.39	51,51,51,51	0
56	MG	1A	3223	1/1	0.92	0.20	46,46,46,46	0
56	MG	1a	1663	1/1	0.92	0.12	46,46,46,46	0
56	MG	2A	3567	1/1	0.92	0.16	42,42,42,42	0
56	MG	1A	3282	1/1	0.92	0.29	48,48,48,48	0
56	MG	1a	1666	1/1	0.92	0.15	69,69,69,69	0
56	MG	1a	1668	1/1	0.92	0.10	71,71,71,71	0
56	MG	2a	3017	1/1	0.92	0.16	76,76,76,76	0
56	MG	2A	3272	1/1	0.92	0.40	54,54,54,54	0
56	MG	2A	3577	1/1	0.92	0.30	54,54,54,54	0
56	MG	1A	3537	1/1	0.92	0.15	36,36,36,36	0
56	MG	2A	3579	1/1	0.92	0.14	36,36,36,36	0
56	MG	1A	4043	1/1	0.92	0.10	66,66,66,66	0
56	MG	1A	3183	1/1	0.92	0.31	43,43,43,43	0
56	MG	1A	3230	1/1	0.92	0.37	60,60,60,60	0
56	MG	2a	3029	1/1	0.92	0.12	87,87,87,87	0
56	MG	2a	3032	1/1	0.92	0.18	60,60,60,60	0
56	MG	2A	3280	1/1	0.92	0.11	55,55,55,55	0
56	MG	1A	4055	1/1	0.92	0.34	53,53,53,53	0
56	MG	1a	1676	1/1	0.92	0.08	52,52,52,52	0
56	MG	1A	3884	1/1	0.92	0.12	35,35,35,35	0
56	MG	2A	3286	1/1	0.92	0.51	67,67,67,67	0
56	MG	2A	3609	1/1	0.92	0.07	66,66,66,66	0
56	MG	1A	3696	1/1	0.92	0.18	55,55,55,55	0
56	MG	2A	3290	1/1	0.92	0.12	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	3452	1/1	0.92	0.29	37,37,37,37	0
56	MG	1a	1688	1/1	0.92	0.11	41,41,41,41	0
56	MG	1A	3056	1/1	0.92	0.10	31,31,31,31	0
56	MG	2A	3625	1/1	0.92	0.18	49,49,49,49	0
56	MG	2A	3631	1/1	0.92	0.13	48,48,48,48	0
56	MG	1a	1690	1/1	0.92	0.63	57,57,57,57	0
56	MG	1A	4064	1/1	0.92	0.36	38,38,38,38	0
56	MG	1A	3335	1/1	0.92	0.16	49,49,49,49	0
56	MG	2A	3302	1/1	0.92	0.21	64,64,64,64	0
56	MG	1A	3388	1/1	0.92	0.81	46,46,46,46	0
56	MG	2A	3642	1/1	0.92	0.39	66,66,66,66	0
56	MG	2A	3644	1/1	0.92	0.13	58,58,58,58	0
56	MG	2A	3646	1/1	0.92	0.20	52,52,52,52	0
56	MG	2a	3062	1/1	0.92	0.36	61,61,61,61	0
56	MG	2a	3063	1/1	0.92	0.10	65,65,65,65	0
56	MG	1A	4076	1/1	0.92	0.17	31,31,31,31	0
56	MG	1a	1699	1/1	0.92	0.14	47,47,47,47	0
56	MG	2A	3309	1/1	0.92	0.14	52,52,52,52	0
56	MG	1A	3462	1/1	0.92	0.15	40,40,40,40	0
56	MG	1A	4078	1/1	0.92	0.15	52,52,52,52	0
56	MG	2a	3071	1/1	0.92	0.10	60,60,60,60	0
56	MG	1A	3718	1/1	0.92	0.13	21,21,21,21	0
56	MG	1A	3121	1/1	0.92	0.52	34,34,34,34	0
56	MG	2A	3659	1/1	0.92	0.12	53,53,53,53	0
56	MG	2a	3081	1/1	0.92	0.12	79,79,79,79	0
56	MG	1A	3338	1/1	0.92	0.83	42,42,42,42	0
56	MG	1A	3556	1/1	0.92	0.14	36,36,36,36	0
56	MG	2A	3668	1/1	0.92	0.47	58,58,58,58	0
56	MG	1A	3291	1/1	0.92	0.14	54,54,54,54	0
56	MG	2A	3673	1/1	0.92	0.16	52,52,52,52	0
56	MG	1A	3906	1/1	0.92	0.10	49,49,49,49	0
56	MG	2a	3090	1/1	0.92	0.09	67,67,67,67	0
56	MG	1A	3909	1/1	0.92	0.12	55,55,55,55	0
56	MG	1A	3344	1/1	0.92	0.22	25,25,25,25	0
56	MG	2A	3324	1/1	0.92	0.15	69,69,69,69	0
56	MG	2A	3325	1/1	0.92	0.11	65,65,65,65	0
56	MG	2a	3102	1/1	0.92	0.13	59,59,59,59	0
56	MG	1A	3912	1/1	0.92	0.32	56,56,56,56	0
56	MG	1A	3562	1/1	0.92	0.58	40,40,40,40	0
56	MG	1A	3292	1/1	0.92	0.19	44,44,44,44	0
56	MG	2a	3109	1/1	0.92	0.17	77,77,77,77	0
56	MG	1A	3564	1/1	0.92	0.25	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	3471	1/1	0.92	0.13	56,56,56,56	0
56	MG	2A	3341	1/1	0.92	0.14	53,53,53,53	0
56	MG	1A	3346	1/1	0.92	0.48	49,49,49,49	0
56	MG	2A	3344	1/1	0.92	0.12	66,66,66,66	0
56	MG	1A	3293	1/1	0.92	0.13	44,44,44,44	0
56	MG	1D	308	1/1	0.92	0.31	32,32,32,32	0
56	MG	2a	3120	1/1	0.92	0.31	60,60,60,60	0
56	MG	2A	3697	1/1	0.92	0.11	59,59,59,59	0
56	MG	1a	1727	1/1	0.92	0.12	59,59,59,59	0
56	MG	2A	3703	1/1	0.92	0.17	50,50,50,50	0
56	MG	1A	3294	1/1	0.92	0.10	42,42,42,42	0
56	MG	2A	3104	1/1	0.92	0.13	67,67,67,67	0
56	MG	1A	3574	1/1	0.92	0.15	30,30,30,30	0
56	MG	1A	3578	1/1	0.92	0.12	12,12,12,12	0
56	MG	1A	3581	1/1	0.92	0.09	50,50,50,50	0
56	MG	2a	3137	1/1	0.92	0.15	55,55,55,55	0
56	MG	1F	307	1/1	0.92	0.55	30,30,30,30	0
56	MG	1A	3410	1/1	0.92	0.34	37,37,37,37	0
56	MG	2A	3114	1/1	0.92	0.12	68,68,68,68	0
56	MG	1A	3927	1/1	0.92	0.26	60,60,60,60	0
56	MG	1N	201	1/1	0.92	0.55	50,50,50,50	0
56	MG	2A	3131	1/1	0.92	0.08	59,59,59,59	0
56	MG	2A	3132	1/1	0.92	0.30	63,63,63,63	0
56	MG	2A	3133	1/1	0.92	0.29	68,68,68,68	0
56	MG	1A	3928	1/1	0.92	0.23	67,67,67,67	0
56	MG	1P	204	1/1	0.92	0.58	31,31,31,31	0
56	MG	2a	3155	1/1	0.92	0.10	93,93,93,93	0
56	MG	2a	3156	1/1	0.92	0.10	78,78,78,78	0
56	MG	1A	3752	1/1	0.92	0.12	29,29,29,29	0
56	MG	1A	3591	1/1	0.92	0.12	31,31,31,31	0
56	MG	1A	3754	1/1	0.92	0.18	48,48,48,48	0
56	MG	2A	3152	1/1	0.92	0.15	40,40,40,40	0
56	MG	2A	3157	1/1	0.92	0.37	65,65,65,65	0
56	MG	2A	3388	1/1	0.92	0.12	53,53,53,53	0
56	MG	2A	3159	1/1	0.92	0.16	51,51,51,51	0
56	MG	2A	3753	1/1	0.92	0.18	63,63,63,63	0
56	MG	1A	3057	1/1	0.92	0.14	57,57,57,57	0
56	MG	1Q	206	1/1	0.92	0.41	42,42,42,42	0
56	MG	1R	203	1/1	0.92	0.23	37,37,37,37	0
56	MG	2A	3166	1/1	0.92	0.12	60,60,60,60	0
56	MG	1R	205	1/1	0.92	0.14	39,39,39,39	0
56	MG	2A	3767	1/1	0.92	0.07	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	3178	1/1	0.92	0.14	53,53,53,53	0
56	MG	2A	3768	1/1	0.92	0.08	65,65,65,65	0
56	MG	2a	3181	1/1	0.92	0.11	68,68,68,68	0
56	MG	2a	3183	1/1	0.92	0.23	76,76,76,76	0
56	MG	1A	3595	1/1	0.92	0.14	40,40,40,40	0
56	MG	1A	3487	1/1	0.92	0.17	54,54,54,54	0
56	MG	2a	3190	1/1	0.92	0.20	67,67,67,67	0
56	MG	2A	3172	1/1	0.92	0.27	65,65,65,65	0
56	MG	1A	3358	1/1	0.92	0.51	47,47,47,47	0
56	MG	1W	207	1/1	0.92	0.25	26,26,26,26	0
56	MG	1A	3415	1/1	0.92	0.18	56,56,56,56	0
56	MG	1A	3954	1/1	0.92	0.20	31,31,31,31	0
56	MG	10	102	1/1	0.92	0.34	39,39,39,39	0
56	MG	2A	3412	1/1	0.92	0.20	53,53,53,53	0
56	MG	1A	3156	1/1	0.92	0.16	30,30,30,30	0
56	MG	2A	3789	1/1	0.92	0.24	53,53,53,53	0
56	MG	10	104	1/1	0.92	0.26	63,63,63,63	0
56	MG	1A	3495	1/1	0.92	0.13	48,48,48,48	0
56	MG	1A	3774	1/1	0.92	0.23	27,27,27,27	0
56	MG	1A	3604	1/1	0.92	0.24	57,57,57,57	0
56	MG	2A	3189	1/1	0.92	0.27	60,60,60,60	0
56	MG	2a	3216	1/1	0.92	0.16	65,65,65,65	0
56	MG	2A	3801	1/1	0.92	0.35	44,44,44,44	0
56	MG	18	102	1/1	0.92	0.38	30,30,30,30	0
56	MG	2A	3426	1/1	0.92	0.40	55,55,55,55	0
56	MG	1A	3969	1/1	0.92	0.15	63,63,63,63	0
56	MG	1A	3164	1/1	0.92	0.33	40,40,40,40	0
56	MG	1A	3610	1/1	0.92	0.10	51,51,51,51	0
56	MG	2A	3812	1/1	0.92	0.12	38,38,38,38	0
56	MG	1A	3363	1/1	0.92	0.17	41,41,41,41	0
56	MG	2A	3201	1/1	0.92	0.57	41,41,41,41	0
56	MG	1A	3193	1/1	0.92	0.17	49,49,49,49	0
56	MG	1a	1611	1/1	0.92	0.38	50,50,50,50	0
56	MG	1a	1796	1/1	0.92	0.10	37,37,37,37	0
56	MG	1A	3504	1/1	0.92	0.17	43,43,43,43	0
56	MG	2A	3832	1/1	0.92	0.20	58,58,58,58	0
56	MG	1A	3979	1/1	0.92	0.24	54,54,54,54	0
56	MG	1A	3422	1/1	0.92	0.20	59,59,59,59	0
56	MG	1A	3088	1/1	0.92	0.13	42,42,42,42	0
56	MG	1A	3791	1/1	0.92	0.33	52,52,52,52	0
56	MG	2A	3839	1/1	0.92	0.42	47,47,47,47	0
56	MG	1A	3140	1/1	0.92	0.24	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	2A	3842	1/1	0.92	0.22	66,66,66,66	0
56	MG	2A	3221	1/1	0.92	0.19	68,68,68,68	0
56	MG	1a	1811	1/1	0.92	0.06	80,80,80,80	0
56	MG	2A	3223	1/1	0.92	0.17	52,52,52,52	0
56	MG	1a	1627	1/1	0.92	0.10	32,32,32,32	0
56	MG	1A	3799	1/1	0.92	0.20	49,49,49,49	0
56	MG	2A	3483	1/1	0.92	0.14	65,65,65,65	0
56	MG	1a	1815	1/1	0.92	0.14	73,73,73,73	0
56	MG	1a	1821	1/1	0.92	0.11	57,57,57,57	0
56	MG	2B	209	1/1	0.92	0.18	67,67,67,67	0
56	MG	2B	210	1/1	0.92	0.22	50,50,50,50	0
56	MG	1A	3512	1/1	0.92	0.24	60,60,60,60	0
56	MG	1A	3810	1/1	0.92	0.12	44,44,44,44	0
56	MG	1A	3814	1/1	0.92	0.36	63,63,63,63	0
56	MG	2y	101	1/1	0.92	0.13	57,57,57,57	0
56	MG	1a	1825	1/1	0.92	0.10	51,51,51,51	0
56	MG	1A	3640	1/1	0.92	0.22	40,40,40,40	0
56	MG	1A	3996	1/1	0.92	0.14	18,18,18,18	0
56	MG	1A	3641	1/1	0.92	0.10	30,30,30,30	0
56	MG	1A	3513	1/1	0.92	0.16	36,36,36,36	0
56	MG	2D	303	1/1	0.92	0.16	30,30,30,30	0
56	MG	2E	301	1/1	0.92	0.09	47,47,47,47	0
56	MG	1N	202	1/1	0.93	0.12	33,33,33,33	0
56	MG	2A	3278	1/1	0.93	0.13	39,39,39,39	0
56	MG	1N	204	1/1	0.93	0.37	50,50,50,50	0
56	MG	2V	202	1/1	0.93	0.14	53,53,53,53	0
56	MG	1A	3714	1/1	0.93	0.13	44,44,44,44	0
56	MG	1A	3576	1/1	0.93	0.10	27,27,27,27	0
56	MG	1A	3577	1/1	0.93	0.16	36,36,36,36	0
56	MG	1P	207	1/1	0.93	0.29	37,37,37,37	0
56	MG	1A	3260	1/1	0.93	0.16	19,19,19,19	0
56	MG	1A	3849	1/1	0.93	0.17	42,42,42,42	0
56	MG	1A	3580	1/1	0.93	0.11	28,28,28,28	0
56	MG	2A	3292	1/1	0.93	0.20	46,46,46,46	0
56	MG	2a	3002	1/1	0.93	0.08	52,52,52,52	0
56	MG	1A	3204	1/1	0.93	0.29	51,51,51,51	0
56	MG	1R	202	1/1	0.93	0.56	45,45,45,45	0
56	MG	2a	3007	1/1	0.93	0.16	67,67,67,67	0
56	MG	2A	3595	1/1	0.93	0.23	47,47,47,47	0
56	MG	2A	3597	1/1	0.93	0.14	71,71,71,71	0
56	MG	2A	3602	1/1	0.93	0.09	69,69,69,69	0
56	MG	1A	3864	1/1	0.93	0.41	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3312	1/1	0.93	0.53	40,40,40,40	0
56	MG	2A	3606	1/1	0.93	0.30	36,36,36,36	0
56	MG	2A	3607	1/1	0.93	0.25	57,57,57,57	0
56	MG	1S	202	1/1	0.93	0.08	44,44,44,44	0
56	MG	1A	3506	1/1	0.93	0.18	32,32,32,32	0
56	MG	2A	3610	1/1	0.93	0.43	53,53,53,53	0
56	MG	2A	3611	1/1	0.93	0.24	66,66,66,66	0
56	MG	2A	3303	1/1	0.93	0.40	58,58,58,58	0
56	MG	1T	201	1/1	0.93	0.07	56,56,56,56	0
56	MG	2A	3080	1/1	0.93	0.36	45,45,45,45	0
56	MG	2A	3621	1/1	0.93	0.14	65,65,65,65	0
56	MG	1V	203	1/1	0.93	0.28	31,31,31,31	0
56	MG	2a	3031	1/1	0.93	0.07	64,64,64,64	0
56	MG	1A	3869	1/1	0.93	0.13	39,39,39,39	0
56	MG	1W	201	1/1	0.93	0.18	35,35,35,35	0
56	MG	2A	3628	1/1	0.93	0.20	61,61,61,61	0
56	MG	1a	1735	1/1	0.93	0.17	42,42,42,42	0
56	MG	1A	3872	1/1	0.93	0.18	31,31,31,31	0
56	MG	2A	3313	1/1	0.93	0.20	55,55,55,55	0
56	MG	2A	3087	1/1	0.93	0.14	42,42,42,42	0
56	MG	2A	3088	1/1	0.93	0.14	36,36,36,36	0
56	MG	1A	3091	1/1	0.93	0.32	44,44,44,44	0
56	MG	1A	3268	1/1	0.93	0.53	62,62,62,62	0
56	MG	1A	3320	1/1	0.93	0.08	41,41,41,41	0
56	MG	1Z	303	1/1	0.93	0.16	48,48,48,48	0
56	MG	1A	3047	1/1	0.93	0.23	31,31,31,31	0
56	MG	1A	3213	1/1	0.93	0.27	41,41,41,41	0
56	MG	1A	3214	1/1	0.93	0.15	42,42,42,42	0
56	MG	1A	3278	1/1	0.93	0.32	42,42,42,42	0
56	MG	2A	3331	1/1	0.93	0.29	56,56,56,56	0
56	MG	11	101	1/1	0.93	0.84	40,40,40,40	0
56	MG	1a	1758	1/1	0.93	0.08	65,65,65,65	0
56	MG	2a	3054	1/1	0.93	0.11	70,70,70,70	0
56	MG	2A	3336	1/1	0.93	0.12	49,49,49,49	0
56	MG	1A	3444	1/1	0.93	0.37	24,24,24,24	0
56	MG	2a	3060	1/1	0.93	0.11	82,82,82,82	0
56	MG	2A	3339	1/1	0.93	0.17	65,65,65,65	0
56	MG	2A	3666	1/1	0.93	0.17	69,69,69,69	0
56	MG	1A	3737	1/1	0.93	0.14	41,41,41,41	0
56	MG	1A	4017	1/1	0.93	0.40	41,41,41,41	0
56	MG	1A	3016	1/1	0.93	0.14	31,31,31,31	0
56	MG	2a	3066	1/1	0.93	0.12	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	2A	3125	1/1	0.93	0.19	44,44,44,44	0
56	MG	2A	3130	1/1	0.93	0.54	47,47,47,47	0
56	MG	1A	3609	1/1	0.93	0.12	39,39,39,39	0
56	MG	1a	1603	1/1	0.93	0.06	49,49,49,49	0
56	MG	2A	3348	1/1	0.93	0.13	58,58,58,58	0
56	MG	2a	3074	1/1	0.93	0.13	68,68,68,68	0
56	MG	1A	3185	1/1	0.93	0.15	34,34,34,34	0
56	MG	2A	3134	1/1	0.93	0.20	56,56,56,56	0
56	MG	1A	3897	1/1	0.93	0.14	55,55,55,55	0
56	MG	1A	3151	1/1	0.93	0.52	41,41,41,41	0
56	MG	1a	1778	1/1	0.93	0.16	67,67,67,67	0
56	MG	2A	3360	1/1	0.93	0.29	43,43,43,43	0
56	MG	2A	3144	1/1	0.93	0.18	47,47,47,47	0
56	MG	1A	3334	1/1	0.93	0.47	40,40,40,40	0
56	MG	1A	3227	1/1	0.93	0.18	44,44,44,44	0
56	MG	2A	3148	1/1	0.93	0.09	45,45,45,45	0
56	MG	2a	3091	1/1	0.93	0.20	59,59,59,59	0
56	MG	2A	3151	1/1	0.93	0.20	77,77,77,77	0
56	MG	1a	1782	1/1	0.93	0.14	57,57,57,57	0
56	MG	2a	3098	1/1	0.93	0.16	73,73,73,73	0
56	MG	1A	3391	1/1	0.93	0.35	45,45,45,45	0
56	MG	1A	3634	1/1	0.93	0.13	23,23,23,23	0
56	MG	1a	1785	1/1	0.93	0.14	68,68,68,68	0
56	MG	2A	3710	1/1	0.93	0.12	68,68,68,68	0
56	MG	1A	3907	1/1	0.93	0.12	22,22,22,22	0
56	MG	1a	1787	1/1	0.93	0.20	45,45,45,45	0
56	MG	2A	3715	1/1	0.93	0.10	53,53,53,53	0
56	MG	1a	1624	1/1	0.93	0.11	56,56,56,56	0
56	MG	1A	4041	1/1	0.93	0.24	52,52,52,52	0
56	MG	2A	3168	1/1	0.93	0.18	49,49,49,49	0
56	MG	2A	3385	1/1	0.93	0.17	53,53,53,53	0
56	MG	2a	3114	1/1	0.93	0.21	78,78,78,78	0
56	MG	1A	3454	1/1	0.93	0.10	45,45,45,45	0
56	MG	2a	3116	1/1	0.93	0.36	79,79,79,79	0
56	MG	1A	4044	1/1	0.93	0.15	55,55,55,55	0
56	MG	2A	3723	1/1	0.93	0.07	39,39,39,39	0
56	MG	2A	3724	1/1	0.93	0.10	72,72,72,72	0
56	MG	2A	3726	1/1	0.93	0.17	57,57,57,57	0
56	MG	1A	3455	1/1	0.93	0.43	31,31,31,31	0
56	MG	2A	3173	1/1	0.93	0.44	54,54,54,54	0
56	MG	1A	4048	1/1	0.93	0.12	46,46,46,46	0
56	MG	2A	3393	1/1	0.93	0.36	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	3286	1/1	0.93	0.12	51,51,51,51	0
56	MG	2A	3396	1/1	0.93	0.12	46,46,46,46	0
56	MG	2A	3740	1/1	0.93	0.12	70,70,70,70	0
56	MG	1A	4050	1/1	0.93	0.18	45,45,45,45	0
56	MG	1a	1634	1/1	0.93	0.08	62,62,62,62	0
56	MG	2a	3140	1/1	0.93	0.15	64,64,64,64	0
56	MG	1a	1637	1/1	0.93	0.12	44,44,44,44	0
56	MG	1a	1639	1/1	0.93	0.09	59,59,59,59	0
56	MG	2a	3144	1/1	0.93	0.16	55,55,55,55	0
56	MG	1A	3767	1/1	0.93	0.16	50,50,50,50	0
56	MG	2A	3750	1/1	0.93	0.23	69,69,69,69	0
56	MG	1A	3229	1/1	0.93	0.14	32,32,32,32	0
56	MG	2a	3149	1/1	0.93	0.07	70,70,70,70	0
56	MG	1a	1805	1/1	0.93	0.13	51,51,51,51	0
56	MG	2A	3755	1/1	0.93	0.12	34,34,34,34	0
56	MG	1a	1807	1/1	0.93	0.08	65,65,65,65	0
56	MG	2A	3409	1/1	0.93	0.12	46,46,46,46	0
56	MG	1A	3460	1/1	0.93	0.12	51,51,51,51	0
56	MG	1a	1810	1/1	0.93	0.20	58,58,58,58	0
56	MG	1A	3539	1/1	0.93	0.12	41,41,41,41	0
56	MG	1A	3776	1/1	0.93	0.15	29,29,29,29	0
56	MG	1A	3339	1/1	0.93	0.18	40,40,40,40	0
56	MG	1A	4066	1/1	0.93	0.17	36,36,36,36	0
56	MG	1a	1816	1/1	0.93	0.08	55,55,55,55	0
56	MG	1a	1820	1/1	0.93	0.09	50,50,50,50	0
56	MG	2A	3422	1/1	0.93	0.63	62,62,62,62	0
56	MG	1A	3542	1/1	0.93	0.17	50,50,50,50	0
56	MG	1A	3395	1/1	0.93	0.58	45,45,45,45	0
56	MG	1A	3396	1/1	0.93	0.15	35,35,35,35	0
56	MG	1A	3662	1/1	0.93	0.11	17,17,17,17	0
56	MG	1A	3078	1/1	0.93	0.17	30,30,30,30	0
56	MG	1A	4079	1/1	0.93	0.25	41,41,41,41	0
56	MG	1A	3060	1/1	0.93	0.36	37,37,37,37	0
56	MG	2A	3434	1/1	0.93	0.09	53,53,53,53	0
56	MG	2A	3215	1/1	0.93	0.25	73,73,73,73	0
56	MG	1A	3098	1/1	0.93	0.15	34,34,34,34	0
56	MG	1f	202	1/1	0.93	0.08	59,59,59,59	0
56	MG	1B	201	1/1	0.93	0.26	58,58,58,58	0
56	MG	2A	3444	1/1	0.93	0.23	57,57,57,57	0
56	MG	1A	3929	1/1	0.93	0.10	50,50,50,50	0
56	MG	1A	3126	1/1	0.93	0.53	42,42,42,42	0
56	MG	1B	212	1/1	0.93	0.30	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	1w	102	1/1	0.93	0.44	62,62,62,62	0
56	MG	2a	3196	1/1	0.93	0.14	49,49,49,49	0
56	MG	2A	3810	1/1	0.93	0.12	27,27,27,27	0
56	MG	2a	3198	1/1	0.93	0.15	78,78,78,78	0
56	MG	2A	3231	1/1	0.93	0.49	62,62,62,62	0
56	MG	2A	3455	1/1	0.93	0.11	59,59,59,59	0
56	MG	2A	3814	1/1	0.93	0.21	51,51,51,51	0
56	MG	1w	103	1/1	0.93	0.08	61,61,61,61	0
56	MG	2a	3204	1/1	0.93	0.16	77,77,77,77	0
56	MG	2A	3465	1/1	0.93	0.25	64,64,64,64	0
56	MG	2A	3468	1/1	0.93	0.07	53,53,53,53	0
56	MG	1w	104	1/1	0.93	0.33	82,82,82,82	0
56	MG	2a	3210	1/1	0.93	0.19	64,64,64,64	0
56	MG	1A	3932	1/1	0.93	0.10	28,28,28,28	0
56	MG	2a	3212	1/1	0.93	0.10	84,84,84,84	0
56	MG	1B	215	1/1	0.93	0.17	58,58,58,58	0
56	MG	2A	3831	1/1	0.93	0.15	53,53,53,53	0
56	MG	1A	3157	1/1	0.93	0.41	33,33,33,33	0
56	MG	2a	3217	1/1	0.93	0.17	75,75,75,75	0
56	MG	1A	3934	1/1	0.93	0.14	23,23,23,23	0
56	MG	1a	1669	1/1	0.93	0.11	46,46,46,46	0
56	MG	2A	3485	1/1	0.93	0.19	53,53,53,53	0
56	MG	1x	106	1/1	0.93	0.12	44,44,44,44	0
56	MG	2A	3241	1/1	0.93	0.37	59,59,59,59	0
56	MG	2a	3228	1/1	0.93	0.08	73,73,73,73	0
56	MG	2A	3242	1/1	0.93	0.11	45,45,45,45	0
56	MG	2A	3243	1/1	0.93	0.14	41,41,41,41	0
56	MG	1A	3671	1/1	0.93	0.17	40,40,40,40	0
56	MG	1A	3475	1/1	0.93	0.13	45,45,45,45	0
56	MG	1A	3295	1/1	0.93	0.22	58,58,58,58	0
56	MG	1A	3812	1/1	0.93	0.13	36,36,36,36	0
56	MG	1A	3477	1/1	0.93	0.24	52,52,52,52	0
56	MG	2B	202	1/1	0.93	0.27	69,69,69,69	0
56	MG	1A	3127	1/1	0.93	0.39	31,31,31,31	0
56	MG	1A	3825	1/1	0.93	0.45	21,21,21,21	0
56	MG	1A	3297	1/1	0.93	0.22	39,39,39,39	0
56	MG	1a	1686	1/1	0.93	0.25	55,55,55,55	0
56	MG	2A	3009	1/1	0.93	0.14	44,44,44,44	0
56	MG	2A	3019	1/1	0.93	0.32	55,55,55,55	0
56	MG	2A	3525	1/1	0.93	0.28	69,69,69,69	0
56	MG	2a	3245	1/1	0.93	0.17	63,63,63,63	0
56	MG	1D	307	1/1	0.93	0.36	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	3417	1/1	0.93	0.27	36,36,36,36	0
56	MG	2A	3024	1/1	0.93	0.15	40,40,40,40	0
56	MG	1A	3099	1/1	0.93	0.59	39,39,39,39	0
56	MG	1A	3966	1/1	0.93	0.16	71,71,71,71	0
56	MG	1E	309	1/1	0.93	0.12	22,22,22,22	0
56	MG	1E	310	1/1	0.93	0.20	18,18,18,18	0
56	MG	1A	3299	1/1	0.93	0.28	40,40,40,40	0
56	MG	2A	3267	1/1	0.93	0.15	53,53,53,53	0
56	MG	2A	3035	1/1	0.93	0.10	50,50,50,50	0
56	MG	1F	304	1/1	0.93	0.13	26,26,26,26	0
56	MG	1A	3102	1/1	0.93	0.13	30,30,30,30	0
56	MG	1A	3251	1/1	0.93	0.15	28,28,28,28	0
56	MG	1A	3836	1/1	0.93	0.14	38,38,38,38	0
56	MG	2F	302	1/1	0.93	0.67	42,42,42,42	0
56	MG	1F	310	1/1	0.93	0.41	36,36,36,36	0
56	MG	1A	3135	1/1	0.93	0.81	30,30,30,30	0
56	MG	2A	3559	1/1	0.93	0.09	54,54,54,54	0
56	MG	2A	3561	1/1	0.93	0.13	39,39,39,39	0
56	MG	2A	3275	1/1	0.93	0.38	66,66,66,66	0
56	MG	1A	3046	1/1	0.93	0.10	38,38,38,38	0
56	MG	2A	3566	1/1	0.93	0.12	42,42,42,42	0
59	ZN	29	501	1/1	0.93	0.08	81,81,81,81	0
56	MG	2B	203	1/1	0.94	0.26	73,73,73,73	0
56	MG	2A	3471	1/1	0.94	0.17	40,40,40,40	0
56	MG	1A	3816	1/1	0.94	0.22	39,39,39,39	0
56	MG	1A	3818	1/1	0.94	0.22	31,31,31,31	0
56	MG	2A	3476	1/1	0.94	0.10	33,33,33,33	0
56	MG	1V	208	1/1	0.94	0.24	30,30,30,30	0
56	MG	2B	211	1/1	0.94	0.23	72,72,72,72	0
56	MG	1A	3980	1/1	0.94	0.20	55,55,55,55	0
56	MG	2A	3481	1/1	0.94	0.23	35,35,35,35	0
56	MG	1W	202	1/1	0.94	0.28	49,49,49,49	0
56	MG	2A	3199	1/1	0.94	0.64	43,43,43,43	0
56	MG	1A	3163	1/1	0.94	0.18	35,35,35,35	0
56	MG	1A	3827	1/1	0.94	0.14	55,55,55,55	0
56	MG	1X	102	1/1	0.94	0.21	33,33,33,33	0
56	MG	2A	3498	1/1	0.94	0.20	51,51,51,51	0
56	MG	1A	3243	1/1	0.94	0.47	33,33,33,33	0
56	MG	2D	304	1/1	0.94	0.45	51,51,51,51	0
56	MG	1A	3985	1/1	0.94	0.10	51,51,51,51	0
56	MG	2A	3209	1/1	0.94	0.25	46,46,46,46	0
56	MG	1Y	203	1/1	0.94	0.12	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	2A	3507	1/1	0.94	0.22	43,43,43,43	0
56	MG	2A	3508	1/1	0.94	0.18	65,65,65,65	0
56	MG	1a	1790	1/1	0.94	0.09	65,65,65,65	0
56	MG	1Z	302	1/1	0.94	0.17	47,47,47,47	0
56	MG	2A	3513	1/1	0.94	0.18	39,39,39,39	0
56	MG	1A	3986	1/1	0.94	0.15	30,30,30,30	0
56	MG	1A	3484	1/1	0.94	0.30	33,33,33,33	0
56	MG	2A	3516	1/1	0.94	0.17	58,58,58,58	0
56	MG	1A	3412	1/1	0.94	0.06	50,50,50,50	0
56	MG	2A	3519	1/1	0.94	0.08	64,64,64,64	0
56	MG	1A	3681	1/1	0.94	0.13	43,43,43,43	0
56	MG	1A	3682	1/1	0.94	0.14	38,38,38,38	0
56	MG	2A	3523	1/1	0.94	0.11	57,57,57,57	0
56	MG	1a	1797	1/1	0.94	0.06	64,64,64,64	0
56	MG	2T	203	1/1	0.94	0.10	39,39,39,39	0
56	MG	1a	1798	1/1	0.94	0.06	50,50,50,50	0
56	MG	1A	3083	1/1	0.94	0.16	44,44,44,44	0
56	MG	11	102	1/1	0.94	0.14	45,45,45,45	0
56	MG	20	102	1/1	0.94	0.09	52,52,52,52	0
56	MG	2A	3229	1/1	0.94	0.21	42,42,42,42	0
56	MG	27	101	1/1	0.94	0.24	41,41,41,41	0
56	MG	2A	3230	1/1	0.94	0.22	52,52,52,52	0
56	MG	11	104	1/1	0.94	0.11	43,43,43,43	0
56	MG	11	106	1/1	0.94	0.15	40,40,40,40	0
56	MG	1A	3351	1/1	0.94	0.57	31,31,31,31	0
56	MG	13	103	1/1	0.94	0.11	44,44,44,44	0
56	MG	1a	1806	1/1	0.94	0.10	59,59,59,59	0
56	MG	1A	3837	1/1	0.94	0.14	35,35,35,35	0
56	MG	15	105	1/1	0.94	0.14	54,54,54,54	0
56	MG	17	105	1/1	0.94	0.35	58,58,58,58	0
56	MG	1A	3691	1/1	0.94	0.27	49,49,49,49	0
56	MG	1A	3839	1/1	0.94	0.14	20,20,20,20	0
56	MG	1A	3692	1/1	0.94	0.23	40,40,40,40	0
56	MG	1a	1814	1/1	0.94	0.11	49,49,49,49	0
56	MG	1A	4000	1/1	0.94	0.21	46,46,46,46	0
56	MG	2A	3560	1/1	0.94	0.13	42,42,42,42	0
56	MG	2A	3245	1/1	0.94	0.43	54,54,54,54	0
56	MG	1A	3247	1/1	0.94	0.16	49,49,49,49	0
56	MG	1a	1605	1/1	0.94	0.09	59,59,59,59	0
56	MG	1A	4002	1/1	0.94	0.07	22,22,22,22	0
56	MG	1a	1607	1/1	0.94	0.21	36,36,36,36	0
56	MG	1A	3843	1/1	0.94	0.12	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1a	1610	1/1	0.94	0.10	59,59,59,59	0
56	MG	1A	3698	1/1	0.94	0.07	41,41,41,41	0
56	MG	1A	3845	1/1	0.94	0.11	38,38,38,38	0
56	MG	1A	3355	1/1	0.94	0.52	30,30,30,30	0
56	MG	1A	4014	1/1	0.94	0.29	61,61,61,61	0
56	MG	2a	3030	1/1	0.94	0.10	46,46,46,46	0
56	MG	1a	1619	1/1	0.94	0.14	47,47,47,47	0
56	MG	1a	1620	1/1	0.94	0.08	68,68,68,68	0
56	MG	1A	3571	1/1	0.94	0.15	24,24,24,24	0
56	MG	2A	3584	1/1	0.94	0.41	47,47,47,47	0
56	MG	1A	3030	1/1	0.94	0.72	30,30,30,30	0
56	MG	1A	3851	1/1	0.94	0.20	55,55,55,55	0
56	MG	1A	3706	1/1	0.94	0.14	26,26,26,26	0
56	MG	2A	3594	1/1	0.94	0.30	37,37,37,37	0
56	MG	1A	4025	1/1	0.94	0.41	32,32,32,32	0
56	MG	1A	4026	1/1	0.94	0.19	48,48,48,48	0
56	MG	2A	3600	1/1	0.94	0.20	55,55,55,55	0
56	MG	1A	3856	1/1	0.94	0.17	31,31,31,31	0
56	MG	1a	1630	1/1	0.94	0.16	56,56,56,56	0
56	MG	1a	1631	1/1	0.94	0.21	42,42,42,42	0
56	MG	1A	3858	1/1	0.94	0.71	29,29,29,29	0
56	MG	1A	3249	1/1	0.94	0.20	32,32,32,32	0
56	MG	1A	3090	1/1	0.94	0.44	42,42,42,42	0
56	MG	1a	1635	1/1	0.94	0.21	51,51,51,51	0
56	MG	2a	3050	1/1	0.94	0.12	69,69,69,69	0
56	MG	1A	3064	1/1	0.94	0.11	45,45,45,45	0
56	MG	2a	3052	1/1	0.94	0.18	48,48,48,48	0
56	MG	1A	4035	1/1	0.94	0.12	32,32,32,32	0
56	MG	2A	3612	1/1	0.94	0.59	52,52,52,52	0
56	MG	2A	3613	1/1	0.94	0.40	66,66,66,66	0
56	MG	1A	3426	1/1	0.94	0.14	52,52,52,52	0
56	MG	2a	3059	1/1	0.94	0.10	65,65,65,65	0
56	MG	1x	112	1/1	0.94	0.15	57,57,57,57	0
56	MG	2A	3619	1/1	0.94	0.13	47,47,47,47	0
56	MG	1A	3427	1/1	0.94	0.55	36,36,36,36	0
56	MG	1A	3583	1/1	0.94	0.13	40,40,40,40	0
56	MG	1A	3586	1/1	0.94	0.17	34,34,34,34	0
56	MG	1A	3254	1/1	0.94	0.56	50,50,50,50	0
56	MG	2A	3624	1/1	0.94	0.12	54,54,54,54	0
56	MG	2A	3005	1/1	0.94	0.08	41,41,41,41	0
56	MG	2A	3626	1/1	0.94	0.09	65,65,65,65	0
56	MG	1A	3590	1/1	0.94	0.11	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	3630	1/1	0.94	0.13	63,63,63,63	0
56	MG	1A	3880	1/1	0.94	0.13	30,30,30,30	0
56	MG	2A	3014	1/1	0.94	0.31	45,45,45,45	0
56	MG	2a	3076	1/1	0.94	0.16	65,65,65,65	0
56	MG	2A	3017	1/1	0.94	0.16	50,50,50,50	0
56	MG	2a	3079	1/1	0.94	0.10	72,72,72,72	0
56	MG	2A	3018	1/1	0.94	0.23	42,42,42,42	0
56	MG	1A	3881	1/1	0.94	0.11	25,25,25,25	0
56	MG	1A	3366	1/1	0.94	0.23	61,61,61,61	0
56	MG	2a	3083	1/1	0.94	0.07	66,66,66,66	0
56	MG	1A	3209	1/1	0.94	0.33	48,48,48,48	0
56	MG	1A	3726	1/1	0.94	0.14	23,23,23,23	0
56	MG	2A	3645	1/1	0.94	0.15	30,30,30,30	0
56	MG	2A	3299	1/1	0.94	0.25	55,55,55,55	0
56	MG	1A	3305	1/1	0.94	0.16	29,29,29,29	0
56	MG	1A	3259	1/1	0.94	0.12	32,32,32,32	0
56	MG	1A	3141	1/1	0.94	0.39	21,21,21,21	0
56	MG	1A	3892	1/1	0.94	0.13	58,58,58,58	0
56	MG	1A	3175	1/1	0.94	0.57	28,28,28,28	0
56	MG	1A	3005	1/1	0.94	0.27	55,55,55,55	0
56	MG	1A	3375	1/1	0.94	0.26	60,60,60,60	0
56	MG	1A	4072	1/1	0.94	0.16	62,62,62,62	0
56	MG	2A	3660	1/1	0.94	0.08	52,52,52,52	0
56	MG	1A	3265	1/1	0.94	0.12	37,37,37,37	0
56	MG	1A	3739	1/1	0.94	0.20	22,22,22,22	0
56	MG	1A	3740	1/1	0.94	0.07	41,41,41,41	0
56	MG	2A	3314	1/1	0.94	0.06	65,65,65,65	0
56	MG	2A	3669	1/1	0.94	0.38	63,63,63,63	0
56	MG	2A	3315	1/1	0.94	0.17	46,46,46,46	0
56	MG	1A	3902	1/1	0.94	0.06	37,37,37,37	0
56	MG	1A	3111	1/1	0.94	0.30	31,31,31,31	0
56	MG	1A	3608	1/1	0.94	0.12	27,27,27,27	0
56	MG	1A	3746	1/1	0.94	0.14	23,23,23,23	0
56	MG	1A	3750	1/1	0.94	0.13	17,17,17,17	0
56	MG	1A	3908	1/1	0.94	0.21	44,44,44,44	0
56	MG	1A	3215	1/1	0.94	0.65	23,23,23,23	0
56	MG	1A	3321	1/1	0.94	0.11	48,48,48,48	0
56	MG	2A	3683	1/1	0.94	0.21	44,44,44,44	0
56	MG	1a	1678	1/1	0.94	0.25	42,42,42,42	0
56	MG	2a	3126	1/1	0.94	0.25	42,42,42,42	0
56	MG	2A	3327	1/1	0.94	0.47	46,46,46,46	0
56	MG	1A	3614	1/1	0.94	0.17	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	2A	3688	1/1	0.94	0.18	66,66,66,66	0
56	MG	1A	3618	1/1	0.94	0.14	38,38,38,38	0
56	MG	1a	1683	1/1	0.94	0.13	59,59,59,59	0
56	MG	1A	3273	1/1	0.94	0.15	41,41,41,41	0
56	MG	2A	3068	1/1	0.94	0.38	65,65,65,65	0
56	MG	1A	3915	1/1	0.94	0.08	45,45,45,45	0
56	MG	2A	3696	1/1	0.94	0.14	58,58,58,58	0
56	MG	1A	3621	1/1	0.94	0.08	21,21,21,21	0
56	MG	2a	3142	1/1	0.94	0.16	65,65,65,65	0
56	MG	2A	3073	1/1	0.94	0.23	57,57,57,57	0
56	MG	2A	3701	1/1	0.94	0.15	63,63,63,63	0
56	MG	1B	224	1/1	0.94	0.26	44,44,44,44	0
56	MG	1A	3623	1/1	0.94	0.09	51,51,51,51	0
56	MG	1a	1691	1/1	0.94	0.45	42,42,42,42	0
56	MG	2A	3079	1/1	0.94	0.26	44,44,44,44	0
56	MG	2A	3711	1/1	0.94	0.18	51,51,51,51	0
56	MG	1A	3758	1/1	0.94	0.10	49,49,49,49	0
56	MG	1A	3382	1/1	0.94	0.53	46,46,46,46	0
56	MG	2A	3714	1/1	0.94	0.10	76,76,76,76	0
56	MG	1B	231	1/1	0.94	0.09	56,56,56,56	0
56	MG	1A	3216	1/1	0.94	0.54	31,31,31,31	0
56	MG	1A	3038	1/1	0.94	0.13	30,30,30,30	0
56	MG	1A	3768	1/1	0.94	0.18	59,59,59,59	0
56	MG	1D	303	1/1	0.94	0.18	23,23,23,23	0
56	MG	1D	304	1/1	0.94	0.22	28,28,28,28	0
56	MG	2A	3089	1/1	0.94	0.18	46,46,46,46	0
56	MG	1A	3222	1/1	0.94	0.17	51,51,51,51	0
56	MG	2A	3091	1/1	0.94	0.12	56,56,56,56	0
56	MG	2A	3096	1/1	0.94	0.12	51,51,51,51	0
56	MG	1A	3326	1/1	0.94	0.16	49,49,49,49	0
56	MG	2A	3728	1/1	0.94	0.14	71,71,71,71	0
56	MG	2A	3098	1/1	0.94	0.10	59,59,59,59	0
56	MG	1a	1706	1/1	0.94	0.17	39,39,39,39	0
56	MG	1A	3328	1/1	0.94	1.12	42,42,42,42	0
56	MG	2a	3173	1/1	0.94	0.06	72,72,72,72	0
56	MG	1A	3184	1/1	0.94	0.17	21,21,21,21	0
56	MG	2a	3177	1/1	0.94	0.08	74,74,74,74	0
56	MG	2A	3737	1/1	0.94	0.32	70,70,70,70	0
56	MG	2a	3179	1/1	0.94	0.16	52,52,52,52	0
56	MG	1D	311	1/1	0.94	0.14	28,28,28,28	0
56	MG	1E	301	1/1	0.94	0.47	29,29,29,29	0
56	MG	1a	1713	1/1	0.94	0.17	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	2a	3184	1/1	0.94	0.17	59,59,59,59	0
56	MG	2a	3185	1/1	0.94	0.09	73,73,73,73	0
56	MG	2A	3377	1/1	0.94	0.19	33,33,33,33	0
56	MG	2a	3188	1/1	0.94	0.26	81,81,81,81	0
56	MG	2A	3110	1/1	0.94	0.10	50,50,50,50	0
56	MG	2A	3381	1/1	0.94	0.31	44,44,44,44	0
56	MG	1a	1714	1/1	0.94	0.19	63,63,63,63	0
56	MG	1E	302	1/1	0.94	0.61	34,34,34,34	0
56	MG	1A	3331	1/1	0.94	0.16	47,47,47,47	0
56	MG	1A	3147	1/1	0.94	0.40	55,55,55,55	0
56	MG	1A	3781	1/1	0.94	0.27	51,51,51,51	0
56	MG	1E	311	1/1	0.94	0.23	50,50,50,50	0
56	MG	1F	302	1/1	0.94	0.33	28,28,28,28	0
56	MG	2A	3759	1/1	0.94	0.12	49,49,49,49	0
56	MG	1A	3148	1/1	0.94	0.17	39,39,39,39	0
56	MG	2a	3202	1/1	0.94	0.10	58,58,58,58	0
56	MG	1A	3114	1/1	0.94	0.19	28,28,28,28	0
56	MG	1A	3076	1/1	0.94	0.22	30,30,30,30	0
56	MG	1A	3936	1/1	0.94	0.29	44,44,44,44	0
56	MG	1A	3937	1/1	0.94	0.16	60,60,60,60	0
56	MG	1A	3938	1/1	0.94	0.13	31,31,31,31	0
56	MG	2A	3401	1/1	0.94	0.12	46,46,46,46	0
56	MG	2A	3773	1/1	0.94	0.11	47,47,47,47	0
56	MG	2A	3139	1/1	0.94	0.38	48,48,48,48	0
56	MG	1A	3120	1/1	0.94	0.50	33,33,33,33	0
56	MG	2A	3141	1/1	0.94	0.20	46,46,46,46	0
56	MG	1G	202	1/1	0.94	0.39	53,53,53,53	0
56	MG	1A	3941	1/1	0.94	0.17	25,25,25,25	0
56	MG	1A	3548	1/1	0.94	0.21	46,46,46,46	0
56	MG	1A	3659	1/1	0.94	0.08	42,42,42,42	0
56	MG	2A	3786	1/1	0.94	0.15	36,36,36,36	0
56	MG	1a	1739	1/1	0.94	0.16	56,56,56,56	0
56	MG	2A	3149	1/1	0.94	0.40	59,59,59,59	0
56	MG	2a	3227	1/1	0.94	0.09	67,67,67,67	0
56	MG	1A	3289	1/1	0.94	0.42	39,39,39,39	0
56	MG	1a	1745	1/1	0.94	0.16	70,70,70,70	0
56	MG	2A	3155	1/1	0.94	0.13	42,42,42,42	0
56	MG	1A	3051	1/1	0.94	0.09	41,41,41,41	0
56	MG	2a	3232	1/1	0.94	0.09	55,55,55,55	0
56	MG	1A	3793	1/1	0.94	0.11	39,39,39,39	0
56	MG	2A	3160	1/1	0.94	0.20	46,46,46,46	0
56	MG	1P	206	1/1	0.94	0.14	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	1A	3079	1/1	0.94	0.60	34,34,34,34	0
56	MG	1A	3803	1/1	0.94	0.07	48,48,48,48	0
56	MG	1a	1754	1/1	0.94	0.13	43,43,43,43	0
56	MG	1A	3554	1/1	0.94	0.16	29,29,29,29	0
56	MG	1A	3806	1/1	0.94	0.25	47,47,47,47	0
56	MG	2A	3429	1/1	0.94	0.39	56,56,56,56	0
56	MG	1A	3967	1/1	0.94	0.06	49,49,49,49	0
56	MG	2A	3815	1/1	0.94	0.12	53,53,53,53	0
56	MG	2A	3818	1/1	0.94	0.30	46,46,46,46	0
56	MG	1R	201	1/1	0.94	0.43	38,38,38,38	0
56	MG	2A	3433	1/1	0.94	0.29	48,48,48,48	0
56	MG	2f	201	1/1	0.94	0.21	66,66,66,66	0
56	MG	1A	3343	1/1	0.94	0.26	30,30,30,30	0
56	MG	2A	3822	1/1	0.94	0.38	61,61,61,61	0
56	MG	1a	1763	1/1	0.94	0.14	76,76,76,76	0
56	MG	2A	3174	1/1	0.94	0.39	55,55,55,55	0
56	MG	1A	3811	1/1	0.94	0.19	50,50,50,50	0
56	MG	2A	3829	1/1	0.94	0.23	67,67,67,67	0
56	MG	2A	3440	1/1	0.94	0.33	56,56,56,56	0
56	MG	2t	201	1/1	0.94	0.07	60,60,60,60	0
56	MG	2A	3176	1/1	0.94	0.14	42,42,42,42	0
56	MG	2A	3443	1/1	0.94	0.28	49,49,49,49	0
56	MG	1a	1766	1/1	0.94	0.12	63,63,63,63	0
56	MG	1a	1767	1/1	0.94	0.11	50,50,50,50	0
56	MG	2A	3179	1/1	0.94	0.46	53,53,53,53	0
56	MG	1A	3010	1/1	0.94	0.23	39,39,39,39	0
56	MG	1S	201	1/1	0.94	0.31	40,40,40,40	0
56	MG	1A	3813	1/1	0.94	0.19	40,40,40,40	0
56	MG	1A	3409	1/1	0.94	0.16	37,37,37,37	0
56	MG	1A	3558	1/1	0.94	0.08	39,39,39,39	0
56	MG	2A	3464	1/1	0.94	0.14	38,38,38,38	0
56	MG	1U	204	1/1	0.94	0.51	39,39,39,39	0
58	A1AIX	2A	3851	43/43	0.94	0.43	43,53,66,72	0
56	MG	2A	3848	1/1	0.94	0.15	40,40,40,40	0
56	MG	1a	1776	1/1	0.94	0.40	74,74,74,74	0
56	MG	1U	206	1/1	0.94	0.37	30,30,30,30	0
56	MG	2A	3390	1/1	0.95	0.29	48,48,48,48	0
56	MG	1A	3349	1/1	0.95	0.12	44,44,44,44	0
56	MG	2A	3650	1/1	0.95	0.23	64,64,64,64	0
56	MG	1A	3646	1/1	0.95	0.10	24,24,24,24	0
56	MG	1A	3877	1/1	0.95	0.09	28,28,28,28	0
56	MG	2A	3195	1/1	0.95	0.34	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	3395	1/1	0.95	0.71	46,46,46,46	0
56	MG	1F	311	1/1	0.95	0.40	42,42,42,42	0
56	MG	1A	3647	1/1	0.95	0.11	18,18,18,18	0
56	MG	1A	3992	1/1	0.95	0.14	22,22,22,22	0
56	MG	1A	3493	1/1	0.95	0.49	36,36,36,36	0
56	MG	1A	3559	1/1	0.95	0.40	36,36,36,36	0
56	MG	1a	1677	1/1	0.95	0.24	51,51,51,51	0
56	MG	1N	203	1/1	0.95	0.22	40,40,40,40	0
56	MG	1x	103	1/1	0.95	0.12	41,41,41,41	0
56	MG	2A	3670	1/1	0.95	0.10	58,58,58,58	0
56	MG	1a	1679	1/1	0.95	0.18	48,48,48,48	0
56	MG	1A	3390	1/1	0.95	0.15	47,47,47,47	0
56	MG	1A	3561	1/1	0.95	0.37	62,62,62,62	0
56	MG	1A	3246	1/1	0.95	0.28	22,22,22,22	0
56	MG	2A	3212	1/1	0.95	0.10	49,49,49,49	0
56	MG	1a	1685	1/1	0.95	0.16	56,56,56,56	0
56	MG	1A	3168	1/1	0.95	0.14	31,31,31,31	0
56	MG	1A	3887	1/1	0.95	0.08	40,40,40,40	0
56	MG	1A	3764	1/1	0.95	0.17	34,34,34,34	0
56	MG	1Q	201	1/1	0.95	0.09	33,33,33,33	0
56	MG	1Q	202	1/1	0.95	0.10	29,29,29,29	0
56	MG	2A	3421	1/1	0.95	0.09	45,45,45,45	0
56	MG	1A	3499	1/1	0.95	0.47	27,27,27,27	0
56	MG	1A	3319	1/1	0.95	0.45	37,37,37,37	0
56	MG	1a	1694	1/1	0.95	0.09	61,61,61,61	0
56	MG	1A	3769	1/1	0.95	0.13	25,25,25,25	0
56	MG	1A	3052	1/1	0.95	0.13	33,33,33,33	0
56	MG	2A	3016	1/1	0.95	0.16	46,46,46,46	0
56	MG	2A	3694	1/1	0.95	0.45	46,46,46,46	0
56	MG	1A	3080	1/1	0.95	0.18	19,19,19,19	0
56	MG	1A	3067	1/1	0.95	0.60	29,29,29,29	0
56	MG	1a	1700	1/1	0.95	0.15	32,32,32,32	0
56	MG	1A	3082	1/1	0.95	0.09	50,50,50,50	0
56	MG	1A	3898	1/1	0.95	0.10	43,43,43,43	0
56	MG	1A	3899	1/1	0.95	0.12	51,51,51,51	0
56	MG	2A	3026	1/1	0.95	0.31	64,64,64,64	0
56	MG	2A	3705	1/1	0.95	0.15	38,38,38,38	0
56	MG	2A	3438	1/1	0.95	0.12	36,36,36,36	0
56	MG	2A	3708	1/1	0.95	0.13	61,61,61,61	0
56	MG	1A	3572	1/1	0.95	0.08	45,45,45,45	0
56	MG	1A	4023	1/1	0.95	0.26	35,35,35,35	0
56	MG	1A	3398	1/1	0.95	0.35	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	2A	3442	1/1	0.95	0.09	46,46,46,46	0
56	MG	1U	202	1/1	0.95	0.53	30,30,30,30	0
56	MG	1a	1708	1/1	0.95	0.16	50,50,50,50	0
56	MG	1U	203	1/1	0.95	0.45	39,39,39,39	0
56	MG	2A	3036	1/1	0.95	0.15	52,52,52,52	0
56	MG	2A	3450	1/1	0.95	0.16	51,51,51,51	0
56	MG	1A	3510	1/1	0.95	0.59	27,27,27,27	0
56	MG	1A	3676	1/1	0.95	0.08	45,45,45,45	0
56	MG	2a	3077	1/1	0.95	0.15	57,57,57,57	0
56	MG	1A	4028	1/1	0.95	0.14	45,45,45,45	0
56	MG	1A	4029	1/1	0.95	0.26	58,58,58,58	0
56	MG	2A	3456	1/1	0.95	0.09	50,50,50,50	0
56	MG	2A	3458	1/1	0.95	0.15	51,51,51,51	0
56	MG	1A	3226	1/1	0.95	0.12	47,47,47,47	0
56	MG	2A	3463	1/1	0.95	0.25	57,57,57,57	0
56	MG	1A	3784	1/1	0.95	0.15	29,29,29,29	0
56	MG	2A	3730	1/1	0.95	0.12	54,54,54,54	0
56	MG	1A	3401	1/1	0.95	0.22	46,46,46,46	0
56	MG	2A	3466	1/1	0.95	0.13	41,41,41,41	0
56	MG	1A	3365	1/1	0.95	0.11	49,49,49,49	0
56	MG	2A	3254	1/1	0.95	0.10	58,58,58,58	0
56	MG	1W	205	1/1	0.95	0.18	35,35,35,35	0
56	MG	1W	206	1/1	0.95	0.12	31,31,31,31	0
56	MG	1A	3101	1/1	0.95	0.35	24,24,24,24	0
56	MG	2A	3742	1/1	0.95	0.14	59,59,59,59	0
56	MG	1A	3518	1/1	0.95	0.15	29,29,29,29	0
56	MG	2A	3477	1/1	0.95	0.09	45,45,45,45	0
56	MG	2a	3101	1/1	0.95	0.09	35,35,35,35	0
56	MG	1X	105	1/1	0.95	0.09	31,31,31,31	0
56	MG	1A	3407	1/1	0.95	0.23	40,40,40,40	0
56	MG	1A	3687	1/1	0.95	0.13	38,38,38,38	0
56	MG	2A	3751	1/1	0.95	0.10	55,55,55,55	0
56	MG	1A	3688	1/1	0.95	0.10	20,20,20,20	0
56	MG	1A	3796	1/1	0.95	0.17	45,45,45,45	0
56	MG	1A	3797	1/1	0.95	0.13	38,38,38,38	0
56	MG	2A	3065	1/1	0.95	0.20	56,56,56,56	0
56	MG	2A	3067	1/1	0.95	0.20	53,53,53,53	0
56	MG	2A	3495	1/1	0.95	0.16	42,42,42,42	0
56	MG	2A	3496	1/1	0.95	0.09	48,48,48,48	0
56	MG	2A	3497	1/1	0.95	0.08	37,37,37,37	0
56	MG	10	101	1/1	0.95	0.12	25,25,25,25	0
56	MG	1A	3798	1/1	0.95	0.26	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3918	1/1	0.95	0.17	65,65,65,65	0
56	MG	2a	3121	1/1	0.95	0.29	49,49,49,49	0
56	MG	2A	3502	1/1	0.95	0.11	40,40,40,40	0
56	MG	2A	3771	1/1	0.95	0.09	33,33,33,33	0
56	MG	1A	3456	1/1	0.95	0.96	33,33,33,33	0
56	MG	2A	3505	1/1	0.95	0.11	43,43,43,43	0
56	MG	2A	3774	1/1	0.95	0.07	33,33,33,33	0
56	MG	2a	3129	1/1	0.95	0.17	51,51,51,51	0
56	MG	2a	3130	1/1	0.95	0.07	60,60,60,60	0
56	MG	1A	3801	1/1	0.95	0.24	29,29,29,29	0
56	MG	2A	3776	1/1	0.95	0.31	65,65,65,65	0
56	MG	2a	3134	1/1	0.95	0.11	50,50,50,50	0
56	MG	10	106	1/1	0.95	0.07	60,60,60,60	0
56	MG	1A	4051	1/1	0.95	0.09	43,43,43,43	0
56	MG	2A	3509	1/1	0.95	0.20	58,58,58,58	0
56	MG	2A	3077	1/1	0.95	0.09	50,50,50,50	0
56	MG	1a	1747	1/1	0.95	0.14	58,58,58,58	0
56	MG	1A	3258	1/1	0.95	0.26	53,53,53,53	0
56	MG	2A	3279	1/1	0.95	0.14	54,54,54,54	0
56	MG	1A	3327	1/1	0.95	0.90	51,51,51,51	0
56	MG	1A	3695	1/1	0.95	0.10	49,49,49,49	0
56	MG	2A	3793	1/1	0.95	0.13	55,55,55,55	0
56	MG	2a	3146	1/1	0.95	0.04	63,63,63,63	0
56	MG	2A	3517	1/1	0.95	0.26	48,48,48,48	0
56	MG	2A	3283	1/1	0.95	0.39	61,61,61,61	0
56	MG	1A	4059	1/1	0.95	0.31	41,41,41,41	0
56	MG	1A	3592	1/1	0.95	0.06	17,17,17,17	0
56	MG	1A	3697	1/1	0.95	0.08	49,49,49,49	0
56	MG	2A	3287	1/1	0.95	0.19	58,58,58,58	0
56	MG	2A	3802	1/1	0.95	0.12	46,46,46,46	0
56	MG	15	101	1/1	0.95	0.26	34,34,34,34	0
56	MG	15	104	1/1	0.95	0.92	49,49,49,49	0
56	MG	1A	3524	1/1	0.95	0.11	39,39,39,39	0
56	MG	2A	3535	1/1	0.95	0.05	62,62,62,62	0
56	MG	17	104	1/1	0.95	0.12	32,32,32,32	0
56	MG	1A	4065	1/1	0.95	0.32	35,35,35,35	0
56	MG	2a	3161	1/1	0.95	0.21	65,65,65,65	0
56	MG	2A	3092	1/1	0.95	0.37	50,50,50,50	0
56	MG	2A	3541	1/1	0.95	0.07	33,33,33,33	0
56	MG	2A	3095	1/1	0.95	0.25	60,60,60,60	0
56	MG	1A	3699	1/1	0.95	0.16	19,19,19,19	0
56	MG	1A	4067	1/1	0.95	0.29	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	19	102	1/1	0.95	0.15	50,50,50,50	0
56	MG	2A	3099	1/1	0.95	0.14	57,57,57,57	0
56	MG	1a	1768	1/1	0.95	0.25	67,67,67,67	0
56	MG	2A	3823	1/1	0.95	0.27	50,50,50,50	0
56	MG	2A	3101	1/1	0.95	0.37	56,56,56,56	0
56	MG	1a	1769	1/1	0.95	0.12	47,47,47,47	0
56	MG	2A	3307	1/1	0.95	0.24	59,59,59,59	0
56	MG	1A	3700	1/1	0.95	0.24	29,29,29,29	0
56	MG	1A	3176	1/1	0.95	0.30	29,29,29,29	0
56	MG	2A	3555	1/1	0.95	0.18	55,55,55,55	0
56	MG	1A	3931	1/1	0.95	0.09	19,19,19,19	0
56	MG	1A	4074	1/1	0.95	0.17	49,49,49,49	0
56	MG	1A	3125	1/1	0.95	0.35	35,35,35,35	0
56	MG	2A	3837	1/1	0.95	0.46	35,35,35,35	0
56	MG	1A	3597	1/1	0.95	0.10	18,18,18,18	0
56	MG	1A	3821	1/1	0.95	0.09	33,33,33,33	0
56	MG	1A	3823	1/1	0.95	0.67	45,45,45,45	0
56	MG	1A	3041	1/1	0.95	0.24	40,40,40,40	0
56	MG	1a	1612	1/1	0.95	0.07	52,52,52,52	0
56	MG	2A	3120	1/1	0.95	0.09	55,55,55,55	0
56	MG	2A	3570	1/1	0.95	0.13	56,56,56,56	0
56	MG	2a	3195	1/1	0.95	0.18	62,62,62,62	0
56	MG	1A	3071	1/1	0.95	0.15	19,19,19,19	0
56	MG	1A	3710	1/1	0.95	0.09	20,20,20,20	0
56	MG	2A	3574	1/1	0.95	0.16	43,43,43,43	0
56	MG	2B	201	1/1	0.95	0.14	60,60,60,60	0
56	MG	2A	3129	1/1	0.95	0.23	62,62,62,62	0
56	MG	1B	203	1/1	0.95	0.30	48,48,48,48	0
56	MG	1A	3600	1/1	0.95	0.12	51,51,51,51	0
56	MG	2B	205	1/1	0.95	0.32	71,71,71,71	0
56	MG	2B	206	1/1	0.95	0.12	70,70,70,70	0
56	MG	2a	3206	1/1	0.95	0.08	56,56,56,56	0
56	MG	1A	3416	1/1	0.95	0.21	36,36,36,36	0
56	MG	1a	1621	1/1	0.95	0.21	47,47,47,47	0
56	MG	2A	3581	1/1	0.95	0.08	34,34,34,34	0
56	MG	1B	207	1/1	0.95	0.31	41,41,41,41	0
56	MG	2A	3583	1/1	0.95	0.14	62,62,62,62	0
56	MG	1A	3942	1/1	0.95	0.18	22,22,22,22	0
56	MG	1A	3264	1/1	0.95	0.12	51,51,51,51	0
56	MG	1A	3947	1/1	0.95	0.09	50,50,50,50	0
56	MG	1A	3535	1/1	0.95	0.08	36,36,36,36	0
56	MG	1A	3949	1/1	0.95	0.17	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3105	1/1	0.95	0.11	36,36,36,36	0
56	MG	1A	3607	1/1	0.95	0.13	39,39,39,39	0
56	MG	2A	3598	1/1	0.95	0.24	56,56,56,56	0
56	MG	2A	3599	1/1	0.95	0.15	73,73,73,73	0
56	MG	1A	3300	1/1	0.95	0.17	50,50,50,50	0
56	MG	2a	3225	1/1	0.95	0.09	57,57,57,57	0
56	MG	1B	228	1/1	0.95	0.16	31,31,31,31	0
56	MG	1A	3955	1/1	0.95	0.18	16,16,16,16	0
56	MG	1A	3961	1/1	0.95	0.16	54,54,54,54	0
56	MG	1A	3074	1/1	0.95	0.12	29,29,29,29	0
56	MG	2E	305	1/1	0.95	0.20	40,40,40,40	0
56	MG	2A	3153	1/1	0.95	0.30	62,62,62,62	0
56	MG	1A	3238	1/1	0.95	0.13	42,42,42,42	0
56	MG	1A	3541	1/1	0.95	0.12	43,43,43,43	0
56	MG	1a	1640	1/1	0.95	0.07	71,71,71,71	0
56	MG	1A	3615	1/1	0.95	0.16	26,26,26,26	0
56	MG	1B	235	1/1	0.95	0.13	61,61,61,61	0
56	MG	1B	238	1/1	0.95	0.32	48,48,48,48	0
56	MG	2A	3615	1/1	0.95	0.75	55,55,55,55	0
56	MG	2A	3356	1/1	0.95	0.24	41,41,41,41	0
56	MG	1A	3239	1/1	0.95	0.63	46,46,46,46	0
56	MG	1A	3424	1/1	0.95	0.12	37,37,37,37	0
56	MG	1D	305	1/1	0.95	0.38	26,26,26,26	0
56	MG	2Q	201	1/1	0.95	0.13	44,44,44,44	0
56	MG	2R	201	1/1	0.95	0.21	58,58,58,58	0
56	MG	2a	3246	1/1	0.95	0.17	70,70,70,70	0
56	MG	2T	201	1/1	0.95	0.15	55,55,55,55	0
56	MG	2e	202	1/1	0.95	0.12	57,57,57,57	0
56	MG	1A	3478	1/1	0.95	0.27	34,34,34,34	0
56	MG	1A	3622	1/1	0.95	0.18	16,16,16,16	0
56	MG	1a	1651	1/1	0.95	0.13	59,59,59,59	0
56	MG	2j	201	1/1	0.95	0.05	81,81,81,81	0
56	MG	2l	201	1/1	0.95	0.96	72,72,72,72	0
56	MG	1A	3240	1/1	0.95	0.47	33,33,33,33	0
56	MG	2Y	201	1/1	0.95	0.23	43,43,43,43	0
56	MG	1A	3972	1/1	0.95	0.08	51,51,51,51	0
56	MG	1A	3973	1/1	0.95	0.26	47,47,47,47	0
56	MG	2q	202	1/1	0.95	0.08	76,76,76,76	0
56	MG	21	101	1/1	0.95	0.89	54,54,54,54	0
56	MG	21	103	1/1	0.95	0.13	61,61,61,61	0
56	MG	1A	3482	1/1	0.95	0.21	50,50,50,50	0
56	MG	23	102	1/1	0.95	0.19	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	25	101	1/1	0.95	0.21	45,45,45,45	0
56	MG	1A	3342	1/1	0.95	0.13	44,44,44,44	0
56	MG	27	102	1/1	0.95	0.33	45,45,45,45	0
56	MG	1A	3631	1/1	0.95	0.14	43,43,43,43	0
56	MG	1E	304	1/1	0.95	0.47	28,28,28,28	0
56	MG	1A	3062	1/1	0.95	0.14	47,47,47,47	0
56	MG	1A	3743	1/1	0.95	0.15	45,45,45,45	0
56	MG	1A	3242	1/1	0.95	0.11	37,37,37,37	0
56	MG	1A	3077	1/1	0.95	0.23	36,36,36,36	0
56	MG	1A	3311	1/1	0.95	0.28	36,36,36,36	0
58	A1AIX	1A	4085	43/43	0.95	0.35	22,41,58,59	0
56	MG	1A	3490	1/1	0.95	0.14	31,31,31,31	0
56	MG	1A	3008	1/1	0.95	0.08	23,23,23,23	0
56	MG	1l	201	1/1	0.95	0.22	61,61,61,61	0
56	MG	2A	3647	1/1	0.95	0.18	56,56,56,56	0
56	MG	2A	3359	1/1	0.96	0.22	49,49,49,49	0
56	MG	16	101	1/1	0.96	0.47	48,48,48,48	0
56	MG	2A	3138	1/1	0.96	0.07	61,61,61,61	0
56	MG	17	101	1/1	0.96	0.20	33,33,33,33	0
56	MG	2A	3629	1/1	0.96	0.21	65,65,65,65	0
56	MG	17	103	1/1	0.96	0.11	37,37,37,37	0
56	MG	28	103	1/1	0.96	0.12	43,43,43,43	0
56	MG	1A	3285	1/1	0.96	0.34	35,35,35,35	0
56	MG	2A	3142	1/1	0.96	0.25	74,74,74,74	0
56	MG	1A	3425	1/1	0.96	0.14	39,39,39,39	0
56	MG	2a	3001	1/1	0.96	0.10	53,53,53,53	0
56	MG	2A	3635	1/1	0.96	0.14	63,63,63,63	0
56	MG	2A	3637	1/1	0.96	0.12	51,51,51,51	0
56	MG	2A	3371	1/1	0.96	0.08	56,56,56,56	0
56	MG	1A	3664	1/1	0.96	0.14	22,22,22,22	0
56	MG	2A	3640	1/1	0.96	0.10	68,68,68,68	0
56	MG	1A	3207	1/1	0.96	0.12	44,44,44,44	0
56	MG	2A	3146	1/1	0.96	0.18	45,45,45,45	0
56	MG	1A	4068	1/1	0.96	0.14	27,27,27,27	0
56	MG	1A	4069	1/1	0.96	0.23	43,43,43,43	0
56	MG	2a	3013	1/1	0.96	0.10	63,63,63,63	0
56	MG	2a	3014	1/1	0.96	0.07	62,62,62,62	0
56	MG	1A	3173	1/1	0.96	0.60	42,42,42,42	0
56	MG	2A	3378	1/1	0.96	0.14	46,46,46,46	0
56	MG	2A	3379	1/1	0.96	0.21	42,42,42,42	0
56	MG	1A	3138	1/1	0.96	0.09	27,27,27,27	0
56	MG	2a	3019	1/1	0.96	0.19	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	1A	3245	1/1	0.96	0.09	35,35,35,35	0
56	MG	1A	3795	1/1	0.96	0.14	42,42,42,42	0
56	MG	2A	3383	1/1	0.96	0.10	46,46,46,46	0
56	MG	2A	3654	1/1	0.96	0.29	50,50,50,50	0
56	MG	1A	3670	1/1	0.96	0.11	56,56,56,56	0
56	MG	1A	3020	1/1	0.96	0.13	35,35,35,35	0
56	MG	2a	3028	1/1	0.96	0.09	79,79,79,79	0
56	MG	2A	3657	1/1	0.96	0.16	53,53,53,53	0
56	MG	2A	3386	1/1	0.96	0.16	47,47,47,47	0
56	MG	1a	1609	1/1	0.96	0.20	55,55,55,55	0
56	MG	1A	3494	1/1	0.96	0.49	40,40,40,40	0
56	MG	1A	3109	1/1	0.96	0.15	22,22,22,22	0
56	MG	1A	4080	1/1	0.96	0.08	56,56,56,56	0
56	MG	2A	3664	1/1	0.96	0.10	36,36,36,36	0
56	MG	1A	3800	1/1	0.96	0.15	12,12,12,12	0
56	MG	1A	3567	1/1	0.96	0.24	38,38,38,38	0
56	MG	1A	3015	1/1	0.96	0.13	47,47,47,47	0
56	MG	1A	3072	1/1	0.96	0.32	32,32,32,32	0
56	MG	1A	3570	1/1	0.96	0.13	48,48,48,48	0
56	MG	1A	3808	1/1	0.96	0.56	34,34,34,34	0
56	MG	1a	1802	1/1	0.96	0.28	64,64,64,64	0
56	MG	1B	206	1/1	0.96	0.12	38,38,38,38	0
56	MG	1A	3182	1/1	0.96	0.13	34,34,34,34	0
56	MG	1A	3500	1/1	0.96	0.31	27,27,27,27	0
56	MG	2A	3679	1/1	0.96	0.08	52,52,52,52	0
56	MG	1A	3573	1/1	0.96	0.14	20,20,20,20	0
56	MG	1A	3501	1/1	0.96	0.16	23,23,23,23	0
56	MG	2A	3405	1/1	0.96	0.15	33,33,33,33	0
56	MG	1B	216	1/1	0.96	0.21	44,44,44,44	0
56	MG	2A	3684	1/1	0.96	0.16	57,57,57,57	0
56	MG	1A	3575	1/1	0.96	0.09	41,41,41,41	0
56	MG	1A	3217	1/1	0.96	0.66	33,33,33,33	0
56	MG	2a	3055	1/1	0.96	0.10	66,66,66,66	0
56	MG	2A	3182	1/1	0.96	0.28	44,44,44,44	0
56	MG	1B	220	1/1	0.96	0.12	27,27,27,27	0
56	MG	2a	3058	1/1	0.96	0.28	73,73,73,73	0
56	MG	1B	221	1/1	0.96	0.11	28,28,28,28	0
56	MG	1A	3946	1/1	0.96	0.09	33,33,33,33	0
56	MG	1A	3093	1/1	0.96	0.11	56,56,56,56	0
56	MG	1A	3505	1/1	0.96	0.66	42,42,42,42	0
56	MG	1a	1819	1/1	0.96	0.27	53,53,53,53	0
56	MG	1B	227	1/1	0.96	0.14	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	3419	1/1	0.96	0.06	44,44,44,44	0
56	MG	2A	3191	1/1	0.96	0.30	39,39,39,39	0
56	MG	1A	3255	1/1	0.96	0.15	30,30,30,30	0
56	MG	2A	3700	1/1	0.96	0.14	57,57,57,57	0
56	MG	2A	3193	1/1	0.96	0.19	47,47,47,47	0
56	MG	2a	3070	1/1	0.96	0.15	59,59,59,59	0
56	MG	2A	3702	1/1	0.96	0.10	58,58,58,58	0
56	MG	1A	3950	1/1	0.96	0.15	53,53,53,53	0
56	MG	1A	3440	1/1	0.96	0.48	50,50,50,50	0
56	MG	1a	1642	1/1	0.96	0.09	43,43,43,43	0
56	MG	1A	3824	1/1	0.96	0.39	29,29,29,29	0
56	MG	1A	3582	1/1	0.96	0.20	28,28,28,28	0
56	MG	1b	301	1/1	0.96	0.03	76,76,76,76	0
56	MG	2A	3200	1/1	0.96	0.15	45,45,45,45	0
56	MG	1A	3826	1/1	0.96	0.41	33,33,33,33	0
56	MG	1A	3957	1/1	0.96	0.11	37,37,37,37	0
56	MG	1f	201	1/1	0.96	0.21	50,50,50,50	0
56	MG	1A	3220	1/1	0.96	0.10	35,35,35,35	0
56	MG	2A	3436	1/1	0.96	0.12	56,56,56,56	0
56	MG	1B	236	1/1	0.96	0.09	35,35,35,35	0
56	MG	2A	3207	1/1	0.96	0.15	52,52,52,52	0
56	MG	2a	3088	1/1	0.96	0.12	50,50,50,50	0
56	MG	1A	3585	1/1	0.96	0.13	43,43,43,43	0
56	MG	1l	202	1/1	0.96	0.10	61,61,61,61	0
56	MG	2A	3721	1/1	0.96	0.15	73,73,73,73	0
56	MG	1D	301	1/1	0.96	0.37	43,43,43,43	0
56	MG	1A	3442	1/1	0.96	0.26	32,32,32,32	0
56	MG	2a	3097	1/1	0.96	0.15	62,62,62,62	0
56	MG	1A	3587	1/1	0.96	0.29	57,57,57,57	0
56	MG	2A	3725	1/1	0.96	0.09	59,59,59,59	0
56	MG	1A	3965	1/1	0.96	0.12	49,49,49,49	0
56	MG	1A	3221	1/1	0.96	0.09	46,46,46,46	0
56	MG	2A	3448	1/1	0.96	0.14	42,42,42,42	0
56	MG	1A	3832	1/1	0.96	0.09	23,23,23,23	0
56	MG	2A	3219	1/1	0.96	0.13	63,63,63,63	0
56	MG	1A	3009	1/1	0.96	0.09	46,46,46,46	0
56	MG	2A	3732	1/1	0.96	0.12	56,56,56,56	0
56	MG	1w	106	1/1	0.96	0.11	64,64,64,64	0
56	MG	1A	3116	1/1	0.96	0.34	42,42,42,42	0
56	MG	1A	3117	1/1	0.96	0.13	54,54,54,54	0
56	MG	1A	3593	1/1	0.96	0.14	19,19,19,19	0
56	MG	1A	3711	1/1	0.96	0.09	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3713	1/1	0.96	0.21	44,44,44,44	0
56	MG	1A	3515	1/1	0.96	0.70	41,41,41,41	0
56	MG	2A	3743	1/1	0.96	0.09	64,64,64,64	0
56	MG	1A	3516	1/1	0.96	0.14	40,40,40,40	0
56	MG	1A	3717	1/1	0.96	0.19	35,35,35,35	0
56	MG	1A	3450	1/1	0.96	0.24	32,32,32,32	0
56	MG	2A	3747	1/1	0.96	0.16	43,43,43,43	0
56	MG	1A	3262	1/1	0.96	0.16	46,46,46,46	0
56	MG	1x	111	1/1	0.96	0.09	45,45,45,45	0
56	MG	1A	3059	1/1	0.96	0.37	35,35,35,35	0
56	MG	1A	3520	1/1	0.96	0.54	35,35,35,35	0
56	MG	1A	3983	1/1	0.96	0.35	58,58,58,58	0
56	MG	2A	3754	1/1	0.96	0.14	46,46,46,46	0
56	MG	2a	3131	1/1	0.96	0.07	49,49,49,49	0
56	MG	1F	306	1/1	0.96	0.38	24,24,24,24	0
56	MG	1A	3350	1/1	0.96	0.34	47,47,47,47	0
56	MG	1A	3850	1/1	0.96	0.10	27,27,27,27	0
56	MG	2A	3479	1/1	0.96	0.13	52,52,52,52	0
56	MG	1F	309	1/1	0.96	0.10	50,50,50,50	0
56	MG	2A	3761	1/1	0.96	0.17	39,39,39,39	0
56	MG	2A	3762	1/1	0.96	0.22	40,40,40,40	0
56	MG	2A	3763	1/1	0.96	0.08	62,62,62,62	0
56	MG	1A	3036	1/1	0.96	0.63	34,34,34,34	0
56	MG	2A	3765	1/1	0.96	0.13	50,50,50,50	0
56	MG	2A	3010	1/1	0.96	0.06	45,45,45,45	0
56	MG	2A	3013	1/1	0.96	0.43	45,45,45,45	0
56	MG	2A	3489	1/1	0.96	0.13	46,46,46,46	0
56	MG	1A	3852	1/1	0.96	0.34	31,31,31,31	0
56	MG	2A	3492	1/1	0.96	0.14	37,37,37,37	0
56	MG	1A	3602	1/1	0.96	0.07	17,17,17,17	0
56	MG	1F	313	1/1	0.96	0.11	41,41,41,41	0
56	MG	1G	201	1/1	0.96	0.22	34,34,34,34	0
56	MG	1A	3352	1/1	0.96	0.57	32,32,32,32	0
56	MG	1G	204	1/1	0.96	0.29	56,56,56,56	0
56	MG	1H	201	1/1	0.96	0.24	32,32,32,32	0
56	MG	2a	3154	1/1	0.96	0.19	75,75,75,75	0
56	MG	1A	3190	1/1	0.96	0.29	26,26,26,26	0
56	MG	1A	3050	1/1	0.96	0.27	55,55,55,55	0
56	MG	1A	3122	1/1	0.96	0.71	46,46,46,46	0
56	MG	2A	3783	1/1	0.96	0.17	40,40,40,40	0
56	MG	1A	3404	1/1	0.96	0.40	54,54,54,54	0
56	MG	1A	3866	1/1	0.96	0.13	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	1693	1/1	0.96	0.14	47,47,47,47	0
56	MG	1P	202	1/1	0.96	0.52	29,29,29,29	0
56	MG	1P	203	1/1	0.96	0.45	23,23,23,23	0
56	MG	2A	3791	1/1	0.96	0.08	52,52,52,52	0
56	MG	2A	3263	1/1	0.96	0.15	55,55,55,55	0
56	MG	2A	3510	1/1	0.96	0.12	46,46,46,46	0
56	MG	1A	3529	1/1	0.96	0.18	46,46,46,46	0
56	MG	1A	3313	1/1	0.96	0.35	28,28,28,28	0
56	MG	1A	3613	1/1	0.96	0.09	37,37,37,37	0
56	MG	1A	3873	1/1	0.96	0.10	33,33,33,33	0
56	MG	1A	3531	1/1	0.96	0.36	52,52,52,52	0
56	MG	1A	3875	1/1	0.96	0.10	53,53,53,53	0
56	MG	2a	3176	1/1	0.96	0.07	65,65,65,65	0
56	MG	2A	3043	1/1	0.96	0.15	34,34,34,34	0
56	MG	1A	3314	1/1	0.96	0.11	51,51,51,51	0
56	MG	1A	4006	1/1	0.96	0.06	35,35,35,35	0
56	MG	1A	4007	1/1	0.96	0.11	12,12,12,12	0
56	MG	1A	3004	1/1	0.96	0.21	24,24,24,24	0
56	MG	1A	3742	1/1	0.96	0.18	33,33,33,33	0
56	MG	1A	4012	1/1	0.96	0.09	26,26,26,26	0
56	MG	1A	3362	1/1	0.96	0.10	36,36,36,36	0
56	MG	2A	3526	1/1	0.96	0.09	24,24,24,24	0
56	MG	2a	3187	1/1	0.96	0.09	70,70,70,70	0
56	MG	2A	3816	1/1	0.96	0.11	45,45,45,45	0
56	MG	2A	3817	1/1	0.96	0.44	55,55,55,55	0
56	MG	2A	3529	1/1	0.96	0.09	48,48,48,48	0
56	MG	1R	204	1/1	0.96	0.16	19,19,19,19	0
56	MG	2A	3533	1/1	0.96	0.06	57,57,57,57	0
56	MG	2A	3534	1/1	0.96	0.35	43,43,43,43	0
56	MG	1A	3467	1/1	0.96	0.18	39,39,39,39	0
56	MG	1A	3063	1/1	0.96	0.08	27,27,27,27	0
56	MG	2A	3281	1/1	0.96	0.13	46,46,46,46	0
56	MG	1A	3538	1/1	0.96	0.21	41,41,41,41	0
56	MG	2A	3062	1/1	0.96	0.17	47,47,47,47	0
56	MG	1A	3747	1/1	0.96	0.13	78,78,78,78	0
56	MG	2A	3830	1/1	0.96	0.09	58,58,58,58	0
56	MG	1A	3364	1/1	0.96	0.22	38,38,38,38	0
56	MG	1T	202	1/1	0.96	0.18	35,35,35,35	0
56	MG	1A	4021	1/1	0.96	0.21	37,37,37,37	0
56	MG	2A	3288	1/1	0.96	0.14	54,54,54,54	0
56	MG	1A	3625	1/1	0.96	0.11	33,33,33,33	0
56	MG	1a	1721	1/1	0.96	0.17	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3071	1/1	0.96	0.12	53,53,53,53	0
56	MG	1A	3626	1/1	0.96	0.10	34,34,34,34	0
56	MG	1A	3890	1/1	0.96	0.05	44,44,44,44	0
56	MG	1V	202	1/1	0.96	0.69	38,38,38,38	0
56	MG	1A	3627	1/1	0.96	0.11	22,22,22,22	0
56	MG	2A	3556	1/1	0.96	0.15	27,27,27,27	0
56	MG	1V	205	1/1	0.96	0.07	35,35,35,35	0
56	MG	2A	3558	1/1	0.96	0.56	59,59,59,59	0
56	MG	2a	3218	1/1	0.96	0.21	77,77,77,77	0
56	MG	1V	206	1/1	0.96	0.34	33,33,33,33	0
56	MG	2A	3849	1/1	0.96	0.09	35,35,35,35	0
56	MG	1A	3470	1/1	0.96	0.38	33,33,33,33	0
56	MG	1a	1730	1/1	0.96	0.14	50,50,50,50	0
56	MG	1a	1731	1/1	0.96	0.11	50,50,50,50	0
56	MG	1A	3893	1/1	0.96	0.10	42,42,42,42	0
56	MG	2A	3565	1/1	0.96	0.11	53,53,53,53	0
56	MG	1A	3630	1/1	0.96	0.10	37,37,37,37	0
56	MG	1A	3318	1/1	0.96	0.12	41,41,41,41	0
56	MG	1A	3235	1/1	0.96	0.18	55,55,55,55	0
56	MG	2A	3086	1/1	0.96	0.17	76,76,76,76	0
56	MG	1a	1737	1/1	0.96	0.13	50,50,50,50	0
56	MG	1A	3474	1/1	0.96	0.25	31,31,31,31	0
56	MG	1A	4034	1/1	0.96	0.18	33,33,33,33	0
56	MG	1a	1740	1/1	0.96	0.06	64,64,64,64	0
56	MG	1A	3039	1/1	0.96	0.26	31,31,31,31	0
56	MG	1a	1742	1/1	0.96	0.13	43,43,43,43	0
56	MG	2A	3093	1/1	0.96	0.22	48,48,48,48	0
56	MG	1a	1743	1/1	0.96	0.08	33,33,33,33	0
56	MG	1A	4036	1/1	0.96	0.20	46,46,46,46	0
56	MG	1X	103	1/1	0.96	0.19	35,35,35,35	0
56	MG	2D	301	1/1	0.96	0.20	54,54,54,54	0
56	MG	1A	3065	1/1	0.96	0.17	26,26,26,26	0
56	MG	1A	3546	1/1	0.96	0.17	39,39,39,39	0
56	MG	1A	3639	1/1	0.96	0.09	56,56,56,56	0
56	MG	2A	3586	1/1	0.96	0.52	47,47,47,47	0
56	MG	2A	3588	1/1	0.96	0.17	52,52,52,52	0
56	MG	2e	201	1/1	0.96	0.07	75,75,75,75	0
56	MG	2A	3590	1/1	0.96	0.09	51,51,51,51	0
56	MG	1A	3370	1/1	0.96	0.11	31,31,31,31	0
56	MG	1A	4042	1/1	0.96	0.08	52,52,52,52	0
56	MG	1A	3281	1/1	0.96	0.19	45,45,45,45	0
56	MG	1A	3479	1/1	0.96	0.12	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	1A	4045	1/1	0.96	0.14	34,34,34,34	0
56	MG	1A	4046	1/1	0.96	0.14	59,59,59,59	0
56	MG	1A	3480	1/1	0.96	0.32	30,30,30,30	0
56	MG	1a	1759	1/1	0.96	0.12	53,53,53,53	0
56	MG	1A	3551	1/1	0.96	0.20	35,35,35,35	0
56	MG	2A	3338	1/1	0.96	0.15	34,34,34,34	0
56	MG	2A	3604	1/1	0.96	0.25	54,54,54,54	0
56	MG	1A	3775	1/1	0.96	0.35	34,34,34,34	0
56	MG	1A	3133	1/1	0.96	0.58	30,30,30,30	0
56	MG	1A	3653	1/1	0.96	0.13	20,20,20,20	0
56	MG	2A	3342	1/1	0.96	0.29	42,42,42,42	0
56	MG	2A	3117	1/1	0.96	0.14	44,44,44,44	0
56	MG	1A	3778	1/1	0.96	0.27	33,33,33,33	0
56	MG	1A	3013	1/1	0.96	0.34	27,27,27,27	0
56	MG	2x	106	1/1	0.96	0.13	70,70,70,70	0
56	MG	1A	3483	1/1	0.96	0.24	56,56,56,56	0
56	MG	2A	3126	1/1	0.96	0.16	44,44,44,44	0
56	MG	2V	201	1/1	0.96	0.39	54,54,54,54	0
56	MG	2A	3128	1/1	0.96	0.23	41,41,41,41	0
56	MG	13	102	1/1	0.96	0.24	38,38,38,38	0
56	MG	1A	3042	1/1	0.96	0.11	35,35,35,35	0
56	MG	1A	4060	1/1	0.96	0.26	29,29,29,29	0
56	MG	1A	3423	1/1	0.96	0.14	73,73,73,73	0
56	MG	2A	3354	1/1	0.96	0.28	39,39,39,39	0
56	MG	1A	4062	1/1	0.96	0.18	50,50,50,50	0
59	ZN	26	501	1/1	0.96	0.15	67,67,67,67	0
56	MG	1A	3661	1/1	0.96	0.09	12,12,12,12	0
56	MG	2A	3181	1/1	0.97	0.11	57,57,57,57	0
56	MG	2A	3400	1/1	0.97	0.17	27,27,27,27	0
56	MG	1A	4005	1/1	0.97	0.14	40,40,40,40	0
56	MG	1A	3357	1/1	0.97	0.12	29,29,29,29	0
56	MG	2a	3004	1/1	0.97	0.14	50,50,50,50	0
56	MG	1A	3234	1/1	0.97	0.13	40,40,40,40	0
56	MG	1m	3001	1/1	0.97	0.18	60,60,60,60	0
56	MG	1A	3087	1/1	0.97	0.17	36,36,36,36	0
56	MG	1A	4009	1/1	0.97	0.11	19,19,19,19	0
56	MG	1A	3650	1/1	0.97	0.10	12,12,12,12	0
56	MG	1w	101	1/1	0.97	0.51	66,66,66,66	0
56	MG	2A	3190	1/1	0.97	0.60	37,37,37,37	0
56	MG	2A	3665	1/1	0.97	0.17	48,48,48,48	0
56	MG	1A	3651	1/1	0.97	0.08	21,21,21,21	0
56	MG	2A	3667	1/1	0.97	0.11	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3885	1/1	0.97	0.09	44,44,44,44	0
56	MG	1A	3760	1/1	0.97	0.16	26,26,26,26	0
56	MG	1A	4015	1/1	0.97	0.08	22,22,22,22	0
56	MG	2A	3671	1/1	0.97	0.19	75,75,75,75	0
56	MG	1A	3652	1/1	0.97	0.10	52,52,52,52	0
56	MG	1A	3026	1/1	0.97	0.20	64,64,64,64	0
56	MG	1A	3765	1/1	0.97	0.08	43,43,43,43	0
56	MG	1A	3766	1/1	0.97	0.11	47,47,47,47	0
56	MG	2A	3676	1/1	0.97	0.15	42,42,42,42	0
56	MG	1A	3112	1/1	0.97	0.30	23,23,23,23	0
56	MG	2a	3025	1/1	0.97	0.53	59,59,59,59	0
56	MG	1A	4022	1/1	0.97	0.06	39,39,39,39	0
56	MG	1x	105	1/1	0.97	0.10	45,45,45,45	0
56	MG	2A	3423	1/1	0.97	0.16	61,61,61,61	0
56	MG	1A	3144	1/1	0.97	0.31	32,32,32,32	0
56	MG	1A	4024	1/1	0.97	0.38	39,39,39,39	0
56	MG	1a	1680	1/1	0.97	0.22	40,40,40,40	0
56	MG	1A	3188	1/1	0.97	0.14	36,36,36,36	0
56	MG	1A	3428	1/1	0.97	0.39	37,37,37,37	0
56	MG	1A	3771	1/1	0.97	0.10	38,38,38,38	0
56	MG	1a	1684	1/1	0.97	0.19	51,51,51,51	0
56	MG	2A	3431	1/1	0.97	0.29	50,50,50,50	0
56	MG	1A	3772	1/1	0.97	0.13	18,18,18,18	0
56	MG	1A	3145	1/1	0.97	1.03	35,35,35,35	0
56	MG	2A	3691	1/1	0.97	0.17	55,55,55,55	0
56	MG	1A	3027	1/1	0.97	0.45	22,22,22,22	0
56	MG	1A	3068	1/1	0.97	0.40	36,36,36,36	0
56	MG	1A	3115	1/1	0.97	0.38	23,23,23,23	0
56	MG	2A	3217	1/1	0.97	0.10	56,56,56,56	0
56	MG	1A	3304	1/1	0.97	0.95	36,36,36,36	0
56	MG	1A	3149	1/1	0.97	0.32	31,31,31,31	0
56	MG	2A	3220	1/1	0.97	0.08	47,47,47,47	0
56	MG	2A	3699	1/1	0.97	0.14	57,57,57,57	0
56	MG	1A	3779	1/1	0.97	0.12	35,35,35,35	0
56	MG	2A	3011	1/1	0.97	0.17	46,46,46,46	0
56	MG	1A	3040	1/1	0.97	0.71	35,35,35,35	0
56	MG	1A	3668	1/1	0.97	0.11	37,37,37,37	0
56	MG	2A	3445	1/1	0.97	0.15	59,59,59,59	0
56	MG	2A	3225	1/1	0.97	0.16	50,50,50,50	0
56	MG	2A	3447	1/1	0.97	0.17	51,51,51,51	0
56	MG	2A	3707	1/1	0.97	0.08	51,51,51,51	0
56	MG	2A	3226	1/1	0.97	0.07	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	1A	3195	1/1	0.97	0.30	35,35,35,35	0
56	MG	1A	3196	1/1	0.97	0.44	27,27,27,27	0
56	MG	1a	1697	1/1	0.97	0.15	48,48,48,48	0
56	MG	1A	4040	1/1	0.97	0.47	47,47,47,47	0
56	MG	1A	3197	1/1	0.97	0.16	44,44,44,44	0
56	MG	1U	201	1/1	0.97	0.35	30,30,30,30	0
56	MG	1A	3511	1/1	0.97	0.20	31,31,31,31	0
56	MG	2A	3457	1/1	0.97	0.15	65,65,65,65	0
56	MG	2A	3025	1/1	0.97	0.56	56,56,56,56	0
56	MG	2A	3459	1/1	0.97	0.27	40,40,40,40	0
56	MG	2A	3460	1/1	0.97	0.33	54,54,54,54	0
56	MG	2A	3461	1/1	0.97	0.10	69,69,69,69	0
56	MG	1A	3376	1/1	0.97	0.07	28,28,28,28	0
56	MG	1A	3787	1/1	0.97	0.09	41,41,41,41	0
56	MG	1U	205	1/1	0.97	0.17	39,39,39,39	0
56	MG	2A	3029	1/1	0.97	0.18	44,44,44,44	0
56	MG	1A	3674	1/1	0.97	0.09	17,17,17,17	0
56	MG	1U	207	1/1	0.97	0.50	28,28,28,28	0
56	MG	2A	3033	1/1	0.97	0.38	43,43,43,43	0
56	MG	2A	3470	1/1	0.97	0.30	58,58,58,58	0
56	MG	1U	208	1/1	0.97	0.77	30,30,30,30	0
56	MG	1V	201	1/1	0.97	0.25	32,32,32,32	0
56	MG	2A	3473	1/1	0.97	0.08	44,44,44,44	0
56	MG	2A	3733	1/1	0.97	0.09	42,42,42,42	0
56	MG	1A	3789	1/1	0.97	0.09	29,29,29,29	0
56	MG	1A	3584	1/1	0.97	0.09	27,27,27,27	0
56	MG	2A	3038	1/1	0.97	0.14	52,52,52,52	0
56	MG	2A	3738	1/1	0.97	0.23	72,72,72,72	0
56	MG	1A	3055	1/1	0.97	0.09	40,40,40,40	0
56	MG	1a	1712	1/1	0.97	0.24	54,54,54,54	0
56	MG	1A	3252	1/1	0.97	0.35	29,29,29,29	0
56	MG	2a	3092	1/1	0.97	0.28	59,59,59,59	0
56	MG	2a	3093	1/1	0.97	0.30	44,44,44,44	0
56	MG	1A	3118	1/1	0.97	0.12	29,29,29,29	0
56	MG	2A	3482	1/1	0.97	0.17	64,64,64,64	0
56	MG	1A	3794	1/1	0.97	0.07	35,35,35,35	0
56	MG	1A	4053	1/1	0.97	0.09	33,33,33,33	0
56	MG	2A	3487	1/1	0.97	0.18	54,54,54,54	0
56	MG	2A	3488	1/1	0.97	0.13	55,55,55,55	0
56	MG	1A	4054	1/1	0.97	0.14	48,48,48,48	0
56	MG	2A	3749	1/1	0.97	0.13	45,45,45,45	0
56	MG	2a	3103	1/1	0.97	0.14	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2a	3104	1/1	0.97	0.11	60,60,60,60	0
56	MG	1A	3154	1/1	0.97	0.21	45,45,45,45	0
56	MG	1A	3589	1/1	0.97	0.06	39,39,39,39	0
56	MG	2a	3107	1/1	0.97	0.09	62,62,62,62	0
56	MG	1A	4057	1/1	0.97	0.17	50,50,50,50	0
56	MG	1A	3014	1/1	0.97	0.31	30,30,30,30	0
56	MG	1A	3685	1/1	0.97	0.23	41,41,41,41	0
56	MG	2A	3260	1/1	0.97	0.19	43,43,43,43	0
56	MG	2A	3756	1/1	0.97	0.16	45,45,45,45	0
56	MG	2A	3053	1/1	0.97	0.09	65,65,65,65	0
56	MG	2A	3055	1/1	0.97	0.09	45,45,45,45	0
56	MG	1A	3686	1/1	0.97	0.13	47,47,47,47	0
56	MG	1X	104	1/1	0.97	0.12	33,33,33,33	0
56	MG	2A	3501	1/1	0.97	0.14	43,43,43,43	0
56	MG	1A	3926	1/1	0.97	0.13	55,55,55,55	0
56	MG	2A	3059	1/1	0.97	0.16	46,46,46,46	0
56	MG	1A	3447	1/1	0.97	0.21	49,49,49,49	0
56	MG	1A	3203	1/1	0.97	0.42	50,50,50,50	0
56	MG	1A	3257	1/1	0.97	0.15	26,26,26,26	0
56	MG	2a	3124	1/1	0.97	0.19	68,68,68,68	0
56	MG	1Z	301	1/1	0.97	0.14	50,50,50,50	0
56	MG	1A	3073	1/1	0.97	0.21	28,28,28,28	0
56	MG	2A	3769	1/1	0.97	0.11	41,41,41,41	0
56	MG	2A	3066	1/1	0.97	0.16	32,32,32,32	0
56	MG	1A	3205	1/1	0.97	0.65	31,31,31,31	0
56	MG	1A	3807	1/1	0.97	0.11	35,35,35,35	0
56	MG	1A	3012	1/1	0.97	0.63	22,22,22,22	0
56	MG	2A	3070	1/1	0.97	0.23	56,56,56,56	0
56	MG	1a	1736	1/1	0.97	0.10	41,41,41,41	0
56	MG	1A	3158	1/1	0.97	0.46	36,36,36,36	0
56	MG	1A	3159	1/1	0.97	0.29	36,36,36,36	0
56	MG	1A	3211	1/1	0.97	0.36	24,24,24,24	0
56	MG	2A	3780	1/1	0.97	0.10	24,24,24,24	0
56	MG	2a	3139	1/1	0.97	0.18	61,61,61,61	0
56	MG	1A	3043	1/1	0.97	0.12	31,31,31,31	0
56	MG	10	107	1/1	0.97	0.17	55,55,55,55	0
56	MG	1A	3123	1/1	0.97	0.38	29,29,29,29	0
56	MG	2A	3522	1/1	0.97	0.08	32,32,32,32	0
56	MG	2A	3078	1/1	0.97	0.31	56,56,56,56	0
56	MG	1A	3459	1/1	0.97	0.14	15,15,15,15	0
56	MG	2A	3787	1/1	0.97	0.23	32,32,32,32	0
56	MG	1A	3267	1/1	0.97	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	11	105	1/1	0.97	0.15	61,61,61,61	0
56	MG	2A	3790	1/1	0.97	0.17	53,53,53,53	0
56	MG	2A	3527	1/1	0.97	0.11	59,59,59,59	0
56	MG	2A	3792	1/1	0.97	0.13	47,47,47,47	0
56	MG	2A	3528	1/1	0.97	0.14	45,45,45,45	0
56	MG	1A	3461	1/1	0.97	0.10	40,40,40,40	0
56	MG	1A	3943	1/1	0.97	0.07	18,18,18,18	0
56	MG	2A	3532	1/1	0.97	0.09	62,62,62,62	0
56	MG	1A	3820	1/1	0.97	0.19	18,18,18,18	0
56	MG	2A	3798	1/1	0.97	0.20	46,46,46,46	0
56	MG	1A	3705	1/1	0.97	0.08	38,38,38,38	0
56	MG	2A	3800	1/1	0.97	0.26	53,53,53,53	0
56	MG	1A	3165	1/1	0.97	0.30	39,39,39,39	0
56	MG	2A	3293	1/1	0.97	0.06	64,64,64,64	0
56	MG	2A	3804	1/1	0.97	0.10	55,55,55,55	0
56	MG	2a	3164	1/1	0.97	0.08	44,44,44,44	0
56	MG	2A	3538	1/1	0.97	0.09	52,52,52,52	0
56	MG	1A	3534	1/1	0.97	0.12	42,42,42,42	0
56	MG	15	103	1/1	0.97	0.66	40,40,40,40	0
56	MG	1A	3269	1/1	0.97	0.14	27,27,27,27	0
56	MG	2A	3542	1/1	0.97	0.16	61,61,61,61	0
56	MG	1A	3270	1/1	0.97	0.12	37,37,37,37	0
56	MG	1A	3124	1/1	0.97	0.08	34,34,34,34	0
56	MG	16	102	1/1	0.97	0.12	46,46,46,46	0
56	MG	2A	3301	1/1	0.97	0.17	39,39,39,39	0
56	MG	2a	3174	1/1	0.97	0.12	55,55,55,55	0
56	MG	1A	3611	1/1	0.97	0.09	33,33,33,33	0
56	MG	2A	3094	1/1	0.97	0.40	51,51,51,51	0
56	MG	1A	3953	1/1	0.97	0.21	24,24,24,24	0
56	MG	1B	208	1/1	0.97	0.18	63,63,63,63	0
56	MG	1a	1765	1/1	0.97	0.22	68,68,68,68	0
56	MG	1B	209	1/1	0.97	0.18	42,42,42,42	0
56	MG	17	106	1/1	0.97	0.16	44,44,44,44	0
56	MG	2a	3182	1/1	0.97	0.18	54,54,54,54	0
56	MG	18	101	1/1	0.97	0.23	32,32,32,32	0
56	MG	1A	3044	1/1	0.97	0.15	25,25,25,25	0
56	MG	1B	213	1/1	0.97	0.24	44,44,44,44	0
56	MG	1A	3716	1/1	0.97	0.14	40,40,40,40	0
56	MG	1A	3956	1/1	0.97	0.09	17,17,17,17	0
56	MG	1A	3170	1/1	0.97	0.10	37,37,37,37	0
56	MG	1A	3960	1/1	0.97	0.18	42,42,42,42	0
56	MG	2A	3107	1/1	0.97	0.21	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	3109	1/1	0.97	0.19	59,59,59,59	0
56	MG	2A	3319	1/1	0.97	0.31	70,70,70,70	0
56	MG	1A	3031	1/1	0.97	0.50	34,34,34,34	0
56	MG	1A	3616	1/1	0.97	0.08	37,37,37,37	0
56	MG	2A	3568	1/1	0.97	0.20	50,50,50,50	0
56	MG	1A	3834	1/1	0.97	0.17	31,31,31,31	0
56	MG	1A	3617	1/1	0.97	0.15	45,45,45,45	0
56	MG	1B	223	1/1	0.97	0.27	48,48,48,48	0
56	MG	1A	3400	1/1	0.97	0.18	26,26,26,26	0
56	MG	2A	3844	1/1	0.97	0.12	53,53,53,53	0
56	MG	2A	3116	1/1	0.97	0.30	36,36,36,36	0
56	MG	1B	225	1/1	0.97	0.18	45,45,45,45	0
56	MG	2A	3329	1/1	0.97	0.08	42,42,42,42	0
56	MG	2A	3330	1/1	0.97	0.14	53,53,53,53	0
56	MG	2A	3118	1/1	0.97	0.43	41,41,41,41	0
56	MG	2A	3119	1/1	0.97	0.25	41,41,41,41	0
56	MG	2A	3333	1/1	0.97	0.10	57,57,57,57	0
56	MG	2A	3334	1/1	0.97	0.08	52,52,52,52	0
56	MG	1A	3619	1/1	0.97	0.10	36,36,36,36	0
56	MG	2A	3121	1/1	0.97	0.12	39,39,39,39	0
56	MG	1a	1613	1/1	0.97	0.12	55,55,55,55	0
56	MG	2A	3123	1/1	0.97	0.19	38,38,38,38	0
56	MG	1A	3276	1/1	0.97	0.42	52,52,52,52	0
56	MG	1A	3472	1/1	0.97	0.32	32,32,32,32	0
56	MG	1a	1616	1/1	0.97	0.08	66,66,66,66	0
56	MG	2A	3592	1/1	0.97	0.70	39,39,39,39	0
56	MG	1A	3277	1/1	0.97	0.18	45,45,45,45	0
56	MG	1a	1618	1/1	0.97	0.29	49,49,49,49	0
56	MG	1A	3219	1/1	0.97	0.10	37,37,37,37	0
56	MG	2A	3596	1/1	0.97	0.09	55,55,55,55	0
56	MG	1A	3011	1/1	0.97	0.11	30,30,30,30	0
56	MG	1A	3729	1/1	0.97	0.10	27,27,27,27	0
56	MG	2B	217	1/1	0.97	0.07	63,63,63,63	0
56	MG	1A	3730	1/1	0.97	0.18	14,14,14,14	0
56	MG	1a	1623	1/1	0.97	0.09	58,58,58,58	0
56	MG	2A	3137	1/1	0.97	0.11	57,57,57,57	0
56	MG	1A	3974	1/1	0.97	0.08	38,38,38,38	0
56	MG	2A	3351	1/1	0.97	0.16	50,50,50,50	0
56	MG	1A	3846	1/1	0.97	0.20	32,32,32,32	0
56	MG	2D	305	1/1	0.97	0.62	57,57,57,57	0
56	MG	1A	3130	1/1	0.97	0.15	40,40,40,40	0
56	MG	1A	3408	1/1	0.97	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	1A	3103	1/1	0.97	0.40	26,26,26,26	0
56	MG	1D	302	1/1	0.97	0.12	30,30,30,30	0
56	MG	1A	3033	1/1	0.97	0.14	30,30,30,30	0
56	MG	1A	3034	1/1	0.97	0.28	19,19,19,19	0
56	MG	1A	3035	1/1	0.97	0.59	34,34,34,34	0
56	MG	1A	3738	1/1	0.97	0.14	34,34,34,34	0
56	MG	1A	3413	1/1	0.97	0.17	35,35,35,35	0
56	MG	1A	3857	1/1	0.97	0.19	40,40,40,40	0
56	MG	2A	3368	1/1	0.97	0.27	42,42,42,42	0
56	MG	2A	3150	1/1	0.97	0.09	39,39,39,39	0
56	MG	2F	306	1/1	0.97	0.28	42,42,42,42	0
56	MG	1a	1636	1/1	0.97	0.19	44,44,44,44	0
56	MG	1A	3178	1/1	0.97	0.12	39,39,39,39	0
56	MG	1a	1638	1/1	0.97	0.13	53,53,53,53	0
56	MG	2A	3154	1/1	0.97	0.08	45,45,45,45	0
56	MG	1A	3859	1/1	0.97	0.68	22,22,22,22	0
56	MG	2A	3156	1/1	0.97	0.21	40,40,40,40	0
56	MG	1A	3741	1/1	0.97	0.19	41,41,41,41	0
56	MG	1A	3228	1/1	0.97	0.58	52,52,52,52	0
56	MG	1A	3021	1/1	0.97	0.14	17,17,17,17	0
56	MG	2A	3161	1/1	0.97	0.14	55,55,55,55	0
56	MG	2A	3162	1/1	0.97	0.12	42,42,42,42	0
56	MG	2U	201	1/1	0.97	0.08	63,63,63,63	0
56	MG	1A	3180	1/1	0.97	0.07	26,26,26,26	0
56	MG	1E	305	1/1	0.97	0.35	35,35,35,35	0
56	MG	2X	102	1/1	0.97	0.26	53,53,53,53	0
56	MG	1a	1817	1/1	0.97	0.13	40,40,40,40	0
56	MG	2Z	301	1/1	0.97	0.23	54,54,54,54	0
56	MG	2x	102	1/1	0.97	0.30	59,59,59,59	0
56	MG	1a	1818	1/1	0.97	0.13	60,60,60,60	0
56	MG	1E	308	1/1	0.97	0.09	55,55,55,55	0
56	MG	2x	105	1/1	0.97	0.45	66,66,66,66	0
56	MG	1A	3181	1/1	0.97	0.14	29,29,29,29	0
56	MG	1A	3139	1/1	0.97	0.08	43,43,43,43	0
56	MG	1A	3995	1/1	0.97	0.09	43,43,43,43	0
56	MG	1E	312	1/1	0.97	0.50	45,45,45,45	0
56	MG	1A	3870	1/1	0.97	0.10	46,46,46,46	0
56	MG	1A	3871	1/1	0.97	0.05	44,44,44,44	0
56	MG	1A	3489	1/1	0.97	0.61	29,29,29,29	0
56	MG	1A	3642	1/1	0.97	0.12	18,18,18,18	0
56	MG	27	104	1/1	0.97	0.14	60,60,60,60	0
56	MG	1A	3643	1/1	0.97	0.09	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3644	1/1	0.97	0.13	20,20,20,20	0
56	MG	1A	3645	1/1	0.97	0.27	38,38,38,38	0
56	MG	1A	3084	1/1	0.97	0.14	32,32,32,32	0
56	MG	1A	3693	1/1	0.98	0.08	55,55,55,55	0
56	MG	1A	3903	1/1	0.98	0.09	43,43,43,43	0
56	MG	2A	3365	1/1	0.98	0.14	36,36,36,36	0
56	MG	1A	3694	1/1	0.98	0.08	38,38,38,38	0
56	MG	1A	3330	1/1	0.98	0.10	38,38,38,38	0
56	MG	18	103	1/1	0.98	0.15	30,30,30,30	0
56	MG	1A	3075	1/1	0.98	0.36	25,25,25,25	0
56	MG	1A	3369	1/1	0.98	0.59	37,37,37,37	0
56	MG	1A	3763	1/1	0.98	0.42	22,22,22,22	0
56	MG	1a	1602	1/1	0.98	0.12	45,45,45,45	0
56	MG	1A	3108	1/1	0.98	0.19	28,28,28,28	0
56	MG	1A	3987	1/1	0.98	0.20	28,28,28,28	0
56	MG	1A	3910	1/1	0.98	0.16	44,44,44,44	0
56	MG	1A	4070	1/1	0.98	0.08	42,42,42,42	0
56	MG	1A	3271	1/1	0.98	0.14	43,43,43,43	0
56	MG	1A	3198	1/1	0.98	0.20	38,38,38,38	0
56	MG	1N	205	1/1	0.98	0.13	33,33,33,33	0
56	MG	2A	3531	1/1	0.98	0.08	44,44,44,44	0
56	MG	2A	3239	1/1	0.98	0.20	37,37,37,37	0
56	MG	2a	3119	1/1	0.98	0.17	52,52,52,52	0
56	MG	1a	1719	1/1	0.98	0.13	47,47,47,47	0
56	MG	1O	201	1/1	0.98	0.33	46,46,46,46	0
56	MG	2B	219	1/1	0.98	0.13	67,67,67,67	0
56	MG	1A	3701	1/1	0.98	0.10	42,42,42,42	0
56	MG	2A	3536	1/1	0.98	0.44	59,59,59,59	0
56	MG	2a	3125	1/1	0.98	0.28	48,48,48,48	0
56	MG	2A	3108	1/1	0.98	0.28	67,67,67,67	0
56	MG	1O	203	1/1	0.98	0.06	60,60,60,60	0
56	MG	1P	201	1/1	0.98	0.21	28,28,28,28	0
56	MG	1A	3007	1/1	0.98	0.07	21,21,21,21	0
56	MG	1a	1725	1/1	0.98	0.09	44,44,44,44	0
56	MG	1A	4075	1/1	0.98	0.19	34,34,34,34	0
56	MG	1A	3336	1/1	0.98	0.14	41,41,41,41	0
56	MG	2A	3709	1/1	0.98	0.09	60,60,60,60	0
56	MG	1A	3085	1/1	0.98	0.12	16,16,16,16	0
56	MG	2A	3545	1/1	0.98	0.36	62,62,62,62	0
56	MG	1A	3502	1/1	0.98	0.34	31,31,31,31	0
56	MG	1A	3842	1/1	0.98	0.16	24,24,24,24	0
56	MG	1A	3224	1/1	0.98	0.42	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	1A	3086	1/1	0.98	0.17	38,38,38,38	0
56	MG	1A	3709	1/1	0.98	0.15	29,29,29,29	0
56	MG	1A	3340	1/1	0.98	0.14	33,33,33,33	0
56	MG	1B	202	1/1	0.98	0.22	45,45,45,45	0
56	MG	1A	3250	1/1	0.98	0.31	25,25,25,25	0
56	MG	2A	3124	1/1	0.98	0.13	43,43,43,43	0
56	MG	1A	3712	1/1	0.98	0.09	52,52,52,52	0
56	MG	1A	4003	1/1	0.98	0.10	42,42,42,42	0
56	MG	2A	3127	1/1	0.98	0.30	36,36,36,36	0
56	MG	1A	3160	1/1	0.98	0.10	33,33,33,33	0
56	MG	1A	3553	1/1	0.98	0.12	32,32,32,32	0
56	MG	1y	101	1/1	0.98	0.68	62,62,62,62	0
56	MG	1A	3309	1/1	0.98	0.12	29,29,29,29	0
56	MG	1A	3161	1/1	0.98	0.14	19,19,19,19	0
56	MG	1B	210	1/1	0.98	0.34	42,42,42,42	0
56	MG	1a	1744	1/1	0.98	0.14	36,36,36,36	0
56	MG	2A	3413	1/1	0.98	0.09	35,35,35,35	0
56	MG	1B	211	1/1	0.98	0.14	34,34,34,34	0
56	MG	2X	101	1/1	0.98	0.10	62,62,62,62	0
56	MG	2A	3415	1/1	0.98	0.12	49,49,49,49	0
56	MG	2A	3136	1/1	0.98	0.16	40,40,40,40	0
56	MG	2A	3006	1/1	0.98	0.08	47,47,47,47	0
56	MG	2A	3736	1/1	0.98	0.13	60,60,60,60	0
56	MG	2a	3162	1/1	0.98	0.15	44,44,44,44	0
56	MG	1A	3853	1/1	0.98	0.16	65,65,65,65	0
56	MG	2A	3572	1/1	0.98	0.09	54,54,54,54	0
56	MG	21	102	1/1	0.98	0.10	44,44,44,44	0
56	MG	2A	3008	1/1	0.98	0.30	58,58,58,58	0
56	MG	1A	3654	1/1	0.98	0.12	30,30,30,30	0
56	MG	2A	3575	1/1	0.98	0.15	51,51,51,51	0
56	MG	1A	4010	1/1	0.98	0.08	28,28,28,28	0
56	MG	25	102	1/1	0.98	0.33	61,61,61,61	0
56	MG	1A	3655	1/1	0.98	0.13	30,30,30,30	0
56	MG	1A	3280	1/1	0.98	0.27	31,31,31,31	0
56	MG	1a	1752	1/1	0.98	0.12	47,47,47,47	0
56	MG	1A	3466	1/1	0.98	0.06	48,48,48,48	0
56	MG	1B	218	1/1	0.98	0.18	33,33,33,33	0
56	MG	1A	3605	1/1	0.98	0.18	31,31,31,31	0
56	MG	1A	3860	1/1	0.98	0.18	26,26,26,26	0
56	MG	2A	3020	1/1	0.98	0.12	41,41,41,41	0
56	MG	2A	3021	1/1	0.98	0.23	43,43,43,43	0
56	MG	1A	3162	1/1	0.98	0.12	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	2A	3587	1/1	0.98	0.13	41,41,41,41	0
56	MG	1a	1644	1/1	0.98	0.20	56,56,56,56	0
56	MG	2a	3003	1/1	0.98	0.15	56,56,56,56	0
56	MG	2A	3589	1/1	0.98	0.43	53,53,53,53	0
56	MG	1A	3660	1/1	0.98	0.19	21,21,21,21	0
56	MG	1a	1761	1/1	0.98	0.15	41,41,41,41	0
56	MG	1A	3347	1/1	0.98	0.22	37,37,37,37	0
56	MG	1A	3939	1/1	0.98	0.18	35,35,35,35	0
56	MG	1V	204	1/1	0.98	0.47	28,28,28,28	0
56	MG	2A	3158	1/1	0.98	0.31	30,30,30,30	0
56	MG	2A	3294	1/1	0.98	0.09	54,54,54,54	0
56	MG	2a	3192	1/1	0.98	0.06	57,57,57,57	0
56	MG	1A	4020	1/1	0.98	0.06	39,39,39,39	0
56	MG	2A	3030	1/1	0.98	0.11	42,42,42,42	0
56	MG	1A	3069	1/1	0.98	0.08	23,23,23,23	0
56	MG	1A	3206	1/1	0.98	0.11	33,33,33,33	0
56	MG	2A	3601	1/1	0.98	0.24	54,54,54,54	0
56	MG	1A	3868	1/1	0.98	0.32	37,37,37,37	0
56	MG	1A	3100	1/1	0.98	0.66	32,32,32,32	0
56	MG	1A	3728	1/1	0.98	0.07	59,59,59,59	0
56	MG	1A	3945	1/1	0.98	0.14	12,12,12,12	0
56	MG	1W	204	1/1	0.98	0.27	26,26,26,26	0
56	MG	2A	3304	1/1	0.98	0.19	39,39,39,39	0
56	MG	1A	3045	1/1	0.98	0.12	22,22,22,22	0
56	MG	2a	3205	1/1	0.98	0.09	62,62,62,62	0
56	MG	2A	3451	1/1	0.98	0.17	47,47,47,47	0
56	MG	2A	3169	1/1	0.98	0.16	71,71,71,71	0
56	MG	2a	3026	1/1	0.98	0.13	51,51,51,51	0
56	MG	1A	3612	1/1	0.98	0.12	31,31,31,31	0
56	MG	2A	3778	1/1	0.98	0.15	58,58,58,58	0
56	MG	1A	3317	1/1	0.98	0.25	50,50,50,50	0
56	MG	1X	101	1/1	0.98	0.17	29,29,29,29	0
56	MG	1A	3431	1/1	0.98	0.20	46,46,46,46	0
56	MG	1A	3353	1/1	0.98	1.09	42,42,42,42	0
56	MG	2a	3215	1/1	0.98	0.06	66,66,66,66	0
56	MG	1B	237	1/1	0.98	0.13	31,31,31,31	0
56	MG	1a	1780	1/1	0.98	0.07	56,56,56,56	0
56	MG	2a	3035	1/1	0.98	0.19	75,75,75,75	0
56	MG	2a	3219	1/1	0.98	0.15	63,63,63,63	0
56	MG	1a	1664	1/1	0.98	0.13	43,43,43,43	0
56	MG	1A	3167	1/1	0.98	0.23	53,53,53,53	0
56	MG	2A	3048	1/1	0.98	0.14	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	3735	1/1	0.98	0.12	20,20,20,20	0
56	MG	1a	1667	1/1	0.98	0.10	55,55,55,55	0
56	MG	2A	3051	1/1	0.98	0.17	38,38,38,38	0
56	MG	2a	3226	1/1	0.98	0.17	46,46,46,46	0
56	MG	1A	3287	1/1	0.98	0.21	33,33,33,33	0
56	MG	2A	3467	1/1	0.98	0.11	66,66,66,66	0
56	MG	1A	3128	1/1	0.98	0.16	24,24,24,24	0
56	MG	2A	3054	1/1	0.98	0.24	43,43,43,43	0
56	MG	1A	3129	1/1	0.98	0.13	16,16,16,16	0
56	MG	2A	3632	1/1	0.98	0.10	57,57,57,57	0
56	MG	1A	3236	1/1	0.98	0.17	59,59,59,59	0
56	MG	1A	3883	1/1	0.98	0.19	44,44,44,44	0
56	MG	2A	3326	1/1	0.98	0.12	50,50,50,50	0
56	MG	2A	3636	1/1	0.98	0.10	48,48,48,48	0
56	MG	1A	3958	1/1	0.98	0.08	27,27,27,27	0
56	MG	2A	3475	1/1	0.98	0.14	44,44,44,44	0
56	MG	2A	3803	1/1	0.98	0.19	52,52,52,52	0
56	MG	1A	3526	1/1	0.98	0.09	37,37,37,37	0
56	MG	1D	309	1/1	0.98	0.37	14,14,14,14	0
56	MG	2A	3061	1/1	0.98	0.35	46,46,46,46	0
56	MG	2A	3807	1/1	0.98	0.37	50,50,50,50	0
56	MG	1A	3089	1/1	0.98	0.16	23,23,23,23	0
56	MG	1A	3360	1/1	0.98	0.21	48,48,48,48	0
56	MG	1A	3003	1/1	0.98	0.25	28,28,28,28	0
56	MG	1A	3019	1/1	0.98	0.19	17,17,17,17	0
56	MG	1A	3037	1/1	0.98	0.36	47,47,47,47	0
56	MG	2A	3813	1/1	0.98	0.05	63,63,63,63	0
56	MG	2A	3484	1/1	0.98	0.11	37,37,37,37	0
56	MG	1A	3443	1/1	0.98	0.11	53,53,53,53	0
56	MG	2A	3486	1/1	0.98	0.09	41,41,41,41	0
56	MG	11	103	1/1	0.98	0.11	33,33,33,33	0
56	MG	1A	3628	1/1	0.98	0.11	14,14,14,14	0
56	MG	1E	306	1/1	0.98	0.20	37,37,37,37	0
56	MG	1E	307	1/1	0.98	0.14	34,34,34,34	0
56	MG	2A	3491	1/1	0.98	0.20	38,38,38,38	0
56	MG	2A	3203	1/1	0.98	0.35	47,47,47,47	0
56	MG	2a	3075	1/1	0.98	0.13	57,57,57,57	0
56	MG	1A	3748	1/1	0.98	0.13	39,39,39,39	0
56	MG	13	101	1/1	0.98	0.24	32,32,32,32	0
56	MG	1A	3817	1/1	0.98	0.05	29,29,29,29	0
56	MG	2A	3827	1/1	0.98	0.13	60,60,60,60	0
56	MG	1A	3749	1/1	0.98	0.13	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3208	1/1	0.98	0.29	40,40,40,40	0
56	MG	2x	101	1/1	0.98	0.17	65,65,65,65	0
56	MG	2A	3663	1/1	0.98	0.28	59,59,59,59	0
56	MG	13	104	1/1	0.98	0.12	30,30,30,30	0
56	MG	1A	3402	1/1	0.98	0.31	51,51,51,51	0
56	MG	1a	1809	1/1	0.98	0.21	48,48,48,48	0
56	MG	2A	3834	1/1	0.98	0.06	49,49,49,49	0
56	MG	1A	4052	1/1	0.98	0.08	36,36,36,36	0
56	MG	15	102	1/1	0.98	0.53	35,35,35,35	0
56	MG	1F	301	1/1	0.98	0.41	28,28,28,28	0
56	MG	1A	3266	1/1	0.98	0.23	26,26,26,26	0
56	MG	1A	3029	1/1	0.98	0.33	24,24,24,24	0
56	MG	1A	3689	1/1	0.98	0.11	13,13,13,13	0
56	MG	1A	3975	1/1	0.98	0.08	17,17,17,17	0
56	MG	2A	3357	1/1	0.98	0.13	49,49,49,49	0
56	MG	2A	3358	1/1	0.98	0.20	57,57,57,57	0
59	ZN	1n	103	1/1	0.98	0.15	60,60,60,60	0
56	MG	1A	3137	1/1	0.98	0.21	25,25,25,25	0
56	MG	1A	3633	1/1	0.98	0.27	18,18,18,18	0
56	MG	1A	3448	1/1	0.98	0.24	51,51,51,51	0
59	ZN	2n	501	1/1	0.98	0.05	98,98,98,98	0
56	MG	1A	3802	1/1	0.99	0.09	57,57,57,57	0
56	MG	2A	3361	1/1	0.99	0.15	48,48,48,48	0
56	MG	1A	3822	1/1	0.99	0.37	36,36,36,36	0
56	MG	1A	3675	1/1	0.99	0.09	27,27,27,27	0
56	MG	2a	3094	1/1	0.99	0.15	69,69,69,69	0
56	MG	1A	3097	1/1	0.99	0.14	32,32,32,32	0
56	MG	2A	3216	1/1	0.99	0.07	66,66,66,66	0
56	MG	2A	3564	1/1	0.99	0.18	37,37,37,37	0
56	MG	2A	3366	1/1	0.99	0.17	32,32,32,32	0
56	MG	1A	3805	1/1	0.99	0.11	31,31,31,31	0
56	MG	1A	3636	1/1	0.99	0.14	20,20,20,20	0
56	MG	1A	3136	1/1	0.99	0.21	29,29,29,29	0
56	MG	1A	3405	1/1	0.99	0.49	40,40,40,40	0
56	MG	1a	1760	1/1	0.99	0.11	36,36,36,36	0
56	MG	1A	3809	1/1	0.99	0.09	34,34,34,34	0
56	MG	1A	3762	1/1	0.99	0.07	27,27,27,27	0
56	MG	2A	3841	1/1	0.99	0.12	50,50,50,50	0
56	MG	2A	3614	1/1	0.99	0.20	46,46,46,46	0
56	MG	1A	3680	1/1	0.99	0.12	22,22,22,22	0
56	MG	1A	3132	1/1	0.99	0.23	28,28,28,28	0
56	MG	2A	3617	1/1	0.99	0.12	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	3876	1/1	0.99	0.05	41,41,41,41	0
56	MG	1A	3708	1/1	0.99	0.08	31,31,31,31	0
56	MG	1A	3308	1/1	0.99	0.15	28,28,28,28	0
56	MG	2A	3012	1/1	0.99	0.11	53,53,53,53	0
56	MG	1A	3855	1/1	0.99	0.09	36,36,36,36	0
56	MG	1A	3166	1/1	0.99	0.27	53,53,53,53	0
56	MG	2A	3015	1/1	0.99	0.10	68,68,68,68	0
56	MG	1A	3684	1/1	0.99	0.10	45,45,45,45	0
56	MG	1A	3150	1/1	0.99	0.12	23,23,23,23	0
56	MG	2A	3627	1/1	0.99	0.18	60,60,60,60	0
56	MG	2a	3072	1/1	0.99	0.07	70,70,70,70	0
56	MG	2A	3503	1/1	0.99	0.17	41,41,41,41	0
56	MG	1a	1674	1/1	0.99	0.13	55,55,55,55	0
56	MG	1G	203	1/1	0.99	0.30	31,31,31,31	0
56	MG	1A	3579	1/1	0.99	0.14	26,26,26,26	0
56	MG	1A	4081	1/1	0.99	0.26	26,26,26,26	0
56	MG	1A	3819	1/1	0.99	0.38	50,50,50,50	0
56	MG	1A	4083	1/1	0.99	0.09	42,42,42,42	0
56	MG	1A	3861	1/1	0.99	0.14	24,24,24,24	0
56	MG	1X	106	1/1	0.99	0.10	46,46,46,46	0
56	MG	1T	203	1/1	0.99	0.20	24,24,24,24	0
56	MG	1A	3862	1/1	0.99	0.17	17,17,17,17	0
59	ZN	1Y	204	1/1	0.99	0.10	84,84,84,84	0
56	MG	1A	3959	1/1	0.99	0.13	24,24,24,24	0
59	ZN	15	106	1/1	0.99	0.20	52,52,52,52	0
59	ZN	16	103	1/1	0.99	0.13	40,40,40,40	0
59	ZN	19	103	1/1	0.99	0.18	43,43,43,43	0
56	MG	17	102	1/1	0.99	0.12	25,25,25,25	0
59	ZN	2Y	202	1/1	0.99	0.07	109,109,109,109	0
56	MG	1A	3208	1/1	0.99	0.11	44,44,44,44	0
59	ZN	25	103	1/1	0.99	0.15	69,69,69,69	0
56	MG	1a	1751	1/1	0.99	0.06	52,52,52,52	0
56	MG	2A	3824	1/1	0.99	0.10	59,59,59,59	0
56	MG	2A	3643	1/1	0.99	0.10	55,55,55,55	0
60	SF4	1d	302	8/8	0.99	0.17	59,68,73,74	0
60	SF4	2d	302	8/8	0.99	0.12	67,80,92,98	0
56	MG	2A	3651	1/1	1.00	0.14	31,31,31,31	0

6.5 Other polymers (i)

There are no such residues in this entry.